Random Lattice Models

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Zusammenfassung

Diese Arbeit befasst sich mit drei verschiedenen physikalischen Modellen, in denen eine zufällige Komponente in Form eines Potentials bzw. Eichfeldes an ein kubisches Gitter geknüpft ist.

Zuerst wird ein Modell untersucht, das in numerischen Rechnungen der Quantenchromodynamik (Gitter-QCD), also der starken Wechselwirkung zwischen Hadronen, benutzt wird. Die Formulierung dieses Models mit zufälligen Eichfeldern auf den Kanten eines kubischen Gitters wird in den mathematischen Rahmen von ergodischen Operatorfamilien eingefügt. Zunächst wird gezeigt, dass für kleine Kopplungskonstanten die Ergodizität des zu Grunde liegenden Wahrscheinlichkeitsmaßes gegeben ist. In diesem Bereich bilden die Wilson Dirac Operatoren eine ergodische Operatorfamilie und es wird weiterhin gezeigt, dass die zugehörige integrierte Zustandsdichte existiert und fast sicher unabhängig von der gewählten Eichfeldkonfiguration ist.

Die nächsten beiden Modelle sind sich in ihrer physikalischen Situation ähnlich. Beide untersuchen einen kubischen Kristall mit Unreinheiten, welche in Form des typischen Anderson-Modells, also als zufälliges Potential an den Gitterpunkten, modelliert werden. Nun wird allerdings nicht ein einzelnes, sondern ein System von Fermionen in diesem Kristall untersucht. Beide Kapitel sind somit Ideen, das 1-Teilchen Anderson-Modell auf unendlich viele Fermionen auszudehnen.

Zunächst wird die Hartree-Fock Näherung auf ein solches System angewendet. Im Fall der reduzierten Hartree-Fock Theorie bei positiver Temperatur und festem chemischen Potential untersuchen wir den thermodynamischen Limes und zeigen die Existenz und Eindeutigkeit eines Minimierers des Hartree-Fock Funktionals, sowie die Tatsache, dass die Minimierer eine ergodische Operatorfamilie bilden.

Im letzten Modell wird das Fermionensystem algebraisch mittels C^*-Algebren formuliert. Dann wird die Wärmeproduktion unter dem Einfluss eines äußeren,

örtlich und zeitlich inhomogenen aber kompakt getragenen, elektromagnetischen Feldes untersucht. Im Falle kleiner Felder, also im Bereich der linearen Response, wird die Existenz einer Funktion, die als Leitfähigkeit aufgefasst werden kann, gezeigt. Die Wärmeproduktion entspricht dann exakt dem empirisch bekannten Jouleschen Gesetz. Für den Fall des perfekten Leiters sowie des perfekten Isolators erwartet man aus physikalischer Sicht keinerlei Wärmeproduktion. Tatsächlich kann gezeigt werden, dass im Limes sehr kleiner Unreinheiten bzw. unendlich großer Unreinheiten die Leitfähigkeit gegen null konvergiert. Außerdem wird bewiesen, dass in einem Bereich mittelerer Unreinheiten die Wärmeproduktion wie erwartet strikt positiv ist.

Summary

This thesis deals with three different physical models, where each model involves a random component which is linked to a cubic lattice.

First, a model is studied, which is used in numerical calculations of Quantum Chromodynamics (QCD), hence the theory of the strong interaction between hadrons. In these calculations random gauge-fields are distributed on the bonds of the lattice $\mathbb{Z}^d$ according to the so-called Wilson-action. The formulation of the model in lattice QCD is fitted into the mathematical framework of ergodic operator families which has been built up to study random Schrödinger operators. We prove, that for small coupling constants, the ergodicity of the underlying probability measure is indeed ensured. In this regime, the Wilson Dirac operators constitute an ergodic operator family in the probabilistic sense. Then we can prove, that the integrated density of states exists in the thermodynamic limit and is almost surely independent of the chosen gauge field configuration.

The physical situations treated in the next two chapters are more similar to one another. In both cases the principle idea is to study a fermion system in a cubic crystal with impurities, that are modeled by a random potential located at the lattice sites, hence the Anderson setup. Very roughly speaking both chapters can be understood as ideas to extend the 1-particle Anderson model to the case of infinitely many particles.

In the second model we apply the Hartree-Fock approximation to such a system. For the case of reduced Hartree-Fock theory at positive temperatures and a fixed chemical potential we consider the limit of an infinite system. In that case we show the existence and uniqueness of minimizers and that they form an ergodic operator family.

The third model also deals with a system of fermions in a crystal with impurities. The question imposed here is to calculate the heat production of the system under the influence of an outer electromagnetic field. We show that in linear response theory there is a function, the AC-conductivity, such that the heat produc-

tion corresponds exactly to what is empirically predicted by AC-Joule's law. From the physical point of view, one does not expect any heat production in a perfect insulator, as well as for the case of a perfect conductor. In both cases we can show that the AC-conductivity converges to zero. Nevertheless, the AC-conductivity is not always zero. We show that the heat production is indeed strictly positive in a regime of moderate randomness.

Contents

Chapter 1

Introduction

In this thesis different physical models are studied, where the common element of all presented models is a random component connected to a lattice. The lattice under consideration is here $\mathbb{Z}^d$, but any other lattice might be studied as well. Apart from model-specific methods, there are two mathematical components that are used frequently in this work and are explicitly connected with the random component of the models, namely the theory about ergodic operator families and the Ackoglu-Krengel (superadditive) ergodic theorem. The first one ensures the non-randomness of the spectrum of a certain family of random operators, and the second one allows us to replace a mean over infinitely many boxes by an expectation value, and can be seen as an expansion of Birkhoff's Theorem to the lattice $\mathbb{Z}^d$. These two rather simple ingredients turn out to be futile methods in very different physical fields.

The following introduction gives a description of the three different models and the according physical setup as well as a presentation of the obtained results. This introducing part is meant to give an detailed overview over the work.

The next chapters, that is Chapter 2 to 4, then refer to one of the models each and contain again a more precise description, the exact mathematical formulation and all results as well as their proofs.

In order to present the results in short in the introduction, some notations are simplified and not all definitions and results are complete. The precise formulation can always be found in the according chapters.

For a better overview, the three different models are presented separately in the following.

Model 1: Lattice QCD and the Wilson Dirac operator

In Chapter 2 a model is studied which evolves from the theory of the strong interaction, that is Quantum Chromodynamics (QCD). In order to give a rough overview over the idea of *lattice QCD* we recite the associated Lagrangian density, that depends on the fermion field $\overline{\psi}(x)$, $\psi(x)$ and gauge fields $\underline{A} := (A_\mu(x))_{\mu,x}$, where x is a point in the (Minkowski) space-time and $\mu \in \{1, \ldots, 4\}$,

$$\mathcal{L}(x) = \underbrace{-\frac{1}{4} F_{\mu\nu}(x) F^{\mu\nu}(x)}_{\mathcal{L}_g} + \underbrace{\overline{\psi}(x)\big(iD(\underline{A}) - m\big)\psi(x)}_{\mathcal{L}_f}. \tag{1.1}$$

Here, $D(\underline{A}) = \gamma_\mu(\partial_\mu + iA_\mu)$ is the Dirac operator with Dirac matrices γ_μ and $F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) - [A_\mu(x), A_\nu(x)]$ is the field tensor. As it turns out, concrete quantitative predictions are difficult to derive from (1.1) and one uses either calculations in perturbation theory or numerical simulations on a discretized finite space-time, that is made euclidean by a Wick rotation. These numerical studies and simulations are generally summarized under the notion of *lattice QCD* (LQCD) and are a very important and frequently used tool, since several important basic properties of QCD occur in the regime of low energies, where perturbation theory in the QCD coupling constant cannot be applied.

For example the low lying eigenvalues of the (discretized) fermion Dirac operator are of particular interest since they are deeply linked to the value of the chiral condensate $\langle\overline{\psi}\psi\rangle$, c.f. [8], which indicates spontaneous chiral symmetry breaking if it is non-vanishing. Furthermore, the distribution of the low-lying eigenvalues of the fermion Dirac operator is observed to be very close to the one of the corresponding (i.e., respecting symmetries) random matrix ensemble. This idea was put forward in [34, 39, 37] and confirmed by numerous numerical studies, for a review see for example [38].

This is the starting point for our analysis, that can be seen as a first, modest step to enlighten these connections. In Chapter 2 we fit the formulation of the model in LQCD into the mathematical framework of ergodic operator families. This mathematical field has been originally built up to study random Schrödinger operators and, especially, the Anderson model. In contrast to random Schrödinger operators, the randomness in LQCD models lies on the lattice bonds - not on the lattice sites.

We consider the lattice $\mathbb{Z}^d$, $d \geq 2$, with fermion fields supported on the sites and gauge fields supported on the bonds of the lattice. The Hilbert space of the fermion fields is $\mathcal{H} = \ell^2(\mathbb{Z}^d, \mathbb{C}^k)$. The considered operators on $\mathcal{H}$ also depend on the configuration of gauge fields, $\underline{U} = \{U_b\}_{b\in\mathcal{B}}$, on the bonds of $\mathbb{Z}^d$, where the set of bonds is given by $\mathcal{B} := \mathbb{Z}^d \times \{1,\ldots,d\}$. The gauge fields associated to the bonds are elements of a compact Lie group $\mathcal{G}$, the gauge group, that is either $SO(N)$, $SU(N)$, or $U(N)$.

The gauge field configuration is randomly generated with a distribution that is determined by the Wilson action S_W, which is a discretized version of the Young-Mills action $S_{YM} = \int \mathcal{L}_g(x)\mathrm{d}x$. In a finite subset $\Lambda \subset \mathbb{Z}^d$ it is given by

$$S_W(\underline{U}) = \sum_{p\in\mathcal{P}} S_p(U_p), \tag{1.2}$$

where $\mathcal{P}$ is the set of all so-called plaquettes (in Λ), that are plane squares consisting of four points of the form

$$p = p(x;\mu,\nu) = \big\{(x,\mu),(x+\hat{e}_\mu,\nu),(x+\hat{e}_\nu,\mu),(x,\nu)\big\}, \tag{1.3}$$

where $\mu \neq \nu \in \{1,\ldots,d\}$, U_p is the product of the gauge fields along a plaquette p, and

$$S_p(U_p) = \mathrm{Re}\,\mathrm{Tr}(\mathbb{1} - U_p)\ . \tag{1.4}$$

The origin of the plaquettes is the discretization of the field tensor $F_{\mu\nu}$ in the gluonic part $\mathcal{L}_g$ of the Lagrangian density (1.1).

In Chapter 2 the precise setup of the underlying probability space is given in detail. Here we summarize, that for finite regions the probability measure of the distribution of gauge field configuration $\underline{U}$ is given by

$$\mathbb{P}_\Lambda(\underline{U}) := (Z_\Lambda)^{-1} e^{-\beta S_W(\underline{U})}\,\widetilde{\mathbb{P}}_\Lambda(\underline{U}) \tag{1.5}$$

where $\beta > 0$ is a coupling constant, Z_Λ a normalization factor and $\widetilde{\mathbb{P}}_\Lambda(\underline{U}) = \bigtimes_{b\in\mathcal{B}} \mu_H$ is the product measure of all bonds in Λ with μ_H being the normalized Haar measure of the gauge group.

Then we use the *Gibbs formalism* to perform the thermodynamic limit, that means Λ is approaching $\mathbb{Z}^d$. It ensures the existence of a probability measure $\mathbb{P}$ whose 'restrictions' to finite $\Lambda \subset \mathbb{Z}^d$ are exactly the measures $\mathbb{P}_\Lambda$. This measure is known to be unique for small β, in our case for

$$0 < \beta < \frac{1}{12N(d-1)}. \tag{1.6}$$

The first main result of Chapter 2 is that the condition on the uniqueness of $\mathbb{P}$ also ensures its ergodicity, i.e. $\mathbb{P}$ obeys

$$\frac{1}{(2L+1)^d} \sum_{l\in\mathbb{Z}^d,\ \|l\|_\infty\leq L} \mathbb{P}(A\cap T^l A') \to \mathbb{P}(A)\mathbb{P}(A'), \quad \text{as } L\to\infty, \tag{1.7}$$

for all sets A, A' of the underlying σ-algebra $\mathcal{F}$, if $0 < \beta < \frac{1}{12N(d-1)}$.

Then we are ready to start our analysis of the Wilson Dirac Operator $D_W \equiv D_W(\underline{U})$ acting on the Hilbert space $\mathcal{H}$, which is a discretization of the fermion Dirac operator. Here we do not give its explicit form for simplicity, but we remark that it also depends on the gauge field configuration $\underline{U}$ and obeys the covariance condition

$$\tau^\ell D_W(\underline{U}) \tau^{-\ell} = D_W(T^\ell \underline{U}) \,, \tag{1.8}$$

where τ^ℓ is the translation in $\mathcal{H}$ by $\ell \in \mathbb{Z}^d$ and T^ℓ is the according translation of the gauge field configuration. Together with the ergodicity of $\mathbb{P}$ a famous result of Pastur [32] gives the non-randomness of the spectrum of the operator family $\{D_W(\underline{U})\}_{\underline{U} \in \mathcal{G}^{\mathcal{B}}}$.

This observation is crucial to proof the main result of Chapter 2, that is the existence and non-randomness of the integrated density of states of the Wilson Dirac Operator:

Theorem 1.0.1. *Choose $0 < \beta < \frac{1}{12N(d-1)}$ (such that $\mathbb{P}$ is ergodic). Let $(\Omega_n)_{n\in\mathbb{N}}$ be a sequence in $\mathbb{Z}^d$ of nested cubes, $\Omega_n \subseteq \Omega_{n+1}$, with $\Omega_n \nearrow \mathbb{Z}^d$ and $N_{\Omega_n,\underline{U}}(E)$ the number of eigenvalues of $D_W(\underline{U})$ restricted to Ω_n that are smaller than E.*

Then the limit

$$\rho_{\underline{U}}(E) \;:=\; \lim_{n\to\infty} \frac{1}{|\Omega_n|} N_{\Omega_n,\underline{U}}(E) \tag{1.9}$$

exists for all $E \in \mathbb{R}$, $\mathbb{P}$-almost surely, and is independent of the sequence $(\Omega_n)_{n\in\mathbb{N}}$.

Furthermore, for all $E \in \mathbb{R}$, the integrated density of states $\rho_{\underline{U}}(E)$ is independent of $\underline{U}$, $\mathbb{P}$-almost surely.

In Chapter 2 also different boundary conditions for the restriction of $D_W(\underline{U})$to to a finite subset $\Lambda \subset \mathbb{Z}^d$ are considered.

Finally, the author would like to emphasize, that the results of Chapter 2 are common work with Volker Bach and are also published in [4].

Model 2: Hartree Fock Theory for Random Schrödinger Operators

The physical situations treated in Chapter 3 and Chapter 4 are more similar to one another. In both cases the principal idea is to study a fermion system in a cubic crystal with impurities. Very roughly speaking both chapters can be understood as ideas to extend the 1-particle Anderson model to the case of infinitely many fermions.

The idea of random Schrödinger operators is to model a disordered quantum mechanical system, e.g. a crystal with impurities, by introducing a random potential on the lattice sites. For example, the Anderson Hamiltonian h_ω acting on $\mathcal{H} := \ell^2(\mathbb{Z}^d)$ is given by

$$h_\omega = -\Delta_{\mathrm{d}} + V_\omega \, , \tag{1.10}$$

where Δ_{d} is the discrete Laplacian and V_ω the multiplication operator with the random potential $\{V_\omega(x)\}_{x\in\mathbb{Z}^d}$. In the Anderson model $\{V_\omega(x)\}_{x\in\mathbb{Z}^d}$ is assumed to be an independently and identical distributed (i.i.d.) random variable.

As it turns out, those systems show the tendency to have localized states, this effect is the famous Anderson localization. The theory of random Schrödinger operators is very successful and has led to deeper mathematical understanding, as for example the theory of ergodic operator families, which have a non-random (essential, discrete, continuous, absolutely continuous etc) spectrum [32, 29].

The state of the art is to handle systems with finitely many interacting fermions in the thermodynamic limit [1]. At that point, the question of a system of infinitely many interacting fermions, as for example an infinite system with constant fermion density, arises naturally.

In Chapter 3 we apply the Hartree-Fock approximation to a system of electrons in the Anderson setup. Technically, the fermion system is described by elements of the *fermion Fock space* $\mathcal{F}_f$, a special Hilbert space whose construction is described in Chapter 3. For the introduction, let us summarize that the elements of $\mathcal{F}_f$ are wave functions that describe a system of particles that obey the Pauli principle. The number of fermions in such a systems is not necessarily fixed.

The Hartree-Fock functional is an approximation to the energy of the fermion system. It takes into account the energy of each fermion with respect to an external, in our case random, potential. This amount of energy is described by the 1-particle Anderson Hamiltonian h_ω. A second part represents the interaction between the fermions, via a certain, in our case repulsive, interaction potential W, and in the case of positive temperatures a third term is added, which yields the entropy S of the system.

The basic idea of the Hartree-Fock approximation is to give an upper bound to the energy of the ground state by minimizing the Hartree-Fock functional over states evolving from Slater determinants, i.e., product wave functions. As it turns out it is of advantage to run the minimization even over quasi-free, particle conserving states, which contain also Slater determinants. These can be represented by *1-particle density matrices* $\{\gamma \in \mathcal{L}^1(\mathcal{H}) \mid 0 \leq \gamma \leq 1\}$.

First, we consider finite systems, that are finitely many fermions in a finite region $\Lambda \subset \mathbb{Z}^d$. Here, we suppress the dependence on Λ in the notation, where all operators are to be understood as acting on $\ell^2(\Lambda)$ or $\ell^2(\Lambda) \otimes \ell^2(\Lambda)$ in the case of the interaction W and the exchange operator Ex, which exchanges components. In Chapter 3 we study the following functionals, that are to be minimized over the set of 1-particle density matrices and represent different physical cases

- The Hartree-Fock functional, describing a system at zero temperature,

$$\mathcal{E}_\omega^{(\mathrm{HF})}(\gamma) = \mathrm{Tr}_{\,\ell^2(\Lambda)}\{h_\omega \gamma\} + \frac{g}{2}\,\mathrm{Tr}_{\,\ell^2(\Lambda)\otimes\ell^2(\Lambda)}\{W(\mathbb{1} - \mathrm{Ex}\,)(\gamma\otimes\gamma)\}\;, \tag{1.11}$$

- The Hartree-Fock functional for a system at zero temperature and at fixed chemical potential μ

$$\widetilde{\mathcal{E}}_{\omega,\mu}^{(\mathrm{HF})}(\gamma) = \mathcal{E}_\omega^{(\mathrm{HF})}(\gamma) - \mu\,\mathrm{Tr}_{\,\ell^2(\Lambda)}\{\gamma\}\;, \tag{1.12}$$

- the Hartree-Fock pressure functional, for a system at temperature $\beta^{-1} > 0$,

$$-\mathcal{P}_{\omega,\beta}^{(\mathrm{HF})}(\gamma) = \mathcal{E}_\omega^{(\mathrm{HF})}(\gamma) - \beta^{-1}S(\gamma)\;, \tag{1.13}$$

- and the Hartree-Fock grand canonical potential functional for a system at temperature $\beta^{-1} > 0$ and fixed chemical potential $\mu \in \mathbb{R}$

$$\mathcal{M}_{\omega,\beta,\mu}^{(\mathrm{HF})}(\gamma) = \mathcal{E}_\omega^{(\mathrm{HF})}(\gamma) - \beta^{-1}S(\gamma) - \mu\,\mathrm{Tr}_{\,\ell^2(\Lambda)}\{\gamma\}\;. \tag{1.14}$$

For the first and third functional we fix the particle number, that is given by $\mathrm{Tr}\{\gamma\}$ for the minimization. The coupling constant $g > 0$ scales the strength of the interaction. Furthermore, we also consider the case of reduced Hartree-Fock theory, where the exchange operator Ex is neglected, hence the reduced Hartree-Fock functional is defined as

$$\mathcal{E}_\omega^{(\mathrm{rHF})}(\gamma) = \mathrm{Tr}\{h_\omega \gamma\} + \frac{g}{2}\,\mathrm{Tr}\{W(\gamma\otimes\gamma)\}\;, \tag{1.15}$$

and accordingly for $\widetilde{\mathcal{E}}_{\omega,\mu}^{(\mathrm{HF})}$, $-\mathcal{P}_{\omega,\beta}^{(\mathrm{rHF})}$, $\mathcal{M}_{\omega,\beta,\mu}^{(\mathrm{rHF})}$.

For finite regions $\Lambda \subset \mathbb{Z}^d$, the minimizers of the functionals introduced above fulfill *self-consistent equations*, in the full as well as in the reduced case. For example we obtain for $\mathcal{M}_{\omega,\beta,\mu}^{(\mathrm{HF})}$ that any minimizer γ_0 obeys

$$\gamma_0 = \Big(1 + \exp\Big[\beta(H_{\mathrm{eff}}^{(\mathrm{HF})}[\gamma_0] - \mu)\Big]\Big)^{-1}\;, \tag{1.16}$$

where $H_{\text{eff}}^{(\text{HF})}[\gamma_0] \in \mathcal{B}(\ell^2(\Lambda))$ is the *effective Hamiltonian*, that depends on the minimizer γ_0. Note, that the effective Hamiltonian is different for the reduced Hartree-Fock theory.

In the reduced case, we use the a convexity property of $\mathcal{E}_\omega^{(\text{rHF})}$ and the self-consistent equations, to deduce the uniqueness of the minimizers of $-\mathcal{P}_{\omega,\beta}^{(\text{rHF})}$, and $\mathcal{M}_{\omega,\beta,\mu}^{(\text{rHF})}$.

Thus it is reasonable to study the minimizers of these reduced functionals in the thermodynamic limit $\Lambda \nearrow \mathbb{Z}^d$. As in Chapter 2, we assume Λ_n to be the cube of side length $2n+1$ centered at zero and take the limit $n \to \infty$. Then we proof the existence of an accumulation point of minimizers γ_n of $\mathcal{M}_{\omega,\beta,\mu}^{(\text{rHF})}$ in Λ_n in the weak-* sense and show that this accumulation point also fulfills self-consistent equations.

For positive temperatures and fixed chemical potential, hence for minimizers of $\mathcal{M}_{\omega,\beta,\mu}^{(\text{rHF})}$, we can show, that the limit is unique provided that $\beta \cdot g$ is small enough, i.e. for high temperature and small interaction between the fermions. Furthermore, we are able to proof that in this case the minimizers as well as the corresponding effective Hamiltonians form ergodic operator families in the probabilistic sense, hence have a non-random spectrum.

Model 3: Entropy production of fermions in disordered media

The last chapter is common work with Walter de Siqueira Pedra and Jean-Bernard Bru. Only those parts of the in some aspects considerably larger work [15, 17, 16, 18] are presented, where the author has had a major contribution and that were completely finished, when this thesis was done.

As mentioned before, Chapter 4 also deals with a system of fermions in a crystal with impurities. The focus is here to calculate the heat or entropy production of the system, due to the impurities, under the influence of an electromagnetic field.

In general, the electric resistance of conductors is supposed to result from both, the presence of disorder in the host material and interactions between charge carriers. The first aspect is included in our model, we use the Anderson setup as introduced in Chapter 3 to model impurities. The interaction between charge carriers is not fully included. We respect the fermionic nature of the electrons, hence the particles obey the Pauli principle, but do not include any further interaction between them, such as for example the Coulomb repulsion. If the density of charge carriers is low, the effect of a mutual force between them is assumed to be small and hence the setup considered here can be seen as a suitable model in that case.

As mentioned before, the impurities of the crystal are modeled as in the usual Anderson setup. The i.i.d. random potential on the lattice sites is assumed to be bounded, e.g. $V_\omega \in [-1, 1]$ and we scale it by a parameter $\lambda > 0$. This is a preparation to consider also the cases of a perfect conductor, that would be $\lambda \to 0$ as well as a perfect insulator, where the randomness is supposed to be very large, hence $\lambda \to \infty$.

Then we study a fermion system in that setup under the influence of an external electromagnetic potential. The fermion system is infinitely extended and described by the C^*-algebra $\mathcal{U}$, that is generated by the identity and the creation and annihilation operators $\{a_x^*, a_x\}_{x\in\mathbb{Z}^d}$, which obey the canonical anti-commutation relations and thus encode the Pauli exclusion principle. The electromagnetic potential is inhomogeneous, but assumed to be smooth and compactly supported in time- and space,

$$\mathbf{A} = \mathbf{A}(t, x) \in C_0^\infty(\mathbb{R} \times \mathbb{R}^d; \mathbb{R}^d) . \tag{1.17}$$

In the following, we denote by t_0 the time where the electromagnetic potential is switched on and by t_1 the time where it is switched off again. The fact that $\mathbf{A}$ is compactly supported in time induces the so-called *AC-condition* for the electric field $E_{\mathbf{A}}$, which is given by

$$E_{\mathbf{A}}(t, x) := -\partial_t \mathbf{A}(t, x) , \tag{1.18}$$

namely,

$$\int_{t_0}^{t_1} E_{\mathbf{A}}(t, x)\mathrm{d}t = 0 . \tag{1.19}$$

As the main assertion about the heat production in the system caused by $\mathbf{A}$ is formulated for times $t \geq t_1$, one should keep in mind, that we really attend to the AC-case in the following and do not aim to formulate results concerning the DC-case.

As usual, the electromagnetic potential $\mathbf{A}$ is minimally coupled to the fermion system, this amounts to replacing the discrete Laplacian Δ_d in the Anderson Hamiltonian by the minimally coupled one, denoted here by $\Delta_\mathrm{d}^{(\mathbf{A})}$, which is then time-dependent. Then we study the induced dynamics, that means we consider the Schrödinger equation on the one-particle Hilbert space $\ell^2(\mathbb{Z}^d)$ with time-dependent Hamiltonian

$$\Delta_\mathrm{d}^{(\mathbf{A})} + \lambda V_\omega \in \mathcal{B}(\ell^2(\mathbb{Z}^d)) ,$$

which has a unique solution determined by the family $\{U_{t,s}^{(\omega,\lambda,\mathbf{A})}\}_{t\geq s}$ of unitary operators on $\ell^2(\mathbb{Z}^d)$. The family $\{U_{t,s}^{(\omega,\lambda,\mathbf{A})}\}_{t\geq s}$ induces a random two-parameter group $\{\tau_{t,s}^{(\omega,\lambda,\mathbf{A})}\}_{t\geq s}$ of Bogoliubov automorphisms of the CAR algebra $\mathcal{U}$.

Before the electromagnetic field is turned on, i.e. as initial state, we assume the system to be at thermodynamic equilibrium. For infinite systems, this is realized by taking the unique Kubo-Martin-Schwinger-state (KMS-state) $\varrho^{(\beta,\omega,\lambda)} \equiv \varrho^{(\beta)}$ of the system at temperature β^{-1}, random potential configuration ω and scaling parameter λ. The precise definition of KMS-states is given in Section 4.2.4, here we may very roughly summarize, that the finite volume analog of the KMS-state minimizes the free energy of the finite system. Then we take the time evolution of this state under the influence of the electromagnetic potential $\mathbf{A}$, that is

$$\rho_t^{(\beta,\mathbf{A})} := \begin{cases} \varrho^{(\beta)} & , \qquad t \leq t_0 \ , \\ \varrho^{(\beta)} \circ \tau_{t,t_0}^{(\omega,\lambda,\mathbf{A})} & , \qquad t \geq t_0 \ . \end{cases} \tag{1.20}$$

Now we are ready to define the heat production of the system, that is the amount of energy, or more precisely entropy, the system gains under the influence of $\mathbf{A}$. We consider the energy observable in the box of side length $2n+1$, that is

$$\Lambda_n := \{x \in \mathbb{Z}^d \ : \ \|x\|_\infty \leq n\} \ , \tag{1.21}$$

which is given by

$$H_n := \sum_{x,y\in\Lambda_n} \langle \mathfrak{e}_x, (\Delta_{\mathrm{d}} + \lambda V_\omega)\, \mathfrak{e}_y \rangle a_x^* a_y \in \mathcal{U} \ , \tag{1.22}$$

for any $n \in \mathbb{N}$.

The energy increment in the state $\rho_t^{(\beta,\mathbf{A})}$ w.r.t. the equilibrium state $\varrho^{(\beta)} \equiv \rho_{t_0}^{(\beta,\mathbf{A})}$ is then given by

$$\mathfrak{I}_t^{(\beta,\mathbf{A})} := \lim_{n\to\infty} \left\{ \rho_t^{(\beta,\mathbf{A})}(H_n) - \rho_{t_0}^{(\beta,\mathbf{A})}(H_n) \right\} \ , \tag{1.23}$$

for any $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $\mathbf{A} \in \mathbf{C}_0^\infty$ and $t \in \mathbb{R}$, whereas it is a priori not clear that the limit above exists. We prove that $\mathfrak{I}_t^{(\beta,\mathbf{A})}$ is indeed well-defined for small fields. Furthermore, we show that the energy increment $\mathfrak{I}_t^{(\beta,\mathbf{A})}$ can also be expressed as an *entropy* production, and hence it is in particular positive.

The main result of Chapter 4 is the following theorem, that we call *AC-Joule's law* in the following. We study the limit of the energy increment $\mathfrak{I}_t^{(\beta,\eta\mathbf{A}_L)}$ for

$(\eta, L^{-1}) \to (0,0)$, where $\mathbf{A}_L(x,t) = \mathbf{A}(L^{-1}x,t)$ is a rescaled version of $\mathbf{A}$. This limit corresponds to analyzing the linear response of the fermion system under the influence of a time-dependent electric field localized in a very small but macroscopic region of the bulk. As it turns out, the energy increment $\mathfrak{I}_t^{(\beta,\eta\mathbf{A}_L)}$ is of order $\mathcal{O}\left(\eta^2 L^d\right)$. This is due to the fact that the electromagnetic energy given to the system, that is the L^2-norms of the fields, is also of order $\mathcal{O}\left(\eta^2 L^d\right)$, by classical electrodynamics.

Theorem 1.0.2.
Let $\beta \in \mathbb{R}^+$ and $\lambda \in \mathbb{R}_0^+$. Then there is a unique function $\sigma \equiv \sigma^{(\beta,\lambda)} \in C(\mathbb{R},\mathbb{R})$ satisfying $\sigma(t) = \sigma(|t|)$ and $\sigma(0) = 0$, and a measurable subset $\tilde{\Omega} \equiv \tilde{\Omega}^{(\beta,\lambda)} \subset \Omega$ of full measure such that, for any $\omega \in \tilde{\Omega}$, $\mathbf{A} \in \mathbf{C}_0^\infty$ and $t \geq t_1$,

$$\begin{aligned}
\mathfrak{I} &:= \lim_{(\eta,L^{-1})\to(0,0)} \left\{ \left(\eta^2 L^d\right)^{-1} \mathfrak{I}_t^{(\beta,\eta\mathbf{A}_L)} \right\} \qquad (1.24)\\
&= \int_{t_0}^{t} \int_{t_0}^{s_1} \left[\sigma(s_1 - s_2) \int_{\mathbb{R}^d} \langle E_{\mathbf{A}}(s_1,x), E_{\mathbf{A}}(s_2,x)\rangle \, \mathrm{d}^d x \right] \mathrm{d}s_2 \mathrm{d}s_1 \\
&= \frac{1}{2} \int_{\mathbb{R}} \int_{\mathbb{R}} \left[\sigma(s_1 - s_2) \int_{\mathbb{R}^d} \langle E_{\mathbf{A}}(s_1,x), E_{\mathbf{A}}(s_2,x)\rangle \, \mathrm{d}^d x \right] \mathrm{d}s_2 \mathrm{d}s_1 \geq 0 \, .
\end{aligned}$$

Note, that in Theorem 1.0.2, we make an assertion for $t \geq t_1$, that means as soon as the electromagnetic field is turned off. For all those times $t, t' \geq t_1$ the energy increment is no longer time-dependent, i.e. $\mathfrak{I}_t = \mathfrak{I}_{t'}$.

The physicist J. P. Joule observed that the heat (per second) within a circuit is proportional to the electric resistance and the square of the current in the DC-regime. Nevertheless, we name Theorem 1.0.2 *AC-Joule's law* because of two clear similarities. Qualitatively like Joule's law, Theorem 1.0.2 describes the rate at which resistance in the fermion system converts electric energy into heat energy for $t \geq t_1$. Quantitatively, Theorem 1.0.2 is an analogue of Joule's law in the AC-regime with currents and resistance replaced by electric fields and AC-conductivity. To see this connection more explicitly, let us assume for the moment, that the AC-conductivity σ in Theorem 1.0.2 would have a Fourier transform $\hat{\sigma}$. Then (1.24) could be rewritten as

$$\mathfrak{I} = \frac{1}{2} \int_{\mathbb{R}} \left[\int_{\mathbb{R}^d} |\widehat{E}_{\mathbf{A}}(\nu,x)|^2 \mathrm{d}^d x \right] \hat{\sigma}(\nu) \mathrm{d}\nu \, , \qquad (1.25)$$

where $\widehat{E}_{\mathbf{A}}(\cdot,x)$ is the Fourier transform of the map $t \mapsto E_{\mathbf{A}}(t,x)$, and the heat production is proportional to the (integrated) square of the absolute value of the electric field, while $\hat{\sigma}$ plays the role of an (inverse) impedance.

However, in general, we can not assume, that σ can be Fourier transformed. This leads us to the notion of an *AC-conductivity measure*. This notion is inspired by the work of Klein, Lenoble and Müller, who introduced in [25] the concept of an AC-conductivity measure for a system of fermions subjected to a random potential for the first time. Let us note here, that the setup in [25] is a bit different than the one presented here, for example we take space inhomogeneous fields instead of homogeneous ones.

During the proof of Theorem 1.0.2, we obtain an explicit expression for the AC-conductivity as an expectation value over certain propagators, from which we deduce by Bochner's Theorem that for any inverse temperature $\beta > 0$ and parameter $\lambda \geq 0$, there is a finite positive measure μ_σ, such that

$$\sigma(t) = \int_{\mathbb{R}} \left(\mathrm{e}^{it\nu} - 1\right) \mathrm{d}\mu_\sigma(\nu) , \qquad t \in \mathbb{R} .$$

Then (1.24) can be written as

$$\mathfrak{I} = \frac{1}{2} \int_{\mathbb{R}\backslash\{0\}} \left[\int_{\mathbb{R}^d} |\widehat{E}_{\mathbf{A}}(\nu, x)|^2 \mathrm{d}^d x\right] \mathrm{d}\mu_\sigma(\nu) . \tag{1.26}$$

We complete Chapter 4 by studying μ_σ for different regimes of randomness. More precisely, we model a perfect conductor by the limit $\lambda \to 0^+$, and a perfect insulator by taking $\lambda \to \infty$. From the physical point of view, one does not expect any heat production in the system for both cases. Indeed, we prove that our model shows exactly the expected behaviour, i.e. the AC-conductivity measure μ_σ converges in the weak*-topology to the trivial measure $(0 \cdot \mathrm{d}\nu)$ on $\mathbb{R}\backslash\{0\}$, as $\lambda \to \infty$ or $\lambda \to 0^+$. The skeptical reader might suspect at that point, that the AC-conductivity measure is the trivial measure for all λ, β. However, this is not the case. We prove that the heat production is generally a strictly positive quantity in a regime of moderate randomness, i.e. for $\lambda \in (\lambda_0/2, \lambda_0)$ with some suitable $\lambda_0 > 0$, we have an almost surely strictly positive heat production.

To conclude the presentation of the main results of Chapter 4 let us remark, that ongoing work shows, that it is possible to extend the model presented here and the used techniques to get much broader results. Especially, the consideration of the electromagnetic free-energy in addition to the entropy increment $\mathfrak{I}_t$ introduced above, allows us to formulate results similar to Theorem 1.0.2 for all times $t \in \mathbb{R}$ and thus also for the DC-case, see [16].

Furthermore, it is to be emphasized, that the inclusion of an additional interaction between the fermions could, in principle, be included in our model. Although the technical treatment is then much more demanding and elaborate, it seems nevertheless possible. This might be the major aspect of this work for further studies and the main advantage in contrast to other publications concerning the concept of an AC-conductivity measure, as for example [25].

Chapter 2

The Integrated Density of States for the Wilson Dirac Operator

In this section a result on the integrated density of states for the Wilson Dirac Operator is presented. It is based on common work with Volker Bach and published in [4]. After the physical motivation in Section 2.1, the precise mathematical description of the model is presented in Section 2.2. Then the main result is formulated in Section 2.3 and proven in Section 2.4.

2.1 Physical motivation

The Standard Model of Elementary Particles provides a common conceptual basis for all elementary forces except gravity. The part which describes the strong nuclear force is called Quantum Chromodynamics (QCD). The associated Lagrangian density has a clear and simple appearance that is

$$\mathcal{L}(x) \;=\; -\frac{1}{4}\, F_{\mu\nu}(x)\, F^{\mu\nu}(x) \;+\; \overline{\psi}(x)\big(iD(\underline{A}) - m\big)\psi(x), \tag{2.1}$$

with $D(\underline{A}) := \gamma_\mu(\partial_\mu + iA_\mu)$ being the Dirac operator of the fermion field $\overline{\psi}(x)$, $\psi(x)$, which depends on the gauge field $\underline{A} := (A_\mu(x))_{\mu,x}$, and $F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x) - [A_\mu(x), A_\nu(x)]$ being the field tensor. In spite of its structural simplicity, concrete quantitative predictions are difficult to derive from (2.1), and one often resorts either to calculations in perturbation theory or numerical simulations on a discretized (Euclidean, after Wick rotation) space-time, known as *lattice QCD* (LQCD, see [30] for an overview).

Several basic properties of QCD, such as the spontaneous breaking of chiral symmetry or the phenomenon of quark confinement, manifest themselves in the regime of low energies, where perturbation theory in the QCD coupling constant cannot be applied. Spontaneous chiral symmetry breaking is signaled by the formation of a non-vanishing chiral condensate $\langle\overline{\psi}\psi\rangle$. In a seminal paper [8], Banks and Casher formulated a link between the value of the condensate and the spectral properties of the Dirac operator D in the deep infra-red. Since the gauge field $\underline{A}$ does not appear explicitly in the observable, it acts as a background field which nonetheless determines the spectral properties in a non-trivial way.

The idea that the distribution of the low-lying eigenvalues of the fermion Dirac operator is very close to the one of the corresponding (i.e., respecting symmetries) random matrix ensemble was put forward in [34, 39, 37] and affirmed by numerous numerical studies, e.g. [24, 9], for a review see for example [38]. In fact, these distributions agree to an accuracy that would, perhaps, allow to replace the derivation of average spectral properties of the fermion Dirac operator by sampling gauge field configurations with the random matrix eigenvalue distribution. The robustness of this phenomenon over a broad range of parameter values, like the underlying gauge group or the system's temperature (in the Boltzmann weight) is also remarkable.

In the following we fit the formulation of the model in LQCD into the mathematical framework of *ergodic operator families* which has been built up over the past three decades or so to study random Schrödinger operators and, especially, the Anderson model. In contrast to random Schrödinger operators, however, the randomness in LQCD models lies on the lattice bonds - not on the lattice sites - and corresponds to a random magnetic field, rather than an alloy or a quenched glass.

We prove that Dirac operators of LQCD which depend on the gauge field indeed constitute ergodic operator families in the probabilistic sense, provided the gauge field itself is ergodic, i.e., has sufficient rapidly decaying correlations (see Section 2.2.2 for a precise formulation). This, in turn, is a fair assumption in many physical situations, e.g., at high temperature. As a consequence of our result the integrated density of states exists in the thermodynamic limit and is almost surely independent of the chosen gauge field configuration.

Many observables can be expressed in terms of derivatives of the QCD partition function with respect to source terms. For example, the chiral condensate is given by [38]

$$\langle\overline{\psi}\psi\rangle \;=\; -\lim_{m\to 0}\lim_{V\to\infty}\frac{1}{V}\partial_m \log Z^{QCD}, \tag{2.2}$$

with the partition function

$$Z^{QCD} \;=\; \int \prod_{x\in V,\mu=1,\ldots,d} dA_\mu \;\det\big[iD(\underline{A})+m\big]e^{-S_{YM}(\underline{A})}. \tag{2.3}$$

Here, the integration of the fermionic variables yields the fermion determinant $\det[iD(\underline{A})+m]$, and $S_{YM}(\underline{A})$ is the Euclidean Yang-Mills action.

It is customary to use the *quenched approximation* in numerical simulations, which amounts to setting the fermion determinant is equal to one. This reduces the numerical effort significantly and corresponds to the physical case of infinitely heavy sea quarks.

The discretization of the Dirac operator is also subtle, because the naive discretization leads to the occurrence of fermion doublers, which have no physical meaning. There are several ways to work around this problem. Wilson proposed to add a term that vanishes in the continuum limit and suppresses the doublers on the lattice [40]. Another method is to introduce staggered fermions - the lattice is divided up in sub-lattices where different staggered phases live, that are interpreted as physical phases [27, 36]. We are mainly interested in those two cases, where the Dirac operator still has nearest-neighbour interaction. This is not the case for another elegant solution, the overlap operator proposed in [31].

2.2 Introduction of the model

Now we come to the precise description of the mathematical setting. We consider the lattice $\mathbb{Z}^d$, $d \geq 2$, with *fermion fields* supported on the sites and *gauge fields* supported on the bonds of the lattice. We only take the one-particle case into account. Then the matter fields are complex vectors and the configuration of all matter fields is supposed to be an element of the Hilbert space $\mathcal{H} = \ell^2(\mathbb{Z}^d, \mathbb{C}^k)$ of square summable $\mathbb{Z}^d$-sequences in $\mathbb{C}^k$. $\mathcal{H}$ is equipped with the usual scalar product

$$\langle \varphi, \psi\rangle \;=\; \sum_{x\in\mathbb{Z}^d}\sum_{i=1}^{d} \bar{\varphi}_i(x)\psi_i(x), \quad \varphi,\psi\in\mathcal{H}. \tag{2.4}$$

We will consider operators on $\mathcal{H}$, that also depend on the configuration of gauge fields on the bonds of $\mathbb{Z}^d$. The set of bonds in the lattice $\mathbb{Z}^d$ is denoted by

$$\mathcal{B} \;:=\; \mathbb{Z}^d \times \{1,\ldots,d\}. \tag{2.5}$$

The bond $(x, \mu) \in \mathcal{B}$ is the one connecting x and $x + \hat{e}_\mu$, with $\hat{e}_\mu$ the unit vector in $\mathbb{Z}^d$ pointing in direction μ. We give the bond (x, μ) the orientation from x to $x + \hat{e}_\mu$.

The gauge fields associated to the bonds are elements of a compact Lie group $\mathcal{G}$, the gauge group. We assume $\mathcal{G}$ to be either $SO(N)$, $SU(N)$, or $U(N)$ to be explicit and since these are the relevant physical cases. The gauge field on the bond $b = (x, \mu)$ is denoted by $U_{x,\mu}$ or U_b.

It turns out to be necessary to consider the orientation of a bond, the gauge field for going from $x + \hat{e}_\mu$ to x is $U_{x+\hat{e}_\mu,-\mu}$ and we set $U_{x+\hat{e}_\mu,-\mu} = U_{x,\mu}^{-1}$.

A gauge field configuration is the collection $\{U_b\}_{b\in\mathcal{B}}$. As mentioned before, this gauge field configuration is randomly generated. In order to specify the underlying probability space in the next section, we will need the notion of a *plaquette*, a collection of four bonds that form a plane square in $\mathbb{Z}^d$,

$$p(x; \mu, \nu) \;:=\; \big\{(x, \mu), (x + \hat{e}_\mu, \nu), (x + \hat{e}_\nu, \mu), (x, \nu)\big\}, \tag{2.6}$$

with $\mu \neq \nu$. We need the product of the gauge fields along a plaquette $p = p(x; \mu, \nu)$,

$$U_p \;:=\; U_{x;\mu,\nu} \;:=\; U_{x,\nu}^{-1}\, U_{x+\hat{e}_\nu,\mu}^{-1}\, U_{x+\hat{e}_\mu,\nu}\, U_{x,\mu}, \tag{2.7}$$

where the orientation of the bonds leads to the inverse gauge fields. Thus we have $U_{x;\mu,\nu} = U_{x;\nu,\mu}^{-1}$ and define a plaquette as positively orientated if $\mu < \nu$. The set of all positively orientated plaquettes is denoted by

$$\mathcal{P} \;:=\; \big\{p(x; \mu, \nu) \,\big|\, x \in \mathbb{Z}^d,\ \mu, \nu \in \{1, \ldots, d\},\ \mu < \nu\big\}. \tag{2.8}$$

Figure 2.1 shows a plaquette and its associated gauge fields.

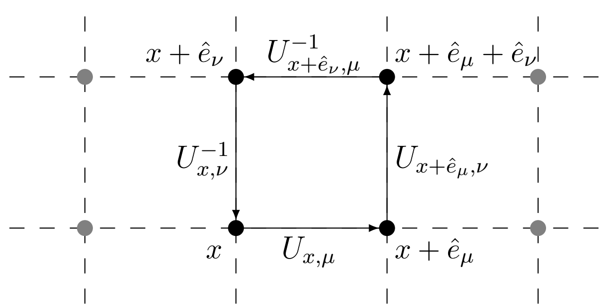

Figure 2.1: The plaquette $p(x; \mu, \nu)$ and the associated gauge fields are sketched in the (μ, ν)-plane of $\mathbb{Z}^d$.

2.2.1 The probability space

We start by specifying the probability space for a single bond. Since $\mathcal{G}$ is a compact Lie group, $\mathcal{G}$ is equipped with a natural measure, the Haar measure μ_H. Because of the compactness of $\mathcal{G}$, the Haar measure μ_H is normalized and we obtain the probability space $(\mathcal{G}, \mathcal{F}_0, \mu_H)$, with $\mathcal{F}_0$ being the σ-algebra of Borel sets of the topological space $\mathcal{G}$. A priori, we let the gauge field U_b on a single bond be a random variable that is uniformly distributed with respect to the Haar measure μ_H of $\mathcal{G}$.

Let $\Omega \subseteq \mathcal{B}$ be a (possibly infinite) subset of $\mathcal{B}$. The gauge field configuration $\mathcal{U} = \{U_b\}_{b\in\Omega}$ can be regarded as an element of the product space $\mathcal{G}^\Omega$. Note that $\mathcal{G}^\Omega$ is compact in the product topology by Tychonov's Theorem. The probability space for gauge field configurations is now constructed by means of cylinder sets as, for example, in [10]. A cylinder set is a subset of $\mathcal{G}^\Omega$ of the form

$$M \;=\; \left\{\mathcal{U} \in \mathcal{G}^\Omega \;\middle|\; U_{b_1} \in A_1, \ldots, U_{b_n} \in A_n\right\} \tag{2.9}$$

with $A_1, \ldots, A_n \in \mathcal{F}_0$ and $b_1, \ldots, b_n \in \Omega$. The set of all cylinder sets is denoted $\mathcal{Z}$. We take as a σ-algebra for $\mathcal{G}^\Omega$ the σ-algebra $\mathcal{F}_\Omega$ generated by the system of all cylinder sets. For finite subsets $\Omega \subset \mathcal{B}$, $\mathcal{F}_\Omega$ is the usual product σ-algebra. The probability measure $\widetilde{\mathbb{P}}_\Omega$ on $\mathcal{G}^\Omega$ is then defined to be the product measure, setting for every cylinder set

$$\widetilde{\mathbb{P}}_\Omega\big(\left\{\mathcal{U} \in \mathcal{G}^\Omega \;\middle|\; U_{b_1} \in A_1, \ldots, U_{b_n} \in A_n\right\}\big) \;=\; \prod_{i=1}^{n} \mu_H(A_i). \tag{2.10}$$

Finally, define $\mathcal{F} := \mathcal{F}_\mathcal{B}$ and $\widetilde{\mathbb{P}} := \widetilde{\mathbb{P}}_\mathcal{B}$.

Now, we modify the measure $\widetilde{\mathbb{P}}_\Omega$ by a weight function that represents the gauge action as it is used in lattice QCD calculations. Those calculations are done on finite lattices, of course. Therefore, let $\Lambda \subset \mathcal{B}$ be a finite region and $\eta \in \mathcal{G}^\mathcal{B}$ a gauge field configuration, that will play the role of a boundary condition, which fixes the gauge field outside of Λ. Then the underlying probability measure is of the form

$$\mathbb{P}^\eta_{\beta,\Lambda}(\mathcal{U}) \;:=\; (Z^\eta_{\beta,\Lambda})^{-1} e^{-\beta S^\eta_\Lambda(\mathcal{U})}\, \widetilde{\mathbb{P}}_\Lambda(\mathcal{U}) \tag{2.11}$$

with $\beta > 0$, Z^η_Λ the normalization factor and S^η_Λ representing the gauge action. We assume in the following that S^η_Λ is the Wilson action, that is often used in lattice QCD calculations, namely

$$S^\eta_\Lambda(\mathcal{U}) \;=\; \sum_{p\in\mathcal{P}, p\cap\Lambda\neq\emptyset} S_p(\{\mathcal{U}_\Lambda, \eta_{\Lambda^c}\}), \tag{2.12}$$

and

$$\begin{aligned} S_p(\{\mathcal{U}_\Lambda, \eta_{\Lambda^c}\}) &:= \frac{1}{2}\operatorname{Tr}\{(\mathbb{1} - U_p(\{\mathcal{U}_\Lambda, \eta_{\Lambda^c}\}))(\mathbb{1} - U_p(\{\mathcal{U}_\Lambda, \eta_{\Lambda^c}\}))^*\} \\ &= \operatorname{Re}\operatorname{Tr}\{\mathbb{1} - U_p(\{\mathcal{U}_\Lambda, \eta_{\Lambda^c}\})\} \end{aligned} \tag{2.13}$$

with $U_p(\{\mathcal{U}_\Lambda, \eta_{\Lambda^c}\})$ the plaquette variable as defined in (2.7) for the gauge field configuration that equals $\mathcal{U}$ inside Λ and η outside Λ. In the following we will use this notation in general for composed gauge field configurations. Note that $S_p(\mathcal{U}) \geq 0$ for all $\mathcal{U} \in \mathcal{G}$.

Let us also formally define the unrestricted gauge action $S(\mathcal{U})$,

$$S(\mathcal{U}) = \sum_{p\in\mathcal{P}} S_p(\{\mathcal{U}\}), \tag{2.14}$$

although this infinite sum might be divergent. If the unrestricted gauge action S converges for a certain gauge field configuration $\mathcal{U} \in \mathcal{G}^{\mathcal{B}}$, it is invariant under translations. Denoting by T^ℓ the translation in $\mathbb{Z}^d$ by $\ell \in \mathbb{Z}^d$, i.e. $T^\ell x := x - \ell$, and defining the translation of a gauge field by $\ell \in \mathbb{Z}^d$ to be

$$T^\ell U_{x,\mu} := U_{T^\ell x,\mu} = U_{x-\ell,\mu}, \tag{2.15}$$

for any $U_{x,\mu} \in \mathcal{G}$ and $(x,\mu) \in \mathcal{B}$, we have

$$S(\mathcal{U}) = S(T^\ell \mathcal{U}) \tag{2.16}$$

for all $\ell \in \mathbb{Z}^d$, with $T^\ell\mathcal{U} := \{U_{x-\ell,\mu}\}_{(x,\mu)\in\mathcal{B}}$

Since we are interested in the integrated density of states, we would like to pass to the thermodynamic limit, hence $\Lambda \nearrow \mathcal{B}$. We use the *Gibbs formalism*, following [12, 35], to establish the existence of such a limit for the probability measure and later its uniqueness and ergodicity for small β. Therefore, the gauge action S_p for a single plaquette is interpreted as an *interaction* between four bonds. Note that in [12] the lattice $\mathbb{Z}^d$ is used as underlying lattice. This is no restriction for our application. For example, we may regard $\mathcal{B} = \mathbb{Z}^d \times \{1, \ldots, d\}$ as a sublattice of $\frac{1}{2}\mathbb{Z}^d$ by identifying each bond $b = (x,\mu)$ with the point $x + \frac{1}{2}\hat{e}_m u$. Then we take the lattice $\frac{1}{2}\mathbb{Z}^d$ and set the interaction equal to zero for all subsets of points, except those that correspond to a plaquette in the original lattice.

For each finite $\Lambda \subset \mathcal{B}$ and $\eta \in \mathcal{G}^{\mathcal{B}}$, $\mathbb{P}^\eta_{\beta,\Lambda}$ is a probability measure on $(\mathcal{G}^{\mathcal{B}}, \mathcal{F})$. These probability measures fulfill the following compatibility condition.

Lemma 2.2.1. *For any two finite subsets $\Lambda \subset \Lambda' \subset \mathcal{B}$, all $\eta \in \mathcal{G}^{\mathcal{B}}$ and any $\mathcal{F}$-measurable function $f : \mathcal{G}^{\mathcal{B}} \to \mathbb{R}$ we have*

$$\begin{aligned} &\int_{\mathcal{G}^{\mathcal{B}}} \mathrm{d}\mathbb{P}^{\eta}_{\beta,\Lambda'}(\mathcal{U}') \int_{\mathcal{G}^{\mathcal{B}}} \mathrm{d}\mathbb{P}^{\{\mathcal{U}'_{\Lambda'},\eta_{\Lambda'^c}\}}_{\beta,\Lambda}(\mathcal{U}) f(\{\mathcal{U}_{\Lambda}, \mathcal{U}'_{\Lambda'\setminus\Lambda}, \eta_{\Lambda'^c}\}) \\ &= \int_{\mathcal{G}^{\mathcal{B}}} \mathrm{d}\mathbb{P}^{\eta}_{\beta,\Lambda'}(\mathcal{U}') f(\{\mathcal{U}'_{\Lambda'}, \eta_{\Lambda'^c}\}). \end{aligned} \tag{2.17}$$

Proof. The result follows by a simple renaming of variables, e.g. set for $b \in \Lambda$ $\tilde{U}_b = U_b$, $\hat{U}_b = U'_b$ and for $b \in \Lambda'\setminus\Lambda$, $\tilde{U}_b = U'_b$. Then the integration over $\hat{\mathcal{U}}$ cancels with $Z^{\{\hat{\mathcal{U}}_{\Lambda},\tilde{\mathcal{U}}_{\Lambda'\setminus\Lambda},\eta_{\Lambda'^c}\}}_{\beta,\Lambda} = Z^{\{\tilde{\mathcal{U}}_{\Lambda'},\eta_{\Lambda'^c}\}}_{\beta,\Lambda}$. □

This compatibility condition is the same as for conditional expectations of some (yet unknown) probability measure. Indeed, this inspires the notion of a *Gibbs measure* as a measure for which the conditional distributions, given the configuration η in the complement of any finite set Λ, are given by $\mathbb{P}^{\eta}_{\beta,\Lambda'}$.

Definition 2.2.2. *[12, Definition 4.2.12] A probability measure $\mathbb{P}_{\beta}$ on $(\mathcal{G}^{\mathcal{B}}, \mathcal{F})$ is a Gibbs measure for the gauge interaction S and $\beta > 0$, if and only if, for any finite $\Lambda \in \mathbb{Z}^d$ and all bounded $\mathcal{F}$-measurable functions $f : \mathcal{G}^{\mathcal{B}} \to \mathbb{R}$ we have*

$$\mathbb{P}_{\beta}(f|\mathcal{F}_{\Lambda^c}) = \mathbb{P}^{(\cdot)}_{\Lambda}. \tag{2.18}$$

The existence of such a Gibbs measure is guaranteed by rather weak assumptions on the underlying probability space and the interaction, [12, Cor. 4.2.17]. It suffices that $\mathcal{G}$ is compact, $S_p : \mathcal{G}^{\mathcal{B}} \to \mathbb{R}$ is continuous for all $p \in \mathcal{P}$ and that for any $b \in \mathcal{B}$ there is a constant $c_b < \infty$ such that

$$\sum_{p\in\mathcal{P}:b\in p} \|S_p\|_{\infty} \leq c_b\,. \tag{2.19}$$

Indeed, we have the uniform constant

$$\sum_{p\in\mathcal{P}:b\in p} \|S_p\|_{\infty} = \sum_{p\in\mathcal{P}:b\in p} \|\operatorname{Re}\operatorname{Tr}(\mathbb{1} - U_p)\| \leq 2(d-1)\cdot 2N \tag{2.20}$$

since any bond $b \in \mathcal{B}$ is part of $2(d-1)$ plaquettes and $U_p \in \mathcal{G}$, that is $U_p \in SO(N), SU(N)$ or $U(N)$. Therefore we obtain by [12, Theorem 4.2.15, Corollary 4.2.17]:

Lemma 2.2.3. *Let $\eta \in \mathcal{G}^{\mathcal{B}}$, $\beta > 0$ and $(\Lambda_n)_{n\in\mathbb{N}}$ be an increasing and absorbing sequence of finite subsets of $\mathcal{B}$, that means $\Lambda_n \subseteq \Lambda_{n+1}$ and for each finite $B \subset \mathcal{B}$ there is Λ_n such that $B \subset \Lambda_n$. Then there is a weakly converging subsequence of $(\mathbb{P}^{\eta}_{\beta,\Lambda_n})_{n\in\mathbb{N}}$ that converges to a Gibbs measure $\mathbb{P}_\beta$ on $(\mathcal{G}^{\mathcal{B}}, \mathcal{F})$ for the gauge interaction S and $\beta > 0$.*

Now, Dobrushin's uniqueness criterion (see for example [12, Theorem 4.3.1 and Equation (4.46)] or [35, Theorem V.1.1]) ensures the uniqueness of the Gibbs measure, provided

$$\sup_{b\in\mathcal{B}} \sum_{p\in\mathcal{P}:b\in p} (|p|-1)\, \|\mathrm{Re}\,\mathrm{Tr}(\mathbb{1}-U_p)\|_\infty \;<\; \beta^{-1}. \tag{2.21}$$

Applying this result we obtain:

Lemma 2.2.4. *Let $\eta \in \mathcal{G}^{\mathcal{B}}$,*

$$0 \;<\; \beta \;<\frac{1}{12N(d-1)} \tag{2.22}$$

and $(\Lambda_n)_{n\in\mathbb{N}}$ be an increasing and absorbing sequence of finite subsets of $\mathcal{B}$. Then the Gibbs measure $\mathbb{P}_\beta$ on $(\mathcal{G}^{\mathcal{B}}, \mathcal{F})$ from Lemma 2.2.3 is unique.

We note in passing, that the translations are measure preserving transformations with respect to $\widetilde{\mathbb{P}}$ and $\mathbb{P}_\beta$, that means for all $A \in \mathcal{F}$, $\ell \in \mathbb{Z}^d$

$$\widetilde{\mathbb{P}}(T^\ell A) = \widetilde{\mathbb{P}}(A) \quad \text{and} \quad \mathbb{P}_\beta(T^\ell A) = \mathbb{P}_\beta(A). \tag{2.23}$$

Put differently, $\mathbb{P}_\beta$ and $\widetilde{\mathbb{P}}$ are stationary w.r.t. the group $\mathbb{Z}^d$ of translations.

2.2.2 Ergodic probability measures

A stationary probability measure $\mathbb{P}$ is called *ergodic* iff, for all $A, A' \in \mathcal{F}$,

$$\frac{1}{(2L+1)^d} \sum_{l\in\mathbb{Z}^d,\ \|l\|_\infty \le L} \mathbb{P}(A \cap T^l A') \to \mathbb{P}(A)\mathbb{P}(A'), \quad \text{as } L \to \infty, \tag{2.24}$$

with $\|l\|_\infty = \max\big\{|l_1|, \dots, |l_d|\big\}$.

A random variable $f : (\mathcal{G}^{\mathcal{B}}, \mathcal{F}) \to (\mathbb{R}, B)$ is called *invariant* iff $f(T^\ell \mathcal{U}) = f(\mathcal{U})$, for all $\ell \in \mathbb{Z}^d$ and almost all $\mathcal{U} \in \mathcal{G}^{\mathcal{B}}$. The importance of the notion of ergodicity lies in the fact that any invariant random variable is $\mathbb{P}$-almost surely constant.

In the following, we show that the measure $\mathbb{P}_\beta$ is ergodic, provided (2.22) holds true.

Lemma 2.2.5. *Assume*

$$0 \ < \ \beta \ < \frac{1}{12N(d-1)}, \tag{2.25}$$

such that the Gibbs measure $\mathbb{P}_\beta$ on $(\mathcal{G}^{\mathcal{B}}, \mathcal{F})$ is unique according to Lemma 2.2.4. Then $\mathbb{P}_\beta$ is also ergodic.

Proof. First, we specify the decay of correlations. We define a metric $d : \mathcal{B}\times\mathcal{B} \to \mathbb{R}_0^+$ on $\mathcal{B}$ by setting $d(b, b) := 0$ and

$$\begin{aligned} &d(b, b') := \\ &\min\big\{n|\exists\{p_1, \ldots, p_n\} \subset \mathcal{P} : b \in p_1,\ p_1 \cap p_2 \neq \emptyset, \ldots, p_{n-1} \cap p_n \neq \emptyset,\ b' \in p_n\big\}, \end{aligned} \tag{2.26}$$

for $b, b' \in \mathcal{B}$, $b \neq b'$. I.e. $d(b, b')$ is the minimal number of plaquettes to connect b and b'.

If $p = (x; \mu, \nu)$, $\tilde{p} = (\tilde{x}; \tilde{\mu}, \tilde{\nu})$, and $p\cap\tilde{p} \neq \emptyset$ then $\|x-\tilde{x}\|_\infty \leq 1$. Therefore, the minimal number of plaquettes connecting $b = (x, \mu) \in \mathcal{B}$ and $b' = (y, \nu) \in \mathcal{B}$ is at least $\|x-y\|_\infty$. Observing that, for all $x \in \mathbb{Z}^d$, $\mu, \nu, \tau \in \{1, \ldots, d\}$, $\nu \neq \mu \neq \tau$,

$$\begin{aligned} p(x; \mu, \nu) \cap p(x + \hat{e}_\mu; \mu, \nu) &\neq \emptyset \\ p(x; \mu, \nu) \cap p(x - \hat{e}_\mu; \mu, \nu) &\neq \emptyset \\ p(x; \mu, \nu) \cap p(x; \mu, \tau) &\neq \emptyset, \end{aligned} \tag{2.27}$$

we obtain, with $b = (x, \mu)$, $b' = (y, \nu) \in \mathcal{B}$ as above, that

$$\|x - y\|_\infty \ \leq \ d(b, b') \ \leq \ \|x - y\|_1 + d, \tag{2.28}$$

with $\|x - y\|_1 = \sum_{i=1}^d |x_i - y_i|$.
A modified version of the metric d called $\tilde{d}$ is obtained by multiplying d with $\ln(\frac{c}{\beta})$, where $c > \beta$,

$$\tilde{d}(\cdot, \cdot) := \ln(\frac{c}{\beta})d(\cdot, \cdot). \tag{2.29}$$

Now, we take two cylinder sets $A, A' \in \mathcal{F}$ and show that condition (2.24) is fulfilled for A and A'. Since the sigma-algebra $\mathcal{F}$ is generated by $\mathcal{Z}$, (2.24) extends to all $\mathcal{F}$ by a monotone class argument. There are two finite sets $\Lambda_A, \Lambda_{A'} \subset \mathcal{B}$ and $A_b, A'_{b'} \in \mathcal{F}_0$ for all $b \in \Lambda_A$, $b' \in \Lambda_{A'}$ such that

$$A = \bigtimes_{b\in\Lambda_A} A_b \times \mathcal{G}^{\mathcal{B}\setminus\Lambda_A}, \ \ A' = \bigtimes_{b'\in\Lambda_{A'}} A'_{b'} \times \mathcal{G}^{\mathcal{B}\setminus\Lambda_{A'}} \tag{2.30}$$

Let us choose $\chi_{A,\epsilon}, \chi_{A',\epsilon} \in C(\mathcal{G}^{\mathcal{B}}, [0,1])$ such that $\chi_{A,\epsilon}, \chi_{A',\epsilon}$ depend only on the variables U_b with $b \in \Lambda_A$ or $b \in \Lambda_{A'}$, respectively, $\chi_{A,\epsilon}(\mathcal{U}) = 1$, $\chi_{A',\epsilon}(\mathcal{U}') = 1$, for all $\mathcal{U} \in A, \mathcal{U}' \in A'$, and

$$\mathbb{P}_\beta\big\{\mathcal{U} \in A^C \mid \chi_{A,\epsilon}(\mathcal{U}) > 0\big\} < \epsilon\,, \quad \mathbb{P}_\beta\big\{\mathcal{U}' \in A'^C \mid \chi_{A',\epsilon}(\mathcal{U}') > 0\big\} < \epsilon. \tag{2.31}$$

Then $\chi_{A,\epsilon}, \chi_{A',\epsilon}$ are continuous functions that differ from the characteristic function of A, A' only on a set of measure less than ϵ.

Now, we use a result of [21] summarized in [35, Theorem V.2.1]. It states that, if $\gamma < 1$, where γ is a constant depending on the interaction, one gets for any two bonds $i, j \in \mathcal{B}$ that

$$\begin{aligned}\left|\int_{\mathcal{G}^{\mathcal{B}}} \chi_{A,\epsilon}\, \chi_{A',\epsilon}\, \mathrm{d}\mathbb{P}_\beta - \int_{\mathcal{G}^{\mathcal{B}}} \chi_{A,\epsilon}\, \mathrm{d}\mathbb{P}_\beta \int_{\mathcal{G}^{\mathcal{B}}} \chi_{A',\epsilon}\, \mathrm{d}\mathbb{P}_\beta\right| & \\ \leq \frac{1}{4}\, e^{-\tilde{d}(i,j)}(1-\gamma)^{-1}\, \Delta_i(\chi_{A,\epsilon})\, \Delta_j(\chi_{A',\epsilon}), &\end{aligned} \tag{2.32}$$

where

$$\Delta_j(f) := \sum_{i\in\mathcal{B}} e^{\tilde{d}(i,j)} \sup\left\{\, |f(\mathcal{U}) - f(\mathcal{U}')| \;\middle|\; U_b = U_b',\ b \neq i\,\right\} \tag{2.33}$$

and

$$\gamma = \sup_j \sum_{i\in\mathcal{B}, i\neq j} e^{\tilde{d}(i,j)} \rho_{ij}. \tag{2.34}$$

In our case ρ_{ij} for $i \neq j$, can be estimated as [35, page 403]

$$\rho_{ij} \leq \sum_{p\in\mathcal{P}: i,j\in p} \|\beta\, \mathrm{Re}\, \mathrm{Tr}(\mathbb{1} - U_p)\| \leq 2N\beta\; \mathbb{1}[d(i,j) = 1], \tag{2.35}$$

such that we get by inserting (2.35) into (2.34)

$$\gamma \leq 3 \cdot 2(d-1) 2N\beta \cdot \frac{c}{\beta}, \tag{2.36}$$

and $\gamma < 1$ corresponds to

$$c \;<\; \frac{1}{12N(d-1)}. \tag{2.37}$$

Since $\beta < \frac{1}{12N(d-1)}$ we can always find a c with $\beta < c < \frac{1}{12N(d-1)}$, such that $\gamma < 1$.

We denote the *distance* of A and A' by

$$\mathrm{dist}(A, A') := \min\{d(i,j) | i \in \Lambda_A, j \in \Lambda_{A'}\} \tag{2.38}$$

and the *diameter* of A by

$$D_A := \max\{d(i,j) | i, j \in \Lambda_A\}. \tag{2.39}$$

If $i \in \Lambda_A$ then

$$\Delta_i(\chi_{A,\epsilon}) \ \leq \ \sum_{k \in \mathcal{B}} e^{\tilde{d}(i,k)} \mathbb{1}[k \in \Lambda_A] \ \leq \ |\Lambda_A| (\frac{c}{\beta})^{D_A} \tag{2.40}$$

and analogously $\Delta_j(\chi_{A',\epsilon}) \leq |\Lambda_{A'}|(\frac{c}{\beta})^{D_{A'}}$, provided $j \in \Lambda_{A'}$. Inserting this into equation (2.32), and choosing $i \in \Lambda_A$ and $j \in \Lambda_{A'}$ such that $d(i,j) = \mathrm{dist}(A, A')$, we estimate

$$\begin{aligned} \Big| \int_{\mathcal{G}^{\mathcal{B}}} \chi_{A,\epsilon}\, \chi_{A',\epsilon}\, \mathrm{d}\mathbb{P}_\beta - \int_{\mathcal{G}^{\mathcal{B}}} \chi_{A,\epsilon}\, \mathrm{d}\mathbb{P}_\beta \int_{\mathcal{G}^{\mathcal{B}}} \chi_{A',\epsilon}\, \mathrm{d}\mathbb{P}_\beta \Big| & \\ \leq \frac{1}{4} \left(\frac{\beta}{c} \right)^{\mathrm{dist}(A,A') - (D_A + D_{A'})} \frac{|\Lambda_A|\, |\Lambda_{A'}|}{1 - 12N(d-1)c}, & \end{aligned} \tag{2.41}$$

for all $0 < \beta < c < (12N(d-1))^{-1}$. In the limit $\epsilon \to 0$, we obtain

$$|\mathbb{P}_\beta(A \cap A') - \mathbb{P}_\beta(A)\mathbb{P}_\beta(A')| \ \leq \ C_{A,A'} \left(\frac{\beta}{c} \right)^{\mathrm{dist}(A,A')}, \tag{2.42}$$

where

$$C_{A,A'} \ = \ \frac{1}{4} \, \frac{1}{1 - 12N(d-1)c} |\Lambda_A||\Lambda_{A'}| \left(\frac{c}{\beta} \right)^{D_A + D_{A'}} \tag{2.43}$$

is a constant independent of the distance of A and A'.

The exponential decay of correlations implies at once,

$$\begin{aligned} & \frac{1}{(2L+1)^d} \sum_{\ell \in \mathbb{Z}^d,\ \|\ell\|_\infty \leq L} \big| \, \mathbb{P}_\beta(A \cap T^\ell A') - \mathbb{P}_\beta(A)\, \mathbb{P}_\beta(A') \, \big| \\ & \qquad \leq \frac{1}{(2L+1)^d} \sum_{\ell \in \mathbb{Z}^d,\ \|\ell\|_\infty \leq L} C_{A,A'} \left(\frac{\beta}{c} \right)^{\mathrm{dist}(A, T^\ell A')} \\ & \qquad \leq \frac{1}{(2L+1)^d} \sum_{m=0}^{L} 2d(2m+1)^{d-1} C_{A,A'} \left(\frac{\beta}{c} \right)^{m - \mathrm{dist}(A,A') - 2(D_A + D_{A'})} \\ & \qquad \leq \frac{2dC_{A,A'}}{2L+1} \left(\frac{\beta}{c} \right)^{-\mathrm{dist}(A,A') - 2(D_A + D_{A'})} \frac{1}{1 - \frac{\beta}{c}} \stackrel{L \to \infty}{\longrightarrow} 0, \end{aligned} \tag{2.44}$$

where we used that $d(k,T^\ell k) \leq d(i,k) + d(i,j) + d(T^\ell k, j)$ and thus

$$\begin{aligned}\operatorname{dist}(A, T^\ell A') &= \min\{d(i,j) | i \in \Lambda_A, j \in T^\ell \Lambda_{A'}\} \\ &\geq \min\{d(k,T^\ell k) | k \in \Lambda_{A'}\} - \max\{d(i,k) | i \in \Lambda_A, k \in \Lambda_{A'}\} \\ &\quad - \max\{d(T^\ell k, j) | k \in \Lambda_{A'}, j \in T^\ell \Lambda_{A'}\} \\ &\geq \|\ell\|_\infty - D_A - 2D_{A'} - \operatorname{dist}(A, A'). \end{aligned} \tag{2.45}$$

□

2.2.3 Ergodic families of Wilson Dirac operators

In this section we specify the considered operators. The dependence of those operators $D_{\mathcal{U}}$ on the gauge field configuration is emphasized by the index $\mathcal{U}$. We consider the corresponding family of operators $\{D_{\mathcal{U}}\}_{\mathcal{U} \in \mathcal{G}^{\mathcal{B}}}$.

Let $\{D_{\mathcal{U}}\}_{\mathcal{U} \in \mathcal{G}^{\mathcal{B}}}$ be a family of bounded, self-adjoint operators on the Hilbert space $\mathcal{H} = \ell^2(\mathbb{Z}^d; \mathbb{C}^k)$. We call this family *stationary* if it depends on the gauge field configuration $\mathcal{U} \in \mathcal{G}^{\mathcal{B}}$ in such a way that translations act transitively, i.e.,

$$\tau^\ell D_{\mathcal{U}} \tau^{-\ell} = D_{T^\ell \mathcal{U}} \tag{2.46}$$

for all $\mathcal{U} \in \mathcal{G}^{\mathcal{B}}$ and $\ell \in \mathbb{Z}^d$, where τ^ℓ denotes the corresponding translation on $\mathcal{H}$, i.e.,

$$[\tau^\ell \phi](x) = \phi(x - \ell), \tag{2.47}$$

for any $\phi \in \mathcal{H}$, $x \in \mathbb{Z}^d$. A stationary family $\{D_{\mathcal{U}}\}_{\mathcal{U} \in \mathcal{G}^{\mathcal{B}}}$ is called *ergodic* if the underlying probability measure $\mathbb{P}$ on $\mathcal{G}^{\mathcal{B}}$ is stationary and ergodic. The crucial fact about ergodic families $\{D_{\mathcal{U}}\}_{\mathcal{U} \in \mathcal{G}^{\mathcal{B}}}$ is the independence of their spectra on $\mathcal{U}$, $\mathbb{P}$-almost surely, see [32].

We assume that $D_{\mathcal{U}}$ includes only nearest-neighbour interaction, i.e., for $\phi \in \mathcal{H}$, $x \in \mathbb{Z}^d$, $[D_{\mathcal{U}}\phi](x)$ depends only on the values of $\phi(x)$, $\phi(y)$ for those y with $|x-y| = 1$ and the gauge fields $U_{x,\mu}$, $U_{x,-\mu}$ for $\mu \in \{1, \ldots, d\}$, where we use the notation $U_{x,-\mu} := U_{x-\hat{e}_\mu,\mu}$.

There are various examples for such operators of physical interest. As mentioned in the introduction, we are mainly interested in the Wilson Dirac operator and the staggered fermions operator. For simplicity, we concentrate our attention to the Wilson Dirac operator int he following. Theorem 2.3.1 can be similarly formulated for every ergodic family of self–adjoint operators of finite range.

In lattice gauge theories the Wilson Dirac operator D is used [30], which is a discretized version of the QCD-Dirac operator. The corresponding matter fields are defined on the hypercubic lattice $\mathbb{Z}^4$ and are assumed to have a Dirac structure labeled by Dirac indices $\alpha \in \{1,2,3,4\}$, as well as a colour structure with labels $c \in \{1,\ldots,N_c\}$. The Dirac structure is represented by the 4×4 Euclidean Dirac matrices $\{\gamma_\mu\}_{\mu=1,\ldots,4}$. A customary explicit representation is

$$\gamma_{1,2,3} = \begin{pmatrix} 0 & -i\sigma_{1,2,3} \\ i\sigma_{1,2,3} & 0 \end{pmatrix} \quad , \quad \gamma_4 = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix} \tag{2.48}$$

with $\sigma_{1,2,3}$ being the Pauli matrices. The Dirac matrices form a Clifford-Algebra since they fulfill $\{\gamma_\mu,\gamma_\nu\} = 2\delta_{\mu\nu}$. Introducing $\gamma_5 := \gamma_1\gamma_2\gamma_3\gamma_4$, i.e.,

$$\gamma_5 = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix}, \tag{2.49}$$

we observe that $\{\gamma_\mu,\gamma_5\} = 0$.

The gauge group is $\mathcal{G} = SU(N_c)$ and acts on the colour structure. Therefore, $k = 4\cdot N_c$, and $\phi = \{\phi_{\alpha,c}\}_{\alpha=1,\ldots,4,\ c=1\ldots,N_c} \in \ell^2(\mathbb{Z}^4,\mathbb{C}^k)$. The Wilson Dirac operator D is defined by

$$\begin{aligned}[D\phi]_{\alpha,c}(x) := \sum_{\beta=1}^{4} \big\{ &(\gamma_5)_{\alpha,\beta}\phi_{\beta,c}(x) \\ - \kappa \sum_{\mu=1}^{4}\sum_{\sigma=\pm1}\sum_{f=1}^{N_c} &\big((r\gamma_5)_{\alpha,\beta} - \sigma(\gamma_5\gamma_\mu)_{\alpha,\beta}\big)\ (U_{x,\sigma\mu})_{c,f}\ \phi_{\beta,f}(x+\sigma\hat{e}_\mu)\big\},\end{aligned} \tag{2.50}$$

in short,

$$[D\phi](x) = \gamma_5\big[\phi(x) - \kappa\sum_{\mu=1}^{4}\sum_{\sigma=\pm1}(r-\sigma\gamma_\mu)U_{x,\sigma\mu}\,\phi(x+\sigma\hat{e}_\mu)\big]\ . \tag{2.51}$$

The parameter $r \in (0,1]$ is the Wilson parameter and $\kappa > 0$ the hopping parameter.

Displaying the dependence of D on the gauge field configuration $\mathcal{U}$ by writing $D_\mathcal{U}$, we observe that $D_\mathcal{U}$ fulfills condition (2.46) for any $\mathcal{U} \in \mathrm{SU}(N_c)^\mathcal{B}$ and any

$\phi \in \mathcal{H}, x \in \mathbb{Z}^d$,

$$
\begin{aligned}
[\tau^{\ell} D_{\mathcal{U}} \tau^{-\ell} \phi](x) &= [D_{\mathcal{U}} \tau^{-\ell} \phi](x-\ell) \\
&= [\tau^{-\ell}\phi](x-\ell) - \kappa \sum_{\mu=1}^{4} \sum_{\sigma=\pm 1} (r+\gamma_{\sigma\mu}) U_{x-\ell,\sigma\mu} \, [\tau^{-\ell}\phi](x-\ell+\sigma\hat{e}_\mu) \\
&= \phi(x) - \kappa \sum_{\mu=1}^{4} \sum_{\sigma=\pm 1} (r+\gamma_{\sigma\mu}) U_{x-\ell,\sigma\mu} \, \phi(x+\sigma\hat{e}_\mu) \\
&= [D_{T^{\ell}\mathcal{U}}\phi](x) \qquad (2.52)
\end{aligned}
$$

and hence we have

$$\tau^{\ell} D_{\mathcal{U}} \tau^{-\ell} = D_{T^{\ell}\mathcal{U}}, \qquad (2.53)$$

for all $\ell \in \mathbb{Z}^d$ and $\mathcal{U} \in SU(N_c)^{\mathcal{B}}$. Thus, if $\mathbb{P}_\beta$ is ergodic, so is $\{D_{\mathcal{U}}\}_{\mathcal{U}\in SU(N_c)^{\mathcal{B}}}$, and its spectrum is $\mathbb{P}_\beta$-almost surely constant.

2.2.4 The integrated density of states

In the following we study the *integrated density of states* of $\{D_{\mathcal{U}}\}_{\mathcal{U}\in\mathcal{G}^{\mathcal{B}}}$, which represents the number of eigenstates per unit volume. For the precise definition of the integrated density of states, we restrict our analysis to a finite subset $\Lambda \subset \mathbb{Z}^d$. Besides, this also allows us to relate our analysis to numerical simulation.

The *boundary* of Λ, denoted $\partial\Lambda$, is defined as

$$\partial\Lambda \;:=\; \big\{ y \in \Lambda \mid \exists\, x \in \Lambda^C,\ |x-y| = 1 \big\} \;\subseteq\; \Lambda. \qquad (2.54)$$

Furthermore we use the canonical orthonormal basis $\mathcal{E}_{\mathcal{H}} := \big\{\hat{s}^{(x,i)}\big\}_{x\in\mathbb{Z}^d, i\in\{1,\ldots,k\}}$ of $\mathcal{H}$ where the $\mathbb{Z}^d$-sequence $\hat{s}^{(x,i)}$ is set to be

$$\hat{s}^{(x,i)}(y) := \begin{cases} \hat{e}_i, & x = y \\ 0, & x \neq y \end{cases} \qquad (2.55)$$

with $\hat{e}_i \in \mathbb{C}^k$ the unit vector in direction i.

Since $D_{\mathcal{U}}$ contains only nearest-neighbour hopping, the value of $D_{\mathcal{U}}\hat{s}^{(x,i)}$ does not change, if we replace $D_{\mathcal{U}}$ by a restriction of $D_{\mathcal{U}}$ to Λ, for any point x in $\Lambda\backslash\partial\Lambda$. Only the boundary $\partial\Lambda$ needs further specification. We present two customary choices for this, namely, Dirichlet boundary conditions and periodic boundary conditions.

Dirichlet boundary conditions

First, we restrict the operators to the finite subset $\Lambda \subset \mathbb{Z}^d$ by means of the projection

$$P_\Lambda^{(dir)} : \mathcal{H} \to \mathcal{H}_\Lambda^{(dir)}, \quad \big[P_\Lambda^{(dir)}\varphi\big](x) := \begin{cases} \varphi(x), & x \in \Lambda, \\ 0, & x \notin \Lambda, \end{cases} \tag{2.56}$$

with

$$\mathcal{H}_\Lambda^{(dir)} \;=\; \ell^2(\Lambda, \mathbb{C}^k) \subset \mathcal{H} \tag{2.57}$$

being the Hilbert space of sequences vanishing outside Λ. Note that

$$P_{T^\ell\Lambda}^{(dir)} = \tau^\ell P_\Lambda^{(dir)} \tau^{-\ell}. \tag{2.58}$$

Then we define

$$D_{\Lambda,\mathcal{U}}^{(dir)} = P_\Lambda^{(dir)} D_{\mathcal{U}} P_\Lambda^{(dir)} : \mathcal{H}_\Lambda^{(dir)} \to \mathcal{H}_\Lambda^{(dir)}. \tag{2.59}$$

Note that, since $\mathcal{H}_\Lambda^{(dir)}$ is finite-dimensional, $D_{\Lambda,\mathcal{U}}^{(dir)}$ can be represented by a matrix of size $(k|\Lambda|) \times (k|\Lambda|)$, where $|\Lambda|$ denotes the number of elements in Λ. Since $D_{\mathcal{U}}$ is self-adjoint, so is $D_{\Lambda,\mathcal{U}}^{(dir)}$. The number of eigenvalues of $D_{\Lambda,\mathcal{U}}^{(dir)}$ smaller than some $E \in \mathbb{R}$, counting multiplicity, is denoted by

$$N_{\Lambda,\mathcal{U}}^{(dir)}(E) \;:=\; \mathrm{Tr}\,\big\{\mathbb{1}[D_{\Lambda,\mathcal{U}}^{(dir)} \;< E]\big\}. \tag{2.60}$$

The integrated density of states of $D_{\Lambda,\mathcal{U}}^{(dir)}$ is defined as the number of eigenvalues smaller than E per unit volume,

$$\rho_{\Lambda,\mathcal{U}}^{(dir)}(E) \;:=\; \frac{1}{|\Lambda|} N_{\Lambda,\mathcal{U}}^{(dir)}(E). \tag{2.61}$$

Clearly, $N_{\Lambda,\mathcal{U}}^{(dir)}(E)$ depends only on the gauge fields on the bonds connecting points in Λ. Note that probabilistic statements about $N_{T^\ell\Lambda,\mathcal{U}}^{(dir)}(E)$ do not depend on $\ell \in \mathbb{Z}^d$, since $\mathbb{P}_\beta$ and $D_{\mathcal{U}}$ are stationary.

Periodic boundary conditions

Another way to restrict $D_{\mathcal{U}}$ to a finite set $\Lambda \subset \mathbb{Z}^d$ is to require periodic boundary conditions, which is often used in numerical simulations. In order to define periodic boundary conditions we assume Λ to be a cube of side length L. Without loss of generality we may assume that $\Lambda = \{1, 2, \ldots, L\}^d$.

We define the Wilson Dirac operator on $\ell^2(\Lambda^{(per)}; \mathbb{C}^k)$ with periodic boundary conditions by

$$\big[D^{(per)}_{\Lambda,\mathcal{U}}\phi\big](x) \ := \ \gamma_5\big[\phi(x) - \kappa \sum_{\mu=1}^{4} \sum_{\sigma=\pm 1} (r - \sigma\gamma_\mu) U_{x,\sigma\mu}\, \phi(x + \sigma\hat{e}_\mu)\big] \ , \tag{2.62}$$

where $\Lambda^{(per)} := (\mathbb{Z}/L\mathbb{Z})^d$ and $x + \sigma\hat{e}_\mu$ is determined only modulo multiples of L in all directions. Similarly

$$U_{x,-\mu} = U^{-1}_{x-\hat{e}_\mu,\mu}, \tag{2.63}$$

where $x - \hat{e}_\mu$ is also defined modulo L. Thus $D^{(per)}_{\Lambda,\mathcal{U}} : \mathcal{H}^{(per)}_\Lambda \to \mathcal{H}^{(per)}_\Lambda$, with

$$\mathcal{H}^{(per)}_\Lambda \ := \ \ell^2(\Lambda^{(per)}; \mathbb{C}^k), \tag{2.64}$$

only depends on the values of $\mathcal{U}$ for bonds $b \in \Lambda \times \{1, \ldots, d\}$, i.e., on

$$\mathcal{U}_\Lambda := \{U_{x,\mu}\}_{x\in\Lambda,\mu=1,\ldots,d}. \tag{2.65}$$

Since $\mathcal{H}^{(per)}_\Lambda$ is finite-dimensional, we can transcribe the definition of the integrated density of states to periodic boundary conditions. We set $N^{(per)}_{\Lambda,\mathcal{U}}(E)$ to be the number of eigenvalues, counting multiplicity, of $D^{(per)}_{\Lambda,\mathcal{U}}$ smaller than $E \in \mathbb{R}$ and define the integrated density of states in the periodic case as

$$\rho^{(per)}_{\Lambda,\mathcal{U}}(E) := \frac{1}{|\Lambda|} N^{(per)}_{\Lambda,\mathcal{U}}(E). \tag{2.66}$$

2.3 Main Theorem

Our aim is the definition of the integrated density of states for $\{D_{\mathcal{U}}\}_{\mathcal{U}\in\Omega}$. A natural way is to let Λ be a cube of side length L and investigate the case $L \to \infty$, the thermodynamic limit. As it turns out, the boundary conditions imposed is immaterial.

Theorem 2.3.1. *Let $(\mathcal{G}^{\mathcal{B}}, \mathcal{F}, \mathbb{P}_\beta)$ be the probability space defined in Section 2.2 and choose $0 < \beta < \frac{1}{12N(d-1)}$ (such that $\mathbb{P}_\beta$ is ergodic). Let $\{D_{\mathcal{U}}\}_{\mathcal{U}\in\mathcal{G}^{\mathcal{B}}}$ be the family of Wilson Dirac operators on $\mathcal{H}$. Let $(\Omega_n)_{n\in\mathbb{N}}$ be a sequence in $\mathbb{Z}^d$ of nested cubes, $\Omega_n \subseteq \Omega_{n+1}$, with $\Omega_n \nearrow \mathbb{Z}^d$.*

(i) Then the limits

$$\rho_{\mathcal{U}}^{(dir)}(E) \;:=\; \lim_{n\to\infty} \frac{1}{|\Omega_n|} N_{\Omega_n,\mathcal{U}}^{(dir)}(E) \tag{2.67}$$

and

$$\rho_{\mathcal{U}}^{(per)}(E) \;:=\; \lim_{n\to\infty} \frac{1}{|\Omega_n|} N_{\Omega_n,\mathcal{U}}^{(per)}(E) \tag{2.68}$$

exist for all $E \in \mathbb{R}$, $\mathbb{P}_\beta$-almost surely, and are independent of the sequence $(\Omega_n)_{n\in\mathbb{N}}$.

(ii) Furthermore, for all $E \in \mathbb{R}$, the <u>integrated density of states</u> $\rho(E)$, defined by

$$\rho_{\mathcal{U}}^{(dir)}(E) = \rho_{\mathcal{U}}^{(per)}(E) =: \rho(E), \tag{2.69}$$

is independent of the chosen boundary condition and of $\mathcal{U} \in \mathcal{G}^{\mathcal{B}}$, $\mathbb{P}_\beta$-almost surely.

We remark that Theorem 2.3.1 implies the existence of the density of states. That means there are measures $\nu, \nu_{\Omega_n,\mathcal{U}}^{(dir)}, \nu_{\Omega_n,\mathcal{U}}^{(per)}$ such that

$$\int_{-\infty}^{E} d\nu(r) = \rho(E)\ , \quad \int_{-\infty}^{E} d\nu_{\Omega_n,\mathcal{U}}^{(dir/per)}(r) = \frac{1}{|\Omega_n|} N_{\Omega_n,\mathcal{U}}^{(dir/per)}(E) \tag{2.70}$$

and $\nu = \mathrm{w} - \lim_{n\to\infty} \nu_{\Omega_n,\mathcal{U}}^{(dir/per)}$ for $\mathcal{U} \in M$, where $M \subset \mathcal{G}^{\mathcal{B}}$ is a set of measure one, such that equation (2.69) holds for all $\mathcal{U} \in M$. The only critical point is to prove the existence of ν, which follows since the family $\{\nu_{\Omega_n,\mathcal{U}}^{(dir/per)}\}_{n\in\mathbb{N}}$ is tight.

2.4 Proof of Theorem 2.3.1

2.4.1 An estimate on eigenvalues

Suppose, we take two disjoint sets $\Omega_1, \Omega_2 \subset \mathbb{Z}^d$ and an operator $D_{\mathcal{U}}$, that fulfills the requirements of Theorem 2.3.1. We can restrict $D_{\mathcal{U}}$ to Ω_1, Ω_2 and $\Omega_1 \cup \Omega_2$ as in (2.59) by means of the projections $P_{\Omega_1}^{(dir)}$, $P_{\Omega_2}^{(dir)}$ and $P_{\Omega_1\cup\Omega_2}^{(dir)}$. To simplify the notation we suppress the superscript (dir) in the following. Then we can determine the number of eigenvalues below some $E \in \mathbb{R}$ for all three restrictions, denoted by $N_{\mathcal{U},\Omega_1}(E)$, $N_{\mathcal{U},\Omega_2}(E)$ and $N_{\mathcal{U},\Omega_1\cup\Omega_2}(E)$, respectively. If $\operatorname{dist}(\Omega_1,\Omega_2) \geq 2$, we know that $N_{\mathcal{U},\Omega_1\cup\Omega_2}(E) = N_{\mathcal{U},\Omega_1}(E) + N_{\mathcal{U},\Omega_2}(E)$, since the operator $D_{\mathcal{U}}$ links only neighbouring sites. Our first goal is the derivation of an upper bound on the difference of $N_{\mathcal{U},\Omega_1}(E) + N_{\mathcal{U},\Omega_2}(E)$ and $N_{\mathcal{U},\Omega_1\cup\Omega_2}(E)$.

To this end, we start with a general observation for finite matrices.

Let A, B be complex, self-adjoint $(M \times M)$-matrices. The rank of B is denoted by b, and the interesting case is $b \ll M$. Since A and B are self-adjoint, so is $A + B$, and all three matrices A, B and $A + B$ have M real eigenvalues counting multiplicity. Due to the fact that $\operatorname{rank}(B) = b$, B has $(M - b)$ eigenvalues equal to zero, and b eigenvalues different from zero. Furthermore, we denote by $N_A \in \mathbb{N}_0$ the number of negative eigenvalues of A, by N_B, N_{-B}, N_{A+B} the number of negative eigenvalues of B, $-B$, and $A + B$, respectively.

Lemma 2.4.1. *Let A, B be self-adjoint $M \times M$-matrices. The difference of the number N_A of negative eigenvalues of A and the number N_{A+B} of negative eigenvalues of $A + B$ is at most* $\operatorname{rank}(B)$*,*

$$|N_A - N_{A+B}| \leq \operatorname{rank}(B). \tag{2.71}$$

Note, that the bound (2.71) is independent of $\|B\|$.

Proof. First, we show that $N_{A+B} - N_A \leq \operatorname{rank}(B)$. Let us assume that $N_{A+B} > N_A + \operatorname{rank}(B)$. Then the min-max principle ensures the existence of a subspace $X \subseteq \mathbb{C}^M$, with dimension $\dim(X) = N_A + \operatorname{rank}(B) + 1$ such that

$$\sup_{\phi \in X, \|\phi\|=1} \langle \phi | (A + B)\phi \rangle < 0. \tag{2.72}$$

In particular we have

$$\sup_{\phi \in X \cap \ker(B), \|\phi\|=1} \langle \phi | (A + B)\phi \rangle = \sup_{\phi \in X \cap \ker(B), \|\phi\|=1} \langle \phi | A\phi \rangle < 0. \tag{2.73}$$

Using the min-max principle again, we obtain

$$N_A \geq \dim(X \cap \ker(B)) \geq \dim(X) - \operatorname{rank}(B) = N_A + 1.$$

Therefore we have that $N_{A+B} - N_A \leq \operatorname{rank}(B)$. Now, we set $A' := A + B$, $B' := -B$ and get analogously $N_{A'+B'} - N_{A'} \leq \operatorname{rank}(B')$ that is $N_A - N_{A+B} \leq \operatorname{rank}(B)$. $\square$

Lemma 2.4.2. *Let $(\mathcal{G}^{\mathcal{B}}, \mathcal{F}, \mathbb{P}_\beta)$ be the probability space defined in Section 2.2.1 and choose $0 < \beta < \frac{1}{12N(d-1)}$ such that $\mathbb{P}_\beta$ is ergodic. Let $\{D_{\mathcal{U}}\}_{\mathcal{U}\in\mathcal{G}^{\mathcal{B}}}$ be the family of Wilson Dirac operators on $\mathcal{H}$. Furthermore let $\Omega_1, \ldots, \Omega_J \subset \mathbb{Z}^d$ be disjoint, finite sets and $\Omega := \bigcup_{j=1}^J \Omega_j$ their union.*

(i) Then we have, for any $\mathcal{U} \in \mathcal{G}^{\mathcal{B}}$ and all $E \in \mathbb{R}$,

$$\frac{1}{|\Omega|}\left| N^{(dir)}_{\Omega,\mathcal{U}}(E) - \sum_{j=1}^{J} N^{(dir)}_{\Omega_j,\mathcal{U}}(E)\right| \;\leq\; k\,\frac{\sum_{j=1}^J |\partial\Omega_j|}{|\Omega|}. \tag{2.74}$$

(ii) If in addition the sets $\Omega_1, \ldots, \Omega_J$ are cubes, such that Ω is also a cube, then

$$\frac{1}{|\Omega|}\left| N^{(per)}_{\Omega,\mathcal{U}}(E) - \sum_{j=1}^{J} N^{(per)}_{\Omega_j,\mathcal{U}}(E)\right| \;\leq\; 3k\,\frac{\sum_{j=1}^J |\partial\Omega_j|}{|\Omega|}, \tag{2.75}$$

for any $\mathcal{U} \in \mathcal{G}^{\mathcal{B}}$ and all $E \in \mathbb{R}$.

Proof. We remark that it is enough to prove the case $E = 0$, because we can replace $D_{\mathcal{U}}$ by $D_{\mathcal{U}} - E$. We start with the case of Dirichlet boundary conditions and define $(k|\Omega| \times k|\Omega|)$-matrices A and C by

$$A := D^{(dir)}_{\Omega,\mathcal{U}},\; C := \sum_{j=1}^{J} P_{\Omega_j} A P_{\Omega_j} \;\; : \; \mathcal{H}^{(dir)}_{\Omega} \to \mathcal{H}^{(dir)}_{\Omega}. \tag{2.76}$$

The matrices are chosen in such a way that we get with counting multiplicity

$$N^{(dir)}_{\Omega,\mathcal{U}}(0) = \mathrm{Tr}\left\{\mathbb{1}[A \geq 0]\right\} \tag{2.77}$$

and

$$\sum_{j=1}^{J} N^{(dir)}_{\Omega_j,\mathcal{U}}(0) = \mathrm{Tr}\left\{\mathbb{1}[C \geq 0]\right\}. \tag{2.78}$$

Now, we set the matrix $B := A - C$ to be the difference of A and C. The rank of B can be estimated as follows

$$\mathrm{rank}(B) \leq k \sum_{j=1}^{J} |\partial\Omega_j|, \tag{2.79}$$

using that $B = \sum_{j \neq l} P_{\Omega_j} A P_{\Omega_l}$. By Lemma 2.4.1, we obtain

$$\frac{1}{|\Omega|} \left| N_{\Omega,\mathcal{U}}(0) - \sum_{j=1}^{J} N_{\Omega_j,\mathcal{U}}(0) \right| \leq k \, \frac{\sum_{j=1}^{J} |\partial \Omega_j|}{|\Omega|} \, , \tag{2.80}$$

and *(i)* is proven.

To prove *(ii)*, we use that, for any cube Λ, we have that

$$\operatorname{rank} \left[D_{\Lambda,\mathcal{U}}^{(per)} - D_{\Lambda,\mathcal{U}}^{(dir)} \right] \ \leq \ k \, |\partial \Lambda| \tag{2.81}$$

Therefore, *(i)* and another application of Lemma 2.4.1 yield (2.75),

$$\begin{aligned} \frac{1}{|\Omega|} & \left| N_{\Omega,\mathcal{U}}^{(per)}(E) - \sum_{j=1}^{J} N_{\Omega_j,\mathcal{U}}^{(per)}(E) \right| \\ & \leq \frac{1}{|\Omega|} \Bigg(\left| N_{\Omega,\mathcal{U}}^{(per)}(E) - N_{\Omega,\mathcal{U}}^{(dir)}(E) \right| + \left| N_{\Omega,\mathcal{U}}^{(dir)}(E) - \sum_{j=1}^{J} N_{\Omega_j,\mathcal{U}}^{(dir)}(E) \right| \\ & \quad + \left| \sum_{j=1}^{J} (N_{\Omega_j,\mathcal{U}}^{(dir)}(E) - N_{\Omega_j,\mathcal{U}}^{(per)}(E)) \right| \Bigg) \\ & \leq 3k \, \frac{\sum_{j=1}^{J} |\partial \Omega_j|}{|\Omega|} . \end{aligned} \tag{2.82}$$

$\square$

Lemma 2.4.2 is an estimate on the change of the integrated density of states as the subset of $\mathbb{Z}^d$ is broken up into smaller pieces. The estimate is, indeed, precise enough to prove the existence of a limit in the sense of Theorem 2.3.1 as is done in the next sections.

2.4.2 Existence of the integrated density of states for a special sequence

In this section it is shown that a limit for the integrated density of states exists almost surely for a sequence of growing cubes in $\mathbb{Z}^d$.

To this end, we define the following sequence of growing cubes,

$$\Lambda_n := \{-l_0 2^{n-1} + 1, \ldots, l_0 2^{n-1}\}^d \, , \tag{2.83}$$

with $l_0 \in \mathbb{N}$ to be fixed later. Note that Λ_n has side length $l_0 2^n$.

The virtue of the sequence $(\Lambda_n)_{n\in\mathbb{N}}$ is, that Λ_{n+1} splits into 2^d disjoint cubes, each of size $|\Lambda_n|$, in a natural way. More precisely, there are $z_1, \ldots, z_{2^d} \in \mathbb{Z}^d$ such that, for

$$\Pi_n := \{T^{z_1}, \ldots, T^{z_{2^d}}\} \tag{2.84}$$

being the set of associated translations,

$$\Lambda_{n+1} = \bigcup_{T\in\Pi_n} T\Lambda_n. \tag{2.85}$$

In order to clarify the notation, we also introduce the sets Π_n^l for $l > n$ that consist of the translations needed to compose Λ_l of translations of Λ_n,

$$\Pi_n^l := \big\{T_n \ldots T_{l-1} : T_n \in \Pi_n, \ldots, T_{l-1} \in \Pi_{l-1}\big\}. \tag{2.86}$$

Thus, $\Pi_n = \Pi_n^{n+1}$ and we have

$$\Lambda_l = \bigcup_{T\in\Pi_n^l} T\Lambda_n, \tag{2.87}$$

see Figure 2.2. Next, we study the integrated density of states of Λ_n, as n grows. We omit the dependence of $N^{(dir)}_{\Lambda_n,\mathcal{U}}(E)$ and $N^{(per)}_{\Lambda_n,\mathcal{U}}(E)$ on E and the gauge field configuration $\mathcal{U}$ and write

$$N^{(dir)}[\Lambda_n] \ := \ N^{(dir)}_{\Lambda_n,\mathcal{U}}(E) \quad \text{and} \quad N^{(per)}[\Lambda_n] \ := \ N^{(per)}_{\Lambda_n,\mathcal{U}}(E) \tag{2.88}$$

instead.

Lemma 2.4.3. *For any $l_0 \in \mathbb{N}$, the sequences $\big(\frac{1}{|\Lambda_n|}N^{(dir)}[\Lambda_n]\big)_{n\in\mathbb{N}}$ and $\big(\frac{1}{|\Lambda_n|}N^{(per)}[\Lambda_n]\big)_{n\in\mathbb{N}}$ converge, $\mathbb{P}_\beta$-almost surely.*

$$\lim_{n\to\infty} \frac{1}{|\Lambda_n|} N^{(dir)}[\Lambda_n] \to \rho^{(dir)}_{l_0}, \qquad \lim_{n\to\infty} \frac{1}{|\Lambda_n|} N^{(per)}[\Lambda_n] \to \rho^{(per)}_{l_0}. \tag{2.89}$$

Furthermore

$$\lim_{n\to\infty} \frac{1}{|\Lambda_n|} \big|N^{(dir)}[\Lambda_n] - N^{(per)}[\Lambda_n]\big| = 0, \tag{2.90}$$

$\mathbb{P}_\beta$-almost surely, and $\rho_{l_0} := \rho^{(dir)}_{l_0} = \rho^{(per)}_{l_0}$.

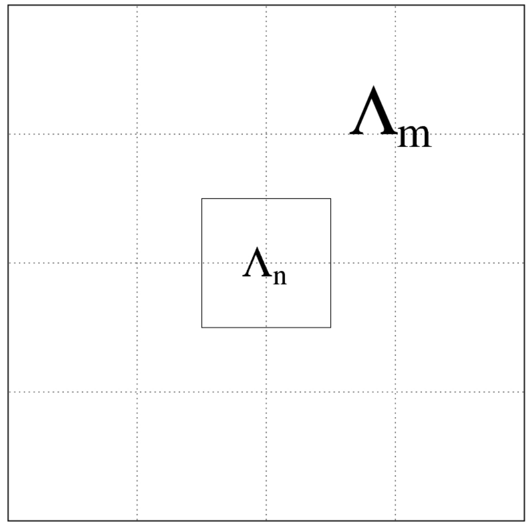

Figure 2.2: Λ_m and Λ_n in $\mathbb{Z}^2$, with $m = n + 2$. The dotted lines indicate the translates of Λ_n whose union gives Λ_m.

Proof. We show that $\left(\frac{1}{|\Lambda_n|} N^{(dir)}[\Lambda_n]\right)_{n\in\mathbb{N}}$ is a Cauchy sequence and in the proof we denote $N^{(dir)}[\Lambda_n] =: N[\Lambda_n]$. The proof for periodic boundary conditions is completely analogous.

Assume that $m > n$. By applying (2.87), one can split Λ_m into $2^{d(m-n)}$ cubes of size $|\Lambda_n|$,

$$\Lambda_m = \bigcup_{T\in\Pi_n^m} T\Lambda_n. \tag{2.91}$$

The mean integrated density of states for these translations of Λ_n is

$$\frac{1}{2^{d(m-n)}} \sum_{T\in\Pi_n^m} \frac{1}{|\Lambda_n|} N[T\Lambda_n] = \frac{1}{|\Lambda_m|} \sum_{T\in\Pi_n^m} N[T\Lambda_n]. \tag{2.92}$$

Thus we can estimate

$$\begin{aligned}
&\left| \frac{1}{|\Lambda_m|} N[\Lambda_m] - \frac{1}{|\Lambda_n|} N[\Lambda_n] \right| \\
&\quad \leq \frac{1}{|\Lambda_m|} \left| N[\Lambda_m] - \sum_{T\in\Pi_n^m} N[T\Lambda_n] \right| + \left| \frac{1}{|\Lambda_m|} \sum_{T\in\Pi_n^m} N[T\Lambda_n] - \frac{1}{|\Lambda_n|} N[\Lambda_n] \right|.
\end{aligned} \tag{2.93}$$

Lemma 2.4.2 directly gives us an upper bound for the first term on the right side of (2.93), since we have

$$\frac{1}{|\Lambda_m|}\left|N[\Lambda_m] - \sum_{T\in\Pi_n^m} N[T\Lambda_n]\right| \le k\,\frac{2^{d(m-n)}|\partial\Lambda_n|}{|\Lambda_m|}$$
$$\le k\,2^{d(m-n)}\,\frac{2d(l_0 2^n)^{d-1}}{(l_0 2^m)^d} \;=\; \frac{2dk}{l_0}\,2^{-n}, \quad (2.94)$$

independently of the gauge field configuration.

The second term on the right side of (2.93) is the difference of the integrated density of states for a cube Λ_n and its spatial mean over $2^{d(m-n)}$ translated disjoint cubes of the same size. As we do not know, yet, whether this term is small with high probability, provided n is large enough, we split Λ_n and its translates into smaller cubes of size $|\Lambda_{n_0}|$ for some $n_0 < n \in \mathbb{N}$, as indicated in Figure 2.3. We

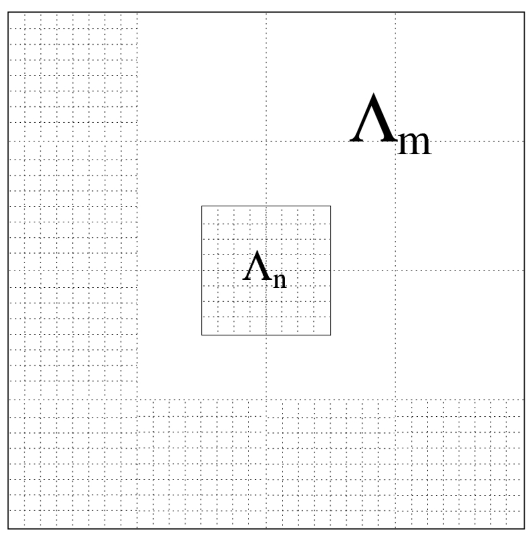

Figure 2.3: Both sets Λ_n and Λ_m are split up in smaller cubes of the same size as Λ_{n_0}. For Λ_m only part of the splitting is sketched.

estimate

$$\begin{aligned}
&\left|\frac{1}{|\Lambda_m|}\sum_{T\in\Pi_n^m} N[T\Lambda_n] - \frac{1}{|\Lambda_n|}N[\Lambda_n]\right| \\
&\leq \frac{1}{|\Lambda_m|}\sum_{T\in\Pi_n^m}\left|N[T\,\Lambda_n] - \sum_{T'\in\Pi_{n_0}^n} N[T'T\Lambda_{n_0}]\right| \\
&\quad + \left|\frac{1}{|\Lambda_m|}\sum_{T\in\Pi_{n_0}^m} N[T\Lambda_{n_0}] - \frac{1}{|\Lambda_n|}\sum_{T\in\Pi_{n_0}^n} N[T\Lambda_{n_0}]\right| \\
&\quad + \frac{1}{|\Lambda_n|}\left|\sum_{T\in\Pi_{n_0}^n} N[T\Lambda_{n_0}] - N[\Lambda_n]\right|, \qquad (2.95)
\end{aligned}$$

using that any $T \in \Pi_{n_0}^m$ is given as a product $T = T'T''$, for unique $T' \in \Pi_n^m$ and $T'' \in \Pi_{n_0}^n$. Then Lemma 2.4.2 yields again an upper bound for the first and the third term on the right side of (2.95), and analogously to (2.94), we obtain that

$$\frac{1}{|\Lambda_m|}\sum_{T\in\Pi_n^m}\left|N[T\Lambda_n] - \sum_{T'\in\Pi_{n_0}^n} N[T'T\Lambda_{n_0}]\right| \;\leq\; \frac{2dk}{l_0}\,2^{-n_0} \qquad (2.96)$$

and

$$\frac{1}{|\Lambda_n|}\left|\sum_{T\in\Pi_{n_0}^n} N[T\Lambda_{n_0}] - N[\Lambda_n]\right| \;\leq\; \frac{2dk}{l_0}\,2^{-n_0}. \qquad (2.97)$$

Thus equations (2.94), (2.95), (2.96), and (2.97) yield

$$\begin{aligned}
&\left|\frac{1}{|\Lambda_m|}N[\Lambda_m] - \frac{1}{|\Lambda_n|}N[\Lambda_n]\right| \\
&\leq \frac{4dk}{l_0}(2^{-n} + 2^{-n_0}) + \left|\frac{1}{|\Lambda_m|}\sum_{T\in\Pi_{n_0}^m} N[T\Lambda_{n_0}] - \frac{1}{|\Lambda_n|}\sum_{T\in\Pi_{n_0}^n} N[T\Lambda_{n_0}]\right|. \qquad (2.98)
\end{aligned}$$

We can choose n_0 and then $n > n_0$ so large that $\frac{4dk}{l_0}(2^{-n} + 2^{-n_0})$ is arbitrarily small. To estimate the remaining term, we view $\{Z_x(\mathcal{U})\}_{x\in\mathbb{Z}^d}$, with

$$Z_x(\mathcal{U}) := N[T^{2^{n_0}l_0x}\Lambda_{n_0}] = N^{(dir)}_{T^{2^{n_0}l_0x}\Lambda_{n_0},\mathcal{U}}(E), \qquad (2.99)$$

to be an invariant family of random variables. By the Ackoglu-Krengel (superadditive) ergodic theorem [20, Theorem VI.1.7, Remark VI.1.8], the mean of these random variables converges $\mathbb{P}_\beta$-almost surely. Hence,

$$\left(\frac{1}{|\Lambda_m|} \sum_{T \in \Pi_{n_0}^m} N[T\Lambda_{n_0}] \right)_{m=n_0+1}^{\infty} \tag{2.100}$$

is a Cauchy sequence, $\mathbb{P}_\beta$-almost surely.

As noted above, we can replace $N[\#]$ by $N^{(per)}[\#]$ and repeat the proof for periodic boundary conditions with exactly the same arguments, since all sets are cubes and Lemma 2.4.2(ii) applies.

Equation (2.90) is similarly proven as Lemma 2.4.2(ii),

$$\frac{1}{|\Lambda_n|} \left| N^{(dir)}[\Lambda_n] - N^{(per)}[\Lambda_n] \right| \;\le\; \frac{k|\partial\Lambda_n|}{|\Lambda_n|} \;\to\; 0, \quad n \to \infty\,. \tag{2.101}$$

□

Note that, while the preceding lemma holds for all $l_0 \in \mathbb{N}_0$, this does not imply the independence of the integrated density of states of the choice of l_0. It turns out, however, that not only the independence holds true, but that furthermore the size of the cubes in the sequence is immaterial, as long as it is monotonically growing.

2.4.3 Proof of main Theorem 2.3.1

The proof is similar to the one of Lemma 2.4.3. We choose $l_0, n_0 \in \mathbb{N}$ arbitrary, but fixed. Given Ω_n, there is an $m \in \mathbb{N}$ such that $\Omega_n \subseteq \Lambda_m$. We define

$$\begin{aligned} \Sigma_n &:= \left\{ T \in \Pi_{n_0}^m \mid T\Lambda_{n_0} \subseteq \Omega_n \right\}, \\ \widetilde{\Omega}_n &:= \bigcup_{T \in \Sigma_n} T\Lambda_{n_0} \;\subseteq\; \Omega_n \end{aligned} \tag{2.102}$$

Note that $\widetilde{\Omega}_n$ is a rectangular box, whose smallest side length is at most two times smaller than its largest side length and all side lengths are multiples of $l_0 2^{n_0}$. Moreover

$$|\Omega_n| - |\widetilde{\Omega}_n| = |\Omega_n \backslash \widetilde{\Omega}_n| \le |\partial\Omega_n| \cdot |\Lambda_{n_0}| \tag{2.103}$$

Now, we estimate for $n > n_0$, $\Omega_n \supseteq \Lambda_{n_0}$

$$\begin{aligned}\left|\frac{1}{|\Lambda_n|}N[\Lambda_n] - \frac{1}{|\Omega_n|}N[\Omega_n]\right| \le & \left|\frac{1}{|\Lambda_n|}N[\Lambda_n] - \frac{1}{|\Lambda_n|}\sum_{T\in\Pi^n_{n_0}} N[T\Lambda_{n_0}]\right| \\ & + \left|\frac{1}{|\Lambda_n|}\sum_{T\in\Pi^n_{n_0}} N[T\Lambda_{n_0}] - \frac{1}{|\widetilde{\Omega}_n|}\sum_{T\in\Sigma_n} N[T\Lambda_{n_0}]\right| \\ & + \left|\frac{1}{|\widetilde{\Omega}_n|}\sum_{T\in\Sigma_n} N[T\Lambda_{n_0}] - \frac{1}{|\widetilde{\Omega}_n|}N[\widetilde{\Omega}_n]\right| \\ & + \left|\frac{1}{|\widetilde{\Omega}_n|}N[\widetilde{\Omega}_n] - \frac{1}{|\Omega_n|}N[\Omega_n]\right|. \end{aligned} \tag{2.104}$$

In the first and third term we can apply Lemma 2.4.2 directly to get upper bounds vanishing in the limit $n \to \infty$. The second term converges $\mathbb{P}_\beta$-almost surely to zero, by the Ackoglu-Krengel ergodic theorem. For the last term we estimate the difference of the integrated density of states of $\widetilde{\Omega}_n$ and Ω_n,

$$\left|\frac{1}{|\widetilde{\Omega}_n|}N[\widetilde{\Omega}_n] - \frac{1}{|\Omega_n|}N[\Omega_n]\right| = \frac{\left||\widetilde{\Omega}_n| \cdot N[\Omega_n] - |\Omega_n| \cdot N[\widetilde{\Omega}_n]\right|}{|\widetilde{\Omega}_n| \cdot |\Omega_n|}. \tag{2.105}$$

First, we estimate

$$\begin{aligned}\Big||\Omega_n| \cdot N[\widetilde{\Omega}_n] - & |\widetilde{\Omega}_n| \cdot N[\Omega_n]\Big| \\ & = \left||\Omega_n|\big(N[\widetilde{\Omega}_n] - N[\Omega_n]\big) + \big(|\Omega_n| - |\widetilde{\Omega}_n|\big)N[\Omega_n]\right| \\ & \le |\Omega_n| \left|N[\Omega_n] - N[\widetilde{\Omega}_n]\right| + \big(|\Omega_n| - |\widetilde{\Omega}_n|\big)N[\Omega_n]. \end{aligned} \tag{2.106}$$

Then we observe that

$$|N[\Omega_n] - N[\widetilde{\Omega}_n]| \ \le \ k|\partial\widetilde{\Omega}_n| + (2d+1)k(|\Omega_n| - |\widetilde{\Omega}_n|) \tag{2.107}$$

holds true because of the following estimate using Lemma 2.4.2

$$
\begin{aligned}
\Big|N[\Omega_n]-N[\widetilde{\Omega}_n]\Big| - \Big|\sum_{x\in\Omega_n\setminus\widetilde{\Omega}_n} N[\{x\}]\Big| \\
&\leq \Big|N[\Omega_n]-\Big(N[\widetilde{\Omega}_n]+\sum_{x\in\Omega_n\setminus\widetilde{\Omega}_n} N[\{x\}]\Big)\Big| \\
&\leq k\Big(|\partial\widetilde{\Omega}_n|+2d(|\Omega_n|-|\widetilde{\Omega}_n|)\Big). \qquad (2.108)
\end{aligned}
$$

Thus we get

$$
\begin{aligned}
\Big|\frac{1}{|\widetilde{\Omega}_n|}N[\widetilde{\Omega}_n]-\frac{1}{|\Omega_n|}N[\Omega_n]\Big| \\
&\leq \frac{1}{|\widetilde{\Omega}_n|}|N[\Omega_n]-N[\widetilde{\Omega}_n]|+\frac{1}{|\Omega_n|}N[\Omega_n]\frac{(|\Omega_n|-|\widetilde{\Omega}_n|)}{|\widetilde{\Omega}_n|} \\
&\leq \frac{k|\partial\widetilde{\Omega}_n|}{|\widetilde{\Omega}_n|}+\frac{(2d+2)k(|\Omega_n|-|\widetilde{\Omega}_n|)}{|\widetilde{\Omega}_n|} \overset{n\to\infty}{\longrightarrow} 0, \qquad (2.109)
\end{aligned}
$$

by using equations (2.106), (2.107) and the fact that $\frac{1}{|\Omega_n|}N[\Omega_n]\leq k$. Altogether we have proven

$$\lim_{n\to\infty}\Big|\frac{1}{|\Lambda_n|}N[\Lambda_n]-\frac{1}{|\Omega_n|}N[\Omega_n]\Big|=0, \qquad (2.110)$$

$\mathbb{P}_\beta$-almost surely. The periodic case is again proven completely analogously.

Recall that Lemma 2.4.3 gives the existence of the limit

$$\rho_{\mathcal{U}}(E):=\lim_{n\to\infty}\frac{1}{|\Lambda_n|}N^{(dir)}_{\Lambda_n,\mathcal{U}}(E)=\lim_{n\to\infty}\frac{1}{|\Lambda_n|}N^{(per)}_{\Lambda_n,\mathcal{U}}(E) \qquad (2.111)$$

with $(\Lambda_n)_{n\in\mathbb{N}}$ as in (2.83), $\mathbb{P}_\beta$-almost surely. Equation (2.110) ensures the independence of this limit of the chosen sequence $(\Omega_n)_{n\in\mathbb{N}}$. Furthermore, Lemma 2.4.3 implies that the limit for periodic boundary conditions is the same.

Since the integrated density of states is invariant under translations, it is $\mathbb{P}_\beta$-almost surely constant, and *(ii)* follows. This finishes the proof of Theorem 2.3.1.

Chapter 3

Hartree–Fock Theory for Random Schrödinger Operators

The theory of random Schrödinger operators has developed since the middle of the last century, going back to the work of Anderson and Mott. The idea is to model a disordered quantum mechanical system, for example a crystal with impurities or dislocations, by introducing a random potential or a random displacement of the lattice sites. As it turns out, those systems show the tendency to have localized states, i.e., there is dense point spectrum, at certain regimes of the spectrum. This effect is the famous Anderson localization. The theory of random Schrödinger operators is very successful and has led to deeper mathematical understanding, as for example the theory of ergodic operator families, which have a non-random spectrum [32, 29].

The state of the art is to handle systems with finitely many interacting fermions in the thermodynamic limit [1]. At that point, the question of a system of infinitely many interacting fermions, as for example a system with constant fermion density in the thermodynamic limit, arises naturally.

The following chapter can be seen as a first modest step in this direction - we aim to apply the Hartree-Fock theory to a system of electrons in a crystal with impurities, which are modeled as in the random Schrödinger operator theory by a random potential, and then take the thermodynamic limit. The principal idea of the Hartree-Fock approximation is to give an upper bound to the energy of the ground state of a quantum mechanical system, that is the lowest eigenvalue of the corresponding Hamiltonian H, by minimizing $\langle \phi, H\phi \rangle$ only over Slater determinants, i.e., product wave functions. We consider finite systems first, and for the case of reduced Hartree-Fock theory at positive temperatures and fixed chemical potential the limit of an infinite system is also considered. We proof the existence of a unique minimizer in the thermodynamic limit in the weak-* sense and show that this minimizers as well as the corresponding effective Hamiltonians form ergodic operator families, hence have a non-random spectrum.

Very recently, a similar setup was also considered by Cancès, Lahbabi and Lewin [19], where some results for the reduced Hartree-Fock case are similar to the ones presented here. The main difference to our work is that we consider general finite range interactions which have a strictly positive Fourier transform, whereas in [19] the Coulomb- and Yukawa-potential are considered more explicitly.

3.1 Introduction of the model

In this section we describe the precise set-up of the model under consideration and give an introduction to (reduced) Hartree-Fock theory for zero temperature and also for positive temperatures. As mentioned above, the Hartree-Fock functional is an approximation for the energy of the ground state of a system with finitely many fermions. It takes into account the energy of each fermion with respect to the external, in our case random, potential. A second part represents the interaction between the fermions, via a certain interaction potential, and in the case of positive temperatures a third term is added, which yields the entropy of the system.

This section is organized as follows: First, we introduce the 1-particle Hamiltonian h_ω, representing the interaction of a single particle with the random potential. Then the interaction W between two fermions is described in Section 3.1.2. We review the formalism of a many-fermion system in Section 3.1.3, before introducing the Hartree-Fock functional and the reduced Hartree-Fock functional for temperature $T = 0$ and $T > 0$ in Section 3.1.4.

3.1.1 Random Schrödinger Operators

The starting point is to describe the propagation and the interaction of a single fermion with the background of impurities in the cubic crystal. This is done by the *1-particle Hamiltonian*. We take as 1-particle Hamiltonian the lattice Anderson-Hamiltonian acting on the Hilbert space $\mathcal{H} = \ell^2(\mathbb{Z}^d)$.

More specifically, we introduce an independently and identically distributed (i.i.d.) random potential in $\mathbb{Z}^d$. Let $(\Omega_0, \mathfrak{A}_0, \mathbb{P}_0)$ be a probability space, where $\Omega_0 \subset \mathbb{R}$ is any bounded subset of $\mathbb{R}$, $\mathfrak{A}_0$ the Borel σ-algebra on Ω_0 w.r.t. the usual metric topology and $\mathbb{P}_0$ a probability measure on $(\Omega_0, \mathfrak{A}_0)$. Now, set $\Omega = \Omega_0^{\mathbb{Z}^d}$ and let $\mathfrak{A}$ be the product σ–algebra generated by the cylinder sets, where a cylinder set is a set of the form $\bigtimes_{x\in\mathbb{Z}^d} A_x$, where $A_x \in \mathfrak{A}$ and $A_x = \Omega_0$ for all but finitely many $x \in \mathbb{Z}^d$. The measure $\mathbb{P}$ is defined to be the product measure, hence for every cylinder set, $\mathbb{P}\left(\bigtimes_{x\in\mathbb{Z}^d} A_x\right) = \prod_{x\in\mathbb{Z}^d} \mathbb{P}_0(A_x)$.

Now, we define the random potential

$$V : \Omega \to \mathcal{B}(\mathcal{H}), \quad \omega = (\omega_x)_{x\in\mathbb{Z}^d} \mapsto V_\omega, \quad [V_\omega(\phi)](x) = \omega_x \phi(x) \;, \tag{3.1}$$

i.e., for every random configuration $\omega = (\omega_x)_{x\in\mathbb{Z}^d} \in \Omega$ the operator V_ω is the multiplication operator by ω.

Then the Anderson Hamiltonian $h_\omega \in \mathcal{B}(\mathcal{H})$ is given as $h_\omega = \Delta_d + V_\omega$, i.e.,

$$[h_\omega(\phi)](x) = (2d + \omega_x)\phi(x) - \sum_{y\in\mathbb{Z}^d,\ |x-y|=1} \phi(y) \;. \tag{3.2}$$

Since we also consider finite systems, let $\mathcal{P}_{\text{fin}}$ be the set of all finite subsets of $\mathbb{Z}^d$, and define for all $\Lambda \in \mathcal{P}_{\text{fin}}$ the Hilbert space $\mathcal{H}_\Lambda := \ell^2(\Lambda)$ and the restriction of h_ω to Λ, that is $h_{\omega,\Lambda} \in \mathcal{B}(\mathcal{H}_\Lambda)$,

$$[h_{\omega,\Lambda}(\phi)](x) := (2d + \omega_x)\phi(x) - \sum_{y\in\Lambda,\ |x-y|=1} \phi(y) \;. \tag{3.3}$$

Note, that the definition above corresponds to Dirichlet boundary conditions.

3.1.2 Interaction between two fermions

The interaction W is assumed to be a self-adjoint, positive semidefinite operator on $\mathcal{H} \otimes \mathcal{H}$, which is symmetric under permutation of the arguments, i.e.,

$$W^* = W \;, \quad \langle \phi \otimes \psi \;,\; W(\phi \otimes \psi)\rangle \geq 0 \;, \quad W(\phi \otimes \psi) = W(\psi \otimes \phi) \tag{3.4}$$

for all $\phi, \psi \in \mathcal{H}$. For our model we assume $W \in \mathcal{B}(\mathcal{H} \otimes \mathcal{H})$ to be bounded.

Furthermore we assume W to be a translation invariant multiplication operator, i.e. W is of the form

$$[W(\psi \otimes \phi)](x, y) = \mathcal{W}(x - y)\psi(x)\phi(y) \tag{3.5}$$

for all $\psi, \phi \in \mathcal{H}$, all $x, y \in \mathbb{Z}^d$ and a suitable function $\mathcal{W} : \mathbb{Z}^d \to \mathbb{R}$. The function $\mathcal{W}$ is supposed to be of finite range, hence there is some $R > 0$ such that $\mathcal{W}(x) = 0$ for all $x \in \mathbb{Z}^d$ with $\|x\| \geq R$. Observe that (3.4) and (3.5) imply $\mathcal{W}(x) = \mathcal{W}(-x)$ for all $x \in \mathbb{Z}^d$. A function $\mathcal{W}$ of finite range is also called a finite range interaction.

To ensure the uniqueness of the minimizer of the reduced Hartree Fock functional (c.f. Section 3.2.2), we also assume that the Fourier transform $\widehat{\mathcal{W}} : \mathbb{T}^d \to \mathbb{R}$ of $\mathcal{W}$ is strictly positive, that is

$$\widehat{\mathcal{W}}(\xi) := \sum_{x\in\mathbb{Z}^d} \mathcal{W}(x)\mathrm{e}^{-i\langle\xi,x\rangle} = \sum_{x\in\mathbb{Z}^d, |x|<R} \mathcal{W}(x)\cos(\langle\xi,x\rangle) > 0 \quad \text{for all } \xi \in \mathbb{T}^d \tag{3.6}$$

where $\mathbb{T}^d = [-\pi, \pi]^d$ is the d-dimensional torus. Note, that the second equality in (3.6) holds, because $\mathcal{W}$ is of finite range and $\mathcal{W}(x) = \mathcal{W}(-x)$ for all $x \in \mathbb{Z}^d$. Since $\widehat{\mathcal{W}}(\xi)$ is in fact a trigonometric polynomial and $\mathbb{T}^d$ is compact, we even have $\widehat{\mathcal{W}}(\xi) \geq c$ for all $\xi \in \mathbb{T}^d$ and some positive constant $c > 0$.

The restriction of W to $\mathcal{H}_\Lambda \otimes \mathcal{H}_\Lambda$ is denoted by W_Λ. When introducing the Hartree-Fock theory in Section 3.1.4, we multiply W by a positive parameter g to rescale the strength of the interaction.

3.1.3 Many fermion systems

In the following, we give a short introduction to the terms used to define the Hartree-Fock functional. Although in the end, the 1-particle density matrix is the main object in the definition, we start slightly more general to motivate the used terms, but omit some details, that are given for example in [14, Section 5.2.1-5.2.3].

In order to describe a system of fermions, we introduce the *fermion Fock space* over a separable, complex Hilbert space $\mathcal{G}$. For $N \in \mathbb{N}$ we define the N-particle Hilbert space $\mathcal{F}^{(N)}[\mathcal{G}]$ to be the N-fold tensor product of $\mathcal{G}$ with itself,

$$\mathcal{F}^{(N)} := \bigotimes_{n=1}^{N} \mathcal{G} \tag{3.7}$$

and set

$$\mathcal{F}^{(0)}[\mathcal{G}] = \mathbb{C}|0\rangle\ , \tag{3.8}$$

where the normalized vector $|0\rangle$ is called vacuum vector.

Furthermore, we define the fermionic N-particle Hilbert space to be

$$\mathcal{F}_f^{(N)}[\mathcal{G}] := \mathcal{A}^{(N)}\left(\mathcal{F}^{(N)}\right)\ , \tag{3.9}$$

where $\mathcal{A}^{(N)} : \mathcal{F}^{(N)}[\mathcal{G}] \to \mathcal{F}^{(N)}[\mathcal{G}]$ is the projection onto antisymmetric elements, i.e.

$$\mathcal{A}^{(N)}(\phi_1 \otimes \ldots \otimes \phi_N) = \frac{1}{N!} \sum_{\pi \in S_N} (-1)^\pi \phi_{\pi(1)} \otimes \ldots \otimes \phi_{\pi(N)} \,. \tag{3.10}$$

Note that this projection ensures that the fermions obey the Pauli principle and that $\mathcal{F}_f^{(N)}[\mathcal{G}]$ is again a Hilbert space. A special class of elements of $\mathcal{F}_f^{(N)}[\mathcal{G}]$ are the *Slater determinants* $\mathcal{S}^{(N)}[\mathcal{G}]$,

$$\mathcal{S}^{(N)}[\mathcal{G}] = \{\phi_1 \wedge \ldots \wedge \phi_N \mid \phi_1, \ldots, \phi_N \in \mathcal{G},\ \langle \phi_i, \phi_j \rangle = \delta_{ij}\} \,, \tag{3.11}$$

with $\phi_1 \wedge \ldots \wedge \phi_N := \sqrt{N!}\mathcal{A}^{(N)}[\phi_1 \otimes \ldots \otimes \phi_N]$, that will be used in the definition of the Hartree-Fock functional.

The fermion Fock space is defined as the direct sum

$$\mathcal{F}_f[\mathcal{G}] := \bigoplus_{N=0}^{\infty} \mathcal{F}_f^{(N)}[\mathcal{G}] \tag{3.12}$$

i.e. $\psi \in \mathcal{F}_f[\mathcal{G}]$ is a sequence $(\psi^{(N)})_{N \in \mathbb{N}_0}$ with $\psi^{(N)} \in \mathcal{F}_f^{(N)}[\mathcal{G}]$ and $\sum_{n=0}^\infty \|\psi^{(n)}\|^2 < \infty$. Then $\mathcal{F}_f[\mathcal{G}]$ is a Hilbert space with scalar product

$$\langle \psi, \phi \rangle_{\mathcal{F}_f[\mathcal{G}]} = \sum_{N \in \mathbb{N}_0} \langle \psi^{(N)}, \phi^{(N)} \rangle_{\mathcal{F}_f[\mathcal{G}]} \tag{3.13}$$

for all $\psi, \phi \in \mathcal{F}_f[\mathcal{G}]$. Therefore we get for $\psi = (\psi^{(N)})_{N \in \mathbb{N}} \in \mathcal{F}_f[\mathcal{G}]$, that $\|\psi\|^2 = \sum_{N=0}^\infty \|\psi^{(N)}\|^2$.

Then we may define creation and annihilation operators $a^*, a : \mathcal{G} \to \mathcal{B}(\mathcal{F}_f[\mathcal{G}])$, by setting for $\phi = (\phi^{(N)})_{N \in \mathbb{N}} \in \mathcal{F}_f[\mathcal{G}]$ $a(f)\phi^{(0)} = 0$, $a^*(f)\phi^{(0)} = f$ and for $\phi_1 \otimes \ldots \otimes \phi_N \in \mathcal{F}_f^{(N)}[\mathcal{G}]$

$$a(f)(\phi_1 \otimes \ldots \otimes \phi_N) = \sqrt{N}\langle f, \phi_1 \rangle \mathcal{A}^{(N-1)}(\phi_2 \otimes \ldots \otimes \phi_N) \tag{3.14}$$

$$a^*(f)(\phi_1 \otimes \ldots \otimes \phi_N) = \sqrt{N+1}\mathcal{A}^{(N+1)}(f \otimes \phi_1 \otimes \ldots \otimes \phi_N). \tag{3.15}$$

Note that $f \mapsto a(f)$ is an anti-linear map, whereas $f \mapsto a^*(f)$ is a linear map and $\|a(f)\|_{\mathrm{op}}, \|a^*(f)\|_{\mathrm{op}} \leq \|f\|_{\mathcal{G}}$. The creation and annihilation operators a^*, a obey the canonical anti-commutation relations (CAR), that is

$$\{a(\phi), a(\psi)\} = 0 \,, \qquad \{a(\phi), a^*(\psi)\} = \langle \phi, \psi \rangle \mathbb{1} \,, \tag{3.16}$$

and constitute the Fock representation of the CAR since

$$a(\psi)|0\rangle = 0 \,, \tag{3.17}$$

for all $\psi \in \mathcal{G}$.

The procedure of the second quantization assigns to an operator $h \in \mathcal{B}(\mathcal{G})$ a corresponding N-particle operator $h^{(N)} \in \mathcal{B}(\mathcal{F}_f^{(N)}[\mathcal{G}])$,

$$h^{(N)} = \sum_{n=1}^{N} \mathbb{1} \otimes \ldots \otimes \mathbb{1} \otimes \underbrace{h}_{n^{th} \text{ factor}} \otimes \mathbb{1} \otimes \ldots \otimes \mathbb{1}. \tag{3.18}$$

As it turns out, $h^{(N)}$ has a very useful representation using creation and annihilation operators,

$$h^{(N)} = \sum_{i,j=1}^{\infty} \langle \phi_i, h\phi_j \rangle a^*(\phi_i) a(\phi_j), \tag{3.19}$$

where $\{\phi_i\}_{i\in\mathbb{N}}$ is any ONB of $\mathcal{G}$.

Similarly, we define for $W \in \mathcal{B}(\mathcal{G} \otimes \mathcal{G})$ a corresponding N-particle operator $W^{(N)} \in \mathcal{B}(\mathcal{F}_f^{(N)}[\mathcal{G}])$ for $N \geq 2$, by setting

$$W^{(N)} = \sum_{1\leq i<j\leq N} \Pi_{i,j} W \underbrace{\otimes \mathbb{1} \otimes \ldots \otimes \mathbb{1}}_{N-2 \text{ factors}} \Pi_{i,j}, \tag{3.20}$$

where $\Pi_{i,j} : \mathcal{F}_f^{(N)}[\mathcal{G}] \to \mathcal{F}_f^{(N)}[\mathcal{G}]$ is the permutation operator, that permutes the first component with component m and the second component with the n-th. Similarly to (3.19) we have

$$W^{(N)} = \frac{1}{2} \sum_{i,j,k,l=1}^{\infty} \langle \phi_i \otimes \phi_j, W(\phi_k \otimes \phi_l) \rangle \; a^*(\phi_j) a^*(\phi_i) a(\phi_k) a(\phi_l), \tag{3.21}$$

for any ONB $\{\phi_n\}_{n\in\mathbb{N}}$ of $\mathcal{G}$.

The physical state of a system is characterized by a functional, that assigns to each observable of the system a real number, which corresponds to the expectation of the measured value for this observable. More precisely, the observables are seen as the C^*-sub-algebra of self-adjoint elements of a C^*-algebra $\mathfrak{C}$, and a *state* is a positive (hence hermetian), normalized linear functional $\rho : \mathfrak{C} \to \mathbb{C}$, that is $\rho(A^*A) \geq 0$ for all $A \in \mathfrak{C}$ and $\|\rho\| = 1$. The set of all states on $\mathfrak{C}$ is thus also denoted by $\mathfrak{C}^*_{+,1}$. In the following, we are, as a first step, solely interested in the value of the energy observable for finitely many degrees of freedom, hence a finite subset $\Lambda \subset \mathbb{Z}^d$, therefore we may simply take $\mathfrak{C} = \mathcal{B}(\mathcal{F}_f[\mathcal{G}]) = \mathcal{B}(\mathcal{F}_f[\mathcal{H}_\Lambda])$.

In the finite dimensional case, any state can be represented by a density matrix, that is a trace-class operator $\hat{\rho} \in \mathcal{L}^1(\mathcal{F}_f[\mathcal{G}])$, that is positive and has trace 1, $\hat{\rho} = \hat{\rho}^*$, $\hat{\rho} \geq 0$ and $\mathrm{Tr}\{\hat{\rho}\} = 1$. The corresponding state $\rho \in \mathcal{B}(\mathcal{F}_f[\mathcal{H}_\Lambda])^*_{+,1}$ is then given by $\rho(\cdot) = \mathrm{Tr}\{\hat{\rho}\ \cdot\}$. Furthermore, we will assume that the states are quasi-free, i.e., that all truncated correlation functions vanish, c.f. [14, p. 42-43]. For example a quasi-free state ρ fulfills

$$\begin{aligned} \rho(a^*(\phi_1)a^*(\phi_2)a(\psi_1)a(\psi_2)) &= \rho(a^*(\phi_1)a^*(\phi_2))\rho(a(\psi_1)a(\psi_2)) \\ &\quad -\rho(a^*(\phi_1)a(\psi_1))\rho(a^*(\phi_2)a(\psi_2)) \\ &\quad +\rho(a^*(\phi_1)a(\psi_2))\rho(a^*(\phi_2)a(\psi_1)) \end{aligned} \tag{3.22}$$

for all $\phi_1, \phi_2, \psi_1, \psi_2 \in \mathcal{G}$. As it turns out, any quasi-free state $\rho \in \mathfrak{C}^*_{+,1}$ is completely characterized by

$$\rho(a^*(\phi_1)a^*(\phi_2)) \quad \text{and} \quad \rho(a^*(\phi_1)a(\phi_2)) \tag{3.23}$$

for all $\phi_1, \phi_2 \in \mathcal{G}$. This observation motivates the definition of the *1-particle density matrix* Γ_ρ, see for example [6], of a quasi-free state $\rho \in \mathfrak{C}^*_{+,1}$ as an operator on $\mathcal{G} \times \mathcal{G}$

$$\Gamma_\rho = \begin{pmatrix} \gamma_\rho & \alpha_\rho \\ \alpha_\rho^* & 1 - \overline{\gamma}_\rho \end{pmatrix} , \tag{3.24}$$

where γ_ρ, α_ρ are bounded operators on $\mathcal{G}$ defined by

$$\langle \phi, \gamma_\rho \psi \rangle := \rho(a^*(\psi)a(\phi)) \quad \text{and} \quad \langle \phi, \alpha_\rho \psi \rangle := \rho(a^*(\psi)a^*(\phi)) \tag{3.25}$$

for all $\phi, \psi \in \mathcal{G}$ and

$$\langle \phi, \overline{\gamma}_\rho \psi \rangle := \overline{\langle \phi, \gamma_\rho \psi \rangle}. \tag{3.26}$$

Note that

$$\gamma_\rho = \gamma_\rho^* \quad \text{and} \quad \alpha_\rho^* = -\alpha_\rho^T . \tag{3.27}$$

One can show that $0 \leq \Gamma_\rho \leq 1$, see [6, Lemma 2.1], and furthermore that any operator Γ on $\mathcal{G} \times \mathcal{G}$ of the form 3.25 obeying 3.27 and $0 \leq \Gamma \leq 1$ is the 1-particle density matrix of a quasi-free state, see [6, Remark after (2b.8), Theorem 2.3].

If a quasi-free state $\rho \in \mathfrak{C}^*_{+,1}$ is *particle conserving*, i.e., $\rho(a^*(\psi)a^*(\phi)) = 0$ for all $\phi, \psi \in \mathcal{G}$, we have $\alpha_\rho = 0$ and hence Γ_ρ is completely characterized by $\gamma_\rho \in \mathcal{B}(\mathcal{G})$, which also obeys $0 \leq \gamma \leq 1$. It will be indeed sufficient to consider quasi-free, particle conserving states in the Hartree-Fock theory introduced in the following section, since we assume the interaction to be repulsive, that is W to be positive, c.f. [6, Theorem 2.11]. Hence all occurring 1-particle density matrices Γ_ρ will be determined by γ_ρ only and we will also call γ_ρ the 1-particle density matrix of the (quasi-free, particle conserving) state ρ.

3.1.4 Hartree–Fock theory

Now we consider an N-Fermion system in a finite crystal with impurities, which is described by the Hamiltonian

$$H_{\omega,\Lambda}^{(N)} := h_{\omega,\Lambda}^{(N)} + gW_\Lambda^{(N)} \in \mathcal{B}(\mathcal{F}_f^{(N)}[\mathcal{H}_\Lambda]), \tag{3.28}$$

where the coupling constant $g > 0$ scales the strength of the repulsive interaction W, $\omega \in \Omega$, and Λ is any finite subset of $\mathbb{Z}^d$.

The ground state energy of such a system is given by

$$E_{\omega,\Lambda}^{(GS)}(N) \quad := \quad \inf \left\{ \langle \phi, H_{\omega,\Lambda}^{(N)} \phi \rangle \;\middle|\; \phi \in \mathcal{F}_f^{(N)}[\mathcal{H}_\Lambda],\ \|\phi\| = 1 \right\} \tag{3.29}$$

The Hartree-Fock approximation is defined by restricting the wave functions in (3.29) to Slater determinants only,

$$E_{\omega,\Lambda}^{(\mathrm{HF})}(N) := \inf \left\{ \langle \phi, H_{\omega,\Lambda}^{(N)} \phi \rangle \;\middle|\; \phi \in \mathcal{S}^{(N)}[\mathcal{H}_\Lambda] \right\}. \tag{3.30}$$

For a Slater determinant $\Phi = \phi_1 \wedge \ldots \wedge \phi_N \in \mathcal{S}^{(N)}[\mathcal{H}_\Lambda]$ the density matrix $\hat{\rho} = |\Phi\rangle\langle\Phi|$ is an orthogonal projection. Let the corresponding state be denoted by ρ. In this case, we get by straightforward computation using (3.16), (3.19) and (3.21), that

$$\begin{aligned} \langle \Phi, H_{\omega,\Lambda}^{(N)} \Phi \rangle &= \rho\left(H_{\omega,\Lambda}^{(N)}\right) \qquad (3.31) \\ &= \mathrm{Tr}_{\mathcal{H}_\Lambda}\{h_{\omega,\Lambda}\gamma_\rho\} + \frac{g}{2}\,\mathrm{Tr}_{\mathcal{H}_\Lambda\otimes\mathcal{H}_\Lambda}\{W_\Lambda(\mathbb{1} - \mathrm{Ex})(\gamma_\rho \otimes \gamma_\rho)\}, \end{aligned}$$

where we exceptionally indicate the space over which the trace is taken. The operator Ex: $\mathcal{H}_\Lambda \otimes \mathcal{H}_\Lambda \to \mathcal{H}_\Lambda \otimes \mathcal{H}_\Lambda$ simply exchanges components, it is determined by

$$\mathrm{Ex}(\phi \otimes \psi) = \psi \otimes \phi \text{ for all } \phi, \psi \in \mathcal{H}_\Lambda\,, \tag{3.32}$$

and is obviously linear and continuous. Note that the right hand side of (3.31) is expressed in terms of the 1-particle operators $h_{\omega,\Lambda}$ and W_Λ. Furthermore, we remark that the second equality of (3.31) is also true if ρ is a quasi-free, particle conserving state because of (3.22).

Introducing the set of 1-particle density matrices on the finite-dimensional Hilbert-space $\mathcal{H}_\Lambda$,

$$\mathcal{Z}_\Lambda := \{\gamma \in \mathcal{B}(\mathcal{H}_\Lambda) \,\big|\, 0 \leq \gamma \leq 1\} \tag{3.33}$$

the Hartree-Fock functional $\mathcal{E}^{(\mathrm{HF})}_{\omega,\Lambda}(\gamma) : \mathcal{Z}_\Lambda \to \mathbb{R}$ is defined as

$$\mathcal{E}^{(\mathrm{HF})}_{\omega,\Lambda}(\gamma) = \mathrm{Tr}\{h_{\omega,\Lambda}\gamma\} + \frac{g}{2}\,\mathrm{Tr}\{W_\Lambda(\mathbb{1} - \text{ Ex })(\gamma \otimes \gamma)\} \tag{3.34}$$

and exists since $\mathcal{B}(\mathcal{H}_\Lambda) = \mathcal{L}^1(\mathcal{H}_\Lambda)$ for $|\Lambda| < \infty$. Then the Hartree-Fock ground state energy (3.30) can also be expressed in terms of 1-particle density matrices,

$$E^{(\mathrm{HF})}_{\omega,\Lambda}(N) = \inf\left\{\mathcal{E}^{(\mathrm{HF})}_{\omega,\Lambda}(\gamma) \,\big|\, \gamma = \gamma^* = \gamma^2, \mathrm{Tr}\{\gamma\} = N\right\}. \tag{3.35}$$

Unfortunately, the set of Slater determinants over which the minimization is taken, does not have a linear or convex structure, which is a basic assumption for most results of the calculus of variations. Lieb's variational principle gives a very elegant solution. Indeed, in [28, 3] it is shown that the infimum $E^{(\mathrm{HF})}_{\omega,\Lambda}(N)$ does not change, if the condition $\gamma = \gamma^* = \gamma^2$ is replaced by the weaker assumption $0 \leq \gamma \leq 1$, that is

$$E^{(\mathrm{HF})}_{\omega,\Lambda}(N) = \inf\left\{\mathcal{E}^{(\mathrm{HF})}_{\omega,\Lambda}(\gamma) \,\big|\, 0 \leq \gamma \leq 1, \mathrm{Tr}\{\gamma\} = N\right\}. \tag{3.36}$$

Physically, this amounts to minimizing over all quasi-free, particle conserving states with particle number expectation value equal to N. Note that, in general, the expectation value of the particle number is possibly not an integer. It is shown in [6, Theorem 2.11], that for repulsive interactions, i.e., if W is positive, even minimizing over all quasi-free states (with particle expectation value N) does not change the infimum $E^{(\mathrm{HF})}_{\omega,\Lambda}(N)$.

Although we originally defined the Hartree-Fock ground state energy for N particles, it is now natural, regarding (3.31) and (3.36), to allow all positive particle numbers $N > 0$,

$$E^{(\mathrm{HF})}_{\omega,\Lambda}(N) = \inf\left\{\mathcal{E}^{(\mathrm{HF})}_{\omega,\Lambda}(\gamma) \,\big|\, \gamma \in \mathcal{Z}_{\Lambda,N}\right\}, \tag{3.37}$$

where

$$\mathcal{Z}_{\Lambda,N} := \left\{\gamma \in \mathcal{B}(\mathcal{H}_\Lambda) \,\big|\, 0 \leq \gamma \leq 1, \mathrm{Tr}\{\gamma\} = N\right\}. \tag{3.38}$$

Let us also define the so-called reduced Hartree-Fock functional. It is given by minimizing $\mathcal{E}^{(\mathrm{rHF})}_{\omega,\Lambda}(\gamma) : \mathcal{Z}_\Lambda \to \mathbb{R}$

$$\mathcal{E}^{(\mathrm{rHF})}_{\omega,\Lambda}(\gamma) = \mathrm{Tr}\{h_{\omega,\Lambda}\gamma\} + \frac{g}{2}\,\mathrm{Tr}\{W_\Lambda(\gamma\otimes\gamma)\}, \tag{3.39}$$

this corresponds to neglecting the exchange term $\frac{g}{2}\,\mathrm{Tr}\{W_\Lambda\,\mathrm{Ex}\,(\gamma\otimes\gamma)\}$ in $\mathcal{E}^{(\mathrm{HF})}_{\omega,\Lambda}$. Analogously, we define the reduced Hartree-Fock ground state energy for $N > 0$

$$E^{(\mathrm{rHF})}_{\omega,\Lambda}(N) = \inf\left\{\mathcal{E}^{(\mathrm{rHF})}_{\omega,\Lambda}(\gamma)\;\middle|\;\gamma\in\mathcal{Z}_{\Lambda,N}\right\}. \tag{3.40}$$

The advantage of the reduced functional is a special convexity property which ensures the uniqueness of the minimizer in some cases, see Section 3.2.2. This can not be guaranteed for the full Hartree-Fock functional by the methods used in the following.

From the physical point of view it is also interesting to fix the chemical potential of the system instead of fixing the particle number. This is the reason why we define the following functionals $\widetilde{\mathcal{E}}^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\mu}(\gamma) : \mathcal{Z} \to \mathbb{R}$ as

$$\widetilde{\mathcal{E}}^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\mu}(\gamma) = \mathcal{E}^{(\mathrm{HF/rHF})}_{\omega,\Lambda}(\gamma) - \mu\,\mathrm{Tr}\{\gamma\}\,, \tag{3.41}$$

which we call (reduced) Hartree-Fock functional at chemical potential μ. Recall that $\mathrm{Tr}\{\gamma\}$ is well-defined since $|\Lambda| < \infty$. The according ground state energy is then given by

$$\widetilde{E}^{(\mathrm{HF/rHF})}_{\omega,\Lambda}(\mu) = \inf\left\{\widetilde{\mathcal{E}}^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\mu}(\gamma)\;\middle|\;\gamma\in\mathcal{Z}_\Lambda\right\}\,. \tag{3.42}$$

Up to now, all our considerations were done for temperature equal to zero. For results at positive temperatures we have to take the entropy $S_\Lambda : \mathcal{Z}_\Lambda \to \mathbb{R}$ of the system into account, that is given in terms of 1-particle density matrices $\gamma \in \mathcal{Z}_\Lambda$ by

$$S_\Lambda(\gamma) = -\frac{1}{2}\,\mathrm{Tr}\left\{\gamma\ln(\gamma)\right\} - \frac{1}{2}\,\mathrm{Tr}\left\{(\mathbb{1}-\gamma)\ln(\mathbb{1}-\gamma)\right\}. \tag{3.43}$$

see for example [7]. In the following, we consider the canonical ensemble and grand canonical ensemble, at fixed positive temperature and a certain particle number or chemical potential, respectively.

We define the (reduced) Hartree-Fock pressure functional $\mathcal{P}^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\beta}$ at inverse temperature β by

$$-\mathcal{P}^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\beta}(\gamma) = \mathcal{E}^{(\mathrm{HF/rHF})}_{\omega,\Lambda}(\gamma) - \beta^{-1}S_\Lambda(\gamma) \tag{3.44}$$

and the supremum of the (reduced) Hartree-Fock pressure functional is denoted as

$$P^{(\mathrm{HF}/\mathrm{rHF})}_{\omega,\Lambda,\beta}(N) = \sup\left\{\mathcal{P}^{(\mathrm{HF}/\mathrm{rHF})}_{\omega,\Lambda,\beta}(\gamma) \;\middle|\; \gamma \in \mathcal{Z}_{\Lambda,N}\right\} . \tag{3.45}$$

Again, we also consider the case where the chemical potential instead of the particle number is fixed. That amounts to considering the grand canonical ensemble, and minimize the (reduced) Hartree-Fock grand canonical potential, given by

$$\mathcal{M}^{(\mathrm{HF}/\mathrm{rHF})}_{\omega,\Lambda,\beta,\mu}(\gamma) = \mathcal{E}^{(\mathrm{HF}/\mathrm{rHF})}_{\omega,\Lambda}(\gamma) - \beta^{-1}S_\Lambda(\gamma) - \mu\,\mathrm{Tr}\{\gamma\} . \tag{3.46}$$

The corresponding infimum is defined as

$$M^{(\mathrm{HF}/\mathrm{rHF})}_{\omega,\Lambda,\beta}(\mu) = \inf\left\{\mathcal{M}^{(\mathrm{HF}/\mathrm{rHF})}_{\omega,\Lambda,\beta,\mu}(\gamma) \;\middle|\; \gamma \in \mathcal{Z}_{\Lambda}\right\} . \tag{3.47}$$

In the thermodynamic limit we are mainly interested in the minimizers of the reduced Hartree-Fock grand canonical potential $\mathcal{M}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta,\mu}$, see Section 3.3.

3.2 Minimizers for finite systems

As a preparation to study the limit $\Lambda \nearrow \mathbb{Z}^d$, we summarize in this section some results for finite systems. For finite systems, i.e., $\Lambda \in \mathcal{P}_{\mathrm{fin}}$, the Hilbert space $\mathcal{H}_\Lambda$ is finite dimensional and so is the fermion Fock space $\mathcal{F}_f(\mathcal{H}_\Lambda)$. Therefore the sets $\mathcal{Z}_\Lambda$ and $\mathcal{Z}_{\Lambda,N}$ are compact for all $N \in \mathbb{R}^+$ and the continuous functionals $\mathcal{E}^{(\mathrm{HF})}_{\omega,\Lambda}$, $\mathcal{E}^{(\mathrm{rHF})}_{\omega,\Lambda}$, $\widetilde{\mathcal{E}}^{(\mathrm{HF})}_{\omega,\Lambda,\mu}$, $\widetilde{\mathcal{E}}^{(\mathrm{rHF})}_{\omega,\Lambda,\mu}$, $\mathcal{M}^{(\mathrm{HF})}_{\omega,\Lambda,\beta,\mu}$ and $\mathcal{M}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta,\mu}$ have indeed a minimizer, likewise $\mathcal{P}^{(\mathrm{HF})}_{\omega,\Lambda,\beta}$ and $\mathcal{P}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta}$ have maximizers. Starting from the existence, we show in Section 3.2.1 that the mini- or maximizers obey self-consistent equations. For the full Hartree Fock Theory mini- or maximizers may turn out to be degenerated, but in the reduced case the uniqueness can be shown by using the self-consistent equations and a convexity property of the reduced Hartree Fock functional, see Section 3.2.2.

3.2.1 Self-consistent equations

The minimizers of $\mathcal{E}^{(\mathrm{HF}/\mathrm{rHF})}_{\omega,\Lambda}$, $\widetilde{\mathcal{E}}^{(\mathrm{HF}/\mathrm{rHF})}_{\omega,\Lambda,\mu}$, $-\mathcal{P}^{(\mathrm{HF}/\mathrm{rHF})}_{\omega,\Lambda,\beta}$, and $\mathcal{M}^{(\mathrm{HF}/\mathrm{rHF})}_{\omega,\Lambda,\beta,\mu}$, no matter whether these are unique or not, fulfill certain self-consistent equations, that we deduce in the following. The self-consistent equations are a useful tool to study the minimizers in the thermodynamic limit, see Section 3.3.

In preparation, we define the *effective Hamiltonians* $H^{(\mathrm{HF})}_{\omega,\Lambda,\mathrm{eff}}[\gamma], H^{(\mathrm{rHF})}_{\omega,\Lambda,\mathrm{eff}}[\gamma] \in \mathcal{B}(\mathcal{H}_\Lambda)$ for all $\gamma \in \mathcal{Z}_\Lambda$ by

$$\begin{aligned}\langle e_i, H^{(\mathrm{HF})}_{\omega,\Lambda,\mathrm{eff}}[\gamma] e_j\rangle &= \langle e_i, h_{\omega,\Lambda} e_j\rangle + g\,\mathrm{Tr}\{W_\Lambda(\mathbb{1} - \mathrm{Ex})(\gamma \otimes |\, e_j\rangle\langle e_i|)\} \\ \langle e_i, H^{(\mathrm{rHF})}_{\omega,\Lambda,\mathrm{eff}}[\gamma] e_j\rangle &= \langle e_i, h_{\omega,\Lambda} e_j\rangle + g\,\mathrm{Tr}\{W_\Lambda(\gamma \otimes |\, e_j\rangle\langle e_i|)\}\,, \end{aligned} \tag{3.48}$$

where $\{e_i\}$ is any orthonormal basis of $\mathcal{H}_\Lambda$.

Remark 3.2.1. *Using* (3.5) *and the canonical ONB $\{e_x\}_{x\in\Lambda}$ of $\mathcal{H}_\Lambda$, the effective Hamiltonian in the reduced case can be rewritten as*

$$\langle e_x, H^{(\mathrm{rHF})}_{\omega,\Lambda,\mathrm{eff}}[\gamma] e_y\rangle = \langle e_x, h_{\omega,\Lambda} e_y\rangle + g \sum_{z\in\Lambda} \mathcal{W}(x-z)\gamma(z,z)\delta_{xy}\,, \tag{3.49}$$

where $\gamma(x,y) := \langle e_x, \gamma e_y\rangle$. In particular $H^{(\mathrm{rHF})}_{\omega,\Lambda,\mathrm{eff}}[\gamma]$ only depends on the diagonal entries of γ. Thus we define the density $\rho_\gamma : \mathbb{Z}^d \to \mathbb{R}$ for all $\gamma \in \mathcal{Z}_\Lambda$ to be

$$\rho_\gamma(x) := \begin{cases} \gamma(x,x), & x \in \Lambda \\ 0, & x \notin \Lambda \end{cases}. \tag{3.50}$$

Then the effective Hamiltonian is of the form

$$H^{(\mathrm{rHF})}_{\omega,\Lambda,\mathrm{eff}}[\gamma] = h_{\omega,\Lambda} + g[W_\Lambda * \rho_\gamma] \tag{3.51}$$

where $[W_\Lambda * \rho_\gamma] \in \mathcal{B}(\mathcal{H}_\Lambda)$ is the multiplication operator

$$\left[[W_\Lambda * \rho_\gamma](\phi)\right](x) = \sum_{y\in\Lambda} \mathcal{W}(x-y)\rho_\gamma(y)\phi(x) \tag{3.52}$$

for every $\gamma \in \mathbb{Z}_\Lambda$, $\phi \in \mathcal{H}_\Lambda$, and $x \in \Lambda$. Emphasizing this observation we also write $H^{(\mathrm{rHF})}_{\omega,\Lambda,\mathrm{eff}}[\rho_\gamma] \equiv H^{(\mathrm{rHF})}_{\omega,\Lambda,\mathrm{eff}}[\gamma]$.

Lemma 3.2.2 (Self-consistent equations for minimizers of $\mathcal{E}^{(\mathrm{HF})}_{\omega,\Lambda}$ and $\mathcal{E}^{(\mathrm{rHF})}_{\omega,\Lambda}$)**.** *Let $\Lambda \in \mathcal{P}_{\mathrm{fin}}$, $\omega \in \Omega$ and $N \in (0, |\Lambda|)$. If $\gamma^{(\mathrm{HF/rHF})}_{\omega,\Lambda,N} \in \mathcal{Z}_{\Lambda,N}$ is a minimizer of $\mathcal{E}^{(\mathrm{HF/rHF})}_{\omega,\Lambda}$ on $\mathcal{Z}_{\Lambda,N}$, then there are $E_F^{(\mathrm{HF/rHF})} \in \mathbb{R}$ and $P^{(\mathrm{HF/rHF})} \in \mathcal{B}(\mathcal{H}_\Lambda)$ with*

$$0 \le P^{(\mathrm{HF/rHF})} \le \mathbb{1}\left[H^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\mathrm{eff}}[\gamma^{(\mathrm{HF/rHF})}_{\omega,\Lambda,N}] = E_F^{(\mathrm{HF/rHF})}\right]$$

such that

$$\gamma^{(\mathrm{HF/rHF})}_{\omega,\Lambda,N} = \mathbb{1}\left[H^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\mathrm{eff}}[\gamma^{(\mathrm{HF/rHF})}_{\omega,\Lambda,N}] < E_F^{(\mathrm{HF/rHF})}\right] + P^{(\mathrm{HF/rHF})} \tag{3.53}$$

Proof. The proof is completely analogous for both cases. We omit the superscripts $^{(\mathrm{HF})}$ and $^{(\mathrm{rHF})}$ for $\mathcal{E}_\Lambda \equiv \mathcal{E}_{\omega,\Lambda}, \gamma_0 \equiv \gamma_{\omega,\Lambda,N}, E_F, P$ and $H_{\mathrm{eff}}[\gamma_0] \equiv H_{\omega,\Lambda,\mathrm{eff}}[\gamma_0]$ to shorten the notation.

First, note that $H_{\mathrm{eff}}[\gamma_0]$ is a self-adjoint operator on the finite dimensional Hilbert space $\mathcal{H}_\lambda$. We denote by $\lambda_1 \leq \lambda_2 \leq \ldots \lambda_{|\Lambda|}$ the eigenvalues (counting multiplicity) of $H_{\mathrm{eff}}[\gamma_0]$ and by $\{\phi_i\}_{i=1,\ldots,|\Lambda|}$ the corresponding ONB of eigenvectors of $H_{\mathrm{eff}}[\gamma_0]$. Let us already fix the Fermi energy E_F by choosing $\widetilde{N} \in \mathbb{N}$ such that $\widetilde{N} \leq N < \widetilde{N}+1$ and setting

$$E_F = \lambda_{\widetilde{N}+1}\,.$$

Furthermore, let m be the degree of degeneration of the eigenvalue E_F, i.e.

$$m = |\{i \in \{1,\ldots,|\Lambda|\} \mid \lambda_i = E_F\}|\,,$$

and n the number of eigenvalues smaller than E_F,

$$n = |\{i \in \{1,\ldots,|\Lambda|\} \mid \lambda_i < E_F\}|\,.$$

Then we define the functional $f : \mathcal{Z}_{\Lambda,N} \to \mathbb{R}$ as

$$f(\gamma) := \frac{\mathrm{d}}{\mathrm{d}t}\left(\mathcal{E}_\Lambda(t\gamma + (1-t)\gamma_0)\right)\bigg|_{t=0}\,. \tag{3.54}$$

A straightforward computation yields for any $\gamma \in \mathcal{Z}_{\Lambda,N}$

$$f(\gamma) = \mathrm{Tr}\{H_{\mathrm{eff}}[\gamma_0](\gamma - \gamma_0)\}. \tag{3.55}$$

Observe that $f(\gamma) \geq 0$ for all $\gamma \in \mathcal{Z}_{\Lambda,N}$ since γ_0 is the minimizer. In particular we have

$$\mathrm{Tr}\,\{(H_{\mathrm{eff}}[\gamma_0] - E_F)\gamma\} \geq \mathrm{Tr}\{(H_{\mathrm{eff}}[\gamma_0] - E_F)\gamma_0\}, \tag{3.56}$$

for all $\gamma \in \mathcal{Z}_{\Lambda,N}$, hence γ_0 also minimizes the functional $g_{E_F}|_{\mathcal{Z}_{\Lambda,N}}$, with $g_{E_F} : \mathcal{Z}_\Lambda \to \mathbb{R}$,

$$g_{E_F}(\gamma) = \mathrm{Tr}\{(H_{\mathrm{eff}}[\gamma_0] - E_F)\gamma\}. \tag{3.57}$$

Recalling that $H_{\mathrm{eff}}[\gamma_0]$ is nothing but a finite self-adjoint matrix, we observe that any minimizer $\widetilde{\gamma} \in \mathcal{Z}_\Lambda$, i.e. $0 \leq \widetilde{\gamma} \leq 1$, of g_{E_F} is of the form

$$\widetilde{\gamma} = \widetilde{\gamma}_{E_F,\underline{\alpha}} := \sum_{i=1}^{n} |\phi_i\rangle\langle\phi_i| + \sum_{j=1}^{m} \alpha_j |\phi_{n+j}\rangle\langle\phi_{n+j}| \tag{3.58}$$

for some $\underline{\alpha} = (\alpha_1, \ldots, \alpha_m)$ with $0 \leq \alpha_j \leq 1$ for $j = 1, \ldots, m$.

Now we choose $\alpha_1, \ldots, \alpha_m \in [0, 1]$ such that

$$\mathrm{Tr}\{\widetilde{\gamma}_{E_F,\underline{\alpha}}\} = N \; . \tag{3.59}$$

Then $\widetilde{\gamma}_{E_F,\underline{\alpha}}$ minimizes g_{E_F} (on $\mathcal{Z}_\Lambda$) as well as $g_{E_F}|_{\mathcal{Z}_{\Lambda,N}}$ and we obtain $g_{E_F}(\widetilde{\gamma}_{E_F,\underline{\alpha}}) = g_{E_F}(\gamma_0)$. But then γ_0 is also a minimizer of g_{E_F} (on $\mathcal{Z}_\Lambda$) and hence of the form (3.58). □

In the proof presented above we choose E_F to be an eigenvalue of $H_{\mathrm{eff}}[\gamma_0]$, and in that case even obtained that $0 \leq P < \mathbb{1}\,[H_{\mathrm{eff}}[\gamma_0] = E_F]$. If $P = 0$ we may also choose E_F slightly smaller (for example as small as the next eigenvalue of $H_{\mathrm{eff}}[\gamma_0]$) and thus get $\gamma_0 = \mathbb{1}\,[H_{\mathrm{eff}}[\gamma_0] \leq E_F]$.

If the interaction W is strictly positive and $N \in \mathbb{N}$, it is known from Lieb's variational principle [28] that any minimizer of the Hartree-Fock functional is necessarily a projection. Furthermore it is shown in [5], that under these conditions one always gets $P^{(HF)} = 0$.

We can not show such a general result, since we only assume the Fourier transform of the interaction potential $\widehat{\mathcal{W}}$ to be strictly positive, but not the interaction itself. Nevertheless, we can prove for finite $\Lambda \subset \mathbb{Z}^d$, that there is at least one minimizer which is a projection.

Lemma 3.2.3.
Let $\Lambda \in \mathcal{P}_{\mathrm{fin}}$, $\omega \in \Omega$ and $N \in \mathbb{N}$ be such that $0 < N < |\Lambda|$. Then there is a projection $\gamma_{\omega,\Lambda,N} = \gamma_{\omega,\Lambda,N}^2 \in \mathcal{Z}_{\Lambda,N}$, which also minimizes $\mathcal{E}_{\omega,\Lambda}^{(\mathrm{HF})}$ on $\mathcal{Z}_{\Lambda,N}$.

Proof. We replace the interaction W_Λ in the Hartree-Fock functional (3.34) by the interaction $W_\varepsilon \equiv W_{\Lambda,\varepsilon}$ defined by

$$W_\varepsilon := W_\Lambda + \varepsilon V \; , \tag{3.60}$$

where V is the interaction that is equally repulsive between any two points in Λ, i.e.

$$[V(\psi \otimes \phi)](x, y) = \mathcal{V}(x - y)\psi(x)\phi(y) = \psi(x)\phi(y) \tag{3.61}$$

for all $\psi, \phi \in \mathcal{H}$ and all $x, y \in \mathbb{Z}^d$, hence $\mathcal{V} \equiv 1$. For any $\varepsilon > 0$ the interaction W_ε is strictly positive and thus we get, following [28, 5], that there is a projection $\gamma_\varepsilon = \gamma_\varepsilon^2 \in \mathcal{Z}_{\Lambda,N}$ which minimizes the following Hartree-Fock functional

$$\mathcal{E}_\varepsilon(\gamma) := \mathrm{Tr}\{h_{\omega,\Lambda}\gamma\} + \frac{g}{2}\,\mathrm{Tr}\{W_\varepsilon(\mathbb{1} - \mathrm{Ex}\,)(\gamma \otimes \gamma)\} \tag{3.62}$$

on $\mathcal{Z}_{\Lambda,N}$. Now we choose the sequence $(\gamma_n)_{n\in\mathbb{N}}$ in $\mathcal{Z}_{\Lambda,N}$ such that

$$\gamma_n^2 = \gamma_n \quad \text{and} \quad \mathcal{E}_{n^{-1}}(\gamma_n) = \inf\left\{\mathcal{E}_{n^{-1}}(\gamma) \mid \gamma \in \mathcal{Z}_{\Lambda,N}\right\} . \tag{3.63}$$

Recall, that γ_n is a sequence of finite matrices. This sequence is bounded and $\mathcal{Z}_{\Lambda,N}$ is closed. Thus we can find a convergent subsequence, which, for the sake of simplicity, we also denote by $(\gamma_n)_{n\in\mathbb{N}}$ and w.l.o.g. we assume (3.63) to hold. Then the limit $\gamma_\infty := \lim_{n\to\infty}\gamma_n \in \mathcal{Z}_{\Lambda,N}$ is obviously also a projection, $\gamma_\infty^2 = \gamma_\infty$. Thus it remains to show that

$$\mathcal{E}_0(\gamma_\infty) = \inf\{\mathcal{E}_0(\gamma) \mid \gamma \in \mathcal{Z}_{\Lambda,N}\} . \tag{3.64}$$

This is achieved via the following two observations: First, the map $\gamma \to \mathcal{E}_0(\gamma)$ is continuous, and second, the sequence of functions $\{\mathcal{E}_{n^{-1}}\}_{n\in\mathbb{N}}$ is uniformly convergent, i.e.

$$\begin{aligned}
\|\mathcal{E}_{n^{-1}} - \mathcal{E}_0\|_\infty &:= \sup_{\gamma\in\mathcal{Z}_{\Lambda,N}} \{|\mathcal{E}_{n^{-1}}(\gamma) - \mathcal{E}_0(\gamma)|\} \\
&= \sup_{\gamma\in\mathcal{Z}_{\Lambda,N}} \left\{ \frac{g}{2n} \left| \sum_{x,y\in\Lambda} \gamma(x,x)\gamma(y,y) - |\gamma(x,y)|^2 \right| \right\} \\
&\leq \frac{2g}{n}|\Lambda|^2 .
\end{aligned} \tag{3.65}$$

Then, for any $\varepsilon > 0$ we may choose $n_0 \in \mathbb{N}$ such that for all $n \geq n_0$

$$|\mathcal{E}_0(\gamma_\infty) - \mathcal{E}(\gamma_n)| \leq \frac{\varepsilon}{3} \quad \text{and} \quad \|\mathcal{E}_{n^{-1}} - \mathcal{E}_0\|_\infty \leq \frac{\varepsilon}{3} . \tag{3.66}$$

Then we get for all $n \geq n_0$

$$\begin{aligned}
0 &\leq \mathcal{E}_0(\gamma_\infty) - \inf_{\gamma\in\mathcal{Z}_{\Lambda,N}}\{\mathcal{E}_0(\gamma)\} \\
&\leq [\mathcal{E}_0(\gamma_\infty) - \mathcal{E}_0(\gamma_n)] + [\mathcal{E}_0(\gamma_n) - \mathcal{E}_{n^{-1}}(\gamma_n)] \\
&\quad + \mathcal{E}_{n^{-1}}(\gamma_n) + \sup_{\gamma\in\mathcal{Z}_{\Lambda,N}}\{-\mathcal{E}_{n^{-1}}(\gamma) + [\mathcal{E}_{n^{-1}}(\gamma) - \mathcal{E}_0(\gamma)]\} \\
&\leq \frac{\varepsilon}{3} + \frac{\varepsilon}{3} + \mathcal{E}_{n^{-1}}(\gamma_n) + \sup_{\gamma\in\mathcal{Z}_{\Lambda,N}}\{-\mathcal{E}_{n^{-1}}(\gamma)\} + \sup_{\gamma\in\mathcal{Z}_{\Lambda,N}}\{\mathcal{E}_{n^{-1}}(\gamma) - \mathcal{E}_0(\gamma)\} \\
&\leq \varepsilon + \mathcal{E}_{n^{-1}}(\gamma_n) - \inf_{\gamma\in\mathcal{Z}_{\Lambda,N}}\{\mathcal{E}_{n^{-1}}(\gamma)\} \\
&= \varepsilon .
\end{aligned} \tag{3.67}$$

Thus we have shown $0 \leq \mathcal{E}(\gamma_\infty) - \inf\{\mathcal{E}_0(\gamma) \mid \gamma \in \mathcal{Z}_{\Lambda,N}\} \leq \varepsilon$ for arbitrarily small $\varepsilon > 0$ and hence we obtain $\mathcal{E}(\gamma_\infty) = \inf\{\mathcal{E}_0(\gamma) \mid \gamma \in \mathcal{Z}_{\Lambda,N}\}$. □

The minimizers of $\widetilde{\mathcal{E}}^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\mu}$ of the Hartree-Fock functional at chemical potential μ fulfill similar self-consistent equations. As it turns out, the Fermi energy is, of course, fixed at μ.

Lemma 3.2.4 (Self-consistent equations for minimizers of $\widetilde{\mathcal{E}}^{(\mathrm{HF})}_{\omega,\Lambda,\mu}$ and $\widetilde{\mathcal{E}}^{(\mathrm{rHF})}_{\omega,\Lambda,\mu}$). *Let $\Lambda \in \mathcal{P}_{\mathrm{fin}}$, $\omega \in \Omega$ and $\mu \in \mathbb{R}$. If $\gamma^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\mu} \in \mathcal{Z}_\Lambda$ is a minimizer of $\widetilde{\mathcal{E}}^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\mu}$ on $\mathcal{Z}_\Lambda$, then there is $P^{(\mathrm{HF/rHF})} \in \mathcal{B}(\mathcal{H}_\Lambda)$ with*

$$0 \leq P^{(\mathrm{HF/rHF})} \leq \mathbb{1}\left[H^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\mathrm{eff}}[\gamma^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\mu}] = \mu\right]$$

such that

$$\gamma^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\mu} = \mathbb{1}\left[H^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\mathrm{eff}}[\gamma^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\mu}] < \mu\right] + P^{(\mathrm{HF/rHF})} \tag{3.68}$$

Proof. Again, the proof is completely analogous for both cases. As before we omit the superscripts $^{(\mathrm{HF})}$ and $^{(\mathrm{rHF})}$, and shorten the notation by setting $\widetilde{\mathcal{E}}_\Lambda \equiv \widetilde{\mathcal{E}}^{(HF/rHF)}_{\omega,\Lambda,\mu}, \gamma_0 \equiv \gamma^{(HF/rHF)}_{\omega,\Lambda,\mu}, P \equiv P^{(HF/rHF)}$ and $H_{\mathrm{eff}}[\gamma_0] \equiv H^{(HF/rHF)}_{\omega,\Lambda,\mathrm{eff}}[\gamma_0]$. Basically, the proof is a simplification of the proof of Lemma 3.2.2. We define the functional $f : \mathcal{Z}_\Lambda \to \mathbb{R}$ as

$$f(\gamma) := \frac{\mathrm{d}}{\mathrm{d}t}\left(\widetilde{\mathcal{E}}_\Lambda(t\gamma + (1-t)\gamma_0)\right)\bigg|_{t=0}, \tag{3.69}$$

and obtain that for any $\gamma \in \mathcal{Z}_\Lambda$

$$f(\gamma) = \mathrm{Tr}\{(H_{\mathrm{eff}}[\gamma_0] - \mu)(\gamma - \gamma_0)\}. \tag{3.70}$$

Obviously, we have $f(\gamma) \geq 0$ for all $\gamma \in \mathcal{Z}_\Lambda$ since γ_0 is the minimizer, and therefore

$$\mathrm{Tr}\left\{(H_{\mathrm{eff}}[\gamma_0] - \mu)\gamma\right\} \geq \mathrm{Tr}\{(H_{\mathrm{eff}}[\gamma_0] - \mu)\gamma_0\}, \tag{3.71}$$

for all $\gamma \in \mathcal{Z}_\Lambda$, and γ_0 also minimizes the functional $g : \mathcal{Z}_\Lambda \to \mathbb{R}$,

$$g(\gamma) = \mathrm{Tr}\{(H_{\mathrm{eff}}[\gamma_0] - \mu)\gamma\}\ . \tag{3.72}$$

Recalling that $H_{\mathrm{eff}}[\gamma_0]$ is nothing but a finite self-adjoint matrix, we observe that any minimizer $\widetilde{\gamma} \in \mathcal{Z}_\Lambda$, i.e. $0 \leq \widetilde{\gamma} \leq 1$, of g is of the form

$$\widetilde{\gamma} = \mathbb{1}[(H_{\mathrm{eff}}[\gamma_0] - \mu) < 0] + P \tag{3.73}$$

for some $P \in \mathcal{B}(\mathcal{H}_\Lambda)$ with $0 \leq P \leq \mathbb{1}[(H_{\mathrm{eff}}[\gamma_0] - \mu) = 0]$. $\square$

For the case of positive temperature, we obtain slightly different self-consistent equations. As one might expect from the physical point of view, the step function $\mathbb{1}[H_{\text{eff}}[\gamma_0] < E_F]$ is replaced by the Fermi-function $(1 + \exp[\beta(H_{\text{eff}}[\gamma_0] - E_F)])^{-1}$. The results for the maximizers of the unrestricted Hartree-Fock and the reduced Hartree-Fock pressure are again completely analogous.

Lemma 3.2.5 (Self-consistent equations for maximizers of $\mathcal{P}^{(\text{HF})}_{\omega,\Lambda,\beta}$ and $\mathcal{P}^{(\text{rHF})}_{\omega,\Lambda,\beta}$**).** *Let $\Lambda \in \mathcal{P}_{\text{fin}}$, $\omega \in \Omega$, $\beta \in (0,\infty)$ and $N \in (0, |\Lambda|)$. If $\gamma^{(\text{HF/rHF})}_{\omega,\Lambda,\beta,N} \in \mathcal{Z}_{\Lambda,N}$ is a maximizer of $\mathcal{P}^{(\text{HF/rHF})}_{\omega,\Lambda,\beta}$ on $\mathcal{Z}_{\Lambda,N}$, then there is $E_F^{(\text{HF/rHF})} \in \mathbb{R}$ such that*

$$\gamma^{(\text{HF/rHF})}_{\omega,\Lambda,\beta,N} = \Big(1 + \exp\Big[\beta(H^{(\text{HF/rHF})}_{\omega,\Lambda,\text{eff}}[\gamma^{(\text{HF/rHF})}_{\omega,\Lambda,\beta,N}] - E_F^{(\text{HF})})\Big]\Big)^{-1} \tag{3.74}$$

Here, $H_{\omega,\Lambda,\text{eff}}(\text{HF/rHF})[\gamma^{(\text{HF/rHF})}_{\omega,\Lambda,\beta,N}] \in \mathcal{B}(\mathcal{H}_\Lambda)$ are the effective Hamiltonians defined in (3.48).

Proof. The proof is again completely analogous for both cases, as before we omit the superscripts $^{(\text{HF})}$ and $^{(\text{rHF})}$. Furthermore, the proof is similar to that of Lemma 3.2.2.

We define the functional $f : \mathcal{Z}_\Lambda \to \mathbb{R}$,

$$f(\gamma) := \frac{\mathrm{d}}{\mathrm{d}t} \left(-\mathcal{P}_{\Lambda,\beta}(t\gamma + (1-t)\gamma_0)\right)\Big|_{t=0}, \tag{3.75}$$

with $\gamma_0 \equiv \gamma_{\omega,\Lambda,\beta,N}$. As before, we have $f(\gamma) \geq 0$ for all $\gamma \in \mathcal{Z}_{\Lambda,N}$ and $f(\gamma_0) = 0$ Furthermore we obtain for any $\gamma \in \mathcal{Z}_{\Lambda,N}$

$$f(\gamma) = \mathrm{Tr}\left\{\left[H_{\text{eff}}[\gamma_0] + \frac{\beta^{-1}}{2}\left(\ln(\gamma_0) - \ln(\mathbb{1} - \gamma_0)\right)\right](\gamma - \gamma_0)\right\} \geq 0. \tag{3.76}$$

In particular we have for any $E \in \mathbb{R}$ and $\gamma \in \mathcal{Z}_{\Lambda,N}$ that

$$\begin{aligned} g_E(\gamma) &\geq \mathrm{Tr}\left\{(H_{\text{eff}}[\gamma_0] - E)\gamma + \frac{\beta^{-1}}{2}(\gamma\ln(\gamma_0) + (\mathbb{1} - \gamma)\ln(\mathbb{1} - \gamma_0))\right\} \\ &\geq \mathrm{Tr}\left\{(H_{\text{eff}}[\gamma_0] - E)\gamma_0 + \frac{\beta^{-1}}{2}(\gamma_0\ln(\gamma_0) + (\mathbb{1} - \gamma_0)\ln(\mathbb{1} - \gamma_0))\right\} \\ &= g_E(\gamma_0) \end{aligned} \tag{3.77}$$

where $g_E : \mathcal{Z}_\Lambda \to \mathbb{R}$

$$g_E(\gamma) := \mathrm{Tr}\left\{(H_{\text{eff}}[\gamma_0] - E)\gamma + \beta^{-1}S_\Lambda(\gamma)\right\}. \tag{3.78}$$

Note that in order to derive the first inequality in (3.77), we used the technical lemma [14, Lemma 6.2.21]. Hence γ_0 also minimizes the functional $g_E|_{\mathcal{Z}_{\Lambda,N}}$. Now, it is a straightforward computation to show that

$$\widetilde{\gamma}_E = (1 + \exp[\beta(H_{\text{eff}}[\gamma_0] - E)])^{-1} \tag{3.79}$$

is the unique minimizer of g_E on $\mathcal{Z}_\Lambda$, c.f. [7]. Obviously, we may choose $E_F \in \mathbb{R}$ such that $\mathrm{Tr}\{\widetilde{\gamma}_{E_F}\} = N$ and obtain the assertion. $\square$

Instead of computing $\widetilde{\gamma}_E$ in (3.79) directly, we may also observe, that the function $g_E(\gamma)$ defined in (3.78) is the free energy of the system with Hamiltonian $H_{\text{eff}}[\gamma_0] - E$ at inverse temperature β in the state with 1-particle density matrix γ. But the unique minimizer of the free energy is known to be the Gibbs-state, see for example [14, Proposition 6.2.22]. As it turns out its corresponding 1-particle density matrix is given by $\widetilde{\gamma}_E$.

Lemma 3.2.6 (Self-consistent equations for minimizers of $\mathcal{M}^{(\mathrm{HF})}_{\omega,\Lambda,\beta,\mu}$ and $\mathcal{M}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta,\mu}$)**.**

Let $\Lambda \in \mathcal{P}_{\text{fin}}$, $\omega \in \Omega$, $\beta \in (0,\infty)$ and $\mu \in \mathbb{R}$. If $\gamma^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\beta,\mu} \in \mathcal{Z}_\Lambda$ is a minimizer of $\mathcal{M}^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\beta,\mu}$, then

$$\gamma^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\beta,\mu} = \left(1 + \exp\left[\beta(H^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\text{eff}}[\gamma^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\beta,\mu}] - \mu)\right]\right)^{-1} \tag{3.80}$$

Here, $H^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\text{eff}}[\gamma^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\mu}] \in \mathcal{B}(\mathcal{H}_\Lambda)$ are the effective Hamiltonians, defined in (3.48).

Proof. The proof is a simplification of the proof of Lemma 3.2.5, we use the same simplified notation in the following. More precisely, let the functional $f : \mathcal{Z}_\Lambda \to \mathbb{R}$ be now given by

$$f(\gamma) := \frac{\mathrm{d}}{\mathrm{d}t}\left(\mathcal{M}_{\omega,\Lambda,\beta,\mu}(t\gamma + (1-t)\gamma_0)\right)\Big|_{t=0}, \tag{3.81}$$

Note that with f as above, (3.76) and (3.77) with $E = \mu$ are valid for all $\gamma \in \mathcal{Z}_\Lambda$. That means, we obtain, now for any $\gamma \in \mathcal{Z}_\Lambda$,

$$f(\gamma) = \mathrm{Tr}\left\{\left[(H_{\text{eff}}[\gamma_0] - \mu) + \frac{\beta^{-1}}{2}(\ln(\gamma_0) - \ln(\mathbb{1} - \gamma_0))\right](\gamma - \gamma_0)\right\} \geq 0. \tag{3.82}$$

and therefore with g_μ as in (3.78),

$$\begin{aligned} g_\mu(\gamma) &\geq \operatorname{Tr}\left\{(H_{\mathrm{eff}}[\gamma_0]-\mu)\gamma + \frac{\beta^{-1}}{2}(\gamma\ln(\gamma_0)+(\mathbb{1}-\gamma)\ln(\mathbb{1}-\gamma_0))\right\} \\ &\geq \operatorname{Tr}\left\{(H_{\mathrm{eff}}[\gamma_0]-\mu)\gamma_0 + \frac{\beta^{-1}}{2}(\gamma_0\ln(\gamma_0)+(\mathbb{1}-\gamma_0)\ln(\mathbb{1}-\gamma_0))\right\} \\ &= g_\mu(\gamma_0) \end{aligned} \tag{3.83}$$

for all $\gamma \in \mathcal{Z}_\Lambda$. The assertion follows by the same argument as in Lemma 3.2.5. □

3.2.2 Uniqueness

Now we are able to prove the uniqueness of the minimizers of $-\mathcal{P}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta}$ and $\mathcal{M}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta,\mu}$, using the self-consistent equations deduced in Section 3.2.1. Before proving the uniqueness, we show the following auxiliary lemma that asserts a special convexity property of $\mathcal{E}^{(\mathrm{rHF})}_{\omega,\Lambda}$:

Lemma 3.2.7. *Let $\gamma, \widetilde{\gamma} \in \mathcal{Z}_\Lambda$ be such that their corresponding densities, defined in* (3.50)*, differ, i.e. $\rho_\gamma \neq \rho_{\widetilde{\gamma}}$. Then*

$$\alpha\mathcal{E}^{(\mathrm{rHF})}_{\omega,\Lambda}(\gamma) + (1-\alpha)\mathcal{E}^{(\mathrm{rHF})}_{\omega,\Lambda}(\widetilde{\gamma}) - \mathcal{E}^{(\mathrm{rHF})}_{\omega,\Lambda}(\alpha\gamma+(1-\alpha)\widetilde{\gamma}) > 0 \tag{3.84}$$

for all $\alpha \in (0,1)$.

Proof. Let $\gamma, \widetilde{\gamma} \in \mathcal{Z}_\Lambda$ be such that $\rho_\gamma \neq \rho_{\widetilde{\gamma}}$. Recall that the Fourier transform of $\mathcal{W}$ is strictly positive by assumption, see (3.6). Hence we get for any $\alpha \in (0,1)$

$$\begin{aligned} &\alpha\mathcal{E}^{(\mathrm{rHF})}_{\omega,\Lambda}(\gamma) + (1-\alpha)\mathcal{E}^{(\mathrm{rHF})}_{\omega,\Lambda}(\widetilde{\gamma}) - \mathcal{E}^{(\mathrm{rHF})}_{\omega,\Lambda}(\alpha\gamma+(1-\alpha)\widetilde{\gamma}) \\ &\quad = \frac{g}{2}\sum_{x,y\in\Lambda}\mathcal{W}(x-y)\left[\alpha\rho_\gamma(x)\rho_\gamma(y)+(1-\alpha)\rho_{\widetilde{\gamma}}(x)\rho_{\widetilde{\gamma}}(y)\right. \\ &\qquad \left. -\left(\alpha\rho_\gamma(x)+(1-\alpha)\rho_{\widetilde{\gamma}}(x)\right)\left(\alpha\rho_\gamma(y)+(1-\alpha)\rho_{\widetilde{\gamma}}(y)\right)\right] \\ &\quad = \frac{g}{2}\left(\alpha-\alpha^2\right)\sum_{x,y\in\Lambda}\mathcal{W}(x-y)(\rho_\gamma-\rho_{\widetilde{\gamma}})(x)(\rho_\gamma-\rho_{\widetilde{\gamma}})(y) \\ &\quad = \frac{g}{2}\left(\alpha-\alpha^2\right)\frac{1}{(2\pi)^d}\int_{[-\pi,\pi]^d} d\xi\, \widehat{\mathcal{W}}(\xi)\,\left|\widehat{[\rho_\gamma-\rho_{\widetilde{\gamma}}]}(\xi)\right|^2 \\ &\quad > 0\,. \end{aligned} \tag{3.85}$$

□

Lemma 3.2.8 (Uniqueness of the minimizers of $-\mathcal{P}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta}$ and $\mathcal{M}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta,\mu}$)**.** *For all $\omega \in \Omega$, $\Lambda \in \mathcal{P}_{\mathrm{fin}}$, $\beta^{-1} > 0$, $N \in (0, |\Lambda|)$, and $\mu \in \mathbb{R}$, there are unique 1-particle density matrices $\gamma_{\omega,\Lambda,\beta,N} \in \mathcal{Z}_{\Lambda,N}$, $\gamma_{\omega,\Lambda,\beta,\mu} \in \mathcal{Z}_{\Lambda}$ such that*

$$
\begin{aligned}
P^{(\mathrm{rHF})}_{\omega,\Lambda,\beta}(N) &= \mathcal{P}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta}(\gamma_{\omega,\Lambda,\beta,N}) &\quad (3.86)\\
M^{(\mathrm{rHF})}_{\omega,\Lambda,\beta}(\mu) &= \mathcal{M}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta,\mu}(\gamma_{\omega,\Lambda,\beta,\mu}) . &\quad (3.87)
\end{aligned}
$$

Proof. First, let us prove (3.86). Recall, that $\mathcal{Z}_{\Lambda,N}$ is a convex set. Let $\gamma, \widetilde{\gamma} \in \mathcal{Z}_{\Lambda,N}$ be minimizers of $-\mathcal{P}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta}$ which have identical densities $\rho_\gamma = \rho_{\widetilde{\gamma}}$ and thus identical effective Hamiltonians $H^{(\mathrm{rHF})}_{\omega,\Lambda,\mathrm{eff}}[\gamma] = H^{(\mathrm{rHF})}_{\omega,\Lambda,\mathrm{eff}}[\widetilde{\gamma}] =: H_{\mathrm{eff}}$. By means of the self-consistent equations, i.e. Lemma 3.2.5, we obtain the existence of $E_F, \widetilde{E}_F \in \mathbb{R}$ such that

$$
\begin{aligned}
\gamma &= \left(1 + \exp\left[\beta(H_{\mathrm{eff}} - E_F)\right]\right)^{-1}\\
\widetilde{\gamma} &= \left(1 + \exp\left[\beta(H_{\mathrm{eff}} - \widetilde{E}_F)\right]\right)^{-1} . &\quad (3.88)
\end{aligned}
$$

But, for $\mathrm{Tr}\{\gamma\} = \mathrm{Tr}\{\widetilde{\gamma}\}$, we have in particular

$$
\mathrm{Tr}\left\{\left(1 + \exp\left[\beta(H_{\mathrm{eff}} - E_F)\right]\right)^{-1}\right\} = \mathrm{Tr}\left\{\left(1 + \exp[\beta(H_{\mathrm{eff}} - \widetilde{E}_F)]\right)^{-1}\right\} \quad (3.89)
$$

and hence $E_F = \widetilde{E}_F$, which implies $\gamma = \widetilde{\gamma}$. Again, we conclude, that any two different minimizers $\gamma, \widetilde{\gamma} \in \mathcal{Z}_{\Lambda,N}$ of $-\mathcal{P}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta}$ have different densities $\rho_\gamma \neq \rho_{\widetilde{\gamma}}$. Lemma 3.2.7 together with the observation, that the entropy $S_\Lambda : \mathcal{Z}_\Lambda \to \mathbb{R}$ is (even strictly) convex, imply for any $\alpha \in (0,1)$

$$
\begin{aligned}
-\mathcal{P}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta}(\gamma) &= \alpha\mathcal{E}^{(\mathrm{rHF})}_{\omega,\Lambda}(\gamma) + (1-\alpha)\mathcal{E}^{(\mathrm{rHF})}_{\omega,\Lambda}(\widetilde{\gamma}) - \beta^{-1}(\alpha S_\Lambda(\gamma) + (1-\alpha)S_\Lambda(\widetilde{\gamma}))\\
&> -\mathcal{P}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta}(\alpha\gamma + (1-\alpha)\widetilde{\gamma}) , &\quad (3.90)
\end{aligned}
$$

and thus we get $\gamma = \widetilde{\gamma}$.

The proof of (3.87) is completely analogous to the case discussed above, since the self-consistent equations in Lemma 3.2.6 imply at once, that $\rho_\gamma = \rho_{\widetilde{\gamma}} \Leftrightarrow \gamma = \widetilde{\gamma}$ for any two minimizers $\gamma, \widetilde{\gamma} \in \mathcal{Z}_\Lambda$. $\square$

3.3 Minimizers in the thermodynamic limit

In this section we concentrate on analyzing the thermodynamic limit of minimizers of $\mathcal{M}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta,\mu}$. Some statements in this section are also possible for minimizers of $\mathcal{E}^{(\mathrm{HF/rHF})}_{\omega,\Lambda}$, $\widetilde{\mathcal{E}}^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\mu}$, $-\mathcal{P}^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\beta}$ or $\mathcal{M}^{(\mathrm{HF})}_{\omega,\Lambda,\beta,\mu}$, which will be indicated in the context. Only for minimizers of $\mathcal{M}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta,\mu}$ we obtain the uniqueness of the minimizer in the thermodynamic limit. Note that for each $\Lambda \in \mathcal{P}_{\mathrm{fin}}$ the minimizer of $\mathcal{M}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta,\mu}$ is of course also the minimizer of the density of the grand canonical ensemble, $\frac{1}{|\Lambda|}\mathcal{M}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta,\mu}$, which is the natural quantity in the thermodynamic limit. Since we consider properties of the corresponding minimizers (but not of $\mathcal{M}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta,\mu}$ itself), we do not need to take this distinction into account.

3.3.1 Existence and uniqueness

We define Λ_n to be the box of side length $2n+1$ centered at zero,

$$\Lambda_n := \{x \in \mathbb{Z}^d \,|\, \|x\|_\infty = \sup_{i=1,\ldots,d}\{|x_i|\} \leq n\}\,. \tag{3.91}$$

Fix $\omega \in \Omega$, $\beta \in (0,\infty)$ and $\mu \in \mathbb{R}$. For each $n \in \mathbb{N}$ let $\gamma_n \in \mathcal{Z}_{\Lambda_n}$ be the unique minimizer of $\mathcal{M}^{(\mathrm{rHF})}_{\omega,\Lambda_n,\beta,\mu}$, see Lemma 3.2.8. We define

$$\mathcal{Z} := \{\gamma \in \mathcal{B}(\mathcal{H}) \mid 0 \leq \gamma \leq 1\} \tag{3.92}$$

and continue γ_n to an operator $\widetilde{\gamma}_n \in \mathcal{Z}$ by setting

$$\langle e_x, \widetilde{\gamma}_n e_y\rangle = \begin{cases} \langle e_x, \gamma_n e_y\rangle, & x, y \in \Lambda_n \\ 0, & x \notin \Lambda_n \vee y \notin \Lambda_n. \end{cases} \tag{3.93}$$

In the following we will denote for any operator $A \in \mathcal{H}_\Lambda$ the above continuation also as $A \equiv \widetilde{A} \in \mathcal{H}$ to simplify notation. Note that the elements of $\mathcal{Z}$ are not assumed to be trace-class operators. For $\mathcal{Z}_\Lambda$ as defined in (3.33) this is naturally the case since Λ is a finite subset of $\mathbb{Z}^d$. Recall that the trace of the 1-particle density matrix γ is the expectation value of the particle number in the corresponding state and we may not expect a finite particle number in the thermodynamic limit.

As explained in Section 3.1.3 each 1-particle density matrix γ_n corresponds to a quasi-free, particle conserving state $\rho_n \in (\mathcal{B}[\mathcal{F}_f[\mathcal{H}]])^*_{+,1}$.

Now we deduce the existence of a limit of γ_n for $n \to \infty$. Since this limit will be in the *weak-* topology* on $(\mathcal{B}_[\mathcal{F}_f[\mathcal{H}]])^*$, let us first recall the definition of this topology. The weak-* topology on any dual X^* of a Banach space X is defined as the weakest topology such that all functionals

$$\{\phi_x : X^* \to \mathbb{C}, \phi_x(x^*) = x^*(x) \mid x \in X\} \tag{3.94}$$

are continuous. This is equivalent to the formulation, that the weak-* topology is the locally convex topology on X^* which is induced by the family

$$\{\|\cdot\|_x : X^* \to \mathbb{R}_0^+, \|x^*\|_x = |x(x^*)|\}_{x\in X} \tag{3.95}$$

of semi-norms on X^*. In particular, we deduce from the continuity of all functionals in (3.94), that any sequence $(x_n^*)_{n\in\mathbb{N}}$ which converges in the weak-* topology to some $x_\infty^* \in X^*$ obeys

$$\lim_{n\to\infty} x_n^*(x) = \lim_{n\to\infty} \phi_x(x_n^*) = \phi_x(x_\infty^*) = x_\infty(x) , \tag{3.96}$$

for all $x \in X$.

It is well-known, that the set of states $(\mathcal{B}[\mathcal{F}_f[\mathcal{H}]])^*_{+,1}$ is compact in the weak-*-topology, see for example [13, Theorem 2.3.15]. This induces at once that the sequence $(\rho_n)_{n\in\mathbb{N}}$ has at least one accumulation point in $(\mathcal{B}[\mathcal{F}_f[\mathcal{H}]])^*_{+,1}$. Hence there is a subsequence $(\rho_{n_k})_{k\in\mathbb{N}}$ that converges in the weak-*-topology to some $\rho_\infty \in (\mathcal{B}[\mathcal{F}_f[\mathcal{H}]])^*_{+,1}$. In the following, we denote this convergent subsequence again as $(\rho_n)_{n\in\mathbb{N}}$ to simplify notation.

Recall, that for each quasi-free, particle conserving state $\rho_n \in (\mathcal{B}[\mathcal{F}_f[\mathcal{H}]])^*_{+,1}$ there is a corresponding 1-particle density matrix $\gamma_n \in \mathcal{B}(\mathcal{H})$, see Section 3.1.3. From the continuity of all functionals in (3.94) we obtain at once that the set of quasi-free, particle conserving states is weak-*-closed. Therefore ρ_∞ is also quasi-free and particle conserving. We denote the corresponding 1-particle-density matrix by $\gamma_\infty \in \mathcal{Z}_\Lambda$, and obtain for every $\phi, \psi \in \mathcal{H}$

$$\langle \phi, \gamma_\infty \psi\rangle = \rho_\infty(a^*(\psi)a(\phi)) = \lim_{n\to\infty} \rho_n(a^*(\psi)a(\phi)) = \lim_{n\to\infty} \langle \phi, \gamma_n \psi\rangle . \tag{3.97}$$

The equation above induces $\gamma_n \stackrel{w}{\to} \gamma_\infty$ in the *weak operator topology* of $\mathcal{B}(\mathcal{H})$. Recall, that the weak operator topology on $\mathcal{B}(\mathcal{H})$, with $\mathcal{H}$ being a Hilbert space, is defined as the weakest topology such that all functionals in the set

$$\{\phi_{x,y} : \mathcal{B}(\mathcal{H}) \to \mathbb{C}, \phi_{x,y}(A) = \langle x, Ay\rangle \mid x, y \in \mathcal{H}\} \tag{3.98}$$

are continuous.

Remark 3.3.1. *The construction of a weak-* accumulation point as described above is of course also possible for minimizers (unique or not) of $\mathcal{E}^{(HF/rHF)}_{\omega,\Lambda_n}$, $\widetilde{\mathcal{E}}^{(\mathrm{HF/rHF})}_{\omega,\Lambda,\mu}$, $-\mathcal{P}^{(HF/rHF)}_{\omega,\Lambda_n,\beta}$ or $\mathcal{M}^{(HF)}_{\omega,\Lambda_n,\beta,\mu}$, but the result is in any case rather weak. Especially, if the uniqueness of the minimizers is not clear, the accumulation points may depend on the choice of the minimizers. In addition to this the uniqueness of the limit state is not understood in any of these cases.*

The following Lemma is a preparation to prove the uniqueness of the thermodynamic limit of minimizers of $\mathcal{M}^{(\mathrm{rHF})}_{\omega,\Lambda_n,\beta,\mu}$ in Theorem 3.3.4 by means of the self-consistent equations.

Lemma 3.3.2 (Self-consistent equations for accumulation points)**.**
For $\omega \in \Omega$, $\beta \in (0,\infty)$ and $\mu \in \mathbb{R}$, let $\gamma_n \in \mathcal{Z}$ be a subsequence of the unique minimizers of $\mathcal{M}^{(\mathrm{rHF})}_{\omega,\Lambda_n,\beta,\mu}$, such that the corresponding quasi-free states $\rho_n \in (\mathcal{B}[\mathcal{F}_f[\mathcal{H}]])^*_{+,1}$ converge in the weak--topology to the quasi-free state ρ_∞ with corresponding 1-particle density matrix $\gamma_\infty \in \mathcal{Z}$ given by* (3.97)*.*

Then the effective Hamiltonians $H^{(\mathrm{rHF})}_{\omega,\Lambda_n,\mathrm{eff}}[\gamma_n] \in \mathcal{B}(\mathcal{H})$ converge in the weak operator topology to $H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\gamma_\infty] \in \mathcal{B}(\mathcal{H})$, given by

$$\langle e_x, H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\gamma_\infty] e_y\rangle = \langle e_x, h_\omega e_y\rangle + g\,\mathrm{Tr}\{W(\gamma_\infty \otimes |\, e_y\rangle\langle e_x|)\}. \tag{3.99}$$

Furthermore, γ_∞ fulfills the self-consistent equation,

$$\gamma_\infty = \Big(1 + \exp\Big[\beta(H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\gamma_\infty] - \mu)\Big]\Big)^{-1} \tag{3.100}$$

Remark 3.3.3. *Similar to* (3.51) *the effective Hamiltonian $H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\gamma_\infty]$ can be expressed as*

$$H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\gamma_\infty] = h_\omega + g[W * \gamma_\infty] \tag{3.101}$$

where $[W * \gamma_\infty] \in \mathcal{B}(\mathcal{H})$ is the multiplication operator defined analogously to (3.52)

$$[[W * \gamma_\infty]\phi]\,(x) = \sum_{y\in\mathbb{Z}^d} \mathcal{W}(x-y)\rho_{\gamma_\infty}(y)\phi(x) \tag{3.102}$$

for every $\phi \in \mathcal{H}_\Lambda, x \in \mathbb{Z}^d$. Note that $[W * \gamma_\infty]$ is well-defined, because W is of finite range.

Proof. We show (3.99) by using (3.101). For all $x, y \in \mathbb{Z}^d$ we have

$$\begin{aligned}
&\lim_{n\to\infty} \langle e_x, (H^{(\mathrm{rHF})}_{\omega,\Lambda_n,\mathrm{eff}}[\gamma_n] - H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\gamma_\infty])e_y\rangle \\
&\quad = \lim_{n\to\infty} \langle e_x, (h_{\omega,\Lambda_n} - h_\omega)e_y\rangle + g\langle e_x, [W * (\gamma_n - \gamma_\infty)]e_y\rangle \\
&\quad = g \lim_{n\to\infty} \mathcal{W}(y-x)(\gamma_n(x,x) - \gamma_\infty(x,x)) = 0
\end{aligned}$$

because of (3.97).

Each minimizer γ_n fulfills the self-consistent equation

$$\gamma_n = f\left(\beta(H^{(\mathrm{rHF})}_{\omega,\Lambda_n,\mathrm{eff}}[\gamma_n] - \mu)\right) \tag{3.103}$$

for $f : \mathbb{R} \to \mathbb{R}$, $f(x) = (1 + e^x)^{-1}$.

Therefore we obtain by (3.97) and the continuity of f, the scalar product and the functional calculus w.r.t. the weak operator topology, that for all $x, y \in \mathbb{Z}^d$

$$\begin{aligned}
\langle e_x, \gamma_\infty e_y\rangle &= \lim_{n\to\infty} \langle e_x, \gamma_n e_y\rangle \\
&= \lim_{n\to\infty} \langle e_x, f(\beta(H^{(\mathrm{rHF})}_{\omega,\Lambda_n,\mathrm{eff}}[\gamma_n] - \mu))e_y\rangle \\
&= \langle e_x, f(\beta(H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\gamma_\infty] - \mu))e_y\rangle \ ,
\end{aligned}$$

which proves (3.100). □

Now we are ready to prove the uniqueness of γ_∞:

Theorem 3.3.4 (Uniqueness of the minimizer of $\mathcal{M}^{(\mathrm{rHF})}_{\omega,\Lambda,\beta,\mu}$ in the thermodynamic limit)**.**
If $\beta \in (0,\infty)$, $g > 0$ are such that

$$\frac{\beta g}{4} \|\mathcal{W}\|_1 < 1 \ , \tag{3.104}$$

where

$$\|\mathcal{W}\|_1 = \sum_{x\in\mathbb{Z}^d} |\mathcal{W}(x)| \ , \tag{3.105}$$

then for all $\omega \in \Omega$, $\beta \in (0,\infty)$ and $\mu \in \mathbb{R}$ there is $\gamma_\infty \in \mathcal{Z}$ such that the sequence of unique minimizers $\gamma_n \in \mathcal{Z}$ of $\mathcal{M}^{(\mathrm{rHF})}_{\omega,\Lambda_n,\beta,\mu}$ converges in the weak-operator topology of $\mathcal{B}(\mathcal{H})$ to γ_∞,

$$\lim_{n\to\infty} \langle e_x, \gamma_n e_y\rangle = \langle e_x, \gamma_\infty e_y\rangle \ \textit{for all } x, y \in \mathbb{Z}^d. \tag{3.106}$$

Proof. Note that

$$f(x) = (1 + e^x)^{-1} = \frac{1}{2}\left(1 + \tanh\left(-\frac{x}{2}\right)\right) . \tag{3.107}$$

It follows from the product representation of $\cosh$ that

$$\begin{aligned}
\tanh(x) &= \frac{d}{dx} \ln\cosh(x) \\
&= \sum_{k=0}^{\infty} \left(\frac{1}{\pi i(k+\frac{1}{2}) + x} - \frac{1}{\pi i(k+\frac{1}{2}) - x}\right) \ , \qquad (3.108)
\end{aligned}$$

c.f. [6]. Therefore we can express f as the following series

$$f(x) = \frac{1}{2} + \sum_{k=0}^{\infty} \sum_{\sigma=\pm 1} \frac{1}{2\sigma\pi i(k+\frac{1}{2}) - x} \,. \tag{3.109}$$

Now, we define for any $\beta \in (0,\infty)$ and $\mu \in \mathbb{R}$ the function $F_{\beta,\mu} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$ by setting

$$F_{\beta,\mu}(\gamma) := f\left(\beta(H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\gamma] - \mu)\right) \tag{3.110}$$

and estimate for arbitrary $\gamma, \widetilde{\gamma} \in \mathcal{B}(\mathcal{H})$

$$\begin{aligned}
\|F_{\beta,\mu}(\gamma) - F_{\beta,\mu}(\widetilde{\gamma})\|_{op} &\leq \left\| f(\beta(H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\gamma] - \mu)) - f(\beta(H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\widetilde{\gamma}] - \mu)) \right\|_{op} \\
&\leq \sum_{k=0}^{\infty} \sum_{\sigma=\pm 1} \left\| \frac{1}{2\sigma\pi i(k+\frac{1}{2}) - \beta(H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\gamma] - \mu)} \right. \\
&\qquad \left. - \frac{1}{2\sigma\pi i(k+\frac{1}{2}) - \beta(H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\widetilde{\gamma}] - \mu)} \right\|_{op} \\
&\leq 2\beta g \sum_{k=0}^{\infty} \frac{1}{4\pi^2(k+\frac{1}{2})^2} \|W * (\widetilde{\gamma} - \gamma)\|_{op} \\
&\leq \frac{\beta g}{4} \|\mathcal{W}\|_1 \|(\widetilde{\gamma} - \gamma)\|_{op}
\end{aligned} \tag{3.111}$$

where we used the second resolvent equality and

$$\sum_{k=0}^{\infty} \frac{1}{\pi^2(k+\frac{1}{2})^2} = \frac{1}{2} \,. \tag{3.112}$$

Because $\frac{\beta g}{4} \|\mathcal{W}\|_1 < 1$, $F_{\beta,\mu}$ is a contraction and therefore it has a unique fixed point. But by Lemma 3.3.2 any accumulation point of $\{\gamma_n\}$ is a fixed point of $F_{\beta,\mu}$, hence there is exactly one unique accumulation point. Since the set of quasi-free states is weak-*-compact, the convergence of γ_n in the weak operator topology follows.

□

3.3.2 Ergodicity of the minimizer and the effective Hamiltonian

We show, that the minimizers as well as the effective Hamiltonians in the thermodynamic limit are ergodic operator families w.r.t. the group of translations in $\mathbb{Z}^d$.

The translations are given by $\tau^k : \mathcal{H} \to \mathcal{H}$

$$[\tau^k \phi](x) := \phi(x-k) \tag{3.113}$$

and $T^k : \Omega \to \Omega$

$$[T^k \omega](x) = \omega(x-k) \; , \tag{3.114}$$

respectively.

Theorem 3.3.5. *Let $\omega \in \Omega$, $\mu \in \mathbb{R}$ and $g, \beta \in (0,\infty)$ be such that $\frac{\beta g}{4} \left\| \mathcal{W} \right\|_1 < 1$. Let $\gamma_\omega \in \mathcal{Z}$ be the thermodynamic limit of the unique minimizers $\gamma_{\omega,n} \in \mathcal{Z}$ of $\mathcal{M}^{(\mathrm{rHF})}_{\omega,\Lambda_n,\beta,\mu}$, c.f Theorem 3.3.4. Set $\widetilde{H}_\omega := H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\gamma_\omega]$ to be the corresponding effective Hamiltonian.*

Then $\{\widetilde{H}_\omega\}_{\omega\in\Omega}$ and $\{\gamma_\omega\}_{\omega\in\Omega}$ are ergodic operator families w.r.t the group of translations $\{\tau^k\}_{k\in\mathbb{Z}^d}$, that is for all $k \in \mathbb{Z}^d$

$$\tau^k \gamma_\omega \tau^{-k} = \gamma_{T^k\omega} \; , \tag{3.115}$$

and

$$\tau^k \widetilde{H}_\omega \tau^{-k} = \widetilde{H}_{T^k\omega} \; . \tag{3.116}$$

Proof. Similar to the proof of Theorem 3.3.4 we define for $\omega \in \Omega$, $\beta \in (0,\infty)$, $\mu \in \mathbb{R}$ the function $F_{\omega,\beta,\mu} : \mathcal{B}(\mathcal{H}) \to \mathcal{B}(\mathcal{H})$

$$F_{\omega,\beta,\mu}(\gamma) := f\left(\beta(H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\gamma] - \mu)\right) \tag{3.117}$$

where we explicitly denote the dependence on $\omega \in \Omega$ now and f is given by $f(x) = (1+e^x)^{-1}$ as before. Recall, that (3.111) implies that $F_{\omega,\beta,\mu}(\gamma)$ has a unique fixed point.

The effective Hamiltonian $H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\gamma]$ obeys for all $\phi \in \mathcal{H}$, $x, k \in \mathbb{Z}^d$

$$\begin{aligned}
\left[\left(\tau^k H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\gamma]\tau^{-k}\right)\phi\right](x) &= [h_\omega(\tau^{-k})\phi](x-k) + g\left[[W * \gamma](\tau^{-k}\phi)\right](x-k) \\
&= [h_{T^k\omega}\phi](x) + g\sum_{y\in\mathbb{Z}^d} \mathcal{W}(x-y)\gamma(y-k,y-k)\phi(x) \\
&= [h_{T^k\omega}\phi](x) + g\left[[W * (\tau^k\gamma\tau^{-k})]\phi\right](x) \\
&= \left[H^{(\mathrm{rHF})}_{T^k\omega,\mathrm{eff}}[\tau^k\gamma\tau^{-k}]\phi\right](x) \; ,
\end{aligned} \tag{3.118}$$

hence we have

$$\tau^k H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\gamma]\tau^{-k} = H^{(\mathrm{rHF})}_{T^k\omega,\mathrm{eff}}[\tau^k\gamma\tau^{-k}] \tag{3.119}$$

Now, we use (3.119) and the self-consistent equations and observe that

$$\begin{aligned}
\tau^k \gamma_\omega \tau^{-k} &= \tau^k F_{\omega,\beta,\mu}(\gamma_\omega)\tau^{-k} \\
&= \tau^k \left(1 + \exp\left[\beta(H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\gamma_\omega] - \mu)\right]\right)^{-1} \tau^{-k} \\
&= \left(1 + \exp\left[\beta(\tau^k H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\gamma_\omega]\tau^{-k} - \mu)\right]\right)^{-1} \\
&= \left(1 + \exp\left[\beta(H^{(\mathrm{rHF})}_{T^k\omega,\mathrm{eff}}[\tau^k\gamma_\omega\tau^{-k}] - \mu)\right]\right)^{-1} \\
&= F_{T^k\omega,\beta,\mu}(\tau^k\gamma_\omega\tau^{-k}) \,, \qquad (3.120)
\end{aligned}$$

as well as

$$\gamma_{T^k\omega} = F_{T^k\omega,\beta,\mu}(\gamma_{T^k\omega}) \,. \qquad (3.121)$$

Since the fixed point of $F_{T^k\omega,\beta,\mu}$ is unique, we obtain (3.115). Then (3.116) follows immediately from (3.119) and (3.115).

□

We conclude this section by remarking that Theorem 3.3.5 implies at once:

Corollary 3.3.6. *Under the assertion of Theorem 3.3.5, the spectrum of the operator families $\{\widetilde{H}_\omega := H^{(\mathrm{rHF})}_{\omega,\mathrm{eff}}[\gamma_\omega]\}_{\omega\in\Omega}$ and $\{\gamma_\omega\}_{\omega\in\Omega}$ is $\mathbb{P}$-almost surely constant.*

Chapter 4

The AC–Conductivity Measure from the Entropy Production of Fermions in Disordered Media

In this chapter, the notion of an *AC-conductivity measure* μ_σ in linear response theory for free fermions on the lattice is proposed. The fermions are subjected to a random potential and an electric field that is time- and space-dependent. General properties of μ_σ, as its behavior at large, small and moderate randomness, are also proven. The project is common work together with Jean-Bernard Bru and Walter de Siqueira Pedra, that is to be published [15, 17, 16, 18].

This chapter is organized in the following way: First, we give an introduction to the physical background and a rough overview of the main results in Section 4.1. The precise description of the model is then given in Section 4.2. Next, in Section 4.3 we prove some technical lemmas as a preparation, since these are essential for the following proofs. In Section 4.4 we define and proof the existence of energy increments. These play a major role in the main result, that is presented in the following Section 4.5. Theorem 4.5.1 corresponds to Joule's law of heat production in the AC-case. Finally, in Section 4.6 we define the AC-conductivity measure and study the asymptotics of this measure, that vanishes in the case of very small and very large randomness, as is proven in Theorem 4.6.5, and show that it is strictly positive in a certain regime of randomness and temperature, see Theorem 4.6.10.

4.1 Introduction

It is widely accepted that the electric resistance of conductors results from both, the presence of disorder in the host material and interactions between charge carriers. Here, we only consider effects of disorder for non-interacting fermions. That means physically that the particles obey the Pauli exclusion principle, i.e. the antisymmetry of the many-body wave function, but do not interact with each other via some mutual force. This setup corresponds for example to the case of low electron densities in crystals.

First let us review a result of Klein, Lenoble and Müller, who introduced in [25] the concept of an AC-conductivity measure μ_{KLM} for a system of non-interacting fermions subjected to a random potential for the first time. More precisely, the authors considered the Anderson tight-binding model in presence of a time-dependent spatially homogeneous electric field $\mathcal{E} = \mathcal{E}_t$ that is adiabatically switched on. Then they showed that the in-phase linear response current density is given, at any time $t \in \mathbb{R}$, by

$$J_{\mathrm{lin}}^{\mathrm{in}}(t;\mathcal{E}) = \int_{\mathbb{R}} \widehat{\mathcal{E}}_\nu \, \mathrm{e}^{i\nu t} \, \mu_{\mathrm{KLM}}(\mathrm{d}\nu) \ ,$$

cf. [25, Eq. (2.13)]. Here, $\widehat{\mathcal{E}}_\nu$ is the Fourier transform of the electric field $\mathcal{E}_t$ at frequency $\nu \in \mathbb{R}$ and is compactly supported, see also [11] for further details. The fermionic nature of charge carriers - electrons or holes in crystals - was implemented by choosing the Fermi-Dirac distribution as the initial density matrix of particles at time $t \to -\infty$. In [25] only systems at zero temperature with Fermi energy lying in the localization regime are considered, but it is shown in [26] that an AC-conductivity measure can also be defined without the localization assumption and at any positive temperature.

Although there is no interaction between fermions, we do not restrict our analyses to the one-particle Hilbert space. In contrast to [25] the presented approach is based on the algebraic formulation of fermion systems on lattices. It makes the role played by many-fermion correlations due to the Pauli exclusion principle, i.e., the antisymmetry of the many-body wave function, more transparent. The AC-conductivity in this framework is naturally defined by current-current correlations, i.e. four-point correlation functions. Moreover, in principle, this approach can be used to define the AC-conductivity measure for interacting fermions on the lattice. This work can thus be seen as a mathematical preparation for such further studies.

In the following, we present the mathematical framework we use and our results. We consider the random two-parameter group $\{U_{t,s}^{(\omega)}\}_{t\geq s}$ of unitary operators on $\ell^2(\mathbb{Z}^d)$ generated by the time-dependent Hamiltonian

$$\Delta_{\mathrm{d}}^{(\mathbf{A}(t,\cdot))} + \lambda V_\omega \in \mathcal{B}(\ell^2(\mathbb{Z}^d)) ,$$

where the parameter ω runs in a probability space and λV_ω is a random potential with strength $\lambda \geq 0$.

Here, the vector potential $\mathbf{A} = \mathbf{A}(t,x) \in C_0^\infty(\mathbb{R} \times \mathbb{R}^d; (\mathbb{R}^d)^*)$ represents a time-dependent spatially inhomogeneous electromagnetic field which is minimally coupled to (minus) the discrete Laplacian Δ_{d}. In contrast to [25, 26], the electromagnetic field is inhomogeneous, supported in an arbitrarily large but bounded region of space and is switched off for times outside some finite interval $[t_0, t_1]$.

The family $\{U_{t,s}^{(\omega)}\}_{t\geq s}$ of unitaries on $\ell^2(\mathbb{Z}^d)$ induces a random two-parameter group $\{\tau_{t,s}^{(\omega,\lambda,\mathbf{A})}\}_{t\geq s}$ of Bogoliubov automorphisms of a CAR algebra $\mathcal{U}$ (c.f. Section 4.2.3) associated with non-relativistic fermions in the cubic lattice $\mathbb{Z}^d$. Indeed, the canonical anti-commutation relations (CAR) encode the Pauli exclusion principle. Note that the C^*-algebra $\mathcal{U}$ corresponds to a fermion system which is infinitely extended.

As initial state of the system at time $t_0 \in \mathbb{R}$, we take the unique KMS state (c.f. Section 4.2.4) on $\mathcal{U}$ related to the autonomous dynamics for $\mathbf{A} \equiv 0$ and inverse temperature $\beta > 0$. That means, we assume the system to be in thermal equilibrium before the electromagnetic potential is switched on. Then we analyze the produced entropy or heat $\mathfrak{I}_t$ up to times $t \geq t_1$. We show that, almost surely,

$$\mathfrak{I}_t = \int_{t_0}^{t} \int_{t_0}^{s_1} \left[\sigma(s_1 - s_2) \int_{\mathbb{R}^d} \langle E_{\mathbf{A}}(s_1, x), E_{\mathbf{A}}(s_2, x) \rangle \, \mathrm{d}^d x \right] \mathrm{d}s_2 \mathrm{d}s_1 \geq 0 \quad (4.1)$$

at leading order. Here,

$$E_{\mathbf{A}}(t,x) := -\partial_t \mathbf{A}(t,x) , \quad t \in \mathbb{R},\ x \in \mathbb{R}^d ,$$

is the electric field induced by $\mathbf{A}$ and $\sigma : \mathbb{R} \to \mathbb{R}$ is a deterministic continuous bounded function. As in [26], we do not need any localization assumption. Additionally, we obtain an explicit expression for the function σ.

Since $E_{\mathbf{A}}$ is the electric field, we may interpret the term

$$\int_{t_0}^{s_1} \sigma(s_1 - s_2) E_{\mathbf{A}}(s_2, x) \mathrm{d}s_2$$

as the current density at time s_1 and space position $x \in \mathbb{R}^d$ and σ can be seen as the AC-conductivity of the system. Hence, (4.1) is the energy delivered by the electric field to the system, as predicted by Joule's law.

As is shown in Section 4.6.1, it follows from the explicit form of σ and the use of analyticity properties of correlation functions of KMS states, that σ is, up to a constant, a function of positive type, and then Bochner's Theorem implies that there is a finite, positive measure, such that

$$\sigma(t) = \int_{\mathbb{R}} \left(\mathrm{e}^{it\nu} - 1\right) \mathrm{d}\mu_\sigma(\nu) , \qquad t \in \mathbb{R} . \tag{4.2}$$

The measure μ_σ is naturally named *AC-conductivity measure* of the fermion system in accordance with Joule's law in the AC-case, because we get for $t \geq t_1$

$$\int_{t_0}^{t} \int_{t_0}^{s_1} \sigma(s_2 - s_1) \langle E_{\mathbf{A}}(s_1, x),\ E_{\mathbf{A}}(s_2, x) \rangle \mathrm{d}s_1 \mathrm{d}s_2 = \frac{1}{2} \int_{\mathbb{R}\backslash\{0\}} |\hat{E}_{\mathbf{A}}(\nu, x)|^2 \, \mathrm{d}\mu_\sigma(\nu) , \tag{4.3}$$

with $\hat{E}_{\mathbf{A}}$ being the Fourier transform of $E_{\mathbf{A}}$. Observe, that $|\hat{E}_{\mathbf{A}}(\nu, x)|^2 \, \mathrm{d}\mu_\sigma(\nu)$ is the heat production due to the component of frequency ν of the electric field at position $x \in \mathbb{R}^d$. Furthermore, note that because of $\mathbf{A}$ being compactly supported in time, we have that $\hat{E}_{\mathbf{A}}(0, x) = 0$ at any space position $x \in \mathbb{R}^d$. Thus the exclusion of $\{0\}$ in (4.3) might seem artificial, but it is done to emphasize that we are dealing with the AC-case here.

The AC-conductivity measure μ_σ converges in the weak*-topology to the zero-measure on $\mathbb{R}\backslash\{0\}$ in the case of perfect conductors, that is the absence of randomness, i.e. $\lambda \to 0$, as well as in the case of perfect insulators, corresponding to complete localization, i.e. $\lambda \to \infty$. Note, that the fact that the AC-conductivity measure vanishes in $\mathbb{R}\backslash\{0\}$ does not imply, in general, that there are no currents in presence of electric fields. It only implies that the so-called in-phase current, which is the component of the total current producing heat (active current), is zero. Furthermore, observe that $\mu_\sigma(\mathbb{R}\backslash\{0\})$ is in general non-vanishing: In Section 4.6 it is shown that $\mu_\sigma(\mathbb{R}\backslash\{0\}) > 0$, at least for large temperatures β^{-1} and small randomness $\lambda > 0$.

4.2 Setup of the model

In this section the precise mathematical setup of the model under consideration is presented. We start by giving a short introduction to fermion systems on lattices and go on by inducing first the dynamic due to the randomness or impurities of the crystal and second the dynamics induced by the outer electromagnetic potential. The section is concluded by the characterization of the initial KMS state and its time evolution.

4.2.1 Algebraic formulation of fermion systems on lattices

The host material for the conducting fermions is assumed to be a cubic crystal. Other crystal families could also be studied in the same way, but, for simplicity, we refrain from considering them. We thus use the d-dimensional cubic lattice $\mathfrak{L} := \mathbb{Z}^d$ to represent the crystal and we define $\mathcal{P}_f(\mathfrak{L})$ to be the set of all finite subsets of $\mathfrak{L}$.

Within this framework, an *infinite* system of charged fermions is considered. To simplify notation we restrict to spinless fermions. That means, we refrain from regarding, for example, $\mathbb{Z}^d \times \{-1,+1\}$ instead of $\mathbb{Z}^d$. The case of spinning particles can be treated by exactly the same methods.

For any $\Lambda \in \mathcal{P}_f(\mathfrak{L})$, $\mathcal{U}_\Lambda$ is the C^*-algebra generated by the identity $\mathbf{1}$ and the annihilation operators $\{a_x\}_{x\in\Lambda}$, satisfying the canonical anti-commutation relations (CAR): For any $x, y \in \mathfrak{L}$,

$$a_x a_y + a_y a_x = 0 \ , \qquad a_x a_y^* + a_y^* a_x = \delta_{x,y}\mathbf{1} \ . \tag{4.4}$$

$\mathcal{U}_\Lambda$ is isomorphic to the (finite dimensional) C^*-algebra $\mathcal{B}(\bigwedge \mathcal{H}_\Lambda)$ of all linear operators on the fermion Fock space $\bigwedge \mathcal{H}_\Lambda$, where $\mathcal{H}_\Lambda := \bigoplus_{x\in\Lambda} \mathcal{H}_x$ is the direct sum of copies $\mathcal{H}_x$, $x \in \Lambda$, of the one-dimensional Hilbert space $\mathcal{H} \equiv \mathbb{C}$, see also Section 3.1.3. The CAR C^*-algebra $\mathcal{U}$ is the (separable) C^*-algebra defined by the inductive limit of $\{\mathcal{U}_\Lambda\}_{\Lambda\in\mathcal{P}_f(\mathfrak{L})}$. Note here that $\mathcal{U}_{\Lambda'} \subset \mathcal{U}_\Lambda$ whenever $\Lambda' \subset \Lambda$.

In order to set up the time evolution in the following sections, we define annihilation and creation operators of (spinless) fermions with wave functions $\psi \in \ell^2(\mathfrak{L})$ by

$$a(\psi) := \sum_{x\in\mathfrak{L}} \overline{\psi(x)} a_x \in \mathcal{U} \ , \quad a^*(\psi) := \sum_{x\in\mathfrak{L}} \psi(x) a_x^* \in \mathcal{U} \ . \tag{4.5}$$

These operators are well-defined because of (4.4). Indeed,

$$\|a(\psi)\|^2, \|a^*(\psi)\|^2 \leq \|\psi\|_2^2 \ , \qquad \psi \in \ell^2(\mathfrak{L}) \ , \tag{4.6}$$

and thus, the antilinear map $\psi \mapsto a(\psi)$ and the linear map $\psi \mapsto a^*(\psi)$ from $\ell^2(\mathfrak{L})$ to $\mathcal{U}$ are norm-continuous. Clearly, $a^*(\psi) = a(\psi)^*$ for all $\psi \in \ell^2(\mathfrak{L})$.

4.2.2 Disorder in the crystal and induced dynamics

Disorder in the crystal is modeled as in the usual Anderson model. Therefore we take a random chemical potential coming from a probability space $(\Omega, \mathfrak{A}_\Omega, \mathfrak{a}_\Omega)$ defined as follows: Let $\Omega := [-1,1]^{\mathfrak{L}}$ and Ω_x, $x \in \mathfrak{L}$, be an arbitrary element of the Borel σ-algebra of the interval $[-1,1]$ w.r.t. the usual metric topology. Then $\mathfrak{A}_\Omega$ is the σ-algebra generated by the cylinder sets $\bigtimes_{x\in\mathfrak{L}} \Omega_x$, where $\Omega_x = [-1,1]$ for all but finitely many $x \in \mathfrak{L}$. The measure $\mathfrak{a}_\Omega$ is the product measure

$$\mathfrak{a}_\Omega \left(\bigtimes_{x\in\mathfrak{L}} \Omega_x \right) := \prod_{x\in\mathfrak{L}} \mathfrak{a}_0(\Omega_x) \ , \tag{4.7}$$

where $\mathfrak{a}_0$ is any fixed probability measure on the interval $[-1,1]$. In other words, the random potential is independently and identically distributed (i.i.d.).

For any realization $\omega \in \Omega$, $V_\omega \in \mathcal{B}(\ell^2(\mathfrak{L}))$ is the self-adjoint multiplication operator with the function $\omega : \mathfrak{L} \to [-1,1]$. Note that the potential V_ω is of order $\mathcal{O}(1)$ and we rescale its strength by an additional parameter $\lambda \in \mathbb{R}_0^+$ (i.e., $\lambda \geq 0$), see (4.9).

For simplicity and without loss of generality (w.l.o.g.), we assume that the expectation of the potential at any single site potential is zero:

$$\mathbb{E}\left(\omega(0)\right) = \int_\Omega \omega(0) \mathrm{d}\mathfrak{a}_0(\omega) = 0 \ . \tag{4.8}$$

We can easily remove this condition by replacing ω by $\omega - \mathbb{E}(\omega(0))$ and adding $\mathbb{E}(\omega(0))$ to the discrete Laplacian defined below.

Finally note that the i.i.d. property of the potential is not essential for our results. We could take any ergodic ensemble instead. However, this assumption and (4.8) extremely simplify the proof of the strict positivity of the heat production (Theorem 4.6.10).

Now, for any realization $\omega \in \Omega$ and strength of disorder $\lambda \in \mathbb{R}_0^+$, we define the free dynamics of the lattice fermion system via the unitary group $\{\mathrm{U}_t^{(\omega,\lambda)}\}_{t\in\mathbb{R}}$ with

$$\mathrm{U}_t^{(\omega,\lambda)} := \exp(-it(\Delta_{\mathrm{d}} + \lambda V_\omega)) \in \mathcal{B}(\ell^2(\mathfrak{L})) \ . \tag{4.9}$$

Here, $\Delta_{\mathrm{d}} \in \mathcal{B}(\ell^2(\mathfrak{L}))$ is (up to a minus sign) the usual d-dimensional discrete Laplacian:

$$[\Delta_{\mathrm{d}}(\psi)](x) := 2d\psi(x) - \sum_{z\in\mathfrak{L},\, |z|=1} \psi(x+z) \ , \qquad x \in \mathfrak{L},\ \psi \in \ell^2(\mathfrak{L}) \ . \tag{4.10}$$

For all $\omega \in \Omega$ and $\lambda \in \mathbb{R}_0^+$, the condition

$$\tau_t^{(\omega,\lambda)}(a(\psi)) = a\left((\mathrm{U}_t^{(\omega,\lambda)})^*(\psi)\right) , \qquad t \in \mathbb{R},\ \psi \in \ell^2(\mathfrak{L}) , \tag{4.11}$$

uniquely defines a one-parameter (Bogoliubov) group $\tau^{(\omega,\lambda)} := \{\tau_t^{(\omega,\lambda)}\}_{t\in\mathbb{R}}$ of automorphisms of $\mathcal{U}$, see [14, Theorem 5.2.5]. As $\tau_t^{(\omega,\lambda)}$ is an automorphism of $\mathcal{U}$, we have in particular -per definition - that

$$\tau_t^{(\omega,\lambda)}(B_1B_2) = \tau_t^{(\omega,\lambda)}(B_1)\tau_t^{(\omega,\lambda)}(B_2) , \qquad B_1, B_2 \in \mathcal{U} ,\ t \in \mathbb{R} . \tag{4.12}$$

Physically, (4.11) means that the fermionic particles do not experience any mutual force: They interact with each other via the Pauli exclusion principle only, i.e., they form an ideal lattice fermion system. From (4.6) and the strong continuity of the unitary group $\{\mathrm{e}^{-it(\Delta_{\mathrm{d}}+\lambda V_\omega)}\}_{t\in\mathbb{R}}$ it follows that the (Bogoliubov) group $\tau^{(\omega,\lambda)}$ of automorphisms is strongly continuous. $(\mathcal{U}, \tau^{(\omega,\lambda)})$ is hence a C^*-dynamical system. Its generator is denoted by $\delta^{(\omega,\lambda)}$, which is a symmetric derivation. This means that the domain $\mathrm{Dom}(\delta^{(\omega,\lambda)})$ of $\delta^{(\omega,\lambda)}$ is a dense $*$-subalgebra of $\mathcal{U}$ and, for all $B_1, B_2 \in \mathrm{Dom}(\delta^{(\omega,\lambda)})$,

$$\delta^{(\omega,\lambda)}(B_1)^* = \delta^{(\omega,\lambda)}(B_1^*), \quad \delta^{(\omega,\lambda)}(B_1B_2) = \delta^{(\omega,\lambda)}(B_1)B_2 + B_1\delta^{(\omega,\lambda)}(B_2) .$$

4.2.3 Electromagnetic fields and induced dynamics

The electromagnetic potential is defined by a smooth, compactly supported time-dependent vector potential

$$\mathbf{A} \in \mathbf{C}_0^\infty := C_0^\infty(\mathbb{R} \times \mathbb{R}^d; (\mathbb{R}^d)^*) . \tag{4.13}$$

Here, $(\mathbb{R}^d)^*$ is the set of one-forms[1] on $\mathbb{R}^d$ that take values in $\mathbb{R}$. Using any orthonormal basis $\{e_k\}_{k=1}^d$ of the Euclidian space $\mathbb{R}^d$, we define the scalar product between two fields $E^{(1)}, E^{(2)} \in (\mathbb{R}^d)^*$ as usual by

$$\left\langle E^{(1)}, E^{(2)} \right\rangle := \sum_{k=1}^{d} E^{(1)}(e_k)\, E^{(2)}(e_k) \ . \tag{4.14}$$

Since $\mathbf{A} \in \mathbf{C}_0^\infty$, $\mathbf{A}(t,x) = 0$ for all $t \leq t_0$, where $t_0 \in \mathbb{R}$ is some initial time. Recall also that

$$E_{\mathbf{A}}(t,x) := -\partial_t \mathbf{A}(t,x) , \quad t \in \mathbb{R},\ x \in \mathbb{R}^d , \tag{4.15}$$

[1] In a strict sense, one should take the tangent spaces $T(\mathbb{R}^d)_x$, $x \in \mathbb{R}^d$, and their dual spaces.

is the electric field associated with $\mathbf{A}$.

Since $\mathbf{A}$ is by assumption compactly supported in time, the corresponding electric field satisfies the *AC-condition*

$$\int_{t_0}^{t} E_{\mathbf{A}}(s,x)\mathrm{d}s = 0 \, , \quad x \in \mathbb{R}^d \, , \tag{4.16}$$

for sufficiently large times $t \geq t_1 \geq t_0$. From (4.16)

$$t_1 := \min \left\{ t \geq t_0 : \quad \int_{t_0}^{t'} E_{\mathbf{A}}(s,x)\mathrm{d}s = 0 \quad \text{for all } x \in \mathbb{R}^d \text{and } t' \geq t \right\} \tag{4.17}$$

is the time at which the electric field is turned off.

Below, we rescale the strength of the electromagnetic potential $\mathbf{A}$ by a parameter $\eta > 0$, see Section 4.4.2. Then the limit $\eta \to 0$ corresponds to the *linear response* of the fermion system, which is the regime in which Joule's law holds true.

Remark 4.2.1.
By considering the Fourier transform of $E_{\mathbf{A}}(\cdot, x)$, the property (4.16) corresponds to the fact that the low frequency components of the external electromagnetic field are small. We do not try to remove this condition because, for electric fields slowly varying in time, charge carriers have time to move and significantly change the charge density, producing an additional, self-generated, internal electric field. This contribution is not taken into account in the model presented here.

We consider w.l.o.g. *negatively* charged fermions. Thus, the (minimal) coupling of the vector potential $\mathbf{A} \in \mathbf{C}_0^\infty$ to the fermion system is achieved through a redefinition of the discrete Laplacian. Indeed, we define the self-adjoint operator $\Delta_{\mathrm{d}}^{(\mathbf{A})} \in \mathcal{B}(\ell^2(\mathfrak{L}))$ by

$$\langle \mathfrak{e}_x, \Delta_{\mathrm{d}}^{(\mathbf{A})} \mathfrak{e}_y \rangle = \exp\left(-i \int_0^1 \left[\mathbf{A}(t, \alpha y + (1-\alpha)x) \right] (y-x) \mathrm{d}\alpha \right) \langle \mathfrak{e}_x, \Delta_{\mathrm{d}} \mathfrak{e}_y \rangle \tag{4.18}$$

for all $x, y \in \mathfrak{L}$, where $\langle \cdot, \cdot \rangle$ is here the scalar product in $\ell^2(\mathfrak{L})$ and $\{\mathfrak{e}_x\}_{x \in \mathfrak{L}}$ is the canonical orthonormal basis $\mathfrak{e}_x(y) \equiv \delta_{x,y}$ of $\ell^2(\mathfrak{L})$. Note, that in Equation (4.18) $\alpha y + (1-\alpha)x$ and $y - x$ are seen as vectors in $\mathbb{R}^d$.

Furthermore, there is some $l_0 \in \mathbb{R}^+$ such that

$$\Delta_{\mathrm{d}}^{(\mathbf{A})} - \Delta_{\mathrm{d}} \in \mathcal{B}(\ell^2([-l_0, l_0]^d)) \subset \mathcal{B}(\ell^2(\mathfrak{L}))$$

for all times $t \in \mathbb{R}$, because $\mathbf{A}$ is, by definition, compactly supported. Note also that, for simplicity, the time dependence is often omitted in the notation

$$\Delta_{\mathrm{d}}^{(\mathbf{A})} \equiv \Delta_{\mathrm{d}}^{(\mathbf{A}(t,\cdot))} , \qquad t \in \mathbb{R} ,$$

even if one has to keep in mind that the dynamics is non-autonomous.

In the following the dynamics due to the electromagnetic vector potential $\mathbf{A}$ is studied. We show the existence of the dynamics and give its explicit expression in terms of a series involving multi-commutators. Let $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $\mathbf{A} \in \mathbf{C}_0^\infty$ be arbitrarily fixed.

Indeed, the Schrödinger equation on the one-particle Hilbert space $\ell^2(\mathfrak{L})$ with time-dependent Hamiltonian $(\Delta_{\mathrm{d}}^{(\mathbf{A})} + \lambda V_\omega)$ and initial value $\psi \in \ell^2(\mathfrak{L})$ at $t = t_0$ has a unique solution $\mathrm{U}_{t,t_0}^{(\omega,\lambda,\mathbf{A})}\psi$ for any $t \geq t_0$. Here,

$$\{\mathrm{U}_{t,s}^{(\omega,\lambda,\mathbf{A})}\}_{t\geq s} \subset \mathcal{B}(\ell^2(\mathfrak{L}))$$

is the random two-parameter group of unitary operators on $\ell^2(\mathfrak{L})$ generated by the (anti-self-adjoint) operator $-i(\Delta_{\mathrm{d}}^{(\mathbf{A})} + \lambda V_\omega)$ for any $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $\mathbf{A} \in \mathbf{C}_0^\infty$, i.e.

$$\forall s,t \in \mathbb{R},\ t \geq s : \quad \partial_t \mathrm{U}_{t,s}^{(\omega,\lambda,\mathbf{A})} = -i(\Delta_{\mathrm{d}}^{(\mathbf{A}(t,\cdot))} + \lambda V_\omega)\mathrm{U}_{t,s}^{(\omega,\lambda,\mathbf{A})} , \quad \mathrm{U}_{s,s}^{(\omega,\lambda)} := \mathbf{1} . \tag{4.19}$$

The restriction $t \geq s$ is not essential here and $\mathrm{U}_{t,s}^{(\omega,\lambda,\mathbf{A})}$ could also be defined for all $s, t \in \mathbb{R}$. Indeed, $\Delta_{\mathrm{d}} \in \mathcal{B}(\ell^2(\mathfrak{L}))$ and the map

$$t \mapsto \mathbf{w}_t^{\mathbf{A}} := (\Delta_{\mathrm{d}}^{(\mathbf{A}(t,\cdot))} - \Delta_{\mathrm{d}}) \in \mathcal{B}(\ell^2(\mathfrak{L})) \tag{4.20}$$

from $\mathbb{R}$ to the set $\mathcal{B}(\ell^2(\mathfrak{L}))$ of bounded operators acting on $\ell^2(\mathfrak{L})$ is continuously differentiable for every $\mathbf{A} \in \mathbf{C}_0^\infty$. Hence, $\{\mathrm{U}_{t,s}^{(\omega,\lambda,\mathbf{A})}\}_{t\geq s}$ can be written explicitly as the Dyson-Phillips series

$$\begin{aligned} &\mathrm{U}_{t,s}^{(\omega,\lambda,\mathbf{A})} - \mathrm{U}_{t-s}^{(\omega,\lambda)} \qquad (4.21)\\ &\quad = \sum_{k\in\mathbb{N}} (-i)^k \int_s^t \mathrm{d}s_1 \cdots \int_s^{s_{k-1}} \mathrm{d}s_k \mathrm{U}_{t-s_1}^{(\omega,\lambda)} \mathbf{w}_{s_1}^{\mathbf{A}} \mathrm{U}_{s_1-s_2}^{(\omega,\lambda)} \cdots \mathrm{U}_{s_{k-1}-s_k}^{(\omega,\lambda)} \mathbf{w}_{s_k}^{\mathbf{A}} \mathrm{U}_{s_k-s}^{(\omega,\lambda)} \end{aligned}$$

for any $t \geq s$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $\mathbf{A} \in \mathbf{C}_0^\infty$. Since all operators are bounded, it is easy to check that $\{\mathrm{U}_{t,s}^{(\omega)}\}_{t\geq s}$ is a family of unitary operators.

Therefore, for all $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $\mathbf{A} \in \mathbf{C}_0^\infty$, the condition

$$\tau_{t,s}^{(\omega,\lambda,\mathbf{A})}(a(\psi)) = a\left((\mathrm{U}_{t,s}^{(\omega,\lambda,\mathbf{A})})^*(\psi)\right) , \qquad t \geq s,\ \psi \in \ell^2(\mathfrak{L}) , \tag{4.22}$$

uniquely defines a family $\{\tau_{t,s}^{(\omega,\lambda,\mathbf{A})}\}_{t\geq s}$ of Bogoliubov automorphisms of the C^*-algebra $\mathcal{U}$, see [14, Theorem 5.2.5]. It is a strongly continuous two-parameter family which obeys the non-autonomous evolution equation

$$\forall s,t \in \mathbb{R},\ t \geq s: \quad \partial_t \tau_{t,s}^{(\omega,\lambda,\mathbf{A})} = \tau_{t,s}^{(\omega,\lambda,\mathbf{A})} \circ \delta_t^{(\omega,\lambda,\mathbf{A})}, \quad \tau_{s,s}^{(\omega,\lambda,\mathbf{A})} := \mathbf{1} , \tag{4.23}$$

with $\mathbf{1}$ being the identity map from $\mathcal{U}$ to $\mathcal{U}$. Here, at any *fixed* time $t \in \mathbb{R}$, $\delta_t^{(\omega,\lambda,\mathbf{A})}$ is the infinitesimal generator of the (Bogoliubov) group $\{\tau_s^{(\omega,\lambda,\mathbf{A})}\}_{s\in\mathbb{R}} \equiv \{\tau_s^{(\omega,\lambda,\mathbf{A}(t,\cdot))}\}_{s\in\mathbb{R}}$ of automorphisms defined by replacing Δ_{d} with $\Delta_{\mathrm{d}}^{(\mathbf{A})}$ in (4.9).

The Bogoliubov automorphisms $\tau_{t,s}^{(\omega,\lambda,\mathbf{A})}$ defined by (4.22) can be represented as a Dyson-Phillips series by using the unperturbed dynamics defined by the one-parameter (Bogoliubov) group $\tau^{(\omega,\lambda)} := \{\tau_t^{(\omega,\lambda)}\}_{t\in\mathbb{R}}$, see (4.9) and (4.11). To this end, for every $\mathbf{A} \in \mathbf{C}_0^\infty$, we denote the second quantization of $\mathbf{w}_t^{\mathbf{A}}$ by

$$\begin{aligned} W_t^{\mathbf{A}} \ \ :&= \sum_{x,y\in\mathfrak{L}} \left[\exp\left(-i\int_0^1 \left[\mathbf{A}(t,\alpha y + (1-\alpha)x)\right](y-x)\mathrm{d}\alpha\right) - 1\right] \\ &\quad \times \langle \mathfrak{e}_x, \Delta_{\mathrm{d}} \mathfrak{e}_y \rangle a_x^* a_y , \end{aligned} \tag{4.24}$$

see (4.18) and (4.20). Note that there is a finite subset $\Lambda \in \mathcal{P}_f(\mathfrak{L})$ such that $W_t^{\mathbf{A}} \in \mathcal{U}_\Lambda$ for all $t \in \mathbb{R}$ because $\mathbf{A} \in \mathbf{C}_0^\infty$. We also define the continuously differentiable map

$$t \mapsto L_t^{\mathbf{A}} := i[W_t^{\mathbf{A}},\ \cdot\ ] \in \mathcal{B}(\mathcal{U}) \tag{4.25}$$

from $\mathbb{R}$ to the set $\mathcal{B}(\mathcal{U})$ of bounded operators acting on $\mathcal{U}$.

Lemma 4.2.2.
For any $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $\mathbf{A} \in \mathbf{C}_0^\infty$ and $s,t \in \mathbb{R}$, $t \geq s$,

$$\tau_{t,s}^{(\omega,\lambda,\mathbf{A})} = \tau_{t-s}^{(\omega,\lambda)} + \sum_{k\in\mathbb{N}} \int_s^t \mathrm{d}s_1 \cdots \int_s^{s_{k-1}} \mathrm{d}s_k \tau_{s_k-s}^{(\omega,\lambda)} L_{s_k}^{\mathbf{A}} \tau_{s_{k-1}-s_k}^{(\omega,\lambda)} \cdots \tau_{s_1-s_2}^{(\omega,\lambda)} L_{s_1}^{\mathbf{A}} \tau_{t-s_1}^{(\omega,\lambda)} . \tag{4.26}$$

Proof. Let $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $\mathbf{A} \in \mathbf{C}_0^\infty$ and define

$$\breve{\tau}_{t,s}^{(\omega,\lambda,\mathbf{A})} := \tau_{t-s}^{(\omega,\lambda)} + \sum_{k\in\mathbb{N}} \int_s^t \mathrm{d}s_1 \cdots \int_s^{s_{k-1}} \mathrm{d}s_k \tau_{s_k-s}^{(\omega,\lambda)} L_{s_k}^{\mathbf{A}} \tau_{s_{k-1}-s_k}^{(\omega,\lambda)} \cdots \tau_{s_1-s_2}^{(\omega,\lambda)} L_{s_1}^{\mathbf{A}} \tau_{t-s_1}^{(\omega,\lambda)} \tag{4.27}$$

for any $t \geq s$. This series is well-defined. Indeed, $\tau^{(\omega,\lambda)} := \{\tau_t^{(\omega,\lambda)}\}_{t\in\mathbb{R}}$ is a one-parameter group of contractions, i.e.,

$$\|\tau_t^{(\omega,\lambda)}\|_{\mathrm{op}} \leq 1 , \quad t \in \mathbb{R} ,$$

whereas, for any $\mathbf{A} \in \mathbf{C}_0^\infty$, there is a constant $D \in \mathbb{R}^+$ such that

$$\sup_{t\in\mathbb{R}} \|L_t^{\mathbf{A}}\|_{\mathrm{op}} < D , \tag{4.28}$$

because $W_t^{\mathbf{A}} = 0$ for any $t \notin [t_0, t_1]$ (cf. (4.17) and (4.24)). By (4.27)-(4.28), it follows that

$$\|\breve{\tau}_{t,s}^{(\omega,\lambda,\mathbf{A})}\|_{\mathrm{op}} \leq \mathrm{e}^{D(t-s)} , \quad s,t \in \mathbb{R},\ t \geq s .$$

Now, straightforward computations using (4.20) and (4.25) show that the following "pull through" formula holds:

$$L_t^{\mathbf{A}}(a(\psi)) = a(i\mathbf{w}_t^{\mathbf{A}}\psi) , \qquad t \in \mathbb{R},\ \psi \in \ell^2(\mathfrak{L}) .$$

We therefore infer from (4.11), (4.21) and (4.27) that

$$\breve{\tau}_{t,s}^{(\omega,\lambda,\mathbf{A})}(a(\psi)) = a((\mathrm{U}_{t,s}^{(\omega,\lambda,\mathbf{A})})^*(\psi)) , \qquad t \geq s,\ \psi \in \ell^2(\mathfrak{L}) ,$$

for all $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $\mathbf{A} \in \mathbf{C}_0^\infty$. By [14, Theorem 5.2.5], this condition uniquely defines the automorphisms of $\mathcal{U}$. Direct computations show, for all $t \geq s$, that $\breve{\tau}_{t,s}^{(\omega,\lambda,\mathbf{A})}$ is an automorphism of $\mathcal{U}$. As a consequence, one gets $\breve{\tau}_{t,s}^{(\omega,\lambda,\mathbf{A})} = \tau_{t,s}^{(\omega,\lambda,\mathbf{A})}$, see (4.22). □

It follows that the Dyson-Philips series (4.26) is an explicit expression of the fundamental solution of the Cauchy initial value problem (4.23), where the infinitesimal generator $\delta_t^{(\omega,\lambda,\mathbf{A})}$ of $\tau_{t,s}^{(\omega,\lambda,\mathbf{A})}$ equals

$$\delta_t^{(\omega,\lambda,\mathbf{A})} = \delta^{(\omega,\lambda)} + i[W_t^{\mathbf{A}}, \cdot\,] \tag{4.29}$$

with $\delta^{(\omega,\lambda)}$ being the (time-independent) generator of the one-parameter (Bogoliubov) group $\tau^{(\omega,\lambda)} := \{\tau_t^{(\omega,\lambda)}\}_{t\in\mathbb{R}}$.

We now introduce the abbreviation

$$W_{t,s}^{\mathbf{A}} := \tau_t^{(\omega,\lambda)}(W_s^{\mathbf{A}}) \in \mathcal{U} \tag{4.30}$$

for any $t, s \in \mathbb{R}$ as well as the multi-commutators defined by induction as follows:

$$[B_1, B_2]^{(2)} := [B_1, B_2] , \qquad B_1, B_2 \in \mathcal{U} , \tag{4.31}$$

and, for all integers $k > 2$,

$$[B_1, B_2, \ldots, B_{k+1}]^{(k+1)} := [B_1, [B_2, \ldots, B_{k+1}]^{(k)}] , \qquad B_1, \ldots, B_{k+1} \in \mathcal{U} . \tag{4.32}$$

Then, using (4.12), we rewrite Equation (4.26) as

$$\begin{aligned}&\tau_{t,s}^{(\omega,\lambda,\mathbf{A})}(B) - \tau_{t-s}^{(\omega,\lambda)}(B) \\ &\quad = \sum_{k\in\mathbb{N}} i^k \int_s^t \mathrm{d}s_1 \cdots \int_s^{s_{k-1}} \mathrm{d}s_k [W_{s_k - s, s_k}^{\mathbf{A}}, \ldots, W_{s_1-s,s_1}^{\mathbf{A}}, \tau_{t-s}^{(\omega,\lambda)}(B)]^{(k+1)}\end{aligned} \tag{4.33}$$

for any $B \in \mathcal{U}$ and $t \geq s$.

In Section 4.3 we will study certain bounds on multi-commutators of the above type in detail.

Finally, observe that one can equivalently use either (4.22) or (4.23) to define the dynamics. However, only the second formulation is appropriate to study transport properties of systems of weakly interacting fermions on the lattice in its algebraic formulation.

Remark 4.2.3.
The initial value problem (4.23) can easily be understood in the Heisenberg picture. The time-evolution of any observable $B_s \in \mathcal{B}(\ell^2(\mathfrak{L}))$ at initial time $t = s \in \mathbb{R}$ equals $B_t = (\mathrm{U}_{t,s}^{(\omega,\lambda,\mathbf{A})})^* B_s \mathrm{U}_{t,s}^{(\omega,\lambda,\mathbf{A})}$ for $t \geq s$, which yields

$$\forall t \geq s : \quad \partial_t B_t = (\mathrm{U}_{t,s}^{(\omega,\lambda,\mathbf{A})})^* i[\Delta_{\mathrm{d}}^{(\mathbf{A})} + \lambda V_\omega, B_s] \mathrm{U}_{t,s}^{(\omega,\lambda,\mathbf{A})} .$$

The action of the symmetric derivation $\delta_t^{(\omega,\lambda,\mathbf{A})}$ is related to the above commutator whereas the map $B \mapsto (\mathrm{U}_{t,s}^{(\omega,\lambda,\mathbf{A})})^* B \mathrm{U}_{t,s}^{(\omega,\lambda,\mathbf{A})}$ leads to the evolution family $\{\tau_{t,s}^{(\omega,\lambda,\mathbf{A})}\}_{t\geq s}$ in the second quantization.

4.2.4 The initial KMS state and its time evolution

States on the C^*-algebra $\mathcal{U}$ are, by definition, continuous linear functionals $\rho \in \mathcal{U}^*$ which are normalized and positive, i.e., $\rho(\mathbf{1}) = 1$ and $\rho(A^*A) \geq 0$ for all $A \in \mathcal{U}$.

It is well-known that, at finite volume, the thermodynamic equilibrium of the system is described by the corresponding Gibbs state, which is the unique state minimizing the free-energy. It is stationary and satisfies the so-called KMS condition. The latter also makes sense in infinite volume and is thus used to define the thermodynamic equilibrium of the infinite system.

These thermal equilibrium states of the fermion system under consideration can be defined, for all inverse temperatures $\beta \in \mathbb{R}^+$, any realization $\omega \in \Omega$ of the potential and any strength $\lambda \in \mathbb{R}_0^+$ of the potential V_ω, through the bounded positive operator

$$\mathbf{f}^{(\beta,\omega,\lambda)} := \frac{1}{1+\mathrm{e}^{\beta(\Delta_{\mathrm{d}}+\lambda V_\omega)}} \in \mathcal{B}(\ell^2(\mathfrak{L})). \tag{4.34}$$

Indeed, the so-called *symbol* $\mathbf{f}^{(\beta,\omega,\lambda)}$ uniquely defines a (faithful) *quasi-free* state $\varrho^{(\beta,\omega,\lambda)}$ on the CAR algebra $\mathcal{U}$ by the conditions $\varrho^{(\beta,\omega,\lambda)}(\mathbf{1}) = 1$ and

$$\varrho^{(\beta,\omega,\lambda)}\left(a^*(f_1)\dots a^*(f_m)a(g_n)\dots a(g_1)\right) = \delta_{m,n} \det\left([\langle g_k, \mathbf{f}^{(\beta,\omega,\lambda)} f_j\rangle]_{j,k}\right) \tag{4.35}$$

for all $\{f_j\}_{j=1}^m, \{g_j\}_{j=1}^n \subset \ell^2(\mathfrak{L})$ and $m,n \in \mathbb{N}$. $\langle \cdot,\cdot\rangle$ is the scalar product in $\ell^2(\mathfrak{L})$. $\varrho^{(\beta,\omega,\lambda)} \in \mathcal{U}^*$ is the unique $(\beta, \tau^{(\omega,\lambda)})$-KMS state of the C^*-dynamical system $(\mathcal{U}, \tau^{(\omega,\lambda)})$. The KMS property (4.40) is usually taken as the mathematical characterization of the thermal equilibrium of C^*-dynamical systems. This definition of thermal equilibrium states for infinite systems is rather abstract, but can be physically motivated from an maximum entropy principle by observing that $\varrho^{(\beta,\omega,\lambda)}$ is the unique weak*-limit of Gibbs states, for further details see also Section 4.4.3. Moreover, KMS states are stationary and thus, $\varrho^{(\beta,\omega,\lambda)}$ is invariant under the dynamics defined by the (Bogoliubov) group $\tau^{(\omega,\lambda)}$ of automorphisms:

$$\varrho^{(\beta,\omega,\lambda)} \circ \tau_t^{(\omega,\lambda)} = \varrho^{(\beta,\omega,\lambda)}, \qquad t \in \mathbb{R},\ \beta \in \mathbb{R}^+,\ \omega \in \Omega,\ \lambda \in \mathbb{R}_0^+ . \tag{4.36}$$

Because of the quasi-free property (4.35), the state $\varrho^{(\beta,\omega,\lambda)}$ is uniquely determined by the set of numbers

$$\left\{\varrho^{(\beta,\omega,\lambda)}\left(a^*(f_j)\,a(f_k)\right) = \langle f_k, \mathbf{f}_k^{(\beta,\omega,\lambda)} f_j\rangle\right\}_{j,k\in\mathbb{N}} \subset \mathbb{C} \tag{4.37}$$

for any orthonormal basis $\{f_k\}_{k\in\mathbb{N}} \subset \ell^2(\mathfrak{L})$. For instance, one can take in (4.37) the canonical orthonormal basis $\{\mathfrak{e}_x\}_{x\in\mathfrak{L}}$ of $\ell^2(\mathfrak{L})$ defined by $\mathfrak{e}_x(y) \equiv \delta_{x,y}$ for all $x,y \in \mathfrak{L}$. The state $\varrho^{(\beta,\omega,\lambda)}$ is thus completely determined by its two-point correlation function defined on $\mathfrak{L}^2$ by

$$\mathbf{x} = (x^{(1)}, x^{(2)}) \mapsto \varrho^{(\beta,\omega,\lambda)}(a^*_{x^{(1)}} a_{x^{(2)}}) . \tag{4.38}$$

It turns out to be useful for our results to consider the complex-time evolution $C_{t+i\alpha}^{(\omega)} \equiv C_{t+i\alpha}^{(\beta,\omega,\lambda)}$ of the two-point correlation function (4.38):

$$C_{t+i\alpha}^{(\omega)}(\mathbf{x}) := \varrho^{(\beta,\omega,\lambda)}\left(a^*_{x^{(1)}} \tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(2)}})\right) \qquad \mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2 , \tag{4.39}$$

for all $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$, and $\alpha \in [0, \beta]$. $C_{t+i\alpha}^{(\omega)} : \mathfrak{L}^2 \to \mathbb{C}$ is called *complex-time two-point correlation function* with potential V_ω. This definition makes sense since $\varrho^{(\beta,\omega,\lambda)}$ is a $(\beta, \tau^{(\omega,\lambda)})$-KMS state: For every $x, y \in \mathfrak{L}$, the map

$$t \mapsto \varrho^{(\beta,\omega,\lambda)} \left(a_x^* \tau_t^{(\omega,\lambda)}(a_y) \right)$$

from $\mathbb{R}$ to $\mathbb{C}$ extends uniquely to a continuous map on $\mathbb{R} \times [0, \beta] \subset \mathbb{C}$ which is holomorphic on $\mathbb{R} \times (0, \beta)$. Note that the KMS property of $\varrho^{(\beta,\omega,\lambda)}$, i.e.

$$\varrho^{(\beta,\omega,\lambda)}(B_1 \tau_{i\beta}^{(\omega,\lambda)}(B_2)) = \varrho^{(\beta,\omega,\lambda)}(B_2 B_1) , \qquad B_1, B_2 \in \mathcal{U} , \tag{4.40}$$

together with (4.12) and (4.36), yields

$$C_{-t+i(\beta-\alpha)}^{(\omega)}(\mathbf{x}) = \varrho^{(\beta,\omega,\lambda)}(a_{x^{(2)}} \tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(1)}}^*)) , \qquad \mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2 , \tag{4.41}$$

for all $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$, and $\alpha \in [0, \beta]$.

We assume that, for any realization $\omega \in \Omega$ and strength $\lambda \in \mathbb{R}_0^+$ of disorder, the state of the system before the electric field is switched on is the unique $(\tau^{(\omega,\lambda)}, \beta)$-KMS state $\varrho^{(\beta,\omega,\lambda)}$, see [14, Example 5.3.2.].

Since $\mathbf{A}(t, x) = 0$ for all $t \leq t_0$, the time evolution of the state of the system thus equals

$$\rho_t^{(\beta,\omega,\lambda,\mathbf{A})} := \begin{cases} \varrho^{(\beta,\omega,\lambda)} & , \qquad t \leq t_0 , \\ \varrho^{(\beta,\omega,\lambda)} \circ \tau_{t,t_0}^{(\omega,\lambda,\mathbf{A})} & , \qquad t \geq t_0 . \end{cases} \tag{4.42}$$

Remark that the definition does not depend on the particular choice of initial time t_0 because of the stationarity of the KMS state $\varrho^{(\beta,\omega,\lambda)}$ w.r.t. the unperturbed dynamics (cf. (4.36)). The state $\rho_t^{(\beta,\omega,\lambda,\mathbf{A})}$ is, by construction, a quasi-free state.

Moreover, since $\{\tau_{t,t_0}^{(\omega,\lambda,\mathbf{A})}\}_{t \geq s}$ is defined by (4.19) and (4.22), we infer from (4.42) that the symbol $\mathbf{f}_t^{(\omega)}$, defined analogously to (4.35), of the quasi-free state $\rho_t^{(\beta,\omega,\lambda,\mathbf{A})}$ is the solution of the following (one-particle) non-autonomous Cauchy-problem:

$$\forall t \geq t_0 : \quad i\partial_t \mathbf{f}_t^{(\omega)} = [\Delta_{\mathrm{d}}^{(\mathbf{A})} + \lambda V_\omega, \mathbf{f}_t^{(\omega)}] \quad \mathbf{f}_{t_0}^{(\omega)} := \mathbf{f}^{(\beta,\omega,\lambda)} , \tag{4.43}$$

for every realization $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $\beta \in \mathbb{R}^+$. The latter is known as the *Liouville equation*.

In [11, 25, 26] the authors consider an evolution equation similar to (4.43) with $t_0 = -\infty$ and use the expectation value of the velocity observable w.r.t. the trace per unit volume of $_{\mathbf{t}}^{(\omega)} \in \mathcal{B}(\ell^{\mathbf{2}}(\mathfrak{L}))$ to define a current density, see, e.g., [25, Eqs. (2.5)-(2.6)]. Spatially local perturbations $\mathbf{A} \in \mathbf{C}_0^\infty$ of the electromagnetic field do not influence the mean velocity of an infinite system of particles. Thus, by contrast, the electromagnetic perturbation considered in [11, 25, 26] is infinitely extended as it is space-homogeneous. Indeed, w.r.t. the time-evolving density operator $_{\mathbf{t}}^{(\omega)}$, the main quantity we analyze, the heat production $\mathfrak{I}^{(\omega,\mathbf{A})}(t)$, is *not* a trace *density*, but rather the infinite volume limit of (finite volume) traces. Note however that, by considering space-homogeneous electromagnetic perturbations $\mathbf{A}_L$ in finite boxes Λ_L, $L \in \mathbb{R}^+$, and the corresponding current densities, one can see in the limit $l \to \infty$ that, up to the different convention on $_{\mathbf{t}}^{(\omega)}$ for the initial condition, the notion of AC-conductivity proposed here corresponds quite well to the one introduced in [25, Eqs. (2.5)-(2.6)], even if this correspondence is not totally explicit and the approaches are conceptually different.

4.3 Technical preparation

In preparation for the following proofs, we develop in this section two useful tools. In Section 4.3.1, we compute multi-commutators of products of annihilation and creation operators. These occur for example already in (4.33), see also (4.31)-(4.32) for the precise definition of multi-commutators. Then we introduce the notion of *tree-decay bounds* and show that these bounds hold for the one-parameter group of automorphisms $\tau^{(\omega,\lambda)}$. The second result is given in Section 4.3.2, we show that the complex-time two-point correlation function $C_{t+i\alpha}^{(\omega)}$, defined in (4.39), can be split up into two terms, whereas the first is arbitrarily small in norm and the second one decays fast in space.

4.3.1 Tree-decay bounds

Before going into details, let us first get an intuitive feeling of what will be proved in Lemma 4.3.1. The aim is to simplify an N-fold multi-commutator of products of annihilation and creation operators, as for example

$$[a^*(\psi_1)a(\psi_2)a^*(\psi_3)a^*(\psi_4), a^*(\psi_5)a(\psi_6), \ldots]^{(N)} \tag{4.44}$$

with $\psi_1, \psi_2, \ldots \in \ell^2(\mathfrak{L})$. At a first glance one expects sums over monomials of all occurring annihilation and creation operators. Because of the structure of the multi-commutator, there are certain terms that can be summed up, getting then a monomial of all annihilation and creation operators except two times the anti-commutator of those two annihilation and creation operators. This is useful because the anti-commutator is known to be a multiple of the identity, c.f. (4.4). This procedure can be repeated in order to reduce the number of operators in the remaining monomial. As one might expect, only pairs of creation and annihilation operators that come from *different* entries of the multi-commutator can be removed from the monomial. This is why we consider a special family of trees in the following, similar to [23]. These trees will play the role of an underlying structure between the N entries in the N-fold multi-commutator. Then we need to introduce some notation to express the monomials of annihilation and creation operators in a convenient way before formulating Lemma 4.3.1.

Recall, that a tree is a connected graph that has no loops. Here, we have a finite number of labeled vertices, denoted by $1, \ldots, N$, and (undirected) bonds between these vertices, for example the bond connecting vertices i and j is denoted by $\{i, j\} = \{j, i\}$. A tree with N vertices is thus characterized by the set of its $N-1$ bonds. The family of trees we use is defined as follows: Let $\mathcal{T}_2$ be the set of all trees with exactly two vertices. This set contains a unique tree $T = \{\{1, 2\}\}$ which, in turn, contains the unique bond $\{1, 2\}$, i.e., $\mathcal{T}_2 := \{\{\{1, 2\}\}\}$. Then, for each integer $N \geq 3$, we recursively define the set $\mathcal{T}_N$ of trees with N vertices by

$$\mathcal{T}_N := \Big\{ \{\{k, N\}\} \cup T \ : \ k = 1, \ldots, N-1, \quad T \in \mathcal{T}_{N-1} \Big\} . \tag{4.45}$$

In other words, $\mathcal{T}_N$ is the set of all trees with vertex set $\mathcal{V}_N := \{1, \ldots N\}$ for which $N \in \mathcal{V}_N$ is a leaf, and if the leaf N is removed, the vertex $N-1$ is a leaf in the remaining tree and so on.

Each of the entries of the N-fold multi-commutator is a product of annihilation and creation operators, which we characterize by certain finite index sets $\bar{\Lambda}_1, \Lambda_1, \ldots, \bar{\Lambda}_N, \Lambda_N \subset \mathbb{N}$, where the set $\bar{\Lambda}_i$ refers to creation operators in entry i and Λ_i to annihilation operators in the corresponding entry. For example we choose for

$$[a^*(\psi_1) a(\psi_2) a^*(\psi_3) a^*(\psi_4), a^*(\psi_5) a(\psi_6), \ldots]^{(N)} \tag{4.46}$$

with $\psi_1, \psi_2, \ldots \in \ell^2(\mathfrak{L})$

$$\bar{\Lambda}_1 = \{1, 3, 4\}, \quad \Lambda_1 = \{2\}, \quad \bar{\Lambda}_2 = \{5\}, \quad \Lambda_2 = \{6\}, \ \ldots \tag{4.47}$$

The kind of products we are interested in allows us to restrict our considerations to index sets $\bar{\Lambda}_1, \Lambda_1, \ldots, \bar{\Lambda}_N, \Lambda_N \subset \mathbb{N}$ that are non-empty, mutually disjoint and such that

$$\left|\bar{\Lambda}_j\right| + |\Lambda_j| := 2n_j \in 2\mathbb{N} \ ,$$

for all $j \in \{1, \dots, N\}$. Hence the total number of annihilation and creation operators is even in each entry of the multi-commutator. To shorten the notation we set

$$\Omega_j := (\{+\} \times \bar{\Lambda}_j) \cup (\{-\} \times \Lambda_j) ,$$

for all $j \in \{1, \dots, N\}$. In order to determine the order of annihilation and creation operators in entry j we choose a numbering (that is an bijective map)

$$\pi_j : \{1, \dots, 2n_j\} \to \Omega_j$$

of Ω_j. Furthermore, for all $x \in \bigcup_{j=1}^N \bar{\Lambda}_j \cup \Lambda_j$ let $\psi_x \in \ell^2(\mathfrak{L})$ be the corresponding wave function and denote (only in this subsection) by

$$a(-, x) := a(\psi_x) \qquad \text{and} \qquad a(+, x) := a^*(\psi_x)$$

the annihilation and creation operators, respectively. Using this notation, we then define the monomials

$$\mathfrak{p}_j := \prod_{k=1}^{2n_j} a(\pi_j(k)) \tag{4.48}$$

in $a(\pm, x)$ for all $j \in \{1, \dots, N\}$. Recall, that $\mathfrak{p}_j$ will be the j-th entry in the N-fold multi-commutator.

To formulate the main result of this section, we need one more thing. Recall, that the idea is to replace a sum over monomials of all occurring annihilation and creation operators, by a sum over shorter monomial times anti-commutators of the removed operators. Therefore we need to specify the annihilation and creation operators, that are 'moved' from the monomial to the anti-commutator. The corresponding points in $\Omega_1, \dots, \Omega_N$ are characterized by maps $(\mathbf{x}, \mathbf{y})$ defined in the following.

For every tree $T \in \mathcal{T}_N$ (cf. (4.45)), we define maps $\mathbf{x}, \mathbf{y} : T \to \bigcup_{j=1}^N \Omega_j$, that choose for each bond $\{i, j\} \in T$ a point in the set Ω_i and one point in the set Ω_j. More precisely, we assume for $i < j$ that $\mathbf{x}(\{i, j\}) \in \Omega_i$ and $\mathbf{y}(\{i, j\}) \in \Omega_j$. The induced orientation of the bond is completely arbitrary, and has no deeper meaning here. Furthermore, we do not allow any points to be chosen twice, that means $|\mathbf{x}(T)| = |\mathbf{y}(T)| = N - 1$ and $\mathbf{x}(T) \cap \mathbf{y}(T) = \emptyset$. This assumptions corresponds to the fact that all operators can be removed from the monomial only once. Then the set of all those maps is given by

$$\begin{aligned}\mathcal{K}_T \ := \ & \Bigg\{ (\mathbf{x},\mathbf{y}) \,\Bigg|\, \mathbf{x},\mathbf{y} : T \to \bigcup_{j=1}^{N} \Omega_j \ \text{ with } \mathbf{x}(b) \in \Omega_i, \mathbf{y}(b) \in \Omega_j \\ & \qquad\qquad \text{for } b = \{i,j\} \in T,\ i<j \\ & \qquad\qquad \text{and } |\mathbf{x}(T)| = |\mathbf{y}(T)| = N-1, \mathbf{x}(T) \cap \mathbf{y}(T) = \emptyset \Bigg\} .\end{aligned}$$

Now, we are finally ready to express an N-fold multi-commutator of products of annihilation and creation operators as a sum over trees $T \in \mathcal{T}_N$ of monomials in the annihilation and creation operators:

Lemma 4.3.1 (Multi-commutators as sums over trees)**.**
Let $N \geq 2$. Then, for all $T \in \mathcal{T}_N$ and $(\mathbf{x},\mathbf{y}) \in \mathcal{K}_T$, there are constants

$$\mathrm{m}_T(\mathbf{x},\mathbf{y}) \in \{-1,1\} \tag{4.49}$$

and numberings

$$\pi_T(\mathbf{x},\mathbf{y}) : \left\{1,2,\ldots,2\overline{\mathrm{N}}\right\} \to \bigcup_{j=1}^{N} \Omega_j \backslash \left(\mathbf{x}(T) \cup \mathbf{y}(T)\right)$$

where $\overline{\mathrm{N}} := \sum_{j=1}^{N} n_j - (N-1) \geq 1$, such that

$$[\mathfrak{p}_N,\ldots,\mathfrak{p}_1]^{(N)} \ = \ \sum_{T\in\mathcal{T}_N} \sum_{(\mathbf{x},\mathbf{y})\in\mathcal{K}_T} \mathrm{m}_T(\mathbf{x},\mathbf{y})\, \mathfrak{p}_T(\mathbf{x},\mathbf{y}) \prod_{b\in T} \{a(\mathbf{x}(b)), a(\mathbf{y}(b))\} \ , \tag{4.50}$$

with $\{B_1,B_2\} := B_1B_2 + B_2B_1$ for $B_1,B_2 \in \mathcal{U}$ being the usual anti-commutator, and where

$$\mathfrak{p}_T(\mathbf{x},\mathbf{y}) := \prod_{k=1}^{2\overline{\mathrm{N}}} a(\pi_T(\mathbf{x},\mathbf{y})(k)) \ .$$

Proof. We first observe that, for any two integers $n_1,n_2 \in \mathbb{N}$ and any arbitrary elements $B_1,\ldots,B_{2n_2} \in \mathcal{U}$ and $\tilde{B}_1,\ldots,\tilde{B}_{2n_1} \in \mathcal{U}$,

$$\begin{aligned}&\left[B_1 \ldots B_{2n_2},\ \tilde{B}_1 \ldots \tilde{B}_{2n_1}\right] \\ &\qquad = \sum_{\substack{1\leq k_2\leq 2n_2 \\ 1\leq k_1\leq 2n_1}} (-1)^{k_1+1} B_1 \ldots B_{k_2-1}\tilde{B}_1 \ldots \tilde{B}_{k_1-1} \\ &\qquad\qquad \times \{B_{k_2},\tilde{B}_{k_1}\}\tilde{B}_{k_1+1}\ldots\tilde{B}_{2n_1}B_{k_2+1}\ldots B_{2n_2} \ ,\end{aligned} \tag{4.51}$$

see [23, Eq. (4.18)]. We are now in position to prove the assertion by induction.

For $N = 2$, the set $\mathcal{T}_2$ consists of only one tree $T = \{\{1, 2\}\}$. Using (4.48) and (4.51) we get

$$
\begin{aligned}
[\mathfrak{p}_2, \mathfrak{p}_1] = \sum_{\substack{1 \leq k_2 \leq 2n_2 \\ 1 \leq k_1 \leq 2n_1}} & (-1)^{k_1+1} a(\pi_2(1)) \ldots a(\pi_2(k_2-1)) a(\pi_1(1)) \ldots a(\pi_1(k_1-1)) \\
& \times \{a(\pi_2(k_2)), a(\pi_1(k_1))\} a(\pi_1(k_1+1)) \ldots a(\pi_1(2n_1)) \\
& \times a(\pi_2(k_2+1)) \ldots a(\pi_2(2n_2)) \ . \qquad (4.52)
\end{aligned}
$$

Note that $\{a(\pi_2(k_2)), a(\pi_1(k_1))\}$ is always either zero or a multiple of the identity in $\mathcal{U}$, see (4.4) and (4.5). Therefore, the assertion for $N = 2$ directly follows from the previous equality by observing that the sum over k_1 and k_2 in (4.52) corresponds to the sum over $(\mathbf{x}, \mathbf{y}) \in \mathcal{K}_{\{\{1,2\}\}}$ in (4.50) by choosing

$$
\begin{aligned}
\mathfrak{p}_{\{\{1,2\}\}}(\mathbf{x}, \mathbf{y}) \ := \ & a(\pi_2(1)) \ldots a(\pi_2(k_2-1)) a(\pi_1(1)) \ldots a(\pi_1(k_1-1)) \qquad (4.53) \\
& \times a(\pi_1(k_1+1)) \ldots a(\pi_1(2n_1)) a(\pi_2(k_2+1)) \ldots a(\pi_2(2n_2))
\end{aligned}
$$

for

$$
\begin{aligned}
\mathbf{x}(\{1,2\}) &= \pi_2(k_2) \in \Omega_2 \ , \qquad k_2 \in \{1, \ldots, 2n_2\} \ , \\
\mathbf{y}(\{1,2\}) &= \pi_1(k_1) \in \Omega_1 \ , \qquad k_1 \in \{1, \ldots, 2n_1\} \ .
\end{aligned}
$$

Indeed, for $(\mathbf{x}, \mathbf{y}) \in \mathcal{K}_{\{\{1,2\}\}}$ as above, the constant $\mathrm{m}_{\{\{1,2\}\}}(\mathbf{x}, \mathbf{y})$ equals $(-1)^{k_1+1} \in \{-1, 1\}$, whereas the associated map

$$
\pi_{\{\{1,2\}\}}(\mathbf{x}, \mathbf{y}) : \left\{1, 2, \ldots, 2\overline{\mathrm{N}}\right\} \to \Omega_1 \cup \Omega_2 \backslash \left(\mathbf{x}(\{\{1,2\}\}) \cup \mathbf{y}(\{\{1,2\}\})\right)
$$

with

$$
\overline{\mathrm{N}} := (n_1 + n_2) - 1 \geq 1
$$

depends on the order of the factors on the r.h.s. of (4.53):

$$
\pi_{\{\{1,2\}\}}(\mathbf{x}, \mathbf{y})(k) := \left\{
\begin{array}{ll}
\pi_2(k) \ , & k \in \{1, 2, \ldots, k_2 - 1\} \\
\pi_1(k - k_2 + 1) \ , & k \in \{k_2, \ldots, k_2 + k_1 - 2\} \\
\pi_1(k - k_2 + 2) \ , & k \in \{k_2 + k_1 - 1, \ldots, 2n_1 - 2 + k_2\} \\
\pi_2(k - 2n_1 + 2) \ , & k \in \left\{2n_1 - 2 + k_2 + 1, \ldots, 2\overline{\mathrm{N}}\right\}
\end{array}
\right. .
$$

We assume now that the assertion holds for some fixed integer $N \geq 2$. Recall that N-fold multi-commutators are defined by (4.31)-(4.32). In particular,

$$
[\mathfrak{p}_{N+1}, \ldots, \mathfrak{p}_1]^{(N+1)} = [\mathfrak{p}_{N+1}, [\mathfrak{p}_N, \ldots, \mathfrak{p}_1]^{(N)}]
$$

where, by assumption,

$$[\mathfrak{p}_N, \ldots, \mathfrak{p}_1]^{(N)} = \sum_{T\in\mathcal{T}_N} \sum_{(\mathbf{x},\mathbf{y})\in\mathcal{K}_T} \mathrm{m}_T(\mathbf{x},\mathbf{y})\, \mathfrak{p}_T(\mathbf{x},\mathbf{y}) \prod_{b\in T} \{a(\mathbf{x}(b)), a(\mathbf{y}(b))\} \ ,$$

as stated in the theorem. Therefore,

$$\begin{aligned}[\mathfrak{p}_{N+1}, \ldots, \mathfrak{p}_1]^{(N+1)} &= \sum_{T\in\mathcal{T}_N} \sum_{(\mathbf{x},\mathbf{y})\in\mathcal{K}_T} \mathrm{m}_T(\mathbf{x},\mathbf{y}) [\mathfrak{p}_{N+1}, \mathfrak{p}_T(\mathbf{x},\mathbf{y})] \\ &\qquad \times \prod_{b\in T} \{a(\mathbf{x}(b)), a(\mathbf{y}(b))\} \ , \end{aligned} \tag{4.54}$$

whereas, using again (4.51),

$$\begin{aligned} &[\mathfrak{p}_{N+1}, \mathfrak{p}_T(\mathbf{x},\mathbf{y})] \\ &\quad = \sum_{\substack{1\leq k_2\leq 2n_{N+1} \\ 1\leq k_1\leq 2\overline{\mathrm{N}}}} (-1)^{k_1+1} a(\pi_{N+1}(1)) \ldots a(\pi_{N+1}(k_2-1)) \\ &\quad \times \ a(\pi_T(1)) \ldots a(\pi_T(k_1-1))\, a(\pi_T(k_1+1)) \ldots a(\pi_T(2\overline{\mathrm{N}})) \\ &\quad \times \ a(\pi_{N+1}(k_2+1)) \ldots a(\pi_{N+1}(2n_{N+1}))\, \{a(\pi_{N+1}(k_2)), a(\pi_T(k_1))\} \ . \end{aligned} \tag{4.55}$$

Note that, for simplicity, we used above the notation $\pi_T \equiv \pi_T(\mathbf{x},\mathbf{y})$. To get now the assertion for $(N+1)$-fold multi-commutators, for any $(\mathbf{x},\mathbf{y}) \in \mathcal{K}_T$, we define:

$$\begin{aligned} X &:= \pi_{N+1}(k_2) \in \Omega_{N+1} \ , & k_2 &\in \{1, \ldots, 2n_{N+1}\} \ , \\ Y &:= \pi_T(k_1) \in \textstyle\bigcup_{j=1}^N \Omega_j \backslash (\mathbf{x}(T) \cup \mathbf{y}(T)) \ , & k_1 &\in \left\{1, \ldots, 2\overline{\mathrm{N}}\right\} \ , \end{aligned}$$

as well as

$$\widetilde{\mathrm{m}}_T(X,Y) := (-1)^{k_1+1}$$

and

$$\begin{aligned} &\tilde{\mathfrak{p}}_T(\mathbf{x},\mathbf{y},X,Y) \\ &\quad := a(\pi_{N+1}(1)) \cdots a(\pi_{N+1}(k_2-1))\, a(\pi_T(1)) \cdots a(\pi_T(k_1-1)) \\ &\quad \times a(\pi_T(k_1+1)) \cdots a(\pi_T(2\overline{\mathrm{N}}))\, a(\pi_{N+1}(k_2+1)) \cdots a(\pi_{N+1}(2n_{N+1})) \ . \end{aligned}$$

Then, by (4.54)-(4.55), one has

$$\begin{aligned} [\mathfrak{p}_{N+1}, \ldots, \mathfrak{p}_1]^{(N+1)} = \sum_{T\in\mathcal{T}_N} \sum_{(\mathbf{x},\mathbf{y})\in\mathcal{K}_T} \sum_{X\in(\Omega_1\cup\cdots\cup\Omega_N)\backslash(\mathbf{x}(T)\cup\mathbf{y}(T))} \sum_{Y\in\Omega_{N+1}} \\ \mathrm{m}_T(\mathbf{x},\mathbf{y})\, \widetilde{\mathrm{m}}_T(X,Y)\, \tilde{\mathfrak{p}}_T(\mathbf{x},\mathbf{y},X,Y) \{a(X), a(Y)\} \prod_{b\in T} \{a(\mathbf{x}(b)), a(\mathbf{y}(b))\} \ . \end{aligned}$$

This last equation can clearly be rewritten as

$$
\begin{aligned}
&[\mathfrak{p}_{N+1},\ldots,\mathfrak{p}_1]^{(N+1)} \qquad (4.56)\\
&\quad = \sum_{T\in\mathcal{T}_N}\ \sum_{k\in\{1,\ldots,N\}}\ \sum_{(\mathbf{x},\mathbf{y})\in\mathcal{K}_T}\ \sum_{X_{\{k,N+1\}}\in\Omega_k\backslash(\mathbf{x}(T)\cup\mathbf{y}(T))}\ \sum_{Y_{\{k,N+1\}}\in\Omega_{N+1}}\\
&\qquad \mathrm{m}_T(\mathbf{x},\mathbf{y})\widetilde{\mathrm{m}}_T\left(X_{\{k,N+1\}},Y_{\{k,N+1\}}\right)\tilde{\mathfrak{p}}_T(\mathbf{x},\mathbf{y},X_{\{k,N+1\}},Y_{\{k,N+1\}})\\
&\qquad \times\ \{a(X_{\{k,N+1\}}),a(Y_{\{k,N+1\}})\}\prod_{b\in T}\{a\left(\mathbf{x}(b)\right),a\left(\mathbf{y}(b)\right)\}\ .
\end{aligned}
$$

Note now, that the first two sums on the l.h.s of the equation above can be seen as a sum over $\mathcal{T}_{N+1}$, where k gives the position of the leaf $N+1$, c.f. (4.45). The remaining sums then give exactly the summation over $\mathcal{K}_T$ with $T\in\mathcal{T}_{N+1}$, since $\{\Omega_j\}_{j\in\{1,\ldots,N\}}$ are by definition mutually disjoint sets. For any $T\in\mathcal{T}_{N+1}$ and $(\mathbf{x},\mathbf{y})\in\mathcal{K}_T$ the appropriate constant $\mathrm{m}_T(\mathbf{x},\mathbf{y})\in\{-1,1\}$ as well as the map $\pi_T\left(\mathbf{x},\mathbf{y}\right)$ can directly be deduced from (4.56) and we arrive at the assertion. □

We conclude this section by the notion of tree-decay bounds:

Definition 4.3.2. *Let $\rho\in\mathcal{U}^*$ be any state and $\tau\equiv\{\tau_t\}_{t\in\mathbb{R}}$ be any one-parameter group of automorphisms on the C^*-algebra $\mathcal{U}$. We say that (ρ,τ) satisfies* tree-decay bounds *with parameters $\epsilon\in\mathbb{R}^+$ and $t_0<t$ if there is a finite constant $D\in\mathbb{R}^+$ such that, for any integer $N\geq 2$, $s_1,\ldots,s_N\in[t_0,t]$, $x_1,\ldots,x_N\in\mathfrak{L}$ and all $z_1,\ldots,z_N\in\mathfrak{L}$ satisfying $|z_i|=1$ for $i\in\{1,\ldots,N\}$,*

$$
\left|\rho\left(\left[\tau_{s_1}(a_{x_1}^*a_{x_1+z_1}),\ldots,\tau_{s_N}(a_{x_N}^*a_{x_N+z_N})\right]^{(N)}\right)\right|\leq D^{N-1}\mathbf{q}_N^{(\epsilon)}\left(x_1,\ldots,x_N\right)\ , \qquad (4.57)
$$

where

$$
\mathbf{q}_N^{(\epsilon)}\left(x_1,\ldots,x_N\right)=\sum_{T\in\mathcal{T}_N}\prod_{\{k,l\}\in T}\frac{1}{1+|x_k-x_l|^{d+\epsilon}}\ ,\qquad x_1,\ldots,x_N\in\mathfrak{L}\ . \qquad (4.58)
$$

Such a property has been used many times in the present work for $\tau=\tau^{(\omega,\lambda)}$ and $\rho=\varrho^{(\beta,\omega,\lambda)}$ for $\beta\in\mathbb{R}^+$, $\omega\in\Omega$ and $\lambda\in\mathbb{R}_0^+$. Using Lemma 4.3.1 we show below that the one-parameter Bogoliubov group $\tau^{(\omega,\lambda)}$ of automorphisms defined by (4.11) and any state ρ satisfy tree-decay bounds. Indeed, observe first the following elementary lemma:

Lemma 4.3.3.
For any $T, \epsilon \in \mathbb{R}^+$, there is a finite constant $D \in \mathbb{R}^+$ such that

$$\left|\left\langle \mathfrak{e}_x, \mathrm{e}^{it(\Delta_{\mathrm{d}}+\lambda V_\omega)} \mathfrak{e}_y \right\rangle\right| \leq \frac{D}{1+|x-y|^{d+\epsilon}}$$

for all $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $t \in [-T, T]$ and $x, y \in \mathfrak{L}$. Recall that $\{\mathfrak{e}_x\}_{x\in\mathfrak{L}}$ is the canonical orthonormal basis of $\ell^2(\mathfrak{L})$ defined by $\mathfrak{e}_x(y) \equiv \delta_{x,y}$ for all $x, y \in \mathfrak{L}$.

Proof. Let $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$ and $x, y \in \mathfrak{L}$. Using the Trotter-Kato formula and the canonical orthonormal basis $\{\mathfrak{e}_x\}_{x\in\mathfrak{L}}$ of $\ell^2(\mathfrak{L})$ we first observe that

$$\begin{aligned}\left\langle \mathfrak{e}_x, \mathrm{e}^{it(\Delta_{\mathrm{d}}+\lambda V_\omega)} \mathfrak{e}_y \right\rangle &= \lim_{m\to\infty} \left\langle \mathfrak{e}_x, \left[\mathrm{e}^{\frac{it}{m}\Delta_{\mathrm{d}}} \mathrm{e}^{\frac{it}{m}\lambda V_\omega}\right]^m \mathfrak{e}_y \right\rangle \\ &= \lim_{m\to\infty} \lim_{l\to\infty} \sum_{x_1,\ldots,x_{m-1}\in\Lambda_l} \left\langle \mathfrak{e}_x, \mathrm{e}^{\frac{it}{m}\Delta_{\mathrm{d}}} \mathfrak{e}_{x_1} \right\rangle \cdots \left\langle \mathfrak{e}_{x_{m-1}}, \mathrm{e}^{\frac{it}{m}\Delta_{\mathrm{d}}} \mathfrak{e}_y \right\rangle \\ &\qquad \times \mathrm{e}^{\frac{it}{m}\lambda V_\omega(x_1)} \times \cdots \times \mathrm{e}^{\frac{it}{m}\lambda V_\omega(y)} ,\end{aligned} \tag{4.59}$$

where Λ_l is the finite box (4.74) of side length $2l+1$ for $l \in \mathbb{N}$. Writing now the exponential $\mathrm{e}^{\frac{it}{m}\Delta_{\mathrm{d}}}$ as a power series and using the definition (4.10) of the discrete Laplacian Δ_{d} note that

$$\left|\left\langle \mathfrak{e}_x, \mathrm{e}^{\frac{it}{m}\Delta_{\mathrm{d}}} \mathfrak{e}_y \right\rangle\right| \leq \mathrm{e}^{\frac{4dt}{m}} \left\langle \mathfrak{e}_x, \mathrm{e}^{-\frac{|t|}{m}\Delta_{\mathrm{d}}} \mathfrak{e}_y \right\rangle \qquad x, y \in \mathfrak{L}\ ,\ t, m \in \mathbb{R}\ . \tag{4.60}$$

Therefore, we infer from (4.59) and (4.60) that

$$\left|\left\langle \mathfrak{e}_x, \mathrm{e}^{it(\Delta_{\mathrm{d}}+\lambda V_\omega)} \mathfrak{e}_y \right\rangle\right| \leq \mathrm{e}^{4d|t|} \left\langle \mathfrak{e}_x, \mathrm{e}^{-|t|\Delta_{\mathrm{d}}} \mathfrak{e}_y \right\rangle\ . \tag{4.61}$$

Since Δ_{d} is explicitly given in Fourier space by the dispersion relation $E(p)$ defined by

$$E(p) = 2\left(d - \sum_{in1}^{d} \cos(p_i)\right) \tag{4.62}$$

for $p \in [-\pi, \pi]^d$, explicit computations show that, for all $s \in \mathbb{R}$,

$$\left\langle \mathfrak{e}_x, \mathrm{e}^{s\Delta_{\mathrm{d}}} \mathfrak{e}_y \right\rangle = \frac{1}{(2\pi)^d} \int_{[-\pi,\pi]^d} \mathrm{e}^{sE(p)-ip\cdot(x-y)} \mathrm{d}^d p\ ,$$

which, combined with (4.61), implies the assertion. $\square$

Since, by (4.4) and (4.11),

$$\left\|\{\tau_{s_1}^{(\omega,\lambda)}(a_x^*), \tau_{s_2}^{(\omega,\lambda)}(a_y)\}\right\| = \left|\left\langle \mathfrak{e}_x, \mathrm{e}^{i(s_2-s_1)(\Delta_{\mathrm{d}}+\lambda V_\omega)}\mathfrak{e}_y \right\rangle\right| \ , \qquad (4.63)$$

for any $\epsilon, t \in \mathbb{R}^+$, we infer from Lemma 4.3.3 the existence of a finite constant $D \in \mathbb{R}^+$ (only depending on ϵ, t) such that

$$\left\|\left\{\tau_{s_1}^{(\omega,\lambda)}\left(a_x^*\right), \tau_{s_2}^{(\omega,\lambda)}\left(a_y\right)\right\}\right\| \leq \frac{D}{1+|x-y|^{d+\epsilon}} \qquad (4.64)$$

for all $s_1, s_2 \in [0,t]$, $x, y \in \mathfrak{L}$, $\omega \in \Omega$ and $\lambda \in \mathbb{R}_0^+$. Using this and Lemma 4.3.1 we obtain (4.57) with a uniform constant $D < \infty$ not depending on $\omega \in \Omega$ and $\lambda \in \mathbb{R}_0^+$:

Corollary 4.3.4 (Uniform tree-decay bounds)**.**
Let $\tau = \tau^{(\omega,\lambda)}$ be the one-parameter Bogoliubov group of automorphisms defined by (4.11) for $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and ρ an arbitrary state on $\mathcal{U}$. Then, for any $\epsilon \in \mathbb{R}^+$ and $t_0 < t$, there is $D = D_{\epsilon,t_0,t} \in \mathbb{R}^+$ such that the tree-decay bounds (4.57)-(4.58) hold for all $\omega \in \Omega$ and $\lambda \in \mathbb{R}_0^+$.

Proof. Choose in Lemma 4.3.1 sets $\bar{\Lambda}_j, \Lambda_j$ containing exactly one element and note that, in this case, $|\mathcal{K}_T| = 2^{2|T|} = 2^{2(N-1)}$. Observe also that $\|\mathfrak{p}_T(\mathbf{x},\mathbf{y})\| \leq 1$ as the corresponding vectors ψ_x have norm 1 in this case. The assertion then follows from (4.64) and Lemma 4.3.1. □

4.3.2 Decay of the complex-time two-point correlation functions

In this section, a space-decay property of the complex-time two-point correlation function $C_{t+i\alpha}^{(\omega)}$

$$C_{t+i\alpha}^{(\omega)}(\mathbf{x}) := \varrho^{(\beta,\omega,\lambda)}(a_{x^{(1)}}^* \tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(2)}})) \qquad \mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2 \ , \qquad (4.65)$$

is proven, which turns out to be very useful in the proofs of the following sections.

Lemma 4.3.5 (Decomposition of two-point correlation functions)**.**
For any $\varepsilon, \beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$, $\upsilon \in (0, \beta/2)$ and $\alpha \in [\upsilon, \beta-\upsilon]$, the complex-time two-point correlation function $C_{t+i\alpha}^{(\omega)}$ can be decomposed as

$$C_{t+i\alpha}^{(\omega)}(\mathbf{x}) = A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(\mathbf{x}) + B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(\mathbf{x}) \ , \qquad \mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2 \ ,$$

where $A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(\cdot)$ and $B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(\cdot)$ are kernels (w.r.t. the canonical basis $\{\mathfrak{e}_x\}_{x\in\mathfrak{L}}$) of bounded operators $A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} \equiv A_{t+i\alpha,\upsilon,\varepsilon}^{(\beta,\omega,\lambda)}$ and $B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} \equiv B_{t+i\alpha,\upsilon,\varepsilon}^{(\beta,\omega,\lambda)}$ acting on $\ell^2(\mathfrak{L})$ and satisfying the following properties:
(i) *Boundedness: There is a finite constant $D \in \mathbb{R}^+$ only depending on β, υ such that*

$$\left\| A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} \right\|_{\mathrm{op}} \leq \varepsilon \qquad \text{and} \qquad \left\| B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} \right\|_{\mathrm{op}} \leq D \ .$$

(ii) *Decay: If $T \in \mathbb{R}^+$ and $t \in [-T, T]$, then there is a finite constant $D \in \mathbb{R}^+$ only depending on $\varepsilon, \beta, \upsilon, d, T$ such that*

$$\left| B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(\mathbf{x}) \right| \leq \frac{D}{1 + |x^{(1)} - x^{(2)}|^{d^2+1}} \ , \qquad \mathbf{x} \in \mathfrak{L}^2 \ .$$

(iii) *Continuity: If $T \in \mathbb{R}^+$ and $s_1, s_2 \in [-T, T]$, then there is a finite constant $\eta \in \mathbb{R}^+$ only depending on $\varepsilon, \beta, \upsilon, d, T$ such that*

$$\left| B_{s_1+i\alpha,\upsilon,\varepsilon}^{(\omega)}(\mathbf{x}) - B_{s_2+i\alpha,\upsilon,\varepsilon}^{(\omega)}(\mathbf{x}) \right| \leq \frac{\varepsilon\,(1+\lambda)}{1 + |x^{(1)} - x^{(2)}|^{d^2+1}} \ , \qquad \mathbf{x} \in \mathfrak{L}^2 \ ,$$

whenever $|s_2 - s_1| \leq \eta$.

Proof. (i) Using (4.11), (4.34) and (4.35), for all $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$ and $\alpha \in [0, \beta]$, one gets from (4.39) that

$$C_{t+i\alpha}^{(\omega)}(\mathbf{x}) = \langle \mathfrak{e}_{x^{(2)}}, \mathrm{e}^{-it(\Delta_{\mathrm{d}}+\lambda V_\omega)} F_\alpha^\beta \left(\Delta_{\mathrm{d}} + \lambda V_\omega\right) \mathfrak{e}_{x^{(1)}} \rangle \ , \tag{4.66}$$

where F_α^β is the real function defined, for every $\beta \in \mathbb{R}^+$ and $\alpha \in \mathbb{R}$, by

$$F_\alpha^\beta(\varkappa) := \frac{\mathrm{e}^{\alpha\varkappa}}{1 + \mathrm{e}^{\beta\varkappa}} \ , \qquad \varkappa \in \mathbb{R} \ .$$

In particular, the spectral theorem applied to the bounded self-adjoint operator $(\Delta_{\mathrm{d}} + \lambda V_\omega) \in \mathcal{B}(\ell^2(\mathfrak{L}))$ implies from (4.66) that

$$C_{t+i\alpha}^{(\omega)}(\mathbf{x}) = \int F_\alpha^\beta(\varkappa) \mathrm{e}^{-it\varkappa} \mathrm{d}\kappa_{\mathbf{x}}^{(\omega)}(\varkappa)$$

with $\mathrm{d}\kappa_{\mathbf{x}}^{(\omega)} \equiv \mathrm{d}\kappa_{\mathbf{x}}^{(\omega,\lambda)}$ being the spectral measure of $(\Delta_{\mathrm{d}} + \lambda V_\omega)$ w.r.t. $\mathfrak{e}_{x^{(1)}}, \mathfrak{e}_{x^{(2)}} \in \ell^2(\mathfrak{L})$.

Note that F_α^β is a Schwartz function for all $\beta \in \mathbb{R}^+$ and $\alpha \in (0, \beta)$. Therefore, its Fourier transform $\hat{F}_\alpha^\beta$ is again a Schwartz function. Moreover, for all $\beta > 0$ and

$\upsilon \in (0, \beta/2)$, there is a finite constant $D_{\beta,\upsilon} \in \mathbb{R}^+$ such that, for any $\alpha \in [\upsilon, \beta - \upsilon]$ and all $\nu \in \mathbb{R}$,

$$\left| \hat{F}_\alpha^\beta (\nu) \right| \leq \frac{D_{\beta,\upsilon}}{1+\nu^2} \ . \tag{4.67}$$

In particular, for any $\varepsilon \in \mathbb{R}^+$, there is $M_{\beta,\upsilon,\varepsilon} \in \mathbb{R}^+$ such that

$$\int_{|\nu| \geq M_{\beta,\upsilon,\varepsilon}} \left| \hat{F}_\alpha^\beta (\nu) \right| \mathrm{d}\nu \leq \int_{|\nu| \geq M_{\beta,\upsilon,\varepsilon}} \frac{D_{\beta,\upsilon}}{1+\nu^2} \mathrm{d}\nu < \varepsilon \ . \tag{4.68}$$

For any $\varepsilon, \beta \in \mathbb{R}^+$, $\upsilon \in (0, \beta/2)$ and $\alpha \in [\upsilon, \beta - \upsilon]$, we then decompose the function F_α^β into two orthogonal functions of $\varkappa \in \mathbb{R}$:

$$\begin{aligned} f_{\upsilon,\varepsilon,\alpha}^\beta (\varkappa) &:= \int_{|\nu| \geq M_{\beta,\upsilon,\varepsilon}} \hat{F}_\alpha^\beta (\nu) \, \mathrm{e}^{i\nu\varkappa} \mathrm{d}\nu \ , \\ g_{\upsilon,\varepsilon,\alpha}^\beta (\varkappa) &:= \int_{|\nu| < M_{\beta,\upsilon,\varepsilon}} \hat{F}_\alpha^\beta (\nu) \, \mathrm{e}^{i\nu\varkappa} \mathrm{d}\nu \ . \end{aligned} \tag{4.69}$$

Now, for any $\varepsilon, \beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$, $\upsilon \in (0, \beta/2)$ and $\alpha \in [\upsilon, \beta - \upsilon]$, define the bounded operators $A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} \equiv A_{t+i\alpha,\upsilon,\varepsilon}^{(\beta,\omega,\lambda)}$ and $B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} \equiv B_{t+i\alpha,\upsilon,\varepsilon}^{(\beta,\omega,\lambda)}$ acting on $\ell^2(\mathfrak{L})$ by their kernels

$$\begin{aligned} \langle \mathfrak{e}_{x^{(2)}}, A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} \mathfrak{e}_{x^{(1)}} \rangle &\equiv A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} (\mathbf{x}) := \int f_{\upsilon,\varepsilon,\alpha}^\beta (\varkappa) \, \mathrm{e}^{-it\varkappa} \mathrm{d}\kappa_{\mathbf{x}}^{(\omega)} (\varkappa) \ , \quad \mathbf{x} \in \mathfrak{L}^2 \ , \\ \langle \mathfrak{e}_{x^{(2)}}, B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} \mathfrak{e}_{x^{(1)}} \rangle &\equiv B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} (\mathbf{x}) := \int g_{\upsilon,\varepsilon,\alpha}^\beta (\varkappa) \, \mathrm{e}^{-it\varkappa} \mathrm{d}\kappa_{\mathbf{x}}^{(\omega)} (\varkappa) \ , \quad \mathbf{x} \in \mathfrak{L}^2 \ . \end{aligned} \tag{4.70}$$

Indeed, by construction (cf. (4.68)),

$$\left\| A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} \right\|_{\mathrm{op}} \leq \varepsilon \qquad \text{and} \qquad \left\| B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} \right\|_{\mathrm{op}} \leq \pi D_{\beta,\upsilon}$$

for all $\varepsilon, \beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$, $\upsilon \in (0, \beta/2)$ and $\alpha \in [\upsilon, \beta - \upsilon]$. By (4.67), recall that $D_{\beta,\upsilon}$ only depends on β and $\upsilon \in (0, \beta/2)$.
(ii) We first invoke Fubini's theorem to observe from (4.69) and (4.70) that

$$\begin{aligned} B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} (\mathbf{x}) &= \int_{|\nu| < M_{\beta,\upsilon,\varepsilon}} \hat{F}_\alpha^\beta (\nu) \left(\int \mathrm{e}^{-i\varkappa(t-\nu)} \mathrm{d}\kappa_{\mathbf{x}}^{(\omega)} (\varkappa) \right) \mathrm{d}\nu \\ &= \int_{|\nu| < M_{\beta,\upsilon,\varepsilon}} \hat{F}_\alpha^\beta (\nu) \, \langle \mathfrak{e}_{x^{(2)}}, \mathrm{e}^{-i(t-\nu)(\Delta_{\mathrm{d}} + \lambda V_\omega)} \mathfrak{e}_{x^{(1)}} \rangle \mathrm{d}\nu \end{aligned} \tag{4.71}$$

for all $\mathbf{x} \in \mathfrak{L}^2$. If $T \in \mathbb{R}^+$ and $t \in [-T, T]$ then

$$(t - \nu) \in [-M_{\beta,\upsilon,\varepsilon} - T, M_{\beta,\upsilon,\varepsilon} + T] \ .$$

Thus, by Lemma 4.3.3 with $\epsilon = d^2 - d + 1$ ($d \in \mathbb{N}$), for any $\varepsilon, \beta, T \in \mathbb{R}^+$ and $\upsilon \in (0, \beta/2)$, there is a finite constant $\tilde{D}_{\beta,\upsilon,\varepsilon,T} \in \mathbb{R}^+$ such that

$$\left|\langle \mathfrak{e}_{x^{(2)}}, \mathrm{e}^{-i(t-\nu)(\Delta_{\mathrm{d}}+\lambda V_\omega)} \mathfrak{e}_{x^{(1)}} \rangle\right| \leq \frac{\tilde{D}_{\beta,\upsilon,\varepsilon,T}}{1 + |x^{(1)} - x^{(2)}|^{d^2+1}} \ , \qquad \mathbf{x} \in \mathfrak{L}^2 \ , \tag{4.72}$$

for all $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $t \in [-T, T]$, $\nu \in [-M_{\beta,\upsilon,\varepsilon}, M_{\beta,\upsilon,\varepsilon}]$ and $\mathbf{x} \in \mathfrak{L}^2$. We now combine this last inequality with (4.67) and (4.71) to derive the bound

$$\left|B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(\mathbf{x})\right| \leq \frac{\pi D_{\beta,\upsilon} \tilde{D}_{\beta,\upsilon,\varepsilon,T}}{1 + |x^{(1)} - x^{(2)}|^{d^2+1}} \ , \qquad \mathbf{x} \in \mathfrak{L}^2 \ .$$

(iii) By (4.71), note that

$$\partial_t B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(\mathbf{x}) = -i \int_{|\nu|<M_{\beta,\upsilon,\varepsilon}} \hat{F}_\alpha^\beta(\nu) \left\langle (\Delta_{\mathrm{d}} + \lambda V_\omega) \, \mathfrak{e}_{x^{(2)}}, \mathrm{e}^{-i(t-\nu)(\Delta_{\mathrm{d}}+\lambda V_\omega)} \mathfrak{e}_{x^{(1)}} \right\rangle \mathrm{d}\nu \tag{4.73}$$

for all $\varepsilon, \beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$, $\upsilon \in (0, \beta/2)$, $\alpha \in [\upsilon, \beta - \upsilon]$ and $\mathbf{x} \in \mathfrak{L}^2$. Since, for any $\mathbf{x} \in \mathfrak{L}^2$,

$$\begin{aligned}
&\langle (\Delta_{\mathrm{d}} + \lambda V_\omega) \mathfrak{e}_{x^{(2)}}, \mathrm{e}^{-i(t-\nu)(\Delta_{\mathrm{d}}+\lambda V_\omega)} \mathfrak{e}_{x^{(1)}} \rangle \\
&\qquad = -\sum_{z \in \mathfrak{L}, |z|=1} \langle \mathfrak{e}_{x^{(2)}+z}, \mathrm{e}^{-i(t-\nu)(\Delta_{\mathrm{d}}+\lambda V_\omega)} \mathfrak{e}_{x^{(1)}} \rangle \\
&\qquad\quad + (\lambda V_\omega(x^{(2)}) + 2d) \langle \mathfrak{e}_{x^{(2)}}, \mathrm{e}^{-i(t-\nu)(\Delta_{\mathrm{d}}+\lambda V_\omega)} \mathfrak{e}_{x^{(1)}} \rangle \ ,
\end{aligned}$$

we use again (4.67) and (4.72) together with (4.73) and $|V_\omega(x)| \leq 1$ to arrive at the third assertion. □

Remark 4.3.6.
Better estimates on the complex-time two-point correlation functions $C_{t+i\alpha}^{(\omega)}$ can certainly be obtained by using that the spectrum of the self-adjoint operator $(\Delta_{\mathrm{d}} + \lambda V_\omega)$ belongs to some (λ-dependant) compact set. This property is however not used in Lemma 4.3.5 to get bounds (i)-(ii) that do not depend on $\lambda \in \mathbb{R}_0^+$.

4.4 Energy increments

In this section we introduce the energy increment, that is the amount of energy (or more precisely entropy) the systems gains by the electromagnetic field. After the definition in Section 4.4.1, we show in Section 4.4.2 that the energy increment exists for small enough fields and give an explicit form using multi-commutators. In the next Section 4.4.3 we rewrite the energy increment as a thermodynamic limit of Gibbs-states, hence the equilibrium states for finite volumes.

4.4.1 Definition of energy increments

As explained in the introduction, we use a thermodynamic approach and consider the heat production of the system while imposing a time-dependent electromagnetic field. The energy increment is defined here by the energy that is definitively absorbed by the fermion system from the electromagnetic field.

The energy observable in the box

$$\Lambda_n := \{(x_1, \ldots, x_d) \in \mathfrak{L} \, : \, |x_1|, \ldots, |x_d| \leq n\} \in \mathcal{P}_f(\mathfrak{L}) \tag{4.74}$$

of side length $2n+1$ is given by

$$H_n^{(\omega,\lambda)} := \sum_{x,y \in \Lambda_n} \langle \mathfrak{e}_x, (\Delta_{\mathrm{d}} + \lambda V_\omega)\, \mathfrak{e}_y \rangle a_x^* a_y \in \mathcal{U} \ , \tag{4.75}$$

for any $n \in \mathbb{N}$. It is the second quantization of the one-particle operator $\Delta_{\mathrm{d}} + \lambda V_\omega$ restricted to $\ell^2(\Lambda_n) \subset \ell^2(\mathfrak{L})$.

Then, for any $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $\mathbf{A} \in \mathbf{C}_0^\infty$ and $t \in \mathbb{R}$,

$$\mathfrak{I}_t^{(\beta,\omega,\lambda,\mathbf{A})} := \lim_{n\to\infty} \left\{ \rho_t^{(\beta,\omega,\lambda,\mathbf{A})}(H_n^{(\omega,\lambda)}) - \rho_{t_0}^{(\beta,\omega,\lambda,\mathbf{A})}(H_n^{(\omega,\lambda)}) \right\} \in \overline{\mathbb{R}} \tag{4.76}$$

is the energy increment in the state $\rho_t^{(\beta,\omega,\lambda,\mathbf{A})}$ w.r.t. the equilibrium state $\varrho^{(\beta,\omega,\lambda)} \equiv \rho_{t_0}^{(\beta,\omega,\lambda,\mathbf{A})}$. It is not a priori clear that the limit (4.76) exists because, in general,

$$\rho_t^{(\beta,\omega,\lambda,\mathbf{A})}(H_n^{(\omega,\lambda)}) = \mathcal{O}(n^d) \ .$$

Note that, by definition, $\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)} \equiv 0$ whenever $t \leq t_0$. If $\mathfrak{I}_t^{(\beta,\omega,\lambda,\mathbf{A})} > 0$ for any $t \geq t_1$, we would have a strictly positive amount of energy absorbed by the infinite volume fermion system even if the AC-condition (4.16) holds. This situation is interpreted as a *heat* production. Indeed, we show below, that the energy increment $\mathfrak{I}_t^{(\beta,\omega,\lambda,\mathbf{A})}$ can also be seen as an *entropy* production, see Corollary 4.4.5 for more details.

4.4.2 Existence of energy increments at small fields

The physical situation considered here is as follows: We start with a macroscopic bulk containing conducting fermions. This is idealized by taking an infinite system of non-interacting fermions as explained above. Then the AC-conductivity is measured in a local region which is very small w.r.t. the size of the bulk, but very large w.r.t. the lattice spacing of the crystal.

We implement this hierarchy of space scales by rescaling the vector potentials. That means, for any $L \in \mathbb{R}^+$ and $\mathbf{A} \in \mathbf{C}_0^\infty$, we consider the space-rescaled vector potential

$$\mathbf{A}_L(t,x) := \mathbf{A}(t, L^{-1}x)\ , \quad t \in \mathbb{R},\ x \in \mathbb{R}^d\ . \tag{4.77}$$

Then, to ensure that a macroscopic number of lattice sites is involved, we eventually perform the limit $L \to \infty$. Indeed, the scaling factor L^{-1} used in (4.77) means, at fixed L, that the space scale of the electric field (4.15) is infinitesimal w.r.t. the macroscopic bulk (which is the whole space), whereas the lattice spacing gets infinitesimal w.r.t. the space scale of the vector potential when $L \to \infty$.

Furthermore, Joule's law is a *linear* response to electric fields. Therefore, as explained in Section 4.2.3, we also rescale the strength of the electromagnetic potential $\mathbf{A}_L$ by a strictly positive parameter $\eta \in \mathbb{R}^+$ and eventually take the limit $\eta \to 0$.

Within this framework we prove that the heat production is a well-defined quantity, i.e., the energy increment $\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)}$ exists for small enough $\eta \in \mathbb{R}^+$ and all $L \in \mathbb{R}^+$.

Indeed, using the Dyson-Phillips series of the time evolution, that is Equation (4.33), and (4.36), i.e. the fact that KMS states are stationary, as well as (4.10) and (4.42), we observe that

$$\begin{aligned}
&\rho_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)}(H_l^{(\omega,\lambda)}) - \rho_{t_0}^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)}(H_l^{(\omega,\lambda)}) \\
&\quad = \sum_{x\in\Lambda_l} \sum_{z\in\mathfrak{L},|z|\leq 1} \langle \mathfrak{e}_x, (\Delta_{\mathrm{d}} + \lambda V_\omega)\, \mathfrak{e}_{x+z}\rangle \mathbf{1}[x+z \in \Lambda_l] \sum_{k\in\mathbb{N}} i^k \\
&\qquad \times \int_{t_0}^{t} \mathrm{d}s_1 \int_{t_0}^{s_1} \mathrm{d}s_2 \cdots \int_{t_0}^{s_{k-1}} \mathrm{d}s_k \\
&\qquad \varrho^{(\beta,\omega,\lambda)} \left([W_{s_k-t_0,s_k}^{\eta\mathbf{A}_L}, \ldots, W_{s_1-t_0,s_1}^{\eta\mathbf{A}_L}, \tau_{t-t_0}^{(\omega,\lambda)}(a_x^* a_{x+z})]^{(k+1)} \right)
\end{aligned} \tag{4.78}$$

for any $L, l, \beta, \eta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $\mathbf{A} \in \mathbf{C}_0^\infty$.

In order to obtain the existence of energy increments, we need to bound the r.h.s. of (4.78). To this end, we prove the following lemma by using tree-decay bounds on multi-commutators:

Lemma 4.4.1.
For any $\mathbf{A} \in \mathbf{C}_0^\infty$, there is $\eta_0 \in \mathbb{R}^+$ such that, for $l, \varepsilon \in \mathbb{R}^+$, there is a ball

$$B(0, R) := \{x \in \mathfrak{L} : |x| \leq R\} \tag{4.79}$$

of radius $R \in \mathbb{R}^+$ centered at 0 such that, for all $\eta \in (0, \eta_0]$, $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $t_0 \leq s_1, \ldots, s_k \leq t$ and $L \in \mathbb{R}^+$,

$$\sum_{x \in \Lambda_l \backslash B_R} \sum_{z \in \mathfrak{L}, |z| \leq 1} \sum_{k \in \mathbb{N}} \frac{(t-t_0)^k}{k!} \left| \varrho^{(\beta,\omega,\lambda)} \left([W_{s_k - t_0, s_k}^{\eta \mathbf{A}_L}, \ldots, W_{s_1 - t_0, s_1}^{\eta \mathbf{A}_L}, \tau_{t-t_0}^{(\omega,\lambda)}(a_x^* a_{x+z})]^{(k+1)} \right) \right| \leq \varepsilon \ .$$

Proof. We first need to bound the $(k+1)$-fold multi-commutator

$$[W_{s_k - t_0, s_k}^{\mathbf{A}}, \ldots, W_{s_1 - t_0, s_1}^{\mathbf{A}}, \tau_{t-t_0}^{(\omega,\lambda)}(a_x^* a_{x+z})]^{(k+1)}$$

for any $k \in \mathbb{N}$, $x \in \Lambda_L$ and $z \in \mathfrak{L}$ so that $|z| \leq 1$. This is done by using tree-decay bounds as explained in Section 4.3.1. Indeed, by (4.77), for any $l \in \mathbb{R}^+$ and $\mathbf{A} \in \mathbf{C}_0^\infty$, there exists a finite subset $\widetilde{\Lambda}_l \in \mathcal{P}_f(\mathfrak{L})$ such that $\mathbf{A}_L(t, x) = 0$ for all $x \in \mathfrak{L} \backslash \widetilde{\Lambda}_l$ and $t \in \mathbb{R}$. Then we infer from (4.24) and (4.30) that, for all $l, \eta \in \mathbb{R}^+$, $x, y \in \mathfrak{L}$, $\mathbf{A} \in \mathbf{C}_0^\infty$ and $t \in \mathbb{R}$, there are constants $D_{x,y}^{\eta \mathbf{A}_L}(t) \in \mathbb{C}$ such that

$$W_{s_1, s_2}^{\eta \mathbf{A}_L} = \sum_{x \in \widetilde{\Lambda}_l} \sum_{z \in \mathfrak{L}, |z| \leq 1} D_{x,x+z}^{\eta \mathbf{A}_L}(s_2) \tau_{s_1}^{(\omega,\lambda)} \left(a_x^* a_{x+z}\right) \tag{4.80}$$

for any $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $s_1, s_2 \in \mathbb{R}$. Here, the constants $D_{x,y}^{\eta \mathbf{A}_L}(t)$ are always of order η:

$$\sup_{t \in \mathbb{R}\ ,\ x,y \in \mathfrak{L}} \left| D_{x,y}^{\eta \mathbf{A}_L}(t) \right| \leq K_\eta \tag{4.81}$$

with

$$K_\eta := \|\Delta_{\mathrm{d}}\| \left| \exp\left\{ i\eta \max_{(t,x) \in \mathbb{R} \times \mathbb{R}^d\ ,\ z \in \mathfrak{L}, |z| \leq 1} \left| \left[\mathbf{A}(t,x)\right](z) \right| \right\} - 1 \right| = \mathcal{O}(\eta) \ . \tag{4.82}$$

Therefore, using Corollary 4.3.4 we deduce that, for every $\epsilon \in \mathbb{R}^+$ and $t_0 < t$, there is a constant $D \in \mathbb{R}^+$ such that, for any $k \in \mathbb{N}$, $L, l, \eta, \beta \in \mathbb{R}^+$, $\omega \in \Omega$,

$\lambda \in \mathbb{R}_0^+$, $\mathbf{A} \in \mathbf{C}_0^\infty$, $s_1, \ldots, s_k \in [t_0, t]$ and $R > R_l$,

$$\sum_{x \in \Lambda_l \backslash B_R} \sum_{z \in \mathfrak{L}, |z| \leq 1} \left| \varrho^{(\beta,\omega,\lambda)} \left([W^{\eta \mathbf{A}_L}_{s_k - t_0, s_k}, \ldots, W^{\eta \mathbf{A}_L}_{s_1 - t_0, s_1}, \tau^{(\omega,\lambda)}_{t-t_0}(a_x^* a_{x+z})]^{(k+1)} \right) \right|$$
$$\leq |\widetilde{\Lambda}_l| \, |\mathcal{T}_{k+1}| \left[\sum_{x \in \mathfrak{L}, |x| \geq R - R_l} \frac{K_\eta D}{1 + |x|^{d+\epsilon}} \right] \left[\sum_{x \in \mathfrak{L}} \frac{K_\eta D}{1 + |x|^{d+\epsilon}} \right]^{k-1} , \quad (4.83)$$

with $B(0, R)$ being the ball of radius $R \in \mathbb{R}^+$ centered at 0 and where $|\widetilde{\Lambda}_l|$ is the volume of the finite subset $\widetilde{\Lambda}_l \in \mathcal{P}_f(\mathfrak{L})$ with radius

$$R_l := \max \left\{ |x| : x \in \widetilde{\Lambda}_l \right\} \in \mathbb{R}^+ , \qquad l \in \mathbb{R}^+ . \quad (4.84)$$

Note that there exists a finite constant $D \in \mathbb{R}^+$ such that $R_l \leq lD$ for all $l \in \mathbb{R}^+$.

From (4.24) and (4.30) it follows that $W^{\mathbf{A}}_{t,s} = 0$ for any $t \geq t_1$, where t_1 is the time when the electromagnetic potential is switched off, see (4.17). Therefore, w.l.o.g. we only consider times $t \in (t_0, t_1]$ with $t_1 > t_0$. Thus, take $\eta_0 \in \mathbb{R}^+$ sufficiently small to imply

$$\sum_{x \in \mathfrak{L}} \frac{K_\eta D}{1 + |x|^{d+\epsilon}} \leq \sum_{x \in \mathfrak{L}} \frac{K_{\eta_0} D}{1 + |x|^{d+\epsilon}} \leq \frac{1}{2\,(t_1 - t_0)}$$

for all $\eta \in (0, \eta_0]$. Then, using $|\mathcal{T}_{k+1}| = k!$ and the upper bound (4.83) we arrive at

$$\sum_{x \in \Lambda_l \backslash B_R} \sum_{z \in \mathfrak{L}, |z| \leq 1} \left| \varrho^{(\beta,\omega,\lambda)} \left([W^{\eta \mathbf{A}_L}_{s_k - t_0, s_k}, \ldots, W^{\eta \mathbf{A}_L}_{s_1 - t_0, s_1}, \tau^{(\omega,\lambda)}_{t-t_0}(a_x^* a_{x+z})]^{(k+1)} \right) \right|$$
$$\leq \frac{k!}{2^{k-1}\,(t_1 - t_0)^{k-1}} |\widetilde{\Lambda}_l| \sum_{x \in \mathfrak{L}, |x| \geq R - R_l} \frac{K_\eta D}{1 + |x|^{d+\epsilon}} \quad (4.85)$$

for all $\eta \in (0, \eta_0]$ and any $L, l, \beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $k \in \mathbb{N}$, $t \in (t_0, t_1]$ and $s_1, \ldots, s_k \in [t_0, t]$. Therefore, we get the assertion from (4.85) by choosing $R \in \mathbb{R}^+$ such that

$$2\,(t_1 - t_0)\,|\widetilde{\Lambda}_l| \sum_{x \in \mathfrak{L}, |x| \geq R - R_l} \frac{K_{\eta_0} D}{1 + |x|^{d+\epsilon}} \leq \varepsilon$$

for some fixed arbitrarily chosen parameter $\varepsilon \in \mathbb{R}^+$. $\square$

From (4.78) and Lemma 4.4.1 we deduce:

Theorem 4.4.2 (Existence of energy increments)**.**
For any $\mathbf{A} \in \mathbf{C}_0^\infty$, there is a strictly positive number $\eta_0 \in \mathbb{R}^+$ such that, for all $\eta \in (0, \eta_0]$, $L, \beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $t \geq t_0$, the limit (4.76) exists and equals

$$\begin{aligned}\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)} = & \sum_{x,z\in\mathfrak{L},|z|\leq 1} \langle \mathfrak{e}_x, (\Delta_{\mathrm{d}} + \lambda V_\omega)\, \mathfrak{e}_{x+z}\rangle \sum_{k\in\mathbb{N}} i^k \int_{t_0}^{t} \mathrm{d}s_1 \cdots \int_{t_0}^{s_{k-1}} \mathrm{d}s_k \\ & \varrho^{(\beta,\omega,\lambda)} \left([W_{s_k-t_0,s_k}^{\eta\mathbf{A}_L}, \ldots, W_{s_1-t_0,s_1}^{\eta\mathbf{A}_L}, \tau_{t-t_0}^{(\omega,\lambda)}(a_x^* a_{x+z})]^{(k+1)} \right) .\end{aligned} \tag{4.86}$$

4.4.3 Energy increments as thermodynamic limits

In this section we first review well-known facts about the infinite system considered above as a thermodynamic limit of finite volume systems. This is used to express the energy increment as a thermodynamic limit, which allows us to find other useful representations of the energy increment.

First, fix $n \in \mathbb{R}^+$ and recall that Λ_n is the box (4.74) of side length $2n+1$. Let

$$[\Delta_{\mathrm{d}}^{(n)}(\psi)](x) := 2d\psi(x) - \sum_{|z|=1,x+z\in\Lambda_n} \psi(x+z) , \qquad x \in \Lambda_n,\ \psi \in \ell^2(\Lambda_n) ,$$

be the discrete Laplacian restricted to the box Λ_n with Dirichlet boundary conditions. For any realization $\omega \in \Omega$, we denote by $V_\omega^{(n)}$ the restriction of V_ω to Λ_n:

$$V_\omega^{(n)}(\mathfrak{e}_x) := \mathbf{1}\left[x \in \Lambda_n\right] V_\omega(\mathfrak{e}_x) , \qquad x \in \mathfrak{L} .$$

Recall that $\{\mathfrak{e}_x\}_{x\in\mathfrak{L}}$ is the canonical orthonormal basis $\mathfrak{e}_x(y) \equiv \delta_{x,y}$ of $\ell^2(\mathfrak{L})$. Then, for any $\lambda \in \mathbb{R}_0^+$, define the bounded self-adjoint operator

$$h_n^{(\omega,\lambda)} := \Delta_{\mathrm{d}}^{(n)} + \lambda V_\omega^{(n)} \in \mathcal{B}(\ell^2(\Lambda_n)) . \tag{4.87}$$

Obviously, this operator can also be extended to a bounded operator $\tilde{h}_n^{(\omega,\lambda)}$ on $\ell^2(\mathfrak{L})$ by defining

$$\tilde{h}_n^{(\omega,\lambda)}(\mathfrak{e}_x) := \begin{cases} h_n^{(\omega,\lambda)}(\mathfrak{e}_x) & \text{for } x \in \Lambda_n . \\ 0 & \text{for } x \in \mathfrak{L}\backslash\Lambda_n . \end{cases}$$

Since $\mathcal{U}_{\Lambda_n}$ is isomorphic to the algebra of all bounded linear operators on the fermion Fock space

$$\mathcal{F} := \bigwedge(\ell^2(\Lambda_n)) ,$$

the Hamiltonian (4.75), that is,

$$H_n^{(\omega,\lambda)} = \sum_{x,y\in\Lambda_n} \langle \mathfrak{e}_x, h_n^{(\omega,\lambda)} \mathfrak{e}_y \rangle a_x^* a_y \in \mathcal{U}_{\Lambda_n} , \tag{4.88}$$

can be seen as the *second quantization* of $h_n^{(\omega,\lambda)}$ for all $\omega \in \Omega$ and $\lambda \in \mathbb{R}_0^+$. It is well-known in this case that the one-parameter (Bogoliubov) group $\tau^{(\omega,\lambda,n)} := \{\tau_t^{(\omega,\lambda,n)}\}_{t\in\mathbb{R}}$ of automorphisms uniquely defined by the condition

$$\tau_t^{(\omega,\lambda,n)}(a(\psi)) = a(\mathrm{e}^{it\tilde{h}_n^{(\omega,\lambda)}}(\psi)) , \qquad t \in \mathbb{R},\ \psi \in \ell^2(\mathfrak{L}) ,$$

(cf. [14, Theorem 5.2.5]) satisfies

$$\tau_t^{(\omega,\lambda,n)}(A) = \mathrm{e}^{itH_n^{(\omega,\lambda)}} A \mathrm{e}^{-itH_n^{(\omega,\lambda)}} , \qquad A \in \mathcal{U} ,$$

for each $n \in \mathbb{R}^+$ and all $\omega \in \Omega$ and $\lambda \in \mathbb{R}_0^+$.

Let $\varrho^{(\beta,\omega,\lambda,n)}$ be the unique $(\tau^{(\omega,\lambda,n)}, \beta)$-KMS state for any $\omega \in \Omega$ and $\lambda \in \mathbb{R}_0^+$ at fixed inverse temperature $\beta \in \mathbb{R}^+$. It is again well-known that this state is directly related with the Gibbs state $\mathfrak{g}^{(\beta,\omega,\lambda,n)}$ associated with the Hamiltonian $H_n^{(\omega,\lambda)}$ and defined by

$$\mathfrak{g}^{(\beta,\omega,\lambda,n)}(A) := \mathrm{Tr}_{\mathcal{F}} \left(A \frac{\mathrm{e}^{-\beta H_n^{(\omega,\lambda)}}}{\mathrm{Tr}_{\mathcal{F}}(\mathrm{e}^{-\beta H_n^{(\omega,\lambda)}})} \right) , \qquad A \in \mathcal{U}_{\Lambda_n} , \tag{4.89}$$

for any $n, \beta \in \mathbb{R}^+$, $\omega \in \Omega$ and $\lambda \in \mathbb{R}_0^+$. Indeed,

$$\varrho^{(\beta,\omega,\lambda,n)}(AB) = \mathfrak{g}^{(\beta,\omega,\lambda,n)}(A)\mathrm{tr}(B) , \qquad A \in \mathcal{U}_{\Lambda_n} ,\ B \in \mathcal{U}_{\mathfrak{L}\backslash\Lambda_n} , \tag{4.90}$$

where tr is the normalized trace (state) on $\mathcal{U}$. Note that tr is also named *tracial state* and satisfies a product property, see [2, Section 4.2]. Here, $\mathcal{U}_{\mathfrak{L}\backslash\Lambda_n} \subset \mathcal{U}$ is the C^*-algebra generated by $\{a_x\}_{x\in\mathfrak{L}\backslash\Lambda_n}$ and the identity. In particular,

$$\varrho^{(\beta,\omega,\lambda,n)}(A) = \mathfrak{g}^{(\beta,\omega,\lambda,n)}(A) , \qquad A \in \mathcal{U}_{\Lambda_n} .$$

In the following theorem we summarize well-known results on the infinite volume dynamics.

Theorem 4.4.3.
Let $\beta \in \mathbb{R}^+$, $\omega \in \Omega$ and $\lambda \in \mathbb{R}_0^+$. Then:
(i) *For any $t \in \mathbb{R}$, the localized (quasi-free) automorphism $\tau_t^{(\omega,\lambda,n)}$ converges strongly to $\tau_t^{(\omega,\lambda)}$, as $n \to \infty$.*
(ii) *The $(\tau^{(\omega,\lambda,n)}, \beta)$-KMS states $\varrho^{(\beta,\omega,\lambda,n)}$ converge to the $(\tau^{(\omega,\lambda)}, \beta)$-KMS state $\varrho^{(\beta,\omega,\lambda)}$ in the weak*-topology, as $n \to \infty$.*

Proof. See [14, Chapters 5.2 and 5.3]. □

Let $\mathbf{A} \in \mathbf{C}_0^\infty$, $t \geq t_0$ and $l, \eta \in \mathbb{R}^+$. For any sufficiently large $n \in \mathbb{R}^+$ we have $W_t^{\eta \mathbf{A}_L} \in \mathcal{U}_{\Lambda_n}$. Thus we consider the following finite dimensional initial value problem on $\mathcal{U}_{\Lambda_n}$ for any sufficiently large $n \in \mathbb{R}^+$:

$$\forall s, t \in \mathbb{R},\ t \geq s: \ \partial_t \tau_{t,s}^{(\omega,\lambda,\eta\mathbf{A}_L,n)} = \tau_{t,s}^{(\omega,\lambda,\eta\mathbf{A}_L,n)} \circ \delta_t^{(\omega,\lambda,\eta\mathbf{A}_L,n)}, \quad \tau_{s,s}^{(\omega,\lambda,\eta\mathbf{A}_L,n)} := \mathbf{1}, \tag{4.91}$$

with $\mathbf{1}$ being here the identity in $\mathcal{U}_{\Lambda_n}$. Here, the infinitesimal generator $\delta_t^{(\omega,\lambda,\eta\mathbf{A}_L,n)}$ of $\tau_{t,s}^{(\omega,\lambda,\eta\mathbf{A}_L,n)}$ equals

$$\delta_t^{(\omega,\lambda,\eta\mathbf{A}_L,n)}(\cdot) := i[H_n^{(\omega,\lambda)} + W_t^{\eta\mathbf{A}_L}, \ \cdot\ ] \tag{4.92}$$

and is of course a bounded operator acting on $\mathcal{U}_{\Lambda_n}$. Therefore, using the Dyson-Phillips series one shows, completely analogously to Section 4.2.3, the existence and uniqueness of a (quasi-free) strongly continuous two-parameter group of automorphisms $\{\tau_{t,s}^{(\omega,\lambda,\eta\mathbf{A}_L,n)}\}_{t\geq s}$ of the finite dimensional C^*-algebra $\mathcal{U}_{\Lambda_n}$ satisfying (4.91).

Now, the energy increment $\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)}$ can be expressed as the thermodynamic limit of quantities resulting from the finite volume system above. Indeed, by combining tree-decay bounds (cf. (4.57)-(4.58) and Corollary 4.3.4) with Theorem 4.4.3, one obtains:

Theorem 4.4.4 (Energy increments as thermodynamic limits)**.**
For all $\mathbf{A} \in \mathbf{C}_0^\infty$ and $t \geq t_0$, there is $\eta_0 \in \mathbb{R}^+$ such that

$$\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)} = \lim_{n\to\infty} \left\{ \mathfrak{g}^{(\beta,\omega,\lambda,n)}(\tau_{t,t_0}^{(\omega,\lambda,\eta\mathbf{A}_L,n)}(H_n^{(\omega,\lambda)})) - \mathfrak{g}^{(\beta,\omega,\lambda,n)}(H_n^{(\omega,\lambda)}) \right\} \in \mathbb{R}$$

for all $\eta \in (0, \eta_0]$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $L, \beta \in \mathbb{R}^+$.

Proof. Similar to Equation (4.78),

$$\begin{aligned}
&\mathfrak{g}^{(\beta,\omega,\lambda,n)}(\tau_{t,t_0}^{(\omega,\lambda,\eta\mathbf{A}_L,n)}(H_n^{(\omega,\lambda)})) - \mathfrak{g}^{(\beta,\omega,\lambda,n)}(H_n^{(\omega,\lambda)}) \\
&\quad = \sum_{x\in\Lambda_n} \sum_{z\in\mathfrak{L},|z|\leq 1} \langle \mathfrak{e}_x, h_n^{(\omega,\lambda)} \mathfrak{e}_{x+z}\rangle \mathbf{1}[x+z\in\Lambda_n] \sum_{k\in\mathbb{N}} i^k \\
&\qquad \times \int_{t_0}^{t} \mathrm{d}s_1 \int_{t_0}^{s_1} \mathrm{d}s_2 \cdots \int_{t_0}^{s_{k-1}} \mathrm{d}s_k \\
&\qquad \times \mathfrak{g}^{(\beta,\omega,\lambda,n)} \left([W_{s_k-t_0,s_k}^{\eta\mathbf{A}_L},\ldots,W_{s_1-t_0,s_1}^{\eta\mathbf{A}_L},\tau_{t-t_0}^{(\omega,\lambda,n)}(a_x^* a_{x+z})]^{(k+1)} \right) . \qquad (4.93)
\end{aligned}$$

By Theorem 4.4.3, for any fixed $x,z\in\mathfrak{L}$, $k\in\mathbb{N}$, $\mathbf{A}\in\mathbf{C}_0^\infty$, $s_1,\ldots,s_k\in[t_0,t]$, $\eta,\beta\in\mathbb{R}^+$, $\omega\in\Omega$, $\lambda\in\mathbb{R}_0^+$ and $L\in\mathbb{R}^+$,

$$\begin{aligned}
&\lim_{n\to\infty} \Big\{ \langle \mathfrak{e}_x, h_n^{(\omega,\lambda)} \mathfrak{e}_{x+z}\rangle \mathbf{1}[x+z\in\Lambda_n] \\
&\quad \times \mathfrak{g}^{(\beta,\omega,\lambda,n)} \left([W_{s_k-t_0,s_k}^{\eta\mathbf{A}_L},\ldots,W_{s_1-t_0,s_1}^{\eta\mathbf{A}_L},\tau_{t-t_0}^{(\omega,\lambda,n)}(a_x^* a_{x+z})]^{(k+1)} \right) \Big\} \\
&= \langle \mathfrak{e}_x, (\Delta_{\mathrm{d}}+\lambda V_\omega)\, \mathfrak{e}_{x+z}\rangle \varrho^{(\beta,\omega,\lambda)} \left([W_{s_k-t_0,s_k}^{\eta\mathbf{A}_L},\ldots,W_{s_1-t_0,s_1}^{\eta\mathbf{A}_L},\tau_{t-t_0}^{(\omega,\lambda)}(a_x^* a_{x+z})]^{(k+1)} \right) .
\end{aligned}$$

Therefore, the assertion follows from (4.86) and (4.93) provided one can use Lebesgue's dominated convergence theorem. In fact, the arguments proving Corollary 4.3.4 can be used for the one-parameter groups $\tau^{(\omega,\lambda,n)}$ and the $(\beta,\tau^{(\omega,\lambda,n)})$-KMS states $\varrho^{(\beta,\omega,\lambda,n)}$. In particular, for any $\epsilon\in\mathbb{R}^+$ and $t_0<t$, there is $D=D_{\epsilon,t_0,t}\in\mathbb{R}^+$ such that the tree-decay bounds (4.57)-(4.58) holds for all $\beta\in\mathbb{R}^+$, $\omega\in\Omega$, $\lambda\in\mathbb{R}_0^+$ and $n\in\mathbb{N}$. Note that this constant $D=D_{\epsilon,t_0,t}$ does not depend on $n\in\mathbb{N}$ because of Lemma 4.3.3 and (4.63). Following the proof of Lemma 4.4.1 as a guideline, we obtain absolutely summable upper bounds for (4.93). □

We show in the following, that the theorem above implies that the energy increment $\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)}$ corresponds to a *heat production*, that is, a production of entropy: For any state ρ on the finite dimensional C^*-algebra $\mathcal{U}_{\Lambda_n}$, there is a density matrix $\mathrm{d}_\rho\in\mathcal{U}_{\Lambda_n}$ with $\mathrm{d}_\rho\geq 0$ and $\mathrm{Tr}_{\mathcal{F}}(\mathrm{d}_\rho)=1$. Then we define the *relative entropy*, for any states ρ_1 and ρ_2, by

$$S(\rho_1|\rho_2) = -\,\mathrm{Tr}_{\mathcal{F}}(\mathrm{d}_{\rho_2}\ln \mathrm{d}_{\rho_1}) - S(\rho_2)\,. \qquad (4.94)$$

Here, we assume that $0\notin\sigma(\mathrm{d}_{\rho_1})$ and, for any state ρ,

$$S(\rho) := -\,\mathrm{Tr}_{\mathcal{F}}(\mathrm{d}_\rho \ln \mathrm{d}_\rho) \qquad (4.95)$$

is the von Neumann entropy of the state ρ on the finite dimensional C^*-algebra $\mathcal{U}_{\Lambda_n}$. Observe that the relative entropy is always a non-negative quantity, i.e., $S(\rho_1|\rho_2) \geq 0$ for all states ρ_1 and ρ_2. Now, using Theorem 4.4.4, we can rewrite the energy increment $\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)}$ as the thermodynamic limit of an entropy production, which is in particular a positive quantity:

Corollary 4.4.5.
For any $\mathbf{A} \in \mathbf{C}_0^\infty$, there is $\eta_0 \in \mathbb{R}^+$ such that, for all $\eta \in (0,\eta_0]$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, and $L, \beta \in \mathbb{R}^+$ and $t \geq t_0$, the energy increment $\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)}$ exists and equals

$$\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)} = \lim_{n\to\infty} \beta^{-1} S\left(\mathfrak{g}^{(\beta,\omega,\lambda,n)} |\, \mathfrak{g}^{(\beta,\omega,\lambda,n)} \circ \tau_{t,t_0}^{(\omega,\lambda,\eta\mathbf{A}_L,n)}\right) \in \mathbb{R}_0^+ \ .$$

In particular, the energy increment is positive.

Proof. The arguments follows those of [22]. Note first that

$$\mathfrak{g}^{(\beta,\omega,\lambda,n)} \circ \tau_{t,t_0}^{(\omega,\lambda,\eta\mathbf{A}_L,n)} \in \mathcal{U}_{\Lambda_n}^* \tag{4.96}$$

is obviously a state and

$$S(\mathfrak{g}^{(\beta,\omega,\lambda,n)} \circ \tau_{t,t_0}^{(\omega,\lambda,\eta\mathbf{A}_L,n)}) = S(\mathfrak{g}^{(\beta,\omega,\lambda,n)}) \tag{4.97}$$

for all $t \geq t_0$ because $\tau_{t,t_0}^{(\omega,\lambda,\eta\mathbf{A}_L,n)}$ is an automorphism on $\mathcal{U}_{\Lambda_n}$. Using (4.89), (4.94)-(4.95) and (4.97), we then directly derive the equality

$$\begin{aligned} & S\left(\mathfrak{g}^{(\beta,\omega,\lambda,n)} \mid \mathfrak{g}^{(\beta,\omega,\lambda,n)} \circ \tau_{t,t_0}^{(\omega,\lambda,\eta\mathbf{A}_L,n)}\right) \\ & \qquad = \beta\left(\mathfrak{g}^{(\beta,\omega,\lambda,n)}(\tau_{t,t_0}^{(\omega,\lambda,\eta\mathbf{A}_L,n)}(H_n^{(\omega,\lambda)})) - \mathfrak{g}^{(\beta,\omega,\lambda,n)}(H_n^{(\omega,\lambda)})\right) \ , \end{aligned}$$

provided $t \geq t_0$. The assertion then follows from Theorem 4.4.4. □

Remark 4.4.6.
It is possible to express the energy increment $\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)}$ as a relative entropy of the states $\varrho^{(\beta,\omega,\lambda)}$ and $\varrho^{(\beta,\omega,\lambda)} \circ \tau_{t,t_0}^{(\omega,\lambda,\eta\mathbf{A}_L)}$, this is done in [15]. We refrain here from doing it for technical simplicity.

Meanwhile, Theorem 4.4.4 also allows us to rewrite the energy increment (4.86) as follows:

Corollary 4.4.7.
For any $\mathbf{A} \in \mathbf{C}_0^\infty$, there is $\eta_0 \in \mathbb{R}^+$ such that, for all $\eta \in (0, \eta_0]$, $L, \beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $t \geq t_0$, the energy increment $\mathfrak{I}^{(\omega,\eta\mathbf{A}_L)}(t)$ exists and equals

$$\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)} = \int_{t_0}^t \varrho^{(\beta,\omega,\lambda)} \circ \tau_{s,t_0}^{(\omega,\lambda,\eta\mathbf{A}_L)} \left(\partial_s W_s^{\eta\mathbf{A}_L}\right) \mathrm{d}s - \varrho_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)}(W_t^{\eta\mathbf{A}_L}) \, .$$

Proof. Let $n \in \mathbb{R}^+$ be sufficiently large so that $W_t^{\eta\mathbf{A}_L} \in \mathcal{U}_{\Lambda_n}$. Since $W_t^{\mathbf{A}} = 0$ for any $t \leq t_0$ (cf. (4.24)), we get for any $t \geq t_0$,

$$\begin{aligned}
&\tau_{t,t_0}^{(\omega,\lambda,\eta\mathbf{A}_L,n)}(H_n^{(\omega,\lambda)} + W_t^{\eta\mathbf{A}_L}) - H_n^{(\omega,\lambda)} \\
&\qquad = \tau_{t,t_0}^{(\omega,\lambda,\eta\mathbf{A}_L,n)}(H_n^{(\omega,\lambda)} + W_t^{\eta\mathbf{A}_L}) - \tau_{t_0,t_0}^{(\omega,\lambda,\eta\mathbf{A}_L,n)}(H_n^{(\omega,\lambda)} + W_{t_0}^{\eta\mathbf{A}_L}) \\
&\qquad = \int_{t_0}^t \partial_s \left\{\tau_{s,t_0}^{(\omega,\lambda,\eta\mathbf{A}_L,n)}(H_n^{(\omega,\lambda)} + W_s^{\eta\mathbf{A}_L})\right\} \mathrm{d}s \, .
\end{aligned}$$

Combining this equality with (4.91)-(4.92) we thus arrive at

$$\tau_{t,t_0}^{(\omega,\lambda,\eta\mathbf{A}_L,n)}(H_n^{(\omega,\lambda)} + W_t^{\eta\mathbf{A}_L}) - H_n^{(\omega,\lambda)} = \int_{t_0}^t \tau_{s,t_0}^{(\omega,\lambda,\eta\mathbf{A}_L,n)} \left(\partial_s W_s^{\eta\mathbf{A}_L}\right) \mathrm{d}s \, .$$

Now, by (4.24) observe that $\partial_s W_s^{\eta\mathbf{A}_L}$ is given by an expression of the form (4.80). Hence, the remaining part of the proof uses arguments similar to those used to show Theorem 4.4.4: Dyson-Phillips series to obtain series over multi-commutators, tree-decay bounds, Theorem 4.4.3 and Lebesgue's dominated convergence theorem. □

This corollary turns out to be useful for proving Theorem 4.5.1 in the next section.

4.5 AC-Joule's law and AC-conductivity

In this section we formulate and proof the main result of the chapter, that is Theorem 4.5.1.

We study the limit of the energy increment $\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)}$ for $(\eta, L^{-1}) \to (0,0)$. As explained before, it means that we analyze the linear response of the fermion system under the influence of a time-dependent electric field localized in a very small but macroscopic region of the bulk.

In the limit $(\eta, L^{-1}) \to (0,0)$ it turns out that the energy increment $\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)}$ is of order $\mathcal{O}\left(\eta^2 L^d\right)$. This is to be expected since by classical electrodynamics the electromagnetic energy given to the system, is also of order $\mathcal{O}\left(\eta^2 L^d\right)$.

Theorem 4.5.1 (AC-Joule's law - Heat production)**.**
Let $\beta \in \mathbb{R}^+$ and $\lambda \in \mathbb{R}_0^+$. Then there is a unique function $\sigma \equiv \sigma^{(\beta,\lambda)} \in C(\mathbb{R},\mathbb{R})$ satisfying $\sigma(t) = \sigma(|t|)$ and $\sigma(0) = 0$, and a measurable subset $\tilde{\Omega} \equiv \tilde{\Omega}^{(\beta,\lambda)} \subset \Omega$ of full measure such that, for any $\omega \in \tilde{\Omega}$, $\mathbf{A} \in \mathbf{C}_0^\infty$ and $t \geq t_1$,

$$\begin{aligned}
&\lim_{(\eta,L^{-1})\to(0,0)} \left\{ \left(\eta^2 L^d\right)^{-1} \mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)} \right\} \qquad (4.98)\\
&\quad = \frac{1}{2} \int_{\mathbb{R}} \int_{\mathbb{R}} \left[\sigma(s_1 - s_2) \int_{\mathbb{R}^d} \langle E_{\mathbf{A}}(s_1,x), E_{\mathbf{A}}(s_2,x) \rangle \, \mathrm{d}^d x \right] \mathrm{d}s_2 \mathrm{d}s_1 \\
&\quad = \int_{t_0}^{t} \int_{t_0}^{s_1} \left[\sigma(s_1 - s_2) \int_{\mathbb{R}^d} \langle E_{\mathbf{A}}(s_1,x), E_{\mathbf{A}}(s_2,x) \rangle \, \mathrm{d}^d x \right] \mathrm{d}s_2 \mathrm{d}s_1 \geq 0 \, .
\end{aligned}$$

Thus, (4.98) exactly corresponds to the heat production or the electric power delivered by the electric field $E_{\mathbf{A}}$ (4.15). Note that the physicist J. P. Joule observed that the heat (per second) within a circuit is proportional to the electric resistance and the square of the current in the DC-regime. Nevertheless, we name Theorem 4.5.1 *AC-Joule's law* because of two clear similarities. Qualitatively like Joule's law, Theorem 4.5.1 describes the rate at which resistance in the fermion system converts electric energy into heat energy for $t \geq t_1$, by (4.98). Quantitatively, Theorem 4.5.1 is an analogue of Joule's law in the AC-regime with currents and resistance replaced by electric fields and AC-conductivity. Indeed, the real-valued function σ is interpreted as the AC-conductivity.

Note, that in Theorem 4.5.1, we make an assertion for $t \geq t_1$, that means as soon as the electromagnetic field is turned off. For all those times $t, t' \geq t_1$ we have, of course,

$$\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)} = \mathfrak{I}_{t'}^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)} \, , \qquad (4.99)$$

and the energy increment is no longer time-dependent. Nevertheless, we keep the index t in the notation.

In the following subsections we prove Theorem 4.5.1.

4.5.1 Derivation of local AC-Joule's law

We derive here an asymptotic expression for the energy increment which is similar to the one given by Theorem 4.5.1.

To this end, for any $\mathbf{A} \in \mathbf{C}_0^\infty$, we define the difference of electric potential between $x^{(2)} \in \mathfrak{L}$ and $x^{(1)} \in \mathfrak{L}$ at time $t \in \mathbb{R}$ by

$$V_t^{\mathbf{A}}(\mathbf{x}) := \int_0^1 \left[E_{\mathbf{A}}(t, \alpha x^{(2)} + (1-\alpha) x^{(1)}) \right] (x^{(2)} - x^{(1)}) \mathrm{d}\alpha \qquad (4.100)$$

with $\mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2$ and where we recall that

$$E_{\mathbf{A}}(t,x) := -\partial_t \mathbf{A}(t,x) \ , \quad t \in \mathbb{R}, \ x \in \mathbb{R}^d \ ,$$

see (4.15).

It is also convenient to define the subset $\mathfrak{K} \subset \mathcal{L}^2$ of nearest neighbours in $\mathfrak{L}$, i.e.

$$\mathfrak{K} := \left\{ \mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2 \ : \ |x^{(1)} - x^{(2)}| = 1 \right\} \ , \tag{4.101}$$

as well as the *current observables* $I_{\mathbf{x}} = I_{\mathbf{x}}^*$

$$I_{\mathbf{x}} := i(a_{x^{(2)}}^* a_{x^{(1)}} - a_{x^{(1)}}^* a_{x^{(2)}}) \ , \qquad \mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2 \ . \tag{4.102}$$

Note, that this term is justified because $I_{\mathbf{x}}$ obeys the following discrete continuity equation

$$\partial_t n_x(t) = -\tau_t^{(\omega,\lambda)} \left(\sum_{y \in \mathfrak{L}, |x-y|=1} I_{(x,y)} \right) \ , \text{ for all } x \in \mathfrak{L} \ , \tag{4.103}$$

where

$$n_x(t) := \tau_t^{(\omega,\lambda)}(a_x^* a_x) \tag{4.104}$$

is the particle density observable at lattice site $x \in \mathfrak{L}$ and time $t \in \mathbb{R}$. Observe that the minus sign in the r.h.s. of (4.103) comes from the fact that the particles are negatively charged, $I_{(x,y)}$ being the observable related to the flow of particles from the lattice site x to the lattice site y or the current from y to x without electric field. Positively charged particles can of course be treated in the same way.

Finally, for any $s_1, s_2 \in \mathbb{R}$ and $\mathbf{x}, \mathbf{y} \in \mathfrak{L}^2$, let

$$\zeta_{\mathbf{x},\mathbf{y}}^{(\omega)} \equiv \zeta_{\mathbf{x},\mathbf{y}}^{(\beta,\omega,\lambda)}(s_1, s_2) := \frac{1}{4} \int_{s_1}^{s_2} \varrho^{(\beta,\omega,\lambda)} \left(i[\tau_{s_1}^{(\omega,\lambda)}(I_{\mathbf{y}}), \tau_s^{(\omega,\lambda)}(I_{\mathbf{x}})] \right) \mathrm{d}s \ . \tag{4.105}$$

Since

$$(\tau_t^{(\omega,\lambda)}(I_{\mathbf{x}}))^* = \tau_t^{(\omega,\lambda)}(I_{\mathbf{x}}^*) = \tau_t^{(\omega,\lambda)}(I_{\mathbf{x}}) \ , \qquad t \in \mathbb{R}, \ \mathbf{x} \in \mathfrak{L}^2, \ \omega \in \Omega, \ \lambda \in \mathbb{R}_0^+ \ ,$$

the function $\zeta_{\mathbf{x},\mathbf{y}}^{(\omega)}$ is a map from $\mathbb{R}^2$ to $\mathbb{R}$ which turns out to be a (local) *energy production* coefficient:

Theorem 4.5.2 (Local AC-Joule's law).
For any $\mathbf{A} \in \mathbf{C}_0^\infty$ *, there is* $\eta_0 \in \mathbb{R}^+$ *such that, for all* $\eta \in (0, \eta_0]$, $L, \beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$, $\omega \in \Omega$ *and* $t \geq t_1$ *one has*

$$\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)} = \eta^2 \int_{t_0}^{t} \mathrm{d}s_1 \int_{t_0}^{s_1} \mathrm{d}s_2 \sum_{\mathbf{x},\mathbf{y}\in\mathfrak{K}} \zeta_{\mathbf{x},\mathbf{y}}^{(\omega)}(s_1, s_2) V_{s_2}^{\mathbf{A}_L}(\mathbf{x}) V_{s_1}^{\mathbf{A}_L}(\mathbf{y}) + \mathcal{O}(\eta^3 L^d) .$$

Proof. First, we develop the expression given in Corollary 4.4.7 for the energy increment $\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)}$ in terms of small fields, i.e. small η. Using $W_t^{\eta\mathbf{A}_L} \equiv 0$ for all $t \notin (t_0, t_1)$ and (4.36) note that, in particular for all $t \geq t_1$

$$\begin{aligned}
\rho_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)}(W_t^{\eta\mathbf{A}_L}) &= \varrho^{(\beta,\omega,\lambda)}(W_t^{\eta\mathbf{A}_L}) = \int_{t_0}^{t} \varrho^{(\beta,\omega,\lambda)} \left(\partial_s W_s^{\eta\mathbf{A}_L}\right) \mathrm{d}s \\
&= \int_{t_0}^{t} \varrho^{(\beta,\omega,\lambda)} \circ \tau_{s-t_0}^{(\omega,\lambda)} \left(\partial_s W_s^{\eta\mathbf{A}_L}\right) \mathrm{d}s .
\end{aligned}$$

Furthermore, for all $s \in [t_0, t]$,

$$W_s^{\eta\mathbf{A}_L}, \partial_s W_s^{\eta\mathbf{A}_L} \in \mathcal{U}_{\widetilde{\Lambda}_L}$$

for some finite subset $\widetilde{\Lambda}_L \in \mathcal{P}_f(\mathfrak{L})$ of diameter of order $\mathcal{O}(L)$, see, e.g., (4.84). As a consequence, by Corollary 4.4.7, for any $\mathbf{A} \in \mathbf{C}_0^\infty$, there is $\eta_0 \in \mathbb{R}^+$ such that, for all $\eta \in (0, \eta_0]$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, and $L, \beta \in \mathbb{R}^+$ and $t \geq t_1$, the energy increment $\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)}$ exists and equals

$$\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)} = \int_{t_0}^{t} \varrho^{(\beta,\omega,\lambda)} \circ \left(\tau_{s,t_0}^{(\omega,\lambda,\eta\mathbf{A}_L)} - \tau_{s-t_0}^{(\omega,\lambda)}\right) \left(\partial_s W_s^{\eta\mathbf{A}_L}\right) \mathrm{d}s \tag{4.106}$$

Similar to the proofs of Lemma 4.4.1, Theorem 4.4.4 or Corollary 4.4.7, one can use Corollary 4.3.4 to infer from (4.106) that, for all $\eta \in (0, \eta_0]$,

$$\begin{aligned}
\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)} &= \int_{t_0}^{t} \mathrm{d}s_1 \int_{t_0}^{s_1} \mathrm{d}s_2\, \varrho^{(\beta,\omega,\lambda)} \left(i \left[\tau_{s_2-t_0}^{(\omega,\lambda)} \left(W_{s_2}^{\eta\mathbf{A}_L}\right), \tau_{s_1-t_0}^{(\omega,\lambda)} \left(\partial_{s_1} W_{s_1}^{\eta\mathbf{A}_L}\right)\right]\right) \\
&\quad + \mathcal{O}(\eta^3 L^d) .
\end{aligned} \tag{4.107}$$

This last correction term of order $\mathcal{O}(L^d \eta^3)$ is uniformly bounded in $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $t \geq t_1$.

Recall that $W_{t,s}^{\mathbf{A}}$ is defined by (4.30) for any $t, s \in \mathbb{R}$ as

$$W_{t,s}^{\mathbf{A}} := \tau_t^{(\omega,\lambda)}(W_s^{\mathbf{A}}) \in \mathcal{U} , \qquad t, s \in \mathbb{R} .$$

In particular, due to (4.80)-(4.82), by (4.10), (4.24) and (4.100), there are constants $\tilde{D}_{x,y}^{\eta \mathbf{A}_L}(s) \in \mathbb{C}$ for all $x, y \in \mathfrak{L}$, $s \in [t_0, t]$ and a finite subset $\widetilde{\Lambda}_L \in \mathcal{P}_f(\mathfrak{L})$ such that

$$\begin{aligned} W_{t,s}^{\eta \mathbf{A}_L} &= -i\eta \sum_{x,y \in \mathfrak{L}, |x-y|=1} \left(\int_{t_0}^{s} V_{\alpha}^{\mathbf{A}_L}(x,y) \mathrm{d}\alpha \right) \tau_t^{(\omega,\lambda)} \left(a_x^* a_y \right) \\ &\quad + \eta^2 \sum_{x \in \widetilde{\Lambda}_L} \sum_{z \in \mathfrak{L}, |z| \leq 1} \tilde{D}_{x,x+z}^{\eta \mathbf{A}_L}(s) \tau_t^{(\omega,\lambda)} \left(a_x^* a_{x+z} \right) \end{aligned} \tag{4.108}$$

and

$$\tilde{D}_{x,x+z}^{\eta \mathbf{A}_L}(s) = \mathcal{O}(1) , \qquad \partial_s \tilde{D}_{x,x+z}^{\eta \mathbf{A}_L}(s) = \mathcal{O}(1) , \tag{4.109}$$

uniformly for all $x, z \in \mathfrak{L}$ such that $|z| \leq 1$, any small parameter $\eta \in (0, \eta_0]$, and all $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $\beta, L \in \mathbb{R}^+$ and $\mathbf{A} \in \mathbf{C}_0^\infty$. Therefore, we insert (4.108)-(4.109) in Equation (4.107) and use Corollary 4.3.4 to arrive at the equality

$$\begin{aligned} \mathfrak{I}_t^{(\beta,\omega,\lambda,\eta \mathbf{A}_L)} &= -i\eta^2 \sum_{\mathbf{x},\mathbf{y} \in \mathfrak{K}} \int_{t_0}^{t} \mathrm{d}s_1 \int_{s_1}^{t} \mathrm{d}s_2 \int_{t_0}^{s_2} \mathrm{d}s_3 \\ &\quad \times V_{s_1}^{\mathbf{A}_L}(\mathbf{x}) V_{s_3}^{\mathbf{A}_L}(\mathbf{y}) \varrho^{(\beta,\omega,\lambda)} \left([\tau_{s_2-t_0}^{(\omega,\lambda)}(a_{y^{(1)}}^* a_{y^{(2)}}), \tau_{s_1-t_0}^{(\omega,\lambda)} \left(a_{x^{(1)}}^* a_{x^{(2)}} \right)] \right) \\ &\quad + \mathcal{O}(L^d \eta^3) \end{aligned} \tag{4.110}$$

uniformly for $\beta \in \mathbb{R}^+$, $\omega \in \Omega$ and $\lambda \in \mathbb{R}_0^+$. Note that (4.100) yields

$$V_t^{\mathbf{A}_L}(\mathbf{x}) \equiv V_t^{\mathbf{A}_L}(x^{(1)}, x^{(2)}) = -V_t^{\mathbf{A}_L}(x^{(2)}, x^{(1)}) , \quad \mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2 , \ t \in \mathbb{R} , \tag{4.111}$$

whereas (4.12) and (4.36) combined with the group property of $\tau^{(\omega,\lambda)} = \{\tau_t^{(\omega,\lambda)}\}_{t \in \mathbb{R}}$ imply that

$$\varrho^{(\beta,\omega,\lambda)} \left([\tau_{s_2-t_0}^{(\omega,\lambda)}(B_2), \tau_{s_1-t_0}^{(\omega,\lambda)} (B_1)] \right) = \varrho^{(\beta,\omega,\lambda)} \left([\tau_{s_2}^{(\omega,\lambda)}(B_2), \tau_{s_1}^{(\omega,\lambda)} (B_1)] \right) \tag{4.112}$$

for any $B_1, B_2 \in \mathcal{U}$ and all $s_1, s_2 \in \mathbb{R}$. Therefore, by (4.111) and (4.112), Equation (4.110) is equal to

$$\begin{aligned} \mathfrak{I}_t^{(\beta,\omega,\lambda,\eta \mathbf{A}_L)} &= \frac{\eta^2}{4} \sum_{\mathbf{x},\mathbf{y} \in \mathfrak{K}} \int_{t_0}^{t} \mathrm{d}s_1 \int_{s_1}^{t} \mathrm{d}s_2 \int_{t_0}^{s_2} \mathrm{d}s_3 V_{s_1}^{\mathbf{A}_L}(\mathbf{x}) V_{s_3}^{\mathbf{A}_L}(\mathbf{y}) \\ &\quad \times \varrho^{(\beta,\omega,\lambda)} \left(i[\tau_{s_2}^{(\omega,\lambda)}(I_{\mathbf{y}}), \tau_{s_1}^{(\omega,\lambda)} (I_{\mathbf{x}})] \right) + \mathcal{O}(\eta^3 L^d) , \end{aligned} \tag{4.113}$$

see (4.102). By (4.105) we obtain that

$$\partial_{s_2} \zeta_{\mathbf{x},\mathbf{y}}^{(\omega)} (s_1, s_2) = \frac{1}{4} \varrho^{(\beta,\omega,\lambda)} \left(i[\tau_{s_1}^{(\omega,\lambda)}(I_{\mathbf{y}}), \tau_{s_2}^{(\omega,\lambda)}(I_{\mathbf{x}})] \right)$$

for any $\mathbf{x}, \mathbf{y} \in \mathfrak{L}^2$, $\beta \in \mathbb{R}^+$, $\omega \in \Omega$ and $\lambda \in \mathbb{R}_0^+$. As a consequence, the assertion follows from (4.113) and an integration by parts using the AC-condition (4.16) for $t \geq t_1$. □

4.5.2 Microscopic AC-conductivity

Recall that, for any $\mathbf{x}, \mathbf{y} \in \mathfrak{L}^2$, the map $\zeta_{\mathbf{x},\mathbf{y}}^{(\omega)} \equiv \zeta_{\mathbf{x},\mathbf{y}}^{(\beta,\omega,\lambda)}$ from $\mathbb{R}^2$ to $\mathbb{R}$ defined by (4.105) is an energy production coefficient, by Theorem 4.5.2. First, we observe that the function $\zeta_{\mathbf{x},\mathbf{y}}^{(\omega)}$ can be reduced to a real-valued function defined on the real line, only. This function is called *microscopic AC-conductivity* in the following. Then we relate the microscopic AC-conductivity to the complex-time two-point correlation functions defined in (4.65).

Lemma 4.5.3 (Microscopic AC-conductivity).
For any $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $\mathbf{x}, \mathbf{y} \in \mathfrak{L}^2$, there is a function $\sigma_{\mathbf{x},\mathbf{y}}^{(\omega)} \equiv \sigma_{\mathbf{x},\mathbf{y}}^{(\beta,\omega,\lambda)}$ from $\mathbb{R}$ to $\mathbb{R}$ such that

$$\zeta_{\mathbf{x},\mathbf{y}}^{(\omega)}(s_1, s_2) = \sigma_{\mathbf{x},\mathbf{y}}^{(\omega)}(s_2 - s_1) \ , \qquad s_1, s_2 \in \mathbb{R} \ .$$

Proof. The assertion follows by combining (4.105) with (4.12) and (4.36). □

Therefore, by (4.105) and Lemma 4.5.3, for any $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $\mathbf{x}, \mathbf{y} \in \mathfrak{L}^2$,

$$\sigma_{\mathbf{x},\mathbf{y}}^{(\omega)}(t) = \frac{1}{4} \int_0^t \varrho^{(\beta,\omega,\lambda)} \left(i[I_{\mathbf{y}}, \tau_s^{(\omega,\lambda)}(I_{\mathbf{x}})] \right) \mathrm{d}s \ , \qquad t \in \mathbb{R} \ . \tag{4.114}$$

The latter directly implies that $\sigma_{\mathbf{x},\mathbf{y}}^{(\omega)}$ is symmetric w.r.t. time-reversal, provided one exchanges $\mathbf{x}$ and $\mathbf{y}$:

Corollary 4.5.4.
For any $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $\mathbf{x}, \mathbf{y} \in \mathfrak{L}^2$, the function $\sigma_{\mathbf{x},\mathbf{y}}^{(\omega)} \equiv \sigma_{\mathbf{x},\mathbf{y}}^{(\beta,\omega,\lambda)}$ obeys

$$\sigma_{\mathbf{x},\mathbf{y}}^{(\omega)}(t) = \sigma_{\mathbf{y},\mathbf{x}}^{(\omega)}(-t) \ , \qquad t \in \mathbb{R} \ .$$

Proof. We use again (4.12) and (4.36) in (4.114) to check that, for all $\mathbf{x}, \mathbf{y} \in \mathfrak{L}^2$

and $t \in \mathbb{R}$,

$$\begin{aligned}\sigma_{\mathbf{x},\mathbf{y}}^{(\omega)}(-t) &= \frac{1}{4}\int_0^{-t} \varrho^{(\beta,\omega,\lambda)}\left(i[I_{\mathbf{y}}, \tau_s^{(\omega,\lambda)}(I_{\mathbf{x}})]\right) \mathrm{d}s \\ &= -\frac{1}{4}\int_0^{t} \varrho^{(\beta,\omega,\lambda)}\left(i[I_{\mathbf{y}}, \tau_{-s}^{(\omega,\lambda)}(I_{\mathbf{x}})]\right) \mathrm{d}s \\ &= \frac{1}{4}\int_0^{t} \varrho^{(\beta,\omega,\lambda)}\left(i[I_{\mathbf{x}}, \tau_s^{(\omega,\lambda)}(I_{\mathbf{y}})]\right) \mathrm{d}s = \sigma_{\mathbf{y},\mathbf{x}}^{(\omega)}(t) \ . \qquad (4.115)\end{aligned}$$

□

The microscopic AC-conductivity $\sigma_{\mathbf{x},\mathbf{y}}^{(\omega)} \equiv \sigma_{\mathbf{x},\mathbf{y}}^{(\beta,\omega,\lambda)}$ defined in Lemma 4.5.3 can be expressed in terms of complex-time two-point correlation functions (4.39) $C_{t+i\alpha}^{(\omega)} \equiv C_{t+i\alpha}^{(\beta,\omega,\lambda)}$ defined by

$$C_{t+i\alpha}^{(\omega)}(\mathbf{x}) := \varrho^{(\beta,\omega,\lambda)}(a_{x^{(1)}}^{*}\tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(2)}})) \ , \qquad \mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2 \ , \qquad (4.116)$$

for all $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$ and $\alpha \in [0, \beta]$. This is done in Lemma 4.5.6 below. The space-decay properties of complex-time two-point correlation functions $C_{t+i\alpha}^{(\omega)}$, specified already in Section 4.3.2 and in particular Lemma 4.3.5, turn out to be very convenient in the proof of AC-Joule's Law, i.e. Theorem 4.5.1.

First, we derive a useful identity relating the microscopic AC-conductivity $\sigma_{\mathbf{x},\mathbf{y}}^{(\omega)}$ to Duhamel two-point correlation functions of currents:

Lemma 4.5.5.
Let $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $\mathbf{x}, \mathbf{y} \in \mathfrak{L}^2$. Then, for all $t \in \mathbb{R}$,

$$\begin{aligned}\sigma_{\mathbf{x},\mathbf{y}}^{(\omega)}(t) &= \frac{1}{4}\int_0^{\beta} \left(\varrho^{(\beta,\omega,\lambda)}\left(I_{\mathbf{y}}\tau_{t+i\alpha}^{(\omega,\lambda)}(I_{\mathbf{x}})\right) - \varrho^{(\beta,\omega,\lambda)}\left(I_{\mathbf{y}}\tau_{i\alpha}^{(\omega,\lambda)}(I_{\mathbf{x}})\right)\right) \mathrm{d}\alpha \\ &= \frac{1}{4}\left\{(I_{\mathbf{y}}, \tau_t^{(\omega,\lambda)}(I_{\mathbf{x}}))_{\sim} - (I_{\mathbf{y}}, I_{\mathbf{x}})_{\sim}\right\} \ ,\end{aligned}$$

where, for any self-adjoint $B_1 = B_1^*, B_2 = B_2^* \in \mathcal{U}$,

$$(B_1, B_2)_{\sim} \equiv (B_1, B_2)_{\sim}^{(\beta,\omega,\lambda)} := \int_0^{\beta} \varrho^{(\beta,\omega,\lambda)}\left(B_1\tau_{i\alpha}^{(\omega,\lambda)}(B_2)\right) \mathrm{d}\alpha \ . \qquad (4.117)$$

Proof. The KMS property (4.40) implies that, for any $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $\mathbf{x}, \mathbf{y} \in \mathfrak{L}^2$ and $s_1, s \in \mathbb{R}$,

$$\begin{aligned}&\varrho^{(\beta,\omega,\lambda)}\left([\tau_{s_1}^{(\omega,\lambda)}(I_{\mathbf{y}}), \tau_s^{(\omega,\lambda)}(I_{\mathbf{x}})]\right) \\ &\qquad = \varrho^{(\beta,\omega,\lambda)}\left(\tau_{s_1}^{(\omega,\lambda)}(I_{\mathbf{y}})\tau_s^{(\omega,\lambda)}(I_{\mathbf{x}})\right) - \varrho^{(\beta,\omega,\lambda)}\left(\tau_{s_1}^{(\omega,\lambda)}(I_{\mathbf{y}})\tau_{s+i\beta}^{(\omega,\lambda)}(I_{\mathbf{x}})\right) \ ,\end{aligned}$$

whereas the map

$$z \mapsto \varrho^{(\beta,\omega,\lambda)}\left(\tau_{s_1}^{(\omega,\lambda)}(I_{\mathbf{y}})\tau_{z}^{(\omega,\lambda)}(I_{\mathbf{x}})\right)$$

is holomorphic on the strip $\mathbb{R}+i(0,\beta)$, see for instance [14, Proposition 5.3.7]. As a consequence, by using (4.12) and (4.36), we obtain from (4.114) that

$$\begin{aligned}\sigma_{\mathbf{x},\mathbf{y}}^{(\omega)}(t) &= \frac{1}{4}\int_0^\beta \left(\varrho^{(\beta,\omega,\lambda)}\left(I_{\mathbf{y}}\tau_{t+i\alpha}^{(\omega,\lambda)}(I_{\mathbf{x}})\right)-\frac{1}{4}\varrho^{(\beta,\omega,\lambda)}\left(I_{\mathbf{y}}\tau_{i\alpha}^{(\omega,\lambda)}(I_{\mathbf{x}})\right)\right)\mathrm{d}\alpha \\ &= \frac{1}{4}\int_0^\beta \varrho^{(\beta,\omega,\lambda)}\left(I_{\mathbf{y}}\tau_{t+i\alpha}^{(\omega,\lambda)}(I_{\mathbf{x}})\right)\mathrm{d}\alpha-\frac{1}{4}(I_{\mathbf{y}},I_{\mathbf{x}})_\sim\end{aligned}$$

for any $\beta\in\mathbb{R}^+$, $\omega\in\Omega$, $\lambda\in\mathbb{R}_0^+$ and $\mathbf{x},\mathbf{y}\in\mathfrak{L}^2$. The group property of $\tau^{(\omega,\lambda)}$ yields

$$\varrho^{(\beta,\omega,\lambda)}\left(I_{\mathbf{y}}\tau_{t+z}^{(\omega,\lambda)}(I_{\mathbf{x}})\right)=\varrho^{(\beta,\omega,\lambda)}\left(I_{\mathbf{y}}\tau_{z}^{(\omega,\lambda)}(\tau_{t}^{(\omega,\lambda)}(I_{\mathbf{x}}))\right) \tag{4.118}$$

for all $z\in\mathbb{R}$. On the other hand, the KMS property (4.40) of $\varrho^{(\beta,\omega,\lambda)}$ and the group property of $\tau^{(\omega,\lambda)}$ together with [14, Proposition 5.3.7], that is here,

$$\varrho^{(\beta,\omega,\lambda)}\left(I_{\mathbf{y}}\tau_{t+i\beta}^{(\omega,\lambda)}(I_{\mathbf{x}})\right)=\varrho^{(\beta,\omega,\lambda)}\left(\tau_{t}^{(\omega,\lambda)}(I_{\mathbf{x}})I_{\mathbf{y}}\right)\ ,$$

lead to Equation (4.118) for all $z\in\mathbb{R}+i\beta$. Together with the Phragmen-Lindelöf Theorem [14, Proposition 5.3.5], this implies that, for any $\beta\in\mathbb{R}^+$, $\omega\in\Omega$, $\lambda\in\mathbb{R}_0^+$ and $\mathbf{x},\mathbf{y}\in\mathfrak{L}^2$, (4.118) can be extended to all $z\in\mathbb{R}+i[0,\beta]$. In particular,

$$\int_0^\beta \varrho^{(\beta,\omega,\lambda)}\left(I_{\mathbf{y}}\tau_{t+i\alpha}^{(\omega,\lambda)}(I_{\mathbf{x}})\right)\mathrm{d}\alpha=(I_{\mathbf{y}},\tau_{t}^{(\omega,\lambda)}(I_{\mathbf{x}}))_\sim\ .$$

$\square$

It is not difficult to check that

$$\varrho^{(\beta,\omega,\lambda)}\left(B\tau_{i\alpha}^{(\omega,\lambda)}(B)\right)\geq 0$$

for any selfadjoint $B=B^*\in\mathcal{U}$ and all $\alpha\in[0,\beta]$. So $(B_1,B_2)\mapsto(B_1,B_2)_\sim$ is a positive bilinear form in the real linear space of self-adjoint elements of $\mathcal{U}$. Indeed, the Duhamel two-point function $(\cdot,\cdot)_\sim$ is also called Bogoliubov or Kubo-Mari scalar product for observables. Its use in the context of linear response theory is well-known, see for instance [14, Discussion after Lemma 5.3.16 and Section 5.4]. Note finally that our definition of $(\cdot,\cdot)_\sim$ is slightly different from the usual one because of the missing normalization factor β^{-1} in front of the integral in (4.117).

Now, we can express the microscopic AC-conductivity $\sigma_{\mathbf{x},\mathbf{y}}^{(\omega)} \equiv \sigma_{\mathbf{x},\mathbf{y}}^{(\beta,\omega,\lambda)}$ defined in Lemma 4.5.3 in terms of complex-time two-point correlation functions:

Lemma 4.5.6.
Let $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $\mathbf{x}, \mathbf{y} \in \mathfrak{L}^2$. Then,

$$\sigma_{\mathbf{x},\mathbf{y}}^{(\omega)}(t) = \int_0^\beta \left(\mathfrak{C}_{t+i\alpha}^{(\omega)}(\mathbf{x}, \mathbf{y}) - \mathfrak{C}_{i\alpha}^{(\omega)}(\mathbf{x}, \mathbf{y}) \right) \mathrm{d}\alpha \in \mathbb{R} , \qquad t \in \mathbb{R} ,$$

where $\mathfrak{C}_{t+i\alpha}^{(\omega)} \equiv \mathfrak{C}_{t+i\alpha}^{(\beta,\omega,\lambda)}$ is the map from $\mathfrak{L}^4$ to $\mathbb{C}$ defined by

$$\mathfrak{C}_{t+i\alpha}^{(\omega)}(\mathbf{x}, \mathbf{y}) \ := \ \frac{1}{4} \sum_{\pi,\pi' \in S_2} \varepsilon_\pi \varepsilon_{\pi'} C_{t+i\alpha}^{(\omega)}(y^{\pi'(1)}, x^{\pi(1)}) C_{-t+i(\beta-\alpha)}^{(\omega)}(x^{\pi(2)}, y^{\pi'(2)}) \tag{4.119}$$

for any $\mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2, \mathbf{y} := (y^{(1)}, y^{(2)}) \in \mathfrak{L}^2$. Here, $\pi, \pi' \in S_2$ are by definition permutations of $\{1, 2\}$ with signatures $\varepsilon_\pi, \varepsilon_{\pi'} \in \{-1, 1\}$.

Proof. From Lemma 4.5.5,

$$\sigma_{\mathbf{x},\mathbf{y}}^{(\omega)}(t) = \frac{1}{4} \int_0^\beta \left(\varrho^{(\beta,\omega,\lambda)} \left(I_{\mathbf{y}} \tau_{t+i\alpha}^{(\omega,\lambda)}(I_{\mathbf{x}}) \right) - \varrho^{(\beta,\omega,\lambda)} \left(I_{\mathbf{y}} \tau_{i\alpha}^{(\omega,\lambda)}(I_{\mathbf{x}}) \right) \right) \mathrm{d}\alpha \tag{4.120}$$

for any $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $\mathbf{x}, \mathbf{y} \in \mathfrak{L}^2$ and $s_1, s_2 \in \mathbb{R}$.

By (4.12) and (4.102), for any $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$, $\alpha \in [0, \beta]$, $\mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2$ and $\mathbf{y} := (y^{(1)}, y^{(2)}) \in \mathfrak{L}^2$,

$$\begin{aligned} I_{\mathbf{y}} \tau_{t+i\alpha}^{(\omega,\lambda)}(I_{\mathbf{x}}) \ &= \ \left(a_{y^{(1)}}^* a_{y^{(2)}} - a_{y^{(2)}}^* a_{y^{(1)}} \right) \tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(2)}}^*) \tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(1)}}) \\ &\quad - \left(a_{y^{(1)}}^* a_{y^{(2)}} - a_{y^{(2)}}^* a_{y^{(1)}} \right) \tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(1)}}^*) \tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(2)}}). \end{aligned} \tag{4.121}$$

Note that, for all $\mathbf{x} \in \mathfrak{L}^2$, $x \in \mathfrak{L}$ the maps $z \mapsto \tau_z^{(\omega,\lambda)}(I_{\mathbf{x}})$, $z \mapsto \tau_z^{(\omega,\lambda)}(a_x^*)$, $z \mapsto \tau_z^{(\omega,\lambda)}(a_x)$, $z \in \mathbb{R}$, have unique analytic continuations for z in whole $\mathbb{C}$.

Meanwhile, using the canonical orthonormal basis $\mathfrak{e}_x(y) \equiv \delta_{x,y}$ of $\ell^2(\mathfrak{L})$, we get that, for any $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$, $\alpha \in [0, \beta]$ and $\mathbf{x}, \mathbf{y} \in \mathfrak{L}^2$,

$$\begin{aligned} &\varrho^{(\beta,\omega,\lambda)} \left(a_{y^{(1)}}^* a_{y^{(2)}} \tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(1)}}^*) \tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(2)}}) \right) \\ &\quad = - \, \varrho^{(\beta,\omega,\lambda)} \left(a_{y^{(1)}}^* \tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(1)}}^*) a_{y^{(2)}} \tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(2)}}) \right) \\ &\qquad + \varrho^{(\beta,\omega,\lambda)} \left(\{ a_{y^{(2)}}, \tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(1)}}^*) \} \right) \varrho^{(\beta,\omega,\lambda)} \left(a_{y^{(1)}}^* \tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(2)}}) \right) \end{aligned} \tag{4.122}$$

since the anticommutator is a multiple of the identity, i.e.,

$$\{a_{y^{(2)}}, \tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(1)}}^{*})\} = \left\langle \mathfrak{e}_{y^{(2)}}, \mathrm{U}_{t+i\alpha}^{(\omega,\lambda)}\mathfrak{e}_{x^{(1)}} \right\rangle$$

from the CAR (4.4) and (4.11). Since $\varrho^{(\beta,\omega,\lambda)}$ is by construction a quasi-free state, we use [14, p. 48], that is here,

$$\begin{aligned}
&\varrho^{(\beta,\omega,\lambda)}(a^{*}(f_1)\, a^{*}(f_2)\, a(g_1)\, a(g_2)) \\
&\quad = \varrho^{(\beta,\omega,\lambda)}(a^{*}(f_1)\, a(g_2))\varrho^{(\beta,\omega,\lambda)}(a^{*}(f_2)\, a(g_1)) \\
&\quad\quad - \varrho^{(\beta,\omega,\lambda)}(a^{*}(f_1)\, a(g_1))\varrho^{(\beta,\omega,\lambda)}(a^{*}(f_2)\, a(g_2)) ,
\end{aligned}$$

to infer from (4.122) that

$$\begin{aligned}
&\varrho^{(\beta,\omega,\lambda)}\left(a_{y^{(1)}}^{*} a_{y^{(2)}} \tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(1)}}^{*})\tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(2)}})\right) \\
&\quad = \varrho^{(\beta,\omega,\lambda)}(a_{y^{(1)}}^{*} a_{y^{(2)}})\varrho^{(\beta,\omega,\lambda)}(\tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(1)}}^{*})\tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(2)}})) \\
&\quad\quad + \varrho^{(\beta,\omega,\lambda)}\left(a_{y^{(1)}}^{*}\tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(2)}})\right)\varrho^{(\beta,\omega,\lambda)}\left(a_{y^{(2)}}\tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(1)}}^{*})\right)
\end{aligned} \tag{4.123}$$

for any $\beta \in \mathbb{R}^{+}$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_{0}^{+}$, $t \in \mathbb{R}$, $\alpha \in [0,\beta]$ and $\mathbf{x},\mathbf{y} \in \mathfrak{L}^{2}$. Using (4.36), (4.39) and (4.41), we then deduce from Equation (4.123) that

$$\begin{aligned}
&\varrho^{(\beta,\omega,\lambda)}\left(a_{y^{(1)}}^{*} a_{y^{(2)}} \tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(1)}}^{*})\tau_{t+i\alpha}^{(\omega,\lambda)}(a_{x^{(2)}})\right) \\
&\quad = C_{0}^{(\omega)}(y^{(1)},y^{(2)})C_{0}^{(\omega)}(x^{(1)},x^{(2)}) + C_{t+i\alpha}^{(\omega)}(y^{(1)},x^{(2)})C_{-t+i(\beta-\alpha)}^{(\omega)}(x^{(1)},y^{(2)})
\end{aligned}$$

for any $\beta \in \mathbb{R}^{+}$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_{0}^{+}$, $t \in \mathbb{R}$, $\alpha \in [0,\beta]$ and $\mathbf{x},\mathbf{y} \in \mathfrak{L}^{2}$. We then combine this last equality with (4.121) to arrive at

$$\begin{aligned}
&\varrho^{(\beta,\omega,\lambda)}\left(I_{\mathbf{y}}\tau_{t+i\alpha}^{(\omega,\lambda)}(I_{\mathbf{x}})\right) \\
&\quad = -\sum_{\pi,\pi'\in S_2}\varepsilon_{\pi}\varepsilon_{\pi'}\Big(C_{t+i\alpha}^{(\omega)}(y^{\pi'(1)},x^{\pi(2)})C_{-t+i(\beta-\alpha)}^{(\omega)}(x^{\pi(1)},y^{\pi'(2)}) \\
&\quad\quad + C_{0}^{(\omega)}(y^{\pi'(1)},y^{\pi'(2)})C_{0}^{(\omega)}(x^{\pi(1)},x^{\pi(2)})\Big)
\end{aligned} \tag{4.124}$$

for any $\beta \in \mathbb{R}^{+}$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_{0}^{+}$, $t \in \mathbb{R}$, $\alpha \in [0,\beta]$, $\mathbf{x} := (x^{(1)},x^{(2)}) \in \mathfrak{L}^{2}$ and $\mathbf{y} := (y^{(1)},y^{(2)}) \in \mathfrak{L}^{2}$. Therefore, the assertion follows by combining (4.120) with (4.124). □

Remark 4.5.7.
Observe that, for each $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$ and $\alpha \in [0,\beta]$, the coefficient $\mathfrak{C}_{t+i\alpha}^{(\omega)}$ defined by (4.119) can be seen as the kernel (w.r.t. the canonical basis $\{\mathfrak{e}_x \otimes \mathfrak{e}_x\}_{x,x' \in \mathfrak{L}}$) of a bounded operator on $\ell^2(\mathfrak{L}) \otimes \ell^2(\mathfrak{L})$ that is again denoted by $\mathfrak{C}_{t+i\alpha}^{(\omega)} \equiv \mathfrak{C}_{t+i\alpha}^{(\beta,\omega,\lambda)}$. By (4.66), its operator norm can be uniformly bounded w.r.t. $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$ and $\alpha \in [0,\beta]$:

$$\left\| \mathfrak{C}_{t+i\alpha}^{(\omega)} \right\|_{\mathrm{op}} \leq \left\| \frac{\mathrm{e}^{(-it+\alpha)(\Delta_{\mathrm{d}}+\lambda V_\omega)}}{1+\mathrm{e}^{\beta(\Delta_{\mathrm{d}}+\lambda V_\omega)}} \right\|_{\mathrm{op}} \cdot \left\| \frac{\mathrm{e}^{(it+\beta-\alpha)(\Delta_{\mathrm{d}}+\lambda V_\omega)}}{1+\mathrm{e}^{\beta(\Delta_{\mathrm{d}}+\lambda V_\omega)}} \right\|_{\mathrm{op}} \leq 1\,. \tag{4.125}$$

We are now in position to give the proof of the main result, that is, a rigorous derivation of AC-Joule's law for lattice fermions with random chemical potential.

4.5.3 Derivation of AC-Joule's law

The main aim of this section is to prove Theorem 4.5.1, this is essentially done in Theorem 4.5.19. Its proof uses several arguments. We present them in various lemmata which then yield the final result.

Note that, by Theorem 4.5.2, Lemmata 4.5.3 and 4.5.6 as well as Equation (4.17), we already obtain that for any $\mathbf{A} \in \mathbf{C}_0^\infty$ and $t \geq t_1$, there is $\eta_0 \in \mathbb{R}^+$ such that, for all $\eta \in (0,\eta_0]$ and $L \in \mathbb{R}^+$, the energy increment exists, is positive and equals

$$\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)} = \eta^2 L^d \int_{t_0}^{t} \int_{t_0}^{s_1} \mathbf{X}_{L,0}^{(\omega)}(s_1,s_2)\mathrm{d}s_2\,\mathrm{d}s_1 + \mathcal{O}(\eta^3 L^d) \tag{4.126}$$

uniformly for $\beta \in \mathbb{R}^+$, $\omega \in \Omega$ and $\lambda \in \mathbb{R}_0^+$. Here, $\mathbf{X}_{L,\upsilon}^{(\omega)} \equiv \mathbf{X}_{L,\upsilon}^{(\beta,\omega,\lambda,\mathbf{A})}$ is defined, for any $\upsilon \in [0,\beta/2)$ and $s_1, s_2 \in \mathbb{R}$, by

$$\mathbf{X}_{L,\upsilon}^{(\omega)}(s_1,s_2) := \frac{1}{L^d} \sum_{\mathbf{x},\mathbf{y} \in \mathfrak{K}} \int_{\upsilon}^{\beta-\upsilon} \mathfrak{C}_{s_2-s_1+i\alpha}^{(\omega)}(\mathbf{x},\mathbf{y}) V_{s_2}^{\mathbf{A}_L}(\mathbf{x})\, V_{s_1}^{\mathbf{A}_L}(\mathbf{y})\mathrm{d}\alpha\,. \tag{4.127}$$

Recall that the definition of the set $\mathfrak{K} \subset \mathfrak{L}^2$ of nearest neighbours is given by (4.101). Note also that the integral in (4.127) can be exchanged with the (finite) sum because $\mathbf{A} \in \mathbf{C}_0^\infty$.

The first important result of the present subsection will be a proof that $\mathbf{X}_{L,0}^{(\omega)}$ almost surely converges to a deterministic function, as $L \to \infty$, this is achieved in Corollary 4.5.17. Then we will use Lebesgue's dominated convergence theorem to get the energy increment $\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)}$ in the limit $(\eta, L^{-1}) \to (0,0)$, see Theorem 4.5.19.

By Lemma 4.3.5, note that, for all $\varepsilon, \beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$, $\upsilon \in (0, \beta/2)$ and $\alpha \in [\upsilon, \beta - \upsilon]$, the complex-time two-point correlation functions $C_{t+i\alpha}^{(\omega)} \equiv C_{t+i\alpha}^{(\beta,\omega,\lambda)}$ can be written as the sum

$$C_{t+i\alpha}^{(\omega)}(\mathbf{x}) = A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(\mathbf{x}) + B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(\mathbf{x}) \ , \qquad \mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2 \ , \tag{4.128}$$

of two maps $A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}, B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}$ from $\mathfrak{L}^2$ to $\mathbb{C}$. This decomposition has the following useful property: $A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}$ can be seen as the kernel (w.r.t. the canonical basis $\{\mathfrak{e}_x\}_{x\in\mathfrak{L}}$) of an operator, again denoted by $A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} \in \mathcal{B}(\ell^2(\mathfrak{L}))$, with arbitrarily small operator norm $\|A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}\|_{\mathrm{op}} \leq \varepsilon$, whereas $B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}$ is fast decaying, as $|x^{(1)} - x^{(2)}| \to \infty$. This is however only verified if $\alpha \in [\upsilon, \beta - \upsilon]$ with fixed $\upsilon \in (0, \beta/2)$, cf. Lemma 4.3.5.

As a consequence, the first step is to approximate $\mathbf{X}_{L,0}^{(\omega)}$ with $\mathbf{X}_{L,\upsilon}^{(\omega)}$ for small $\upsilon > 0$. This is done by using the following lemma:

Lemma 4.5.8 (Approximation I)**.**
Let $\mathbf{A} \in \mathbf{C}_0^\infty$. *Then,*

$$\mathbf{X}_{L,0}^{(\omega)}(s_1, s_2) = \mathbf{X}_{L,\upsilon}^{(\omega)}(s_1, s_2) + \mathcal{O}(\upsilon) \ ,$$

uniformly for $L, \beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ *and* $s_1, s_2 \in \mathbb{R}$.

Proof. The canonical orthonormal basis of $\ell^2(\mathfrak{L}) \otimes \ell^2(\mathfrak{L})$ is $\{\mathfrak{e}_{x^{(1)}} \otimes \mathfrak{e}_{x^{(2)}}\}_{(x^{(1)},x^{(2)})\in\mathfrak{L}^2}$ with

$$\mathbf{e}_{\mathbf{x}} := \mathfrak{e}_{x^{(1)}} \otimes \mathfrak{e}_{x^{(2)}} \ , \qquad \mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2 \ .$$

Recall that $\mathfrak{e}_x(y) \equiv \delta_{x,y} \in \ell^2(\mathfrak{L})$. Then, using Remark 4.5.7 observe that

$$\sum_{\mathbf{x},\mathbf{y}\in\mathfrak{K}} \mathfrak{C}_{s_2-s_1+i\alpha}^{(\omega)}(\mathbf{x},\mathbf{y}) V_{s_2}^{\mathbf{A}_L}(\mathbf{x}) V_{s_1}^{\mathbf{A}_L}(\mathbf{y}) = \sum_{\mathbf{x},\mathbf{y}\in\mathfrak{K}} \left\langle \mathbf{e}_{\mathbf{x}}, \mathfrak{C}_{s_2-s_1+i\alpha}^{(\omega)} \mathbf{e}_{\mathbf{y}} \right\rangle V_{s_2}^{\mathbf{A}_L}(\mathbf{x}) V_{s_1}^{\mathbf{A}_L}(\mathbf{y}) \ . \tag{4.129}$$

In particular, via (4.125) we arrive at the upper bound

$$\begin{aligned} &\frac{1}{L^d} \sum_{\mathbf{x},\mathbf{y}\in\mathfrak{K}} \left| \mathfrak{C}_{s_2-s_1+i\alpha}^{(\omega)}(\mathbf{x},\mathbf{y}) V_{s_2}^{\mathbf{A}_L}(\mathbf{x})\, V_{s_1}^{\mathbf{A}_L}(\mathbf{y}) \right| \\ &\qquad \leq 2d \|V^{\mathbf{A}}\|_\infty^2 \max_{t\in\mathbb{R}} |\mathrm{supp}(\mathbf{A}(t,.))| + \mathcal{O}(1) \end{aligned} \tag{4.130}$$

for any $\mathbf{A} \in \mathbf{C}_0^\infty$, $L, \beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $\alpha \in [0, \beta]$, and $s_1, s_2 \in \mathbb{R}$, where

$$\|V^{\mathbf{A}}\|_\infty := \max\left\{|E_{\mathbf{A}_L}(t, x)| \ : \ (t, x) \in \mathrm{supp}(A)\right\} \in \mathbb{R}^+ \ . \tag{4.131}$$

Therefore, the assertion follows from (4.127) combined with (4.130). □

Because of (4.128) and Lemma 4.3.5, it is natural to define, at any $\varepsilon, \beta \in \mathbb{R}^+$, $t \in \mathbb{R}$, $\upsilon \in (0, \beta/2)$ and $\alpha \in [\upsilon, \beta - \upsilon]$, the map $\mathfrak{B}_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} \equiv \mathfrak{B}_{t+i\alpha,\upsilon,\varepsilon}^{(\beta,\omega,\lambda)}$ from $\mathfrak{L}^4$ to $\mathbb{C}$ by

$$\begin{aligned}\mathfrak{B}_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}&(\mathbf{x}, \mathbf{y}) \\ &:= \frac{1}{4} \sum_{\pi, \pi' \in S_2} \varepsilon_\pi \varepsilon_{\pi'} B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(y^{\pi'(1)}, x^{\pi(1)}) B_{-t+i(\beta-\alpha),\upsilon,\varepsilon}^{(\omega)}(x^{\pi(2)}, y^{\pi'(2)})\end{aligned} \tag{4.132}$$

for any $\mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2$ and $\mathbf{y} := (y^{(1)}, y^{(2)}) \in \mathfrak{L}^2$. In other words, this map is defined by replacing in (4.119) the complex-time two-point correlation functions $C_{t+i\alpha}^{(\omega)}$ by their approximations $B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}$ coming from the decomposition (4.128).

Similarly, we define the function $\mathbf{Y}_{L,\upsilon,\varepsilon,0}^{(\omega)} \equiv \mathbf{Y}_{L,\upsilon,\varepsilon,0}^{(\beta,\omega,\lambda,\mathbf{A})}$ of times $s_1, s_2 \in \mathbb{R}$ by

$$\mathbf{Y}_{L,\upsilon,\varepsilon,0}^{(\omega)}(s_1, s_2) := \frac{1}{L^d} \sum_{\mathbf{x},\mathbf{y} \in \mathfrak{K}} \int_\upsilon^{\beta-\upsilon} \mathfrak{B}_{s_2-s_1+i\alpha,\upsilon,\varepsilon}^{(\omega)}(\mathbf{x}, \mathbf{y}) V_{s_2}^{\mathbf{A}_L}(\mathbf{x})\, V_{s_1}^{\mathbf{A}_L}(\mathbf{y}) \mathrm{d}\alpha \ . \tag{4.133}$$

We show in the next lemma that it is a good approximation of (4.127), provided $\upsilon \neq 0$.

Lemma 4.5.9 (Approximation II)**.**
Let $\varepsilon \in \mathbb{R}^+$ and $\mathbf{A} \in \mathbf{C}_0^\infty$. Then,

$$\mathbf{X}_{L,\upsilon}^{(\omega)}(s_1, s_2) = \mathbf{Y}_{L,\upsilon,\varepsilon,0}^{(\omega)}(s_1, s_2) + \mathcal{O}(\varepsilon) \ ,$$

uniformly for $L, \beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $\upsilon \in (0, \beta/2)$ and $s_1, s_2 \in \mathbb{R}$.

Proof. Let $\varepsilon, \beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $\mathbf{A} \in \mathbf{C}_0^\infty$. By Lemma 4.3.5 (i), note that $A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}, B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}$ can be seen as the kernels (w.r.t. the canonical basis $\{\mathfrak{e}_x\}_{x \in \mathfrak{L}}$) of two bounded operators on $\ell^2(\mathfrak{L})$. In particular, similar to (4.129),

$$A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(y, x) = \left\langle \mathfrak{e}_y, A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} \mathfrak{e}_x \right\rangle \ , \quad B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(y, x) = \left\langle \mathfrak{e}_y, B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} \mathfrak{e}_x \right\rangle ,$$

where $\mathfrak{e}_x(y) \equiv \delta_{x,y} \in \ell^2(\mathfrak{L})$. Therefore, Lemma 4.3.5 (i) and the Cauchy-Schwarz inequality yield the existence of a finite constant $D \in \mathbb{R}^+$ independent of $\alpha \in [\upsilon, \beta - \upsilon]$, $t \in \mathbb{R}$, $\omega \in \Omega$ and $\varepsilon \in \mathbb{R}^+$ such that, for all $c_x, c_y' \in \mathbb{C}$, $y \in \mathfrak{L}$,

$$\begin{aligned}
\left| \sum_{x,y\in\mathfrak{L}} \overline{c_x} c_y' A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(y,x) \right| &\leq \left\| A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} \right\|_{\mathrm{op}} \sqrt{\sum_{x,y\in\mathfrak{L}} |c_x|^2 \left| c_y' \right|^2} \\
&\leq \varepsilon \sqrt{\sum_{x,y\in\mathfrak{L}} |c_x|^2 \left| c_y' \right|^2}, \\
\left| \sum_{x,y\in\mathfrak{L}} \overline{c_x} c_y' B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(y,x) \right| &\leq \left\| B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} \right\|_{\mathrm{op}} \sqrt{\sum_{x,y\in\mathfrak{L}} |c_x|^2 \left| c_y' \right|^2} \\
&\leq D \sqrt{\sum_{x,y\in\mathfrak{L}} |c_x|^2 \left| c_y' \right|^2}.
\end{aligned}$$

It obviously follows that, for all $c_{\mathbf{x}} \in \mathbb{C}$, $\mathbf{x} \in \mathfrak{K}$, and some $D \in \mathbb{R}^+$

$$\begin{aligned}
\left| \sum_{\mathbf{x},\mathbf{y}\in\mathfrak{K}} \overline{c_{\mathbf{x}}} c_{\mathbf{y}} B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(y^{(1)},x^{(2)}) A_{-t+i(\beta-\alpha),\upsilon,\varepsilon}^{(\omega)}(x^{(1)},y^{(2)}) \right| &\leq \varepsilon D \sum_{\mathbf{x}\in\mathfrak{K}} |c_x|^2 , \\
\left| \sum_{\mathbf{x},\mathbf{y}\in\mathfrak{K}} \overline{c_{\mathbf{x}}} c_{\mathbf{y}} A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(y^{(1)},x^{(2)}) B_{-t+i(\beta-\alpha),\upsilon,\varepsilon}^{(\omega)}(x^{(1)},y^{(2)}) \right| &\leq \varepsilon D \sum_{\mathbf{x}\in\mathfrak{K}} |c_x|^2 , \\
\left| \sum_{\mathbf{x},\mathbf{y}\in\mathfrak{K}} \overline{c_{\mathbf{x}}} c_{\mathbf{y}} A_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(y^{(1)},x^{(2)}) A_{-t+i(\beta-\alpha),\upsilon,\varepsilon}^{(\omega)}(x^{(1)},y^{(2)}) \right| &\leq \varepsilon^2 D \sum_{\mathbf{x}\in\mathfrak{K}} |c_x|^2 ,
\end{aligned}$$

provided $\alpha \in [\upsilon, \beta - \upsilon]$ with $\upsilon \in (0, \beta/2)$. Here, $\mathbf{x} = (x^{(1)}, x^{(2)})$, $\mathbf{y} = (y^{(1)}, y^{(2)})$. Similar to (4.130), we then use this three above bounds to get the existence of a finite constant $D \in \mathbb{R}^+$ not depending on $\alpha \in [\upsilon, \beta - \upsilon]$, $s_1, s_2 \in \mathbb{R}$, $\omega \in \Omega$, $\varepsilon \in (0,1)$ and $L \in \mathbb{N}$ such that

$$\left| \mathbf{X}_{L,\upsilon}^{(\omega)}(s_1,s_2) - \mathbf{Y}_{L,\upsilon,\varepsilon,0}^{(\omega)}(s_1,s_2) \right| \leq \varepsilon D .$$

$\square$

The (approximating) correlation functions $B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}$ in (4.132) decay fast, as $|y^{\pi'(1)} - x^{\pi(2)}| \to \infty$ or $|x^{\pi(1)} - y^{\pi'(2)}| \to \infty$, see Lemma 4.3.5(ii). This decay is uniform for t on compact intervals. We can divide the (compact) support

$\mathrm{supp}(\mathbf{A}(t,.)) \subset \mathbb{R}^d$ of the vector potential $\mathbf{A} \in \mathbf{C}_0^\infty$ in small regions to use later a piecewise-constant approximation of the smooth electric field $E_{\mathbf{A}}$ (4.15) in (4.133). Then, because of the space decay of $B^{(\omega)}_{t+i\alpha,\upsilon,\varepsilon}$, the contributions to the total heat production coming from each region of constant electric field behave additive, at large L.

To do this, let us assume w.l.o.g. that, for all $t \in \mathbb{R}$,

$$\mathrm{supp}(\mathbf{A}(t,.)) \subset [-1/2, 1/2]^d .$$

For $n \in \mathbb{N}$, we divide the elementary box $[-1/2,1/2]^d$ in n^d boxes $\{b_j\}_{j\in\mathcal{D}_n}$ of side-length $1/n$, where

$$\mathcal{D}_n := \{-(n-1)/2, -(n-3)/2, \cdots, (n-3)/2, (n-1)/2\}^d . \tag{4.134}$$

Explicitly, for any $j \in \mathcal{D}_n$,

$$b_j := jn^{-1} + n^{-1}[-1/2,1/2]^d \quad \text{and} \quad [-1/2,1/2]^d = \bigcup_{j\in\mathcal{D}_n} b_j . \tag{4.135}$$

Then, for all $\varepsilon, L, \beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $\upsilon \in (0,\beta/2)$, we extend the definition of $\mathbf{Y}^{(\omega)}_{L,\upsilon,\varepsilon,0}$ to all $n \in \mathbb{N}$ as

$$\mathbf{Y}^{(\omega)}_{L,\upsilon,\varepsilon,n}(s_1,s_2) \tag{4.136}$$
$$:= \frac{1}{L^d}\sum_{j\in\mathcal{D}_n}\sum_{\mathbf{x},\mathbf{y}\in\mathfrak{K}\cap(Lb_j)^2}\int_\upsilon^{\beta-\upsilon}\mathfrak{B}^{(\omega)}_{s_2-s_1+i\alpha,\upsilon,\varepsilon}(\mathbf{x},\mathbf{y})V^{\mathbf{A}_L}_{s_2}(\mathbf{x})\,V^{\mathbf{A}_L}_{s_1}(\mathbf{y})\mathrm{d}\alpha$$

for all $s_1, s_2 \in \mathbb{R}$. In fact, the acumulation points of $\mathbf{Y}^{(\omega)}_{L,\upsilon,\varepsilon,T,n}$, as $L\to\infty$, do not depend on n:

Lemma 4.5.10 (Approximation III)**.**
Let $n \in \mathbb{N}$, $\varepsilon, L, \beta \in \mathbb{R}^+$, $\omega\in\Omega$, $\lambda \in \mathbb{R}_0^+$, $\upsilon \in (0,\beta/2)$ and $\mathbf{A}\in\mathbf{C}_0^\infty$. Then, for all $s_1, s_2 \in \mathbb{R}$,

$$\lim_{L\to\infty}\left|\mathbf{Y}^{(\omega)}_{L,\upsilon,\varepsilon,0}(s_1,s_2) - \mathbf{Y}^{(\omega)}_{L,\upsilon,\varepsilon,n}(s_1,s_2)\right| = 0 .$$

Proof. We observe from (4.133), (4.135) and (4.136) that

$$\mathbf{Y}^{(\omega)}_{L,\upsilon,\varepsilon,0}(s_1,s_2) - \mathbf{Y}^{(\omega)}_{L,\upsilon,\varepsilon,n}(s_1,s_2)$$
$$= \frac{1}{L^d}\sum_{j,k\in\mathcal{D}_n, j\neq k}\ \sum_{\mathbf{x}\in\mathfrak{K}\cap(Lb_j)^2}\ \sum_{\mathbf{y}\in\mathfrak{K}\cap(Lb_k)^2}$$
$$\int_\upsilon^{\beta-\upsilon}\mathfrak{B}^{(\omega)}_{s_2-s_1+i\alpha,\upsilon,\varepsilon}(\mathbf{x},\mathbf{y})V^{\mathbf{A}_L}_{s_2}(\mathbf{x})\,V^{\mathbf{A}_L}_{s_1}(\mathbf{y})\mathrm{d}\alpha . \tag{4.137}$$

Meanwhile, for any $j,k \in \mathcal{D}_n$, $j \neq k$, every

$$\mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{K} \cap (Lb_j)^2 , \qquad \mathbf{y} := (y^{(1)}, y^{(2)}) \in \mathfrak{K} \cap (Lb_k)^2 ,$$

(cf. (4.101)) and all sufficiently large $L \in \mathbb{R}^+$, one clearly has the lower bound

$$\min_{\pi,\pi' \in S_2} \left| x^{\pi(1)} - y^{\pi'(2)} \right| \geq \left| \left| x^{(1)} - y^{(1)} \right| - 2 \right| .$$

Therefore, we use the last estimate together with (4.131) and Lemma 4.3.5 (ii) to obtain from (4.132) and (4.137) that, for any fixed $T \in \mathbb{R}^+$ and all $s_1, s_2 \in [-T, T]$,

$$\begin{aligned} &\left| \mathbf{Y}^{(\omega)}_{L,\upsilon,\varepsilon,0}\ (s_1, s_2) - \mathbf{Y}^{(\omega)}_{L,\upsilon,\varepsilon,n}(s_1, s_2) \right| \\ &\qquad \leq D \frac{1}{L^d} \sum_{j,k \in \mathcal{D}_n, j \neq k} \ \sum_{x \in \mathfrak{L} \cap (Lb_j)} \ \sum_{y \in \mathfrak{L} \cap (Lb_k)} \frac{1}{(1 + | \, |x-y| - 2|)^{2d^2+2}} , \end{aligned} \tag{4.138}$$

where $D \in \mathbb{R}^+$ is a finite constant only depending on d, ε, T, β, λ, $\upsilon \in (0, \beta/2)$ and $\mathbf{A} \in \mathbf{C}_0^\infty$. Note that, for any small $\delta > 0$,

$$\frac{1}{L^d} \sum_{j,k \in \mathcal{D}_n, j \neq k} \ \sum_{x \in \mathfrak{L} \cap (Lb_j)} \ \sum_{y \in \mathfrak{L} \cap (Lb_k)} \frac{\mathbf{1}\left[|x-y| \geq \delta L \right]}{(1 + | \, |x-y| - 2|)^{2d^2+2}} = \mathcal{O}\left(\frac{1}{L^{2d^2-d+2} \delta^{2d^2+2}} \right)$$

and

$$\frac{1}{L^d} \sum_{j,k \in \mathcal{D}_n, j \neq k} \ \sum_{x \in \mathfrak{L} \cap (Lb_j)} \ \sum_{y \in \mathfrak{L} \cap (Lb_k)} \frac{\mathbf{1}\left[|x-y| \leq \delta L \right]}{(1 + | \, |x-y| - 2|)^{2d^2+2}} = \mathcal{O}\left(\delta^{d+1} L^d \right) .$$

Then, for $\delta = L^{-\frac{2d^2+2}{2d^2+d+3}}$, the last two sums are both of order $\mathcal{O}(L^{-\frac{d^2-d+2}{2d^2+d+3}})$ with $d^2 - d + 2 \geq 2$ for all $d \in \mathbb{N}$. Combining this two asymptotics with (4.138) we arrive at the assertion. □

As already mentioned above, we now consider piecewise-constant approximations of the (smooth) electric field (4.15), that is,

$$E_{\mathbf{A}}(t, x) := -\partial_t \mathbf{A}(t, x) , \quad t \in \mathbb{R}, \ x \in \mathbb{R}^d . \tag{4.139}$$

For any $j \in \mathcal{D}_n$, let $z^{(j)} \in b_j$ be any fixed point of the box b_j. Then, define the function $\bar{\mathbf{Y}}_{L,\upsilon,\varepsilon,n}^{(\omega)} \equiv \bar{\mathbf{Y}}_{L,\upsilon,\varepsilon,n}^{(\beta,\omega,\lambda,\mathbf{A})}$ of times $s_1, s_2 \in \mathbb{R}$ by

$$\begin{aligned}\bar{\mathbf{Y}}_{L,\upsilon,\varepsilon,n}^{(\omega)}(s_1, s_2) \quad := \quad & \frac{1}{L^d} \sum_{j\in\mathcal{D}_n} \sum_{\mathbf{x},\mathbf{y}\in\mathfrak{K}\cap(Lb_j)^2} \int_{\upsilon}^{\beta-\upsilon} \mathrm{d}\alpha \, \mathfrak{B}_{s_2-s_1+i\alpha,\upsilon,\varepsilon}^{(\omega)}(\mathbf{x}, \mathbf{y}) \\ & \times \left[E_{\mathbf{A}}(s_2, z^{(j)})\right](x^{(1)} - x^{(2)}) \left[E_{\mathbf{A}}(s_1, z^{(j)})\right](y^{(1)} - y^{(2)}) \, .\end{aligned} \tag{4.140}$$

Recall that in this definition $\mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2$ and $\mathbf{y} := (y^{(1)}, y^{(2)}) \in \mathfrak{L}^2$, see (4.101). This new function aproximates (4.136) arbitrarily well, as $L \to \infty$ and $n \to \infty$:

Lemma 4.5.11 (Approximation IV)**.**
Let $n \in \mathbb{N}$, $\varepsilon, L, \beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $\upsilon \in (0, \beta/2)$ and $\mathbf{A} \in \mathbf{C}_0^\infty$. Then, for all $s_1, s_2 \in \mathbb{R}$,

$$\lim_{n\to\infty} \left\{ \limsup_{L\to\infty} \left| \mathbf{Y}_{L,\upsilon,\varepsilon,n}^{(\omega)}(s_1, s_2) - \bar{\mathbf{Y}}_{L,\upsilon,\varepsilon,n}^{(\omega)}(s_1, s_2) \right| \right\} = 0 \, .$$

Proof. By taking an orthonormal basis $\{e_k\}_{k=1}^d$ of the lattice $\mathfrak{L}$, we directly infer from (4.77), (4.100) and (4.139) that, for any $L \in \mathbb{R}^+$, $\mathbf{A} \in \mathbf{C}_0^\infty$, $j \in \mathcal{D}_n$, $t \in \mathbb{R}$, $k \in \{1, \cdots, d\}$ and $x \in Lb_j$,

$$\begin{aligned}&\left|V_t^{\mathbf{A}_L}\ (x, x \pm e_k) - \left[E_{\mathbf{A}}(t, z^{(j)})\right](\pm e_k)\right| \\ &\quad \leq \int_0^1 \left| \left[\partial_t \mathbf{A}(t, z^{(j)})\right](e_k) - \left[\partial_t \mathbf{A}_l(t, x \pm (1-\alpha)e_k)\right](e_k) \right| \mathrm{d}\alpha \\ &\quad \leq \sup_{y\in\tilde{b}_{j,l}} \left| \left[\partial_t \mathbf{A}(t, z^{(j)})\right](e_k) - \left[\partial_t \mathbf{A}(t, y)\right](e_k) \right| < \infty \, ,\end{aligned}$$

where

$$\tilde{b}_{j,L} := \left\{ x \in \mathbb{R}^d \ : \ \min_{y\in b_j} |x - y| \leq L^{-1} \right\} \, .$$

In particular, since $\mathbf{A} \in \mathbf{C}_0^\infty$, there is a finite constant D independent of $j \in \mathcal{D}_n$, $t \in \mathbb{R}$, $k \in \{1, \cdots, d\}$ and $x \in b_j$ such that

$$\left|V_t^{\mathbf{A}_L}(x, x \pm e_k) - \left[E_{\mathbf{A}}(t, z^{(j)})\right](\pm e_k)\right| \leq D(n^{-1} + L^{-1}) \, .$$

Therefore, using (4.131) and Lemma 4.3.5(ii) as in (4.138), one gets that, for any fixed $T \in \mathbb{R}^+$ and all $s_1, s_2 \in [-T, T]$,

$$\begin{aligned}&\left|\mathbf{Y}^{(\omega)}_{L,\upsilon,\varepsilon,n}(s_1,s_2) - \bar{\mathbf{Y}}^{(\omega)}_{L,\upsilon,\varepsilon,n}(s_1,s_2)\right| \\ &\qquad \leq D(n^{-1}+L^{-1})^2 \frac{1}{L^d} \sum_{j\in\mathcal{D}_n} \sum_{x,y\in\mathfrak{L}\cap(Lb_j)} \frac{1}{(1+|\,|x-y|-2|)^{2d^2+2}} ,\end{aligned} \tag{4.141}$$

where $D \in \mathbb{R}^+$ is a finite constant depending on d, ε, T, β, λ, $\upsilon \in (0, \beta/2)$ and $\mathbf{A} \in \mathbf{C}_0^\infty$. For all $j \in \mathcal{D}_n$, note that

$$\frac{1}{L^d} \sum_{x,y\in\mathfrak{L}\cap(Lb_j)} \frac{1}{(1+|\,|x-y|-2|)^{2d^2+2}} \leq \frac{1}{n^d} \sum_{x\in\mathfrak{L}} \frac{1}{(1+|\,|x|-2|)^{2d^2+2}} \leq \frac{D}{n^d}$$

for some finite constant $D \in \mathbb{R}^+$. Therefore, we arrive at the assertion by combining this last bound with (4.141). □

By taking again some orthonormal basis $\{e_k\}_{k=1}^d$ of the lattice $\mathfrak{L}$ and setting $e_{-k} := -e_k$ for each $k \in \{1, \cdots, d\}$, we rewrite the function (4.140) as

$$\begin{aligned}\bar{\mathbf{Y}}^{(\omega)}_{L,\upsilon,\varepsilon,n}(s_1,s_2) \;:=\; & \frac{1}{n^d} \sum_{j\in\mathcal{D}_n} \sum_{k,q\in\{1,-1,\cdots,d,-d\}} \mathbf{Z}^{(\omega)}_{L,j,k,q}(s_2-s_1) \\ & \times \left[E_{\mathbf{A}}(s_2, z^{(j)})\right](e_k) \left[E_{\mathbf{A}}(s_1, z^{(j)})\right](e_q)\end{aligned} \tag{4.142}$$

for any $s_1, s_2 \in \mathbb{R}$, where, for all $n \in \mathbb{N}$, $\varepsilon, L, \beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $\upsilon \in (0, \beta/2)$, $j \in \mathcal{D}_n$, $k, q \in \{1, -1, \cdots, d, -d\}$ and $t \in \mathbb{R}$,

$$\mathbf{Z}^{(\omega)}_{L,j,k,q}(t) \equiv \mathbf{Z}^{(\beta,\omega,\lambda)}_{L,\upsilon,\varepsilon,n,j,k,q} := \frac{n^d}{L^d} \sum_{x,y\in\mathfrak{L}\cap(Lb_j)} \int_{\upsilon}^{\beta-\upsilon} \mathfrak{B}^{(\omega)}_{t+i\alpha,\upsilon,\varepsilon}(y, y-e_q, x, x-e_k)\mathrm{d}\alpha\,.$$

Notice that we have neglected terms related to x, y on the boundary of $\mathfrak{L} \cap (Lb_j)$, since these are irrelevant in the limit $L \to \infty$. Here, for any $\mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2$ and $\mathbf{y} := (y^{(1)}, y^{(2)}) \in \mathfrak{L}^2$,

$$\mathfrak{B}^{(\omega)}_{s_2-s_1+i\alpha,\upsilon,\varepsilon}(\mathbf{x}, \mathbf{y}) \equiv \mathfrak{B}^{(\omega)}_{s_2-s_1+i\alpha,\upsilon,\varepsilon}(x^{(1)}, x^{(2)}, y^{(1)}, y^{(2)})\,, \tag{4.143}$$

see (4.132). Hence, it remains to analyze the limit of $\mathbf{Z}^{(\omega)}_{L,j,k,q}$, as $L \to \infty$.

Lemma 4.5.12.
Let $\varepsilon, L, \beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$ and $\upsilon \in (0, \beta/2)$. Then, there is a measurable subset $\tilde{\Omega}_{\upsilon,\varepsilon}(t) \equiv \tilde{\Omega}_{\upsilon,\varepsilon}^{(\beta,\lambda)}(t) \subset \Omega$ of full measure such that, for any $n \in \mathbb{N}$, $j \in \mathcal{D}_n$, $k, q \in \{1, -1, \cdots, d, -d\}$ and any $\omega \in \tilde{\Omega}_{\upsilon,\varepsilon}(t)$,

$$\lim_{L\to\infty} \mathbf{Z}_{L,j,k,q}^{(\omega)}(t) = \sum_{x\in\mathfrak{L}} \mathbb{E}\left(\int_{\upsilon}^{\beta-\upsilon} \mathfrak{B}_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(x, x-e_q, 0, -e_k)\mathrm{d}\alpha\right) < \infty \ .$$

Here, $\mathbb{E}$ is the expectation value associated with the probability measure $\mathfrak{a}_\Omega$ (4.7).

Proof. Fix first in all the proof the parameters $n \in \mathbb{N}$, $\varepsilon, \beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$, $\upsilon \in (0, \beta/2)$, $j \in \mathcal{D}_n$ and $k, q \in \{1, -1, \cdots, d, -d\}$. To avoid trivial technical complications in this proof we will, moreover, assume w.l.o.g. that n is a *odd* natural number. For any $x \in \mathfrak{L}$, let

$$\mathfrak{F}_\omega(\{x\}) := \sum_{y\in\mathfrak{L}} \int_{\upsilon}^{\beta-\upsilon} \mathfrak{B}_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(y, y-e_q, x, x-e_k)\mathrm{d}\alpha < \infty \ .$$

This sum is finite because of (4.132) and Lemma 4.3.5 (ii). We now define an *additive* process $\{\mathfrak{F}_\omega(\Lambda)\}_{\Lambda\in\mathcal{P}_f(\mathfrak{L})}$ (cf. [20, Definition VI.1.6]) by

$$\mathfrak{F}_\omega(\Lambda) := \sum_{x\in\Lambda} \mathfrak{F}_\omega(\{x\})$$

for any finite subset $\Lambda \in \mathcal{P}_f(\mathfrak{L})$ with cardinality $|\Lambda| < \infty$. Indeed, it is not difficult to show that the map $\omega \mapsto \mathfrak{F}_\omega(\Lambda)$ is bounded and measurable w.r.t. the σ-algebra $\mathfrak{A}_\Omega$ for all $\Lambda \in \mathcal{P}_f(\mathfrak{L})$. Obviously, for all $\Lambda \in \mathcal{P}_f(\mathfrak{L})$,

$$|\Lambda|^{-1}\,\mathbb{E}(\mathfrak{F}_\omega(\Lambda)) = \mathbb{E}(\mathfrak{F}_\omega(\{0\})) \ , \tag{4.144}$$

because the probability measure $\mathfrak{a}_\Omega$ (4.7) is translation invariant. Then, for any *regular* sequence $\{\Lambda^{(L)}\}_{L\in\mathbb{N}} \subset \mathcal{P}_f(\mathfrak{L})$ (cf. [20, Remark VI.1.8]), the Ackoglu-Krengel (superadditive) ergodic theorem [20, Theorem VI.1.7, Remark VI.1.8] tells us that, almost surely, the limit

$$\lim_{L\to\infty}\left\{\left|\Lambda^{(L)}\right|^{-1}\mathfrak{F}_\omega\left(\Lambda^{(L)}\right)\right\}$$

exists and, by (4.144), is equal to

$$\lim_{L\to\infty}\left\{\left|\Lambda^{(L)}\right|^{-1}\mathfrak{F}_\omega\left(\Lambda^{(L)}\right)\right\} = \mathbb{E}(\mathfrak{F}_\omega(\{0\})) \ . \tag{4.145}$$

Observe however that $\{\mathfrak{L}\cap(Lb_j)\}_{L\in\mathbb{N}}$ is not a non-decreasing sequence, and is thus a *non-regular* sequence, if $j\neq(0,\ldots,0)$. To overcome this difficulty, we take first the regular sequences $\{\Lambda^{(L,j)}\}_{L\in\mathbb{N}}$ and $\{\tilde{\Lambda}^{(L,j)}\}_{L\in\mathbb{N}}$ defined, for any $L\in\mathbb{N}$ and $j\in\mathcal{D}_n\backslash\{(0,\ldots,0)\}$, by

$$\Lambda^{(L,j)}:=\left\{(x_1,\ldots,x_d)\in\mathfrak{L}\,:\,\forall k\in\{1,\ldots,d\},\ |x_k|\leq L(|j_k|+1/2)n^{-1}+1\right\}$$

and $\tilde{\Lambda}^{(L,j)}:=\Lambda^{(L,j)}\backslash\{\mathfrak{L}\cap(Lb_j)\}$. Notice that $\{\Lambda^{(L,j)}\}_{L\in\mathbb{N}}$ and $\{\tilde{\Lambda}^{(L,j)}\}_{L\in\mathbb{N}}$ are regular sequences for all $j\in\mathcal{D}_n\backslash\{(0,\ldots,0)\}$ because we assumed that n is odd. Note indeed that $\{\mathfrak{L}\cap(Lb_j)\}\subset\Lambda^{(L,j)}$ and hence, for any $j\in\mathcal{D}_n$,

$$\sum_{x\in\mathfrak{L}\cap(Lb_j)}\mathfrak{F}_\omega\left(\{x\}\right)=\sum_{x\in\Lambda^{(L,j)}}\mathfrak{F}_\omega\left(\{x\}\right)-\sum_{x\in\tilde{\Lambda}^{(L,j)}}\mathfrak{F}_\omega\left(\{x\}\right)\ ,$$

see (4.134) and (4.135). Therefore, we apply (4.145) twice to the regular sequences $\{\Lambda^{(L,j)}\}_{L\in\mathbb{N}}$ and $\{\tilde{\Lambda}^{(L,j)}\}_{L\in\mathbb{N}}$, respectively, to get that

$$\lim_{L\to\infty}\left\{\frac{n^d}{L^d}\sum_{x\in\mathfrak{L}\cap(Lb_j)}\sum_{y\in\mathfrak{L}}\int_{\upsilon}^{\beta-\upsilon}\mathfrak{B}^{(\omega)}_{t+i\alpha,\upsilon,\varepsilon}(y,y-e_q,x,x-e_k)\mathrm{d}\alpha\right\}=\mathbb{E}\left(\mathfrak{F}_\omega\left(\{0\}\right)\right) \tag{4.146}$$

for any $j\in\mathcal{D}_n$. Note that we have used here that the intersection of two sets of full measure has of course full measure. In the way one proves Lemma 4.5.10, we obtain

$$\lim_{L\to\infty}\left\{\frac{n^d}{L^d}\sum_{x\in\mathfrak{L}\cap(Lb_j)}\sum_{y\in\mathfrak{L}\backslash\{\mathfrak{L}\cap(Lb_j)\}}\int_{\upsilon}^{\beta-\upsilon}\mathfrak{B}^{(\omega)}_{t+i\alpha,\upsilon,\varepsilon}(y,y-e_q,x,x-e_k)\mathrm{d}\alpha\right\}=0\ .$$

Using this with (4.146) and observing that

$$\mathbb{E}\left(\mathfrak{F}_\omega\left(\{0\}\right)\right)=\sum_{x\in\mathfrak{L}}\mathbb{E}\left(\int_{\upsilon}^{\beta-\upsilon}\mathfrak{B}^{(\omega)}_{t+i\alpha,\upsilon,\varepsilon}(x,x-e_q,0,0-e_k)\mathrm{d}\alpha\right)\ ,$$

we arrive at the assertion for any realization ω within a measurable set

$$\hat{\Omega}_{\upsilon,\varepsilon,n,j,k,q}(t)\equiv\hat{\Omega}^{(\beta,\lambda)}_{\upsilon,\varepsilon,n,j,k,q}(t)\subset\Omega$$

of full measure that still depends on $n\in\mathbb{N}$, $j\in\mathcal{D}_n$, and $k,q\in\{1,-1,\cdots,d,-d\}$. To remove this dependency and obtain the lemma, define

$$\tilde{\Omega}_{\upsilon,\varepsilon}(t):=\bigcap_{n\in\mathbb{N}}\bigcap_{j\in\mathcal{D}_n}\bigcap_{k,q\in\{1,-1,\cdots,d,-d\}}\hat{\Omega}_{\upsilon,\varepsilon,n,j,k,q}(t)$$

and observe that any *countable* intersection of measurable sets of full measure has full measure. □

For all $\varepsilon, \beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$, $\upsilon \in (0, \beta/2)$ and $k, q \in \{1, -1, \cdots, d, -d\}$, define the functions

$$\tilde{\Gamma}_{\upsilon,\varepsilon,k,q}(t) \equiv \tilde{\Gamma}_{\upsilon,\varepsilon,k,q}^{(\beta,\lambda)}(t) = \sum_{x \in \mathfrak{L}} \mathbb{E}\left(\int_{\upsilon}^{\beta-\upsilon} \mathfrak{B}_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(x, x - e_q, 0, -e_k)\mathrm{d}\alpha\right) \tag{4.147}$$

for any $t \in \mathbb{R}$, and

$$\begin{aligned} \mathbf{Y}_{\infty,\upsilon,\varepsilon}(s_1, s_2) \quad := \quad & \sum_{k,q \in \{1,-1,\cdots,d,-d\}} \tilde{\Gamma}_{\upsilon,\varepsilon,k,q}(s_1 - s_2) \\ & \times \int_{\mathbb{R}^d} \left[E_{\mathbf{A}}(s_2, x)\right](e_k) \left[E_{\mathbf{A}}(s_1, x)\right](e_q)\mathrm{d}^d x \end{aligned} \tag{4.148}$$

for any $s_1, s_2 \in \mathbb{R}$. We show next that the function $\mathbf{Y}_{L,\upsilon,\varepsilon,0}^{(\omega)}$ defined by (4.133) almost surely converges to the deterministic function $\mathbf{Y}_{\infty,\upsilon,\varepsilon}$, as $L \to \infty$:

Lemma 4.5.13.
Let $\varepsilon, \beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$, $\upsilon \in (0, \beta/2)$ and $s_1, s_2 \in \mathbb{R}$. Then, there is a measurable subset $\tilde{\Omega}_{\upsilon,\varepsilon}(s_1, s_2) \equiv \tilde{\Omega}_{\upsilon,\varepsilon}^{(\beta,\lambda)}(s_1, s_2) \subset \Omega$ of full measure such that, for any $\mathbf{A} \in \mathbf{C}_0^\infty$ and $\omega \in \tilde{\Omega}_{\upsilon,\varepsilon}(t)$,

$$\lim_{L \to \infty} \mathbf{Y}_{L,\upsilon,\varepsilon,0}^{(\omega)}(s_1, s_2) = \mathbf{Y}_{\infty,\upsilon,\varepsilon}(s_1, s_2) .$$

Proof. Let $\varepsilon, \beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$, $\upsilon \in (0, \beta/2)$, $\mathbf{A} \in \mathbf{C}_0^\infty$ and $s_1, s_2 \in \mathbb{R}$. Using Lemmata 4.5.10-4.5.12 and (4.142), we obtain the existence of a measurable subset $\tilde{\Omega}_{\upsilon,\varepsilon}(s_1, s_2) \equiv \tilde{\Omega}_{\upsilon,\varepsilon}^{(\beta,\lambda)}(s_1, s_2) \subset \Omega$ of full measure such that, for any $\omega \in \tilde{\Omega}_{\upsilon,\varepsilon}(s_1, s_2)$,

$$\begin{aligned} \lim_{L \to \infty} \mathbf{Y}_{L,\upsilon,\varepsilon,0}^{(\omega)}(s_1, s_2) \quad = \quad & \sum_{k,q \in \{1,-1,\cdots,d,-d\}} \tilde{\Gamma}_{\upsilon,\varepsilon,k,q}(s_2 - s_1) \\ & \times \lim_{n \to \infty} \left\{ \frac{1}{n^d} \sum_{j \in \mathcal{D}_n} \left[E_{\mathbf{A}}(s_2, z^{(j)})\right](e_k) \left[E_{\mathbf{A}}(s_1, z^{(j)})\right](e_q) \right\} . \end{aligned}$$

The latter implies the assertion because the term within the limit $n \to \infty$ is a Riemann sum and $E_{\mathbf{A}} \in \mathbf{C}_0^\infty$ for any $\mathbf{A} \in \mathbf{C}_0^\infty$, see (4.139). □

This last limit depends on the two arbitrary parameters $\varepsilon \in \mathbb{R}^+$ and $\upsilon \in (0, \beta/2)$, where $\beta \in \mathbb{R}^+$. Therefore, the next step is to remove this dependency, by considering the limits $\varepsilon \to 0^+$ and $\upsilon \to 0^+$.

As a preliminary, we first observe that the functions $\tilde{\Gamma}_{\upsilon,\varepsilon,k,q}$ (4.147) are approximations of the function $\Gamma_{k,q} \equiv \Gamma_{k,q}^{(\beta,\lambda)}$ defined, for any $\beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$, $k, q \in \{1, -1, \cdots, d, -d\}$ and $t \in \mathbb{R}$, by

$$\Gamma_{k,q}(t) := \lim_{n\to\infty} \frac{1}{|\Lambda_n|} \sum_{x,y\in\Lambda_n} \mathbb{E}\left(\int_0^\beta \mathfrak{C}_{t+i\alpha}^{(\omega)}(x, x-e_q, y, y-e_k)\mathrm{d}\alpha\right) . \quad (4.149)$$

Observe that, for all $x, y \in \mathfrak{L}$, $k, q \in \{1, -1, \cdots, d, -d\}$ and $t \in \mathbb{R}$, the map

$$\omega \mapsto \int_0^\beta \mathfrak{C}_{t+i\alpha}^{(\omega)}(x, x-e_q, y, y-e_k)\mathrm{d}\alpha$$

is bounded and measurable w.r.t. the σ-algebra $\mathfrak{A}_\Omega$. Here, we use the convention for the arguments of $\mathfrak{C}_{t+i\alpha}^{(\omega)}$ as described in (4.143) for $\mathfrak{B}_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}$. Recall also that $\mathbb{E}$ is the expectation value associated with $\mathfrak{a}_\Omega$. This function is well-defined and it is the limit of $\tilde{\Gamma}_{\upsilon,\varepsilon,k,q}$, as $\varepsilon \to 0^+$ and $\upsilon \to 0^+$:

Lemma 4.5.14.
Let $\varepsilon, \beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$ and $k, q \in \{1, -1, \cdots, d, -d\}$. Then $\Gamma_{k,q}(t)$ exists and equals

$$\Gamma_{k,q}(t) = \tilde{\Gamma}_{\upsilon,\varepsilon,k,q}(t) + \mathcal{O}(\upsilon) + \mathcal{O}(\varepsilon) .$$

Proof. Let $\varepsilon, \beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$, $\upsilon \in (0, \beta/2)$, $t \in \mathbb{R}$ and $k, q \in \{1, -1, \cdots, d, -d\}$. Then using similar arguments to the proof of Lemma 4.5.9, one shows that

$$\limsup_{n\to\infty} \frac{1}{|\Lambda_n|} \sum_{x,y\in\Lambda_n} \mathbb{E}\left(\int_\upsilon^{\beta-\upsilon} \Big| \mathfrak{B}_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(x, x-e_q, y, y-e_k) - \mathfrak{C}_{t+i\alpha}^{(\omega)}(x, x-e_q, y, y-e_k) \Big| \mathrm{d}\alpha\right) = \mathcal{O}(\varepsilon)$$

uniformly for any $\upsilon \in (0, \beta/2)$. Moreover, by Lemma 4.3.5 (ii) and the translation invariance of $\mathfrak{a}_\Omega$ observe that

$$\lim_{n\to\infty} \left\{ \frac{1}{|\Lambda_n|} \sum_{x,y\in\Lambda_n} \mathbb{E}\left(\int_\upsilon^{\beta-\upsilon} \mathfrak{B}_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(x, x-e_q, y, y-e_k)\mathrm{d}\alpha\right) - \sum_{x\in\mathfrak{L}} \mathbb{E}\left(\int_\upsilon^{\beta-\upsilon} \mathfrak{B}_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(x, x-e_q, 0, 0-e_k)\mathrm{d}\alpha\right)\right\} = 0 \quad (4.150)$$

for $t \in \mathbb{R}$ and $\upsilon \in (0, \beta/2)$. Then one uses the same arguments as in Lemma 4.5.8 to obtain the assertion, see (4.147) and (4.149). $\square$

We can now consider the limit of the integrand $\mathbf{X}_{L,0}^{(\omega)}$ in (4.126), as $L \to \infty$, see also (4.127). In fact, we show in the theorem below that $\mathbf{X}_{L,0}^{(\omega)}$ converges almost surely to the deterministic function $\mathbf{X}_\infty \equiv \mathbf{X}_\infty^{(\beta,\lambda)}$ defined, for any $\beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$ and $s_1, s_2 \in \mathbb{R}$, by

$$\begin{aligned}\mathbf{X}_\infty(s_1, s_2) \quad := & \sum_{k,q \in \{1,-1,\cdots,d,-d\}} \Gamma_{k,q}(s_2 - s_1) \\ & \times \int_{\mathbb{R}^d} \left[E_{\mathbf{A}}(s_2, x)\right](e_k) \left[E_{\mathbf{A}}(s_1, x)\right](e_q) \mathrm{d}^d x \ . \end{aligned} \quad (4.151)$$

Lemma 4.5.15.
Let $\beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$ and $s_1, s_2 \in \mathbb{R}$. Then there is a measurable subset $\tilde{\Omega}(s_1, s_2) \equiv \tilde{\Omega}^{(\beta,\lambda)}(s_1, s_2) \subset \Omega$ of full measure such that, for any $\mathbf{A} \in \mathbf{C}_0^\infty$ and $\omega \in \tilde{\Omega}(s_1, s_2)$,

$$\lim_{L \to \infty} \mathbf{X}_{L,0}^{(\omega)}(s_1, s_2) = \mathbf{X}_\infty(s_1, s_2) \ .$$

Proof. Fix the parameters $\beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$ and $s_1, s_2 \in \mathbb{R}$. Define also the sequences $\{\upsilon_n\}_{n \in \mathbb{N}}$ and $\{\varepsilon_m\}_{m \in \mathbb{N}}$ by $\upsilon_n := n^{-1}$ and $\varepsilon_m := m^{-1}$ for $n, m \in \mathbb{N}$. Then, by Lemma 4.5.13, for any $n, m \in \mathbb{N}$, there is a measurable subset $\hat{\Omega}_{n,m}(s_1, s_2) \equiv \hat{\Omega}_{n,m}^{(\beta,\lambda)}(s_1, s_2) \subset \Omega$ of full measure such that, for any $\mathbf{A} \in \mathbf{C}_0^\infty$ and $\omega \in \hat{\Omega}_{n,m}(s_1, s_2)$,

$$\lim_{L \to \infty} \mathbf{Y}_{L,\upsilon_n,\varepsilon_m,0}^{(\omega)}(s_1, s_2) = \mathbf{Y}_{\infty,\upsilon_n,\varepsilon_m}(s_1, s_2) \ . \quad (4.152)$$

Thus, we define the subset

$$\tilde{\Omega}(s_1, s_2) := \bigcap_{n,m \in \mathbb{N}} \hat{\Omega}_{n,m}(s_1, s_2) \ . \quad (4.153)$$

It has full measure, since it is a *countable* intersection of measurable sets of full measure. Now, we always assume $\omega \in \tilde{\Omega}(s_1, s_2) \subset \Omega$.

Fix any strictly positive parameter $\epsilon \in \mathbb{R}^+$. Then, by Lemmata 4.5.8, 4.5.9 and 4.5.14, there is $N_\epsilon \in \mathbb{N}$ such that, for all $n, m > N_\epsilon$ and any $L, \beta \in \mathbb{R}^+$, $\omega \in \tilde{\Omega}(s_1, s_2)$ and $\lambda \in \mathbb{R}_0^+$,

$$\left| \mathbf{X}_{L,0}^{(\omega)}(s_1, s_2) - \mathbf{X}_\infty(s_1, s_2) \right| \leq \frac{\epsilon}{2} + \left| \mathbf{Y}_{L,\upsilon_n,\varepsilon_m,0}^{(\omega)}(s_1, s_2) - \mathbf{Y}_{\infty,\upsilon_n,\varepsilon_m}(s_1, s_2) \right| \ .$$

Therefore we prove this theorem by combining the bound above with (4.152)-(4.153) for any realization $\omega \in \tilde{\Omega}\,(s_1, s_2)$. □

In order to obtain the energy increment $\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)}$ given by (4.126) in the limit $(\eta, L^{-1}) \to (0,0)$, we use below Lebesgue's dominated convergence theorem and it is crucial to remove the dependence of the measurable subset $\tilde{\Omega}\,(s_1, s_2)$ on $s_1, s_2 \in \mathbb{R}$, see Lemma 4.5.15. In order to achieve this, we first need to show some uniform boundedness and continuity of the function $\mathbf{X}_{L,0}^{(\omega)}$ defined by (4.127):

Lemma 4.5.16.
Let $T, \beta \in \mathbb{R}^+$ and $\lambda \in \mathbb{R}_0^+$. The family

$$\left\{(s_1, s_2) \mapsto \mathbf{X}_{L,0}^{(\omega)}(s_1, s_2)\right\}_{L\in\mathbb{R}^+,\omega\in\Omega}$$

of maps from $[-T, T] \times [-T, T]$ to $\mathbb{C}$ is uniformly bounded and uniformly continuous.

Proof. The uniform boundedness of this collection of maps is an immediate consequence of (4.130)-(4.131), see (4.127). To prove the uniform continuity on any compact set, it suffices, by Lemmata 4.5.8-4.5.9, to verify that, for any fixed $T, \beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$, $\varepsilon \in \mathbb{R}^+$ and $\upsilon \in (0, \beta/2)$, the family

$$\left\{(s_1, s_2) \mapsto \mathbf{Y}_{L,\upsilon,\varepsilon,0}^{(\omega)}(s_1, s_2)\right\}_{L\in\mathbb{R}^+,\omega\in\Omega}$$

of maps from $[-T, T]$ to $\mathbb{C}$ is uniformly continuous, see (4.133). This property immediately follows from Lemma 4.3.5 (iii). □

Lemma 4.5.15 and Lemma 4.5.16 imply two corollaries: The first one allows us to eliminate the (s_1, s_2)-dependency of the measurable set $\tilde{\Omega}\,(s_1, s_2)$ of Lemma 4.5.15. The second one concerns the continuity of the function $\Gamma_{k,q}$ which is in fact related to a matrix-valued AC-conductivity as explained after Theorem 4.5.19.

Corollary 4.5.17.
Let $\beta \in \mathbb{R}^+$ and $\lambda \in \mathbb{R}_0^+$. Then there is a measurable subset $\tilde{\Omega} \equiv \tilde{\Omega}^{(\beta,\lambda)} \subset \Omega$ of full measure such that, for any $s_1, s_2 \in \mathbb{R}$, $\mathbf{A} \in \mathbf{C}_0^\infty$ and $\omega \in \tilde{\Omega}$,

$$\lim_{L\to\infty} \mathbf{X}_{L,0}^{(\omega)}\,(s_1, s_2) = \mathbf{X}_\infty(s_1, s_2)\,. \tag{4.154}$$

Proof. First, fix $\beta \in \mathbb{R}^+$ and $\lambda \in \mathbb{R}_0^+$. By Lemma 4.5.15, for any $s_1, s_2 \in \mathbb{Q}$, there is a measurable subset $\hat{\Omega}(s_1, s_2) \subset \Omega$ of full measure such that (4.154) holds. Let $\tilde{\Omega}$ be the intersection of all such subsets $\hat{\Omega}(s_1, s_2)$. Since this intersection is countable, $\tilde{\Omega}$ is measurable and has full measure. By Lemma 4.5.16 and the density of $\mathbb{Q}$ in $\mathbb{R}$, it follows that (4.154) holds true for any $s_1, s_2 \in \mathbb{R}$, $\mathbf{A} \in \mathbf{C}_0^\infty$ and $\omega \in \tilde{\Omega}$. □

Corollary 4.5.18.
For any $k, q \in \{1, -1, \cdots, d, -d\}$, the function $\Gamma_{k,q} \equiv \Gamma_{k,q}^{(\beta,\lambda)}$ from $\mathbb{R}$ to $\mathbb{C}$ defined by (4.149) is continuous.

Proof. For each $k, q \in \{1, -1, \cdots, d, -d\}$ and $t \in \mathbb{R}$, choose $\mathbf{A} \in \mathbf{C}_0^\infty$ such that, a fixed neighborhood of t, the map $s \mapsto E_{\mathbf{A}}(s, x)$ is constant for any $x \in \mathbb{R}^d$ and

$$\int_{\mathbb{R}^d} [E_{\mathbf{A}}(t,x)]\,(e_k)\,[E_{\mathbf{A}}(0,x)]\,(e_q)\mathrm{d}^d x \neq 0\ .$$

Then we combine the uniform continuity of the family

$$\left\{ s \mapsto \mathbf{X}_{L,0}^{(\omega)}(s,0) \right\}_{L\in\mathbb{R}^+,\omega\in\Omega}$$

of maps from $\mathbb{R}$ to $\mathbb{C}$ given by Lemma 4.5.16 with Corollary 4.5.17 to show that the function $\Gamma_{k,q}$ is continuous at $t \in \mathbb{R}$ for each $k, q \in \{1, -1, \cdots, d, -d\}$. □

Because of Lemma 4.5.16 and Corollary 4.5.17, we can now use Lebesgue's dominated convergence theorem to get the energy increment $\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)}$ in the limit $(\eta, L^{-1}) \to (0,0)$:

Theorem 4.5.19 (Matrix-valued AC-conductivity)**.**
Let $\beta \in \mathbb{R}^+$ and $\lambda \in \mathbb{R}_0^+$. Then there is a measurable subset $\tilde{\Omega} \equiv \tilde{\Omega}^{(\beta,\lambda)} \subset \Omega$ of full measure such that, for any $t \geq t_1$, $\mathbf{A} \in \mathbf{C}_0^\infty$ and $\omega \in \tilde{\Omega}$,

$$\lim_{(\eta,L^{-1})\to(0,0)} \left\{ \left(\eta^2 L^d\right)^{-1} \mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)} \right\} = \int_{t_0}^{t} \int_{t_0}^{s_1} \mathbf{X}_\infty(s_1, s_2)\mathrm{d}s_2\,\mathrm{d}s_1 \in \mathbb{R}_0^+\ .$$

Proof. Recall (4.126), that is, for any $t \geq t_1$,

$$\left(\eta^2 L^d\right)^{-1} \mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)} = \int_{t_0}^{t} \int_{t_0}^{s_1} \mathbf{X}_{L,0}^{(\omega)}(s_1, s_2)\mathrm{d}s_2\,\mathrm{d}s_1 + \mathcal{O}(\eta)\ .$$

The assertion then follows from Lemma 4.5.16 and Corollary 4.5.17 together with Lebesgue's dominated convergence theorem. Note that $\mathfrak{I}_t^{(\beta,\omega,\lambda,\eta\mathbf{A}_L)} \in \mathbb{R}_0^+$ for all $L \in \mathbb{R}^+$ and sufficiently small $\eta \in \mathbb{R}^+$ because of Corollary 4.4.5. □

Notice at this point that the theorem above together with Equation (4.151) means that the continuous functions $\Gamma_{k,q}$ define the entries of a matrix-valued AC-conductivity. Below we obtain a *scalar* AC-conductivity under the assumption that the probability measure $\mathfrak{a}_\Omega$ is invariant by permutations of the axis, by translations and by reflections.

Indeed, let $\sigma \equiv \sigma^{(\beta,\lambda)}$ be the *deterministic* function defined by

$$\sigma(t) := 4\left(\Gamma_{1,1}(t) - \Gamma_{1,1}(0)\right) \in \mathbb{R}\ , \qquad t \in \mathbb{R}\ , \tag{4.155}$$

and named here the *macroscopic* energy production coefficient. Observe that, by Corollary 4.5.18 and (4.155), for any $\beta \in \mathbb{R}^+$ and $\lambda \in \mathbb{R}_0^+$, $\sigma^{(\beta,\lambda)}$ is a continuous map from $\mathbb{R}$ to $\mathbb{R}$ satisfying $\sigma(0) = 0$. In fact, it is the function appearing in Theorem 4.5.1:

Lemma 4.5.20 (Scalar AC-conductivity)**.**
For any $\beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$ and $\mathbf{A} \in \mathbf{C}_0^\infty$, the (deterministic) function $\mathbf{X}_\infty$ defined by (4.151) equals

$$\mathbf{X}_\infty(s_1,s_2) = \sigma(s_2 - s_1)\int_{\mathbb{R}^d} \langle E_{\mathbf{A}}(s_2,x), E_{\mathbf{A}}(s_1,x)\rangle\, \mathrm{d}^d x\ , \qquad s_1,s_2 \in \mathbb{R}\ .$$

Proof. By (4.7), the probability measure $\mathfrak{a}_\Omega$ is invariant by permutations of the axis and by reflections. Consequently, the functions $\{\Gamma_{k,q}\}_{k,q\in\{1,-1,\cdots,d,-d\}}$ defined by (4.149) satisfy:

$$\Gamma_{k,q}(t) = \Gamma_{q,k}(t)\ ,\ \ \Gamma_{k,k}(t) = \Gamma_{q,q}(t)\ \ \Gamma_{k,k}(t) = \Gamma_{-k,-k}(t)\ ,\ \ \Gamma_{k,-k}(t) = \Gamma_{q,-q}(t)\ , \tag{4.156}$$

for any $k,q \in \{1,-1,\cdots,d,-d\}$ and all $t \in \mathbb{R}$. Straightforward computations using the invariance of $\mathfrak{a}_\Omega$ under translations, reflections and permutations of axes show that the function $\Gamma_{k,q}(t)$ vanishes for all $k,q \in \{1,-1,\cdots,d,-d\}$ with $k \notin \{q,-q\}$ and that

$$\Gamma_{k,k}(t) = -\Gamma_{k,-k}(t)\ . \tag{4.157}$$

Therefore, we deduce from (4.155) that

$$\sigma(t) = 4\left[\Gamma_{1,1}(t) - \Gamma_{1,1}(0)\right] \tag{4.158}$$

for any $t \in \mathbb{R}_0^+$, $\beta \in \mathbb{R}^+$ and $\lambda \in \mathbb{R}_0^+$. Using this together with (4.14), (4.151) and (4.156), we arrive at the assertion. □

Note, that there is an intuitive connection between the (macroscopic) AC-conductivity σ and the microscopic AC-conductivity introduced in Section 4.5.2, which we prove in the following. Therefore, let the averaged microscopic AC-conductivity $\bar{\sigma}_l^{(\omega)}$ in the box Λ_l be defined by

$$\bar{\sigma}_l^{(\omega)}(t) = \frac{4}{|\Lambda_l|} \sum_{x,y\in\Lambda_l} \sigma^{(\omega)}_{(x,x+e_1),(y,y+e_1)}(t) \in \mathbb{R} , \qquad t \in \mathbb{R} , \tag{4.159}$$

for any $l, \beta \in \mathbb{R}^+$, $\omega \in \Omega$ and $\lambda \in \mathbb{R}_0^+$. We show that, at large l, $\bar{\sigma}_l^{(\omega)}$ is the energy production coefficient at macroscopic space scales. Indeed, the pointwise limit $l \to \infty$ of $\bar{\sigma}_l^{(\omega)}$ exists almost surely and it is the deterministic function $\sigma \equiv \sigma^{(\beta,\lambda)}$ defined in (4.155):

Theorem 4.5.21 (Macroscopic AC-conductivity)**.**
Let $\beta \in \mathbb{R}^+$ and $\lambda \in \mathbb{R}_0^+$. Then there is a measurable subset $\tilde{\Omega} \equiv \tilde{\Omega}^{(\beta,\lambda)} \subset \Omega$ of full measure such that, for any $t \in \mathbb{R}$ and $\omega \in \tilde{\Omega}$,

$$\lim_{l\to\infty} \bar{\sigma}_l^{(\omega)}(t) = \sigma(t) \in \mathbb{R} . \tag{4.160}$$

Proof. For any $\beta \in \mathbb{R}^+ \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$ and $\mathbf{x}, \mathbf{y} \in$
fL^2, recall that

$$\sigma^{(\omega)}_{\mathbf{x},\mathbf{y}}(t) = \int_0^\beta \left(\mathfrak{C}^{(\omega)}_{t+i\alpha}(\mathbf{x},\mathbf{y}) - \mathfrak{C}^{(\omega)}_{i\alpha}(\mathbf{x},\mathbf{y}) \right) \mathrm{d}\alpha \in \mathbb{R} , \qquad t \in \mathbb{R} ,$$

see Lemma 4.5.6. Therefore, by (4.159) the pointwise limit of $\bar{\sigma}_l^{(\omega)}$ as $l \to \infty$ follows from Corollary 4.5.17 by taking (smooth approximations of) an electric field $E_{\mathbf{A}}(t,\cdot)$ which is constant in space, supported on the unit box $[-1/2, 1/2]^d$, and such that $[E_{\mathbf{A}}(0,0)]\,(e_k) = 0$ for $k \in \{2, \ldots, d\}$ as well as

$$[E_{\mathbf{A}}(0,0)]\,(e_1)\,[E_{\mathbf{A}}(t,0)]\,(e_1) = 1 .$$

□

Combined with Corollary 4.5.4, Theorem 4.5.21 immediately yields the time-reversal symmetry of the AC-conductivity σ:

Corollary 4.5.22 (Time-reversal symmetry of σ)**.**
For any $\beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$ and $t \in \mathbb{R}$, $\sigma(t) = \sigma(|t|)$.

Thus, Theorem 4.5.1 is a consequence of Corollary 4.5.18, Theorem 4.5.19, Lemma 4.5.20 and Corollary 4.5.22.

4.6 The AC-conductivity measure

In this section we introduce the notion of an *AC-conductivity measure* and show its existence in the model presented here as well as important properties, as the asymptotics for small and large randomness λ and its strict positivity in the case of moderate randomness.

In order to illustrate the physical meaning of our results on the AC-conductivity measure presented below, we first discuss some heuristics: Recall that computations using Drude's model predict that the AC-conductivity $\sigma_{\mathrm{Drude}}(t)$ behaves like

$$D\exp(-\mathrm{T}^{-1}t)\ , \qquad t\in\mathbb{R}_0^+\ ,$$

where $T>0$ is related to the mean time interval between two collisions of a charged carrier with defects in the crystal, whereas $D\in\mathbb{R}^+$ is some positive constant. In particular, for any electromagnetic potential $\mathbf{A}\in\mathbf{C}_0^\infty$, the heat production is in this case equal to

$$D\int_{\mathbb{R}^d}\left[\int_{t_0}^{t}\int_{t_0}^{s_1}\exp\left(-\mathrm{T}^{-1}\left(s_1-s_2\right)\right)\langle E_{\mathbf{A}}(s_1,x),E_{\mathbf{A}}(s_2,x)\rangle\mathrm{d}s_2\mathrm{d}s_1\right]\mathrm{d}^dx \tag{4.161}$$

for any $t\geq t_0$. Then, since $s\mapsto E_{\mathbf{A}}(s,x)$ is smooth and compactly supported for all $x\in\mathbb{R}^d$, we deduce from (4.161) at sufficiently large $t\in\mathbb{R}$ that

$$\begin{aligned}\int_{t_0}^{t}\int_{t_0}^{s_1}&\left[\sigma_{\mathrm{Drude}}(s_1-s_2)\int_{\mathbb{R}^d}\langle E_{\mathbf{A}}(s_1,x),E_{\mathbf{A}}(s_2,x)\rangle\,\mathrm{d}^dx\right]\mathrm{d}s_2\mathrm{d}s_1\\ &=\frac{1}{2}\int_{\mathbb{R}^d}\left[\int_{\mathbb{R}}\langle\hat{E}_{\mathbf{A}}(\nu,x),\hat{E}_{\mathbf{A}}(\nu,x)\rangle\vartheta_{\mathrm{T}}\left(\nu\right)\mathrm{d}\nu\right]\mathrm{d}^dx\ ,\end{aligned}$$

where $\nu\mapsto\hat{E}_{\mathbf{A}}(\nu,x)$ and

$$\nu\mapsto\vartheta_{\mathrm{T}}\left(\nu\right):=\frac{D\sqrt{2}\mathrm{T}}{\pi\left(1+\mathrm{T}^2\nu^2\right)}$$

are the Fourier transforms of the maps

$$s\mapsto E_{\mathbf{A}}(s,x)\qquad\text{and}\qquad s\mapsto\exp\left(-\mathrm{T}^{-1}\left|s\right|\right)\ ,$$

respectively, at any fixed $x\in\mathbb{R}^d$. Thus, the restriction of the (positive) measure $\vartheta_{\mathrm{T}}(\nu)\mathrm{d}\nu$ on $\mathbb{R}\backslash\{0\}$ can be interpreted as the (real part of the) "AC-conductivity measure" of Drude's model. In the limit of the perfect insulator ($\mathrm{T}\rightarrow 0$) and perfect conductor ($\mathrm{T}\rightarrow\infty$) the AC-conductivity measure of Drude's model, as defined above, converges in the weak*-topology to the trivial measure ($0\cdot\mathrm{d}\nu$) on $\mathbb{R}\backslash\{0\}$. The same phenomenology is found in our many-body quantum system.

4.6.1 Derivation of the AC-conductivity measure

In order to derive the AC-conductivity measure, we observe that Theorem 4.5.21 can be combined with Lemma 4.5.5 to prove that the production coefficient σ is - up to a constant - a function of positive type (see, e.g., [33, Section IX.2]):

Theorem 4.6.1.
For any $\beta \in \mathbb{R}^+$ and $\lambda \in \mathbb{R}_0^+$, there is $D \in \mathbb{R}_0^+$ such that $\{\sigma(\mathfrak{t}_i - \mathfrak{t}_j) + D\}_{i,j}$ is a positive matrix on $\mathbb{C}^n$ for each $n \in \mathbb{N}$ and all $(\mathfrak{t}_1, \ldots, \mathfrak{t}_n) \in \mathbb{R}^n$.

Proof. Fix $\beta \in \mathbb{R}^+$ and $\lambda \in \mathbb{R}_0^+$. For any $\omega \in \Omega$ and $l \in \mathbb{R}^+$ define the constant

$$D_l^{(\omega)} := \frac{1}{|\Lambda_l|} (\mathbb{I}_l, \mathbb{I}_l)_\sim \in \mathbb{R}_0^+$$

where $\mathbb{I}_l = \mathbb{I}_l^* \in \mathcal{U}$ is the macroscopic current observable in the box Λ_l defined by

$$\mathbb{I}_l := \sum_{x \in \Lambda_l} I_{(x,x+e_1)} \in \mathcal{U} \tag{4.162}$$

Recall also that $(\cdot, \cdot)_\sim$ is the Duhamel two-point function defined in Lemma 4.5.5. It is a scalar product on the set of self-adjoint elements of $\mathcal{U}$, as discussed after Lemma 4.5.5. Note additionally that we show within the proof of Lemma 4.5.5 that (4.118) can be extended to all $z \in \mathbb{R} + i[0, \beta]$.

Then, using this together with (4.159), (4.12), (4.36) and Lemma 4.5.5, we obtain that, for any $\omega \in \Omega$, $l \in \mathbb{R}^+$, $n \in \mathbb{N}$, $(\mathfrak{t}_1, \ldots, \mathfrak{t}_n) \in \mathbb{R}^n$ and all $(\mathfrak{z}_1, \ldots, \mathfrak{z}_n) \in \mathbb{R}^n$,

$$\begin{aligned}
&\sum_{i,j=1}^{n} \left(\bar{\sigma}_l^{(\omega)}(\mathfrak{t}_i - \mathfrak{t}_j) + D_l^{(\omega)} \right) \mathfrak{z}_j \mathfrak{z}_i \\
&\qquad = \frac{4}{|\Lambda_l|} \left(\sum_{j=1}^{n} \tau_{\mathfrak{t}_j}^{(\omega,\lambda)}(\mathbb{I}_l)\mathfrak{z}_j, \sum_{j=1}^{n} \tau_{\mathfrak{t}_j}^{(\omega,\lambda)}(\mathbb{I}_l)\mathfrak{z}_j \right)_\sim \geq 0 \,.
\end{aligned} \tag{4.163}$$

Note that it suffices to consider n real numbers $\mathfrak{z}_1, \ldots, \mathfrak{z}_n \in \mathbb{R}^n$ instead of complex ones.

From (4.124) observe now that

$$\begin{aligned}
D_l^{(\omega)} &= \frac{1}{|\Lambda_l|} \sum_{x,y \in \Lambda_l} \int_0^\beta \mathfrak{C}_{i\alpha}^{(\omega)}((x, x+e_1), (y, y+e_1)) \mathrm{d}\alpha \\
&\quad - \frac{\beta}{|\Lambda_l|} \sum_{x,y \in \Lambda_l} \mathfrak{C}_0^{(\omega)}((x, x+e_1), (y, y+e_1))
\end{aligned} \tag{4.164}$$

for any $\omega \in \Omega$ and $l \in \mathbb{R}^+$. Thus, in order to compute the limit $l \to \infty$ of the positive constant $D_l^{(\omega)} \in \mathbb{R}_0^+$ we do exactly the same as in the proof of Theorem 4.5.17: One uses approximations like in Lemmata 4.5.8-4.5.9 and 4.5.14 with Lemma 4.3.5 and the Ackoglu-Krengel (superadditive) ergodic theorem [20, Theorem VI.1.7, Remark VI.1.8] to obtain the existence of a measurable subset $\tilde{\Omega} \subset \Omega$ of full measure such that, for all $\omega \in \tilde{\Omega}_1$,

$$\Gamma_{-1,-1}(0) = \lim_{l\to\infty} \frac{1}{|\Lambda_l|} \sum_{x,y\in\Lambda_l} \int_0^\beta \mathfrak{C}_{i\alpha}^{(\omega)}((x, x + e_1), (y, y + e_1))\mathrm{d}\alpha$$

(cf. (4.149)), whereas

$$\lim_{l\to\infty} \frac{\beta}{|\Lambda_l|} \sum_{x,y\in\Lambda_l} \mathfrak{C}_0^{(\omega)}((x, x + e_1), (y, y + e_1))$$
$$= \lim_{l\to\infty} \frac{\beta}{|\Lambda_l|} \sum_{x,y\in\Lambda_l} \mathbb{E}\left(\mathfrak{C}_0^{(\omega)}((x, x + e_1), (y, y + e_1))\right) \in \mathbb{R}$$

for all $\omega \in \tilde{\Omega}_1$. As a consequence, by (4.164), there is a measurable subset $\tilde{\Omega}_1 \subset \Omega$ of full measure such that, for all $\omega \in \tilde{\Omega}_1$,

$$D_\infty := \lim_{l\to\infty} D_l^{(\omega)} \in \mathbb{R}_0^+ \ . \tag{4.165}$$

By Theorem 4.5.21, there is also a measurable subset $\tilde{\Omega}_2 \subset \Omega$ of full measure such that, for all $\omega \in \tilde{\Omega}_2$, the functions $\bar{\sigma}_l^{(\omega)} : \mathbb{R} \to \mathbb{R}$ converge point-wise to σ, as $l \to \infty$. Then the assertion with $D = D_\infty$ follows from (4.163) and (4.165), by using the non-empty measurable subset $\tilde{\Omega} := \tilde{\Omega}_1 \cap \tilde{\Omega}_2$. □

By using $\sigma(0) = 0$ (cf. (4.155)) and Theorem 4.6.1 for $n = 2$, $\mathfrak{t}_1 = t \in \mathbb{R}$ and $\mathfrak{t}_2 = 0$, one obviously obtains:

Corollary 4.6.2.
For any $\beta \in \mathbb{R}^+$ and $\lambda \in \mathbb{R}_0^+$, there is $D \in \mathbb{R}_0^+$ such that $\sigma(t) \in [-2D, 0]$ for all $t \in \mathbb{R}$.

Note that if the constant of Theorem 4.6.1 is zero, i.e., $D = 0$, then clearly $\sigma = 0$.

By Corollary 4.5.18 and (4.155), for any $\beta \in \mathbb{R}^+$ and $\lambda \in \mathbb{R}_0^+$, the non-positive bounded function σ is also continuous. Therefore, we deduce from Theorem 4.6.1 the existence of a non-negative constant $D \in \mathbb{R}_0^+$ such that $(\sigma + D) : \mathbb{R} \to \mathbb{R}$ is a function of positive type. Using Bochner's theorem [33, Theorem IX.9] and the condition $\sigma(0) = 0$, we thus directly obtain the following corollary:

Corollary 4.6.3 (AC-conductivity measure)**.**
For any $\beta \in \mathbb{R}^+$ and $\lambda \in \mathbb{R}_0^+$, there is a positive measure $\mu_\sigma \equiv \mu_\sigma^{(\beta,\lambda)}$ that is finite, i.e., $\mu_\sigma(\mathbb{R}) < \infty$, such that

$$\sigma(t) = \int_{\mathbb{R}} \left(\mathrm{e}^{it\nu} - 1\right) \mathrm{d}\mu_\sigma(\nu) \, , \qquad t \in \mathbb{R} \, .$$

Remark 4.6.4.
It is also possible to obtain the AC-conductivity measure already by the fact that the heat production is positive and $\mathbf{A}$ is compactly supported, see [16] for more details. In this case one uses the Bochner-Schwartz Theorem and obtains the weaker assertion that the measure is of at most polynomial growth.

4.6.2 Asymptotics of the AC-conductivity

In the present section, we study the asymptotics properties of the AC-conductivity $\sigma \equiv \sigma^{(\beta,\lambda)}$ as $\lambda \to 0^+$ and $\lambda \to \infty$, that are summarized in Theorem 4.6.5 below. Physically, the case $\lambda = 0$ can be interpreted as the perfect conductor and the limit $\lambda \to \infty$ corresponds to the perfect insulator. Both cases lead to a vanishing heat production, as will be proved in the following.

Theorem 4.6.5 (AC-conductivity - Asymptotics)**.**
For any $\beta \in \mathbb{R}^+$, $\sigma^{(\beta,\lambda)}(t)$ converges uniformly on compact sets to zero, as $\lambda \to 0^+$. If $\mathfrak{a}_0$ is absolutely continuous w.r.t. the Lebesgue measure, then the same is true for $\lambda \to \infty$. In particular, the AC-conductivity measure $\mu_{\sigma^{(\beta,\lambda)}}$ converges in the weak*-topology to the trivial measure in these two cases.

Proof. The assertion follows from Lemma 4.6.8 and Lemma 4.6.9, that we prove in the following. □

The crucial observation for the proof of Theorem 4.6.5 is that by Lemma 4.5.14 and Equation (4.158), it suffices to obtain the asymptotics of the functions $\tilde{\Gamma}_{\upsilon,\varepsilon,1,1}$ defined for all $\varepsilon, \beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$ and $\upsilon \in (0, \beta/2)$, by (4.147). By (4.150), this functions equals

$$\tilde{\Gamma}_{\upsilon,\varepsilon,1,1}(t) = \lim_{l \to \infty} \frac{1}{|\Lambda_l|} \sum_{x,y \in \Lambda_l} \mathbb{E}\left(\int_\upsilon^{\beta-\upsilon} \mathfrak{B}^{(\omega)}_{t+i\alpha,\upsilon,\varepsilon}(x, x-e_1, y, y-e_1) \mathrm{d}\alpha \right) \tag{4.166}$$

with $\mathfrak{B}_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)} \equiv \mathfrak{B}_{t+i\alpha,\upsilon,\varepsilon}^{(\beta,\omega,\lambda)}$ being defined by (4.132), that is,

$$\mathfrak{B}_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(\mathbf{x},\mathbf{y}) := \frac{1}{4}\sum_{\pi,\pi'\in S_2} \varepsilon_\pi \varepsilon_{\pi'} B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(y^{\pi'(1)}, x^{\pi(1)}) \times B_{-t+i(\beta-\alpha),\upsilon,\varepsilon}^{(\omega)}(x^{\pi(2)}, y^{\pi'(2)})$$

for any $\omega \in \Omega$, $\mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2$ and $\mathbf{y} := (y^{(1)}, y^{(2)}) \in \mathfrak{L}^2$.

Note furthermore that $B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}$ is given by (4.71), that is,

$$B_{t+i\alpha,\upsilon,\varepsilon}^{(\omega)}(\mathbf{x}) = \int_{|\nu|<M_{\beta,\upsilon,\varepsilon}} \hat{F}_\alpha^\beta(\nu)\, \langle \mathfrak{e}_{x^{(2)}}, \mathrm{e}^{-i(t-\nu)(\Delta_{\mathrm{d}}+\lambda V_\omega)} \mathfrak{e}_{x^{(1)}} \rangle \mathrm{d}\nu \qquad (4.167)$$

for all $\mathbf{x} \in \mathfrak{L}^2$. Here, $M_{\beta,\upsilon,\varepsilon}$ is a constant only depending on $\beta, \upsilon, \varepsilon$. To analyze the asymptotics $\lambda \to 0^+$ and $\lambda \to \infty$ we use the finite sum approximation

$$\xi_{\nu,t,N}^{(\omega,\lambda)} := \mathrm{e}^{-i(t-\nu)\lambda V_\omega} + \sum_{n=1}^{N-1} (-i)^n \int_\nu^t \mathrm{d}\nu_1 \cdots \int_\nu^{\nu_{n-1}} \mathrm{d}\nu_n \, \mathrm{e}^{-i(t-\nu_1)\lambda V_\omega} \Delta_{\mathrm{d}} \times \mathrm{e}^{-i(\nu_1-\nu_2)\lambda V_\omega} \Delta_{\mathrm{d}} \mathrm{e}^{-i(\nu_2-\nu_3)\lambda V_\omega} \cdots \mathrm{e}^{-i(\nu_{n-1}-\nu_n)\lambda V_\omega} \Delta_{\mathrm{d}} \mathrm{e}^{-i(\nu_n-\nu)\lambda V_\omega}$$

of the unitary operator $\mathrm{e}^{-i(t-\nu)(\Delta_{\mathrm{d}}+\lambda V_\omega)}$ for any $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $N \in \mathbb{N}$ and $\nu, t \in \mathbb{R}$. Indeed, using Duhamel's formula one gets that

$$\lim_{N\to\infty} \left\| \xi_{\nu,t,N}^{(\omega,\lambda)} - \mathrm{e}^{-i(t-\nu)(\Delta_{\mathrm{d}}+\lambda V_\omega)} \right\|_{\mathrm{op}} = 0 \qquad (4.168)$$

uniformly for $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $\nu \in [-M_{\beta,\upsilon,\varepsilon}, M_{\beta,\upsilon,\varepsilon}]$ and $t \in [-T, T]$, where $T \in \mathbb{R}^+$ is arbitrarily but fixed. Hence, we replace $\mathrm{e}^{-i(t-\nu)(\Delta_{\mathrm{d}}+\lambda V_\omega)}$ by its approximation $\xi_{\nu,t,N}^{(\omega,\lambda)}$ in (4.167) and define

$$\tilde{B}_{t+i\alpha,\upsilon,\varepsilon,N}^{(\omega,\lambda)}(\mathbf{x}) := \int_{|\nu|<M_{\beta,\upsilon,\varepsilon}} \hat{F}_\alpha^\beta(\nu)\, \langle \mathfrak{e}_{x^{(2)}}, \xi_{\nu,t,N}^{(\omega,\lambda)} \mathfrak{e}_{x^{(1)}} \rangle \mathrm{d}\nu \qquad (4.169)$$

and

$$\tilde{\mathfrak{B}}_{t+i\alpha,\upsilon,\varepsilon,N}^{(\omega,\lambda)}(\mathbf{x},\mathbf{y}) := \frac{1}{4}\sum_{\pi,\pi'\in S_2} \varepsilon_\pi \varepsilon_{\pi'} \tilde{B}_{t+i\alpha,\upsilon,\varepsilon,N}^{(\omega)}(y^{\pi'(1)}, x^{\pi(1)}) \times \tilde{B}_{-t+i(\beta-\alpha),\upsilon,\varepsilon,N}^{(\omega)}(x^{\pi(2)}, y^{\pi'(2)})$$

for any $\varepsilon, \beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$ and $\mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2$ and $\mathbf{y} := (y^{(1)}, y^{(2)}) \in \mathfrak{L}^2$. Indeed, one has:

Lemma 4.6.6.
Let $\varepsilon, \beta \in \mathbb{R}^+$, $t \in \mathbb{R}$ and $\upsilon \in (0, \beta/2)$. Then,

$$\lim_{N\to\infty} \frac{1}{|\Lambda_l|} \sum_{x,y\in\Lambda_l} \int_{\upsilon}^{\beta-\upsilon} \Big| \mathfrak{B}^{(\omega)}_{t+i\alpha,\upsilon,\varepsilon}(x, x-e_1, y, y-e_1) \\ - \tilde{\mathfrak{B}}^{(\omega,\lambda)}_{t+i\alpha,\upsilon,\varepsilon,N}(x, x-e_1, y, y-e_1) \Big| \mathrm{d}\alpha = 0$$

uniformly for $l \in \mathbb{R}^+$, $\omega \in \Omega$ and $\lambda \in \mathbb{R}_0^+$.

Proof. The map $(\alpha, \nu) \mapsto \hat{F}^{\beta}_{\alpha}(\nu)$ is absolutely integrable in $(\alpha, \nu) \in [\upsilon, \beta-\upsilon] \times [-M_{\beta,\upsilon,\varepsilon}, M_{\beta,\upsilon,\varepsilon}]$ for any $\varepsilon, \beta \in \mathbb{R}^+$ and $\upsilon \in (0, \beta/2)$. Therefore, the assertion is directly proven by using (4.168) to compute the difference between (4.167) and (4.169). □

As a consequence, we only need to study, for any $\varepsilon, \beta \in \mathbb{R}^+$, $\upsilon \in (0, \beta/2)$, and $l, N \in \mathbb{N}$, the asymptotics of the function

$$\mathfrak{q}^{(\beta,\omega,\lambda)}_{\upsilon,\varepsilon,N,l}(t) := \frac{1}{|\Lambda_l|} \sum_{x,y\in\Lambda_l} \mathbb{E}\left(\int_{\upsilon}^{\beta-\upsilon} \tilde{\mathfrak{B}}^{(\omega,\lambda)}_{t+i\alpha,\upsilon,\varepsilon,N}(x, x-e_1, y, y-e_1)\mathrm{d}\alpha \right),$$

as $\lambda \to 0^+$ and $\lambda \to \infty$.

Lemma 4.6.7.
Let $\varepsilon, \beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$, $\upsilon \in (0, \beta/2)$, and $N \in \mathbb{N}$. Then,

$$\lim_{\lambda\to 0} \mathbb{E}\left(\mathfrak{q}^{(\beta,\omega,\lambda)}_{\upsilon,\varepsilon,N,l}(t) \right) = \mathbb{E}\left(\mathfrak{q}^{(\beta,\omega,0)}_{\upsilon,\varepsilon,N,l}(t) \right)$$

uniformly for all $l \in \mathbb{R}^+$. If the probability measure $\mathfrak{a}_0$ is additionally absolutely continuous w.r.t. the Lebesgue measure, then

$$\lim_{\lambda\to\infty} \mathbb{E}\left(\mathfrak{q}^{(\beta,\omega,\lambda)}_{\upsilon,\varepsilon,N,l}(t) \right) = 0$$

uniformly for all $l \in \mathbb{R}^+$.

Proof. The function $\mathfrak{q}_{\upsilon,\varepsilon,N,l}^{(\beta,\omega,\lambda)}(t)$ is a finite sum of terms of the form

$$\frac{(-i)^{n_1+n_2}}{4}\sum_{x,y\in\Lambda_l}\sum_{\pi,\pi'\in S_2}\varepsilon_\pi\varepsilon_{\pi'}\int_\upsilon^{\beta-\upsilon}\mathrm{d}\alpha\int_{|\nu|<M_{\beta,\upsilon,\varepsilon}}\mathrm{d}\nu\int_{|u|<M_{\beta,\upsilon,\varepsilon}}\mathrm{d}u$$
$$\int_\nu^t\mathrm{d}\nu_1\cdots\int_\nu^{\nu_{n_1-1}}\mathrm{d}\nu_{n_1}\int_u^{-t}\mathrm{d}u_1\cdots\int_u^{u_{n_2-1}}\mathrm{d}u_{n_2}\hat{F}_\alpha^\beta(\nu)\,\hat{F}_{\beta-\alpha}^\beta(u)$$
$$\left\langle\mathfrak{e}_{x_{\pi(1)}},\mathrm{e}^{-i(t-\nu_1)\lambda V_\omega}\Delta_{\mathrm{d}}\mathrm{e}^{-i(\nu_1-\nu_2)\lambda V_\omega}\cdots\mathrm{e}^{-i\left(\nu_{n_1-1}-\nu_{n_1}\right)\lambda V_\omega}\Delta_{\mathrm{d}}\mathrm{e}^{-i(\nu_{n_1}-\nu)\lambda V_\omega}\mathfrak{e}_{y_{\pi'(1)}}\right\rangle$$
$$\times\left\langle\mathfrak{e}_{y_{\pi'(2)}},\mathrm{e}^{-i(-t-u_1)\lambda V_\omega}\Delta_{\mathrm{d}}\mathrm{e}^{-i(u_1-u_2)\lambda V_\omega}\cdots\mathrm{e}^{i\left(u_{n_2-1}-u_{n_2}\right)\lambda V_\omega}\Delta_{\mathrm{d}}\mathrm{e}^{-i(u_{n_2}-u)\lambda V_\omega}\mathfrak{e}_{x_{\pi(2)}}\right\rangle$$

for $n_1,n_2\in\mathbb{N}_0$. Here, $(x_1,x_2):=(x,x-e_1)$, $(y_1,y_2):=(y,y-e_1)$. From this and the translation invariance of the probability measure $\mathfrak{a}_\Omega$, we get that $\mathbb{E}(\mathfrak{q}_{\upsilon,\varepsilon,N,l}^{(\beta,\omega,\lambda)}(t))$ is a finite sum of terms of the form

$$\frac{(-i)^{n_1+n_2}}{4\,|\Lambda_l|}\sum_{x\in\mathfrak{L}}\sum_{\pi,\pi'\in S_2}\varepsilon_\pi\varepsilon_{\pi'}\int_\upsilon^{\beta-\upsilon}\mathrm{d}\alpha\int_{|\nu|<M_{\beta,\upsilon,\varepsilon}}\mathrm{d}\nu\int_{|u|<M_{\beta,\upsilon,\varepsilon}}\mathrm{d}u \tag{4.170}$$
$$\int_\nu^t\mathrm{d}\nu_1\cdots\int_\nu^{\nu_{n_1-1}}\mathrm{d}\nu_{n_1}\int_u^{-t}\mathrm{d}u_1\cdots\int_u^{u_{n_2-1}}\mathrm{d}u_{n_2}\hat{F}_\alpha^\beta(\nu)\,\hat{F}_{\beta-\alpha}^\beta(u)\,\mathbf{1}[x\in\Lambda_l]$$
$$\mathbb{E}\left(\left\langle\mathfrak{e}_{x_{\pi(1)}},\mathrm{e}^{-i(t-\nu_1)\lambda V_\omega}\Delta_{\mathrm{d}}\mathrm{e}^{-i(\nu_1-\nu_2)\lambda V_\omega}\cdots\Delta_{\mathrm{d}}\mathrm{e}^{-i(\nu_{n_1}-\nu)\lambda V_\omega}\mathfrak{e}_{y_{\pi'(1)}}\right\rangle\right.$$
$$\left.\times\left\langle\mathfrak{e}_{y_{\pi'(2)}},\mathrm{e}^{-i(-t-u_1)\lambda V_\omega}\Delta_{\mathrm{d}}\mathrm{e}^{-i(u_1-u_2)\lambda V_\omega}\cdots\Delta_{\mathrm{d}}\mathrm{e}^{-i(u_{n_2}-u)\lambda V_\omega}\mathfrak{e}_{x_{\pi(2)}}\right\rangle\right)\ ,$$

where $(x_1,x_2):=(x,x-e_1)$, $(y_1,y_2):=(0,-e_1)$. Note that

$$\int_\upsilon^{\beta-\upsilon}\mathrm{d}\alpha\int_{|\nu|<M_{\beta,\upsilon,\varepsilon}}\mathrm{d}\nu\int_{|u|<M_{\beta,\upsilon,\varepsilon}}\mathrm{d}u\left|\hat{F}_\alpha^\beta(\nu)\,\hat{F}_{\beta-\alpha}^\beta(u)\right|<\infty$$

and the volume of integration in (4.170) of the ν_a- and u_b-integrals, $a=1,\ldots,n_1$, $b=1,\ldots,n_2$, gives a factor $\frac{|t-\nu|^{n_1}|t+u|^{n_2}}{n_1!n_2!}$. By developing the Laplacians Δ_{d}, note that, whenever $t\neq\nu$, $t\neq-u$,

$$\mathbf{1}[x\in\Lambda_l]\mathbb{E}\left(\left\langle\mathfrak{e}_{x_{\pi(1)}},\mathrm{e}^{-i(t-\nu_1)\lambda V_\omega}\Delta_{\mathrm{d}}\mathrm{e}^{-i(\nu_1-\nu_2)\lambda V_\omega}\cdots\Delta_{\mathrm{d}}\mathrm{e}^{-i(\nu_{n_1}-\nu)\lambda V_\omega}\mathfrak{e}_{y_{\pi'(1)}}\right\rangle\right.$$
$$\left.\times\left\langle\mathfrak{e}_{y_{\pi'(2)}},\mathrm{e}^{-i(-t-u_1)\lambda V_\omega}\Delta_{\mathrm{d}}\mathrm{e}^{-i(u_1-u_2)\lambda V_\omega}\cdots\Delta_{\mathrm{d}}\mathrm{e}^{-i(u_{n_2}-u)\lambda V_\omega}\mathfrak{e}_{x_{\pi(2)}}\right\rangle\right)$$

is a sum of $(2d+1)^{n_1+n_2}$ terms of the form (up to constants bounded in absolut value by $(2d)^{n_1+n_2}$)

$$\mathbf{1}[x\in\Lambda_l]\mathbb{E}\left(\mathrm{e}^{\pm it_1\lambda V_\omega(x_1)}\cdots\mathrm{e}^{\pm it_n\lambda V_\omega(x_n)}\right) \tag{4.171}$$

with $n \in \mathbb{N}$, $n \leq n_1 + n_2$, and where $\mathfrak{t}_1, \ldots, \mathfrak{t}_n \in \mathbb{R}^+$ and $x_1, \ldots, x_n \in \mathfrak{L}$ with $x_j \neq x_p$ for $j \neq p$. By Lebesgue's dominated convergence theorem, it suffices to analyze (4.171) either in the limit $\lambda \to \infty$ or $\lambda \to 0^+$. By (4.7),

$$\mathbb{E}\left(\mathrm{e}^{\pm i\mathfrak{t}_1\lambda V_\omega(x_1)} \cdots \mathrm{e}^{\pm i\mathfrak{t}_n\lambda V_\omega(x_n)}\right) = \mathbb{E}\left(\mathrm{e}^{\pm i\mathfrak{t}_1\lambda V_\omega(x_1)}\right) \cdots \mathbb{E}\left(\mathrm{e}^{\pm i\mathfrak{t}_n\lambda V_\omega(x_n)}\right) \qquad (4.172)$$

for any $n \in \mathbb{N}$, $\mathfrak{t}_1, \ldots, \mathfrak{t}_n \in \mathbb{R}^+$ and $x_1, \ldots, x_n \in \mathfrak{L}$ with $x_j \neq x_p$ for $j \neq p$. Since

$$\lim_{\lambda \to 0} \mathbb{E}\left(\mathrm{e}^{\pm i\mathfrak{t}\lambda V_\omega(x)}\right) = 1$$

for all $x \in \mathfrak{L}$ and $\mathfrak{t} \in \mathbb{R}^+$, we deduce from (4.172) that

$$\lim_{\lambda \to 0} \mathbb{E}\left(\mathrm{e}^{\pm i\mathfrak{t}_1\lambda V_\omega(x_1)} \cdots \mathrm{e}^{\pm i\mathfrak{t}_n\lambda V_\omega(x_n)}\right) = 1 \ .$$

and one gets the first assertion of the lemma by Lebesgue's dominated convergence theorem.

If the probability measure $\mathfrak{a}_0$ is in addition absolutely continuous w.r.t. the Lebesgue measure, then from the Riemann-Lebesgue lemma we have the limit

$$\lim_{\lambda \to \infty} \mathbb{E}\left(\mathrm{e}^{\pm i\mathfrak{t}\lambda V_\omega(x)}\right) = 0$$

for all $x \in \mathfrak{L}$ and $\mathfrak{t} \in \mathbb{R}^+$. From (4.172), we then obtain that

$$\lim_{\lambda \to \infty} \mathbb{E}\left(\mathbf{1}[x \in \Lambda_l]\mathrm{e}^{\pm i\mathfrak{t}_1\lambda V_\omega(x_1)} \cdots \mathrm{e}^{\pm i\mathfrak{t}_n\lambda V_\omega(x_n)}\right) = 0$$

uniformly for all $l \in \mathbb{R}^+$. Using this and Lebesgue's dominated convergence theorem, one thus gets the second assertion. $\square$

We are now in position to compute the asymptotics, as $\lambda \to 0^+$ and $\lambda \to \infty$, of the AC-conductivity $\sigma \equiv \sigma^{(\beta,\lambda)}$, which is defined by (4.158).

Lemma 4.6.8.
Let $\beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$ and $t \in \mathbb{R}$. Then,

$$\lim_{\lambda \to 0} \sigma^{(\beta,\lambda)}(t) = \sigma^{(\beta,0)}(t) \ .$$

If additionally the probability measure $\mathfrak{a}_0$ is absolutely continuous w.r.t. the Lebesgue measure, then

$$\lim_{\lambda \to \infty} \sigma^{(\beta,\lambda)}(t) = 0 \ .$$

Proof. Let $\beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$ and $t \in \mathbb{R}$. By Lemmata 4.6.6 and 4.6.7, one gets that

$$\lim_{\lambda\to 0} \frac{1}{|\Lambda_l|} \sum_{x,y\in\Lambda_l} \mathbb{E}\left(\int_{\upsilon}^{\beta-\upsilon} \mathfrak{B}_{t+i\alpha,\upsilon,\varepsilon}^{(\beta,\omega,\lambda)}(x, x-e_1, y, y-e_1)\mathrm{d}\alpha \right)$$
$$= \frac{1}{|\Lambda_l|} \sum_{x,y\in\Lambda_l} \mathbb{E}\left(\int_{\upsilon}^{\beta-\upsilon} \mathfrak{B}_{t+i\alpha,\upsilon,\varepsilon}^{(\beta,\omega,0)}(x, x-e_1, y, y-e_1)\mathrm{d}\alpha \right)$$

uniformly for all $l \in \mathbb{R}^+$, whereas

$$\lim_{\lambda\to \infty} \frac{1}{|\Lambda_l|} \sum_{x,y\in\Lambda_l} \mathbb{E}\left(\int_{\upsilon}^{\beta-\upsilon} \mathfrak{B}_{t+i\alpha,\upsilon,\varepsilon}^{(\beta,\omega,\lambda)}(x, x-e_1, y, y-e_1)\mathrm{d}\alpha \right) = 0$$

provided the probability measure $\mathfrak{a}_0$ is absolutely continuous w.r.t. the Lebesgue measure. Therefore, by using these limits together with Lemma 4.5.14, (4.158) and (4.166) we arrive at the assertions. □

Finally, to get Theorem 4.6.5, we need to compute explicitly the macroscopic AC-conductivity $\sigma^{(\beta,\lambda)}$ at $\lambda = 0$. This is done in the next lemma:

Lemma 4.6.9 (AC-conductivity at constant potential)**.**
For any $\beta \in \mathbb{R}^+$ and $t \in \mathbb{R}$, $\sigma^{(\beta,0)}(t) = 0$.

Proof. Let $\beta \in \mathbb{R}^+$. By (4.159), Lemma 4.5.6 and Theorem 4.5.21, note that

$$\sigma^{(\beta,0)}(t) = \lim_{l\to\infty} \frac{4}{|\Lambda_l|} \sum_{x,y\in\Lambda_l} \int_0^{\beta} \left(\mathfrak{D}_{t+i\alpha}(x,y) - \mathfrak{D}_{i\alpha}(x,y)\right) \mathrm{d}\alpha \,, \tag{4.173}$$

where

$$\mathfrak{D}_{t+i\alpha}(x,y) := \mathfrak{C}_{t+i\alpha}^{(\beta,\omega,0)}(x, x-e_1, y, y-e_1).$$

Observe also that $\mathfrak{C}_{t+i\alpha}^{(\beta,\omega,0)}$, which is defined by (4.119), does not depend on $\omega \in \Omega$. Explicit computations show that $\mathfrak{D}_{t+i\alpha}(x,y)$ equals

$$\begin{aligned} \mathfrak{D}_{t+i\alpha}(x,y) \;\; = \;\; & \frac{1}{2(2\pi)^{2d}} \int_{[-\pi,\pi]^d} \mathrm{d}^d p \int_{[-\pi,\pi]^d} \mathrm{d}^d p' \frac{\mathrm{e}^{\beta E_{p'}} \mathrm{e}^{(\alpha - it)\left(E_p - E_{p'}\right)}}{\left(1+\mathrm{e}^{\beta E_p}\right)\left(1+\mathrm{e}^{\beta E_{p'}}\right)} \\ & \times \left(1 - \cos\left(p_1 - p_1'\right)\right) \mathrm{e}^{i(p+p')\cdot(x-y)} \end{aligned}$$

for any $t \in \mathbb{R}$, $\alpha \in [0, \beta]$ and $x, y \in \mathfrak{L}$, with E_p being the dispersion relation of Δ_{d}, that is,

$$E_p := 2\left[d - (\cos(p_1) + \cdots + \cos(p_d))\right] \ , \qquad p \in [-\pi, \pi]^d \ , \tag{4.174}$$

Since $E_p = E_{-p}$, it follows that

$$\int_0^\beta \mathfrak{D}_{t+i\alpha}(x, y)\mathrm{d}\alpha = \int_{[-\pi,\pi]^d} \mathfrak{d}_t\left(p\right) \mathrm{e}^{ip\cdot(x-y)}\mathrm{d}^d p \tag{4.175}$$

for all $t \in \mathbb{R}$ and $x, y \in \mathfrak{L}$, with $\mathfrak{d}_t$ being the function defined on $[-\pi, \pi]^d$ by

$$\begin{aligned} \mathfrak{d}_t\left(p\right) \ := \ & \frac{1}{2(2\pi)^{2d}} \int_{[-\pi,\pi]^d} \mathrm{d}^d p' \frac{\mathrm{e}^{\beta E_{p'+\frac{p}{2}}} \mathrm{e}^{-it\left(E_{p'-\frac{p}{2}} - E_{p'+\frac{p}{2}}\right)}}{\left(1 + \mathrm{e}^{\beta E_{p'-\frac{p}{2}}}\right)\left(1 + \mathrm{e}^{\beta E_{p'+\frac{p}{2}}}\right)} \\ & \times \frac{\left(\mathrm{e}^{\beta\left(E_{p'-\frac{p}{2}} - E_{p'+\frac{p}{2}}\right)} - 1\right)}{\left(E_{p'-\frac{p}{2}} - E_{p'+\frac{p}{2}}\right)} \left(1 - \cos\left(2p_1'\right)\right) \ . \end{aligned}$$

Consequently, using (4.175) one gets, for any $l \in \mathbb{R}^+$ and $t \in \mathbb{R}$, the equality

$$\frac{1}{|\Lambda_l|} \sum_{x,y\in\Lambda_l} \int_0^\beta \mathfrak{D}_{t+i\alpha}(x, y)\mathrm{d}\alpha = \int_{[-\pi,\pi]^d} \gamma_l\left(p\right) \mathfrak{d}_t\left(p\right) \mathrm{d}^d p \ , \tag{4.176}$$

where the function γ_l is defined on $[-\pi, \pi]^d$ by

$$\gamma_l\left(p\right) := \left| \frac{1}{|\Lambda_l|^{1/2}} \sum_{x\in\Lambda_l} \mathrm{e}^{ip\cdot x} \right|^2 = \frac{1}{|\Lambda_l|} \sum_{x,y\in\Lambda_l} \mathrm{e}^{ip\cdot(x-y)} \ .$$

Observe that, for any $l \in \mathbb{R}^+$ and all $\varepsilon \in \mathbb{R}^+$,

$$\int_{[-\pi,\pi]^d} \gamma_l\left(p\right) \mathrm{d}^d p = 1 \qquad \text{and} \qquad \lim_{l\to\infty} \int_{[-\pi,\pi]^d\backslash\mathcal{B}(0,\varepsilon)} \gamma_l\left(p\right) \mathrm{d}^d p = 0 \ ,$$

where $\mathcal{B}\left(0, \varepsilon\right) \subset \mathbb{R}^d$ is the ball of radius ε centered at 0. From this we infer that

$$\lim_{l\to\infty} \left| \int_{[-\pi,\pi]^d} \gamma_l\left(p\right) \mathfrak{d}_t\left(p\right) \mathrm{d}^d p - \int_{\mathcal{B}(0,\varepsilon)} \gamma_l\left(p\right) \mathfrak{d}_t\left(p\right) \mathrm{d}^d p \right| = 0 \tag{4.177}$$

for all $\varepsilon \in \mathbb{R}^+$ and any $t \in \mathbb{R}$. Meanwhile, remark that

$$\mathfrak{d}_t(p) - \mathfrak{d}_0(p) = \mathcal{O}(|tp|) \ .$$

Then, using the continuity of the function $\mathfrak{d}_0(\cdot)$ together with (4.173), (4.176) and (4.177), it follows that $\sigma^{(\beta,0)}(t) = 0$ for all $t \in \mathbb{R}$. □

Therefore, Theorem 4.6.5 follows from Lemma 4.6.8 and Lemma 4.6.9.

4.6.3 On the strict positivity of the heat production

In this subsection we show, that the heat production is in general strictly positive. By Theorem 4.5.1, the fermion system cannot transfer any energy to the electromagnetic field, as expected. This is not so, because $\mu_{\sigma^{(\beta,\lambda)}}$ is the trivial measure $\mu_{\sigma^{(\beta,\lambda)}}(\mathbb{R}\backslash\{0\}) \equiv 0$ for any choice of β, λ. In fact, the fermion system generally absorbs some non-vanishing amount of electromagnetic energy:

Theorem 4.6.10 (Absorption of electromagnetic energy)**.**
There are $\beta_0, \lambda_0 \in \mathbb{R}^+$ and a meager set $\mathcal{Z} \subset \mathbf{C}_0^\infty$ such that, for any $\beta \in (0, \beta_0)$, $\lambda \in (\lambda_0/2, \lambda_0)$, all $\mathbf{A} \in \mathbf{C}_0^\infty \backslash \mathcal{Z}$ and every $t \geq t_1$, the AC-conductivity $\sigma \in C(\mathbb{R}, \mathbb{R}_0^+)$ defined in Theorem 4.5.1 satisfies

$$\int_{t_0}^{t} \int_{t_0}^{s_1} \left[\sigma(s_1 - s_2) \int_{\mathbb{R}^d} \langle E_{\mathbf{A}}(s_1, x), E_{\mathbf{A}}(s_2, x) \rangle \, \mathrm{d}^d x \right] \mathrm{d}s_2 \mathrm{d}s_1 > 0 \ .$$

Here, $\mathbf{C}_0^\infty$ is seen as a subspace of the Fréchet space $\mathcal{S}(\mathbb{R}^d)$ (space of Schwartz functions $\mathbb{R}^d \to \mathbb{R}^d$) endowed with the corresponding relative topology.

Proof. Use Lemmata 4.6.11 and 4.6.12. □

To prove Theorem 4.6.10 we expand the AC-conductivity σ at $\beta, \lambda, t = 0$. Then we show that the behavior of σ near this point implies strict positivity of the heat production, at least for short pulses of the electric field and small $\beta, \lambda > 0$. This result corresponds to Lemma 4.6.11. The latter can, at small $\beta, \lambda > 0$, be extended by an analyticity argument to all electric fields outside a meager[2] set, this will be done in Lemma 4.6.12.

[2]in the sense of the usual metric of the space of Schwartz functions.

Lemma 4.6.11.
Let $\mathbf{A} \in \mathbf{C}_0^\infty \backslash \{0\}$ be such that, for some $k \in \{1, \ldots, d\}$,

$$\int_{\mathbb{R}^d} \left(\int_{\mathbb{R}} s E_{\mathbf{A}}(s,x)\,(e_k)\,\mathrm{d}s \right)^2 \mathrm{d}^d x > 0$$

and define, for all $T \in \mathbb{R}^+$, the time-rescaled potential

$$\mathbf{A}^{(T)}(t,x) := \mathbf{A}(T^{-1}t, x) \ , \quad t \in \mathbb{R},\ x \in \mathbb{R}^d \ .$$

There are $\beta_0, \lambda_0, T_0 \in \mathbb{R}^+$ such that, for $\beta \in (0, \beta_0)$, $\lambda \in (\lambda_0/2, \lambda_0)$ and $T \in (T_0/2, T_0)$, the AC-conductivity $\sigma \in C(\mathbb{R};\mathbb{R})$ defined in Theorem 4.5.1 satisfies

$$\int_{t_0}^{t} \int_{t_0}^{s_1} \left[\sigma(s_2 - s_1) \int_{\mathbb{R}^d} \langle E_{\mathbf{A}^{(T)}}(s_1,x), E_{\mathbf{A}^{(T)}}(s_2,x) \rangle \,\mathrm{d}^d x \right] \mathrm{d}s_1 \mathrm{d}s_2 > 0$$

for all $t \geq T t_1$.

Proof. Recall (4.119), (4.149) and (4.158), that are, respectively,

$$\mathfrak{C}_{t+i\alpha}^{(\omega)}(\mathbf{x},\mathbf{y}) := \frac{1}{4} \sum_{\pi,\pi' \in S_2} \varepsilon_\pi \varepsilon_{\pi'} C_{t+i\alpha}^{(\omega)}(y^{\pi'(1)}, x^{\pi(1)}) C_{-t+i(\beta-\alpha)}^{(\omega)}(x^{\pi(2)}, y^{\pi'(2)})$$

for any $\mathbf{x} := (x^{(1)}, x^{(2)}), \mathbf{y} := (y^{(1)}, y^{(2)}) \in \mathfrak{L}^2$,

$$\Gamma_{1,1}(t) := \lim_{l \to \infty} \frac{1}{|\Lambda_l|} \sum_{x,y \in \Lambda_l} \mathbb{E} \left(\int_0^\beta \mathfrak{C}_{t+i\alpha}^{(\omega)}(x, x-e_1, y, y-e_1) \mathrm{d}\alpha \right) \tag{4.178}$$

and

$$\sigma(t) = 4(\Gamma_{1,1}(t) - \Gamma_{1,1}(0)) \tag{4.179}$$

for any $\beta \in \mathbb{R}^+$, $\lambda \in \mathbb{R}_0^+$ and $t \in \mathbb{R}$. In the first equation, $\pi, \pi' \in S_2$ are, by definition, permutations of the elements $\{1, 2\}$ with signatures $\varepsilon_\pi, \varepsilon_{\pi'} \in \{-1, 1\}$. $C_{t+i\alpha}^{(\omega)} \equiv C_{t+i\alpha}^{(\beta,\omega,\lambda)}$ is the complex-time two-point correlation function (4.39). It is equal to (4.66), that is, for all $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$ and $\alpha \in [0, \beta]$,

$$C_{t+i\alpha}^{(\omega)}(\mathbf{x}) = \langle \mathfrak{e}_{x^{(2)}}, \mathrm{e}^{-it(\Delta_{\mathrm{d}} + \lambda V_\omega)} F_\alpha^\beta \left(\Delta_{\mathrm{d}} + \lambda V_\omega \right) \mathfrak{e}_{x^{(1)}} \rangle \ , \quad \mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2 \ ,$$

where the real function F_α^β is defined, for any $\beta \in \mathbb{R}^+$ and $\alpha \in \mathbb{R}$, by

$$F_\alpha^\beta(\varkappa) := \frac{\mathrm{e}^{\alpha\varkappa}}{1 + \mathrm{e}^{\beta\varkappa}} \ , \qquad \varkappa \in \mathbb{R} \ .$$

Using Duhamel's formula note first that

$$\mathrm{e}^{(\alpha-it)(\Delta_{\mathrm{d}}+\lambda V_\omega)}=\mathrm{e}^{(\alpha-it)\Delta_{\mathrm{d}}}+\int_0^1\mathrm{e}^{(\alpha-it)(1-\gamma)\Delta_{\mathrm{d}}}\left(\alpha-it\right)\lambda V_\omega \mathrm{e}^{(\alpha-it)\gamma(\Delta_{\mathrm{d}}+\lambda V_\omega)}\mathrm{d}\gamma \tag{4.180}$$

for any $\alpha\in[0,\beta]$ and $t\in\mathbb{R}$. Since all operators in this last equation are bounded, it follows that, if $\lambda,\beta\in\mathbb{R}^+$ are sufficiently small, the Neumann series for $\left(1+\mathrm{e}^{\beta(\Delta_{\mathrm{d}}+\lambda V_\omega)}\right)^{-1}$ converges absolutely:

$$\begin{aligned}\left(1\right.&\left.+\mathrm{e}^{\beta(\Delta_{\mathrm{d}}+\lambda V_\omega)}\right)^{-1} \qquad (4.181)\\ &=\sum_{n=0}^{\infty}\left\{-\beta\lambda\left(1+\mathrm{e}^{\beta\Delta_{\mathrm{d}}}\right)^{-1}\int_0^1\mathrm{e}^{\beta(1-\gamma)\Delta_{\mathrm{d}}}V_\omega\mathrm{e}^{\beta\gamma(\Delta_{\mathrm{d}}+\lambda V_\omega)}\mathrm{d}\gamma\right\}^n\left(1+\mathrm{e}^{\beta\Delta_{\mathrm{d}}}\right)^{-1}.\end{aligned}$$

By (4.180) and (4.181), one then gets the existence of a constant D such that, for any sufficiently small $\lambda,\beta\in(0,1)$ and any $\alpha\in[0,\beta]$, $\omega\in\Omega$,

$$\left\|F_\alpha^\beta\left(\Delta_{\mathrm{d}}+\lambda V_\omega\right)-F_\alpha^\beta\left(\Delta_{\mathrm{d}}\right)\right\|_{\mathrm{op}}\leq D\beta\lambda\,. \tag{4.182}$$

Therefore, we define the approximated complex-time two-point correlation function $\tilde{C}_{t+i\alpha}^{(\omega)}\equiv\tilde{C}_{t+i\alpha}^{(\beta,\omega,\lambda)}$, for any $\beta\in\mathbb{R}^+$, $\omega\in\Omega$, $\lambda\in\mathbb{R}_0^+$, $t\in\mathbb{R}$ and $\alpha\in[0,\beta]$, by

$$\tilde{C}_{t+i\alpha}^{(\omega)}(\mathbf{x}):=\langle\mathfrak{e}_{x^{(2)}},\mathrm{e}^{-it(\Delta_{\mathrm{d}}+\lambda V_\omega)}F_\alpha^\beta\left(\Delta_{\mathrm{d}}\right)\mathfrak{e}_{x^{(1)}}\rangle\,,\quad \mathbf{x}:=(x^{(1)},x^{(2)})\in\mathfrak{L}^2\,. \tag{4.183}$$

For any $\mathbf{x}:=(x^{(1)},x^{(2)})\in\mathfrak{L}^2$ and $\mathbf{y}:=(y^{(1)},y^{(2)})\in\mathfrak{L}^2$, let

$$\tilde{\mathfrak{C}}_{t+i\alpha}^{(\omega)}(\mathbf{x},\mathbf{y}):=\frac{1}{4}\sum_{\pi,\pi'\in S_2}\varepsilon_\pi\varepsilon_{\pi'}\tilde{C}_{t+i\alpha}^{(\omega)}(y^{\pi'(1)},x^{\pi(1)})\tilde{C}_{-t+i(\beta-\alpha)}^{(\omega)}(x^{\pi(2)},y^{\pi'(2)})\,.$$

From (4.178) and (4.182) we thus deduce that

$$\Gamma_{1,1}(t)=\lim_{l\to\infty}\frac{1}{|\Lambda_l|}\sum_{x,y\in\Lambda_l}\mathbb{E}\left(\int_0^\beta\tilde{\mathfrak{C}}_{t+i\alpha}^{(\omega)}(x,x-e_1,y,y-e_1)\mathrm{d}\alpha\right)+\mathcal{O}(\beta^2\lambda)\,. \tag{4.184}$$

Next, we define an approximation $\hat{C}_{t+i\alpha}^{(\omega)}\equiv\hat{C}_{t+i\alpha}^{(\beta,\omega,\lambda)}$ of $\tilde{C}_{t+i\alpha}^{(\omega)}$ by

$$\begin{aligned}\hat{C}_{t+i\alpha}^{(\omega)}(\mathbf{x}):=&\,\langle\mathfrak{e}_{x^{(2)}},\mathrm{e}^{-it\Delta_{\mathrm{d}}}F_\alpha^\beta\left(\Delta_{\mathrm{d}}\right)\mathfrak{e}_{x^{(1)}}\rangle\\ &-\frac{1}{2}\left\langle\mathfrak{e}_{x^{(2)}},\lambda\left(itV_\omega+\frac{t^2}{2}(V_\omega\Delta_{\mathrm{d}}+\Delta_{\mathrm{d}}V_\omega+\lambda V_\omega^2)\right)\mathfrak{e}_{x^{(1)}}\right\rangle\end{aligned} \tag{4.185}$$

for all $\beta \in \mathbb{R}^+$, $\omega \in \Omega$, $\lambda \in \mathbb{R}_0^+$, $t \in \mathbb{R}$, $\alpha \in [0,\beta]$ and $\mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2$. Indeed, by (4.180) and an expansion of $F_\alpha^\beta(\Delta_\mathrm{d})$ at $\alpha, \beta = 0$, note that there is a constant D such that, for any $\lambda, \beta \in (0,1)$, $\alpha \in [0,\beta]$, $\omega \in \Omega$ and $t \in \mathbb{R}$,

$$\left\| \left(\mathrm{e}^{-it(\Delta_\mathrm{d}+\lambda V_\omega)} - \mathrm{e}^{-it\Delta_\mathrm{d}}\right) F_\alpha^\beta(\Delta_\mathrm{d}) + \frac{1}{2}\int_0^1 \mathrm{e}^{-it(1-\gamma)\Delta_\mathrm{d}} it\lambda V_\omega \mathrm{e}^{-it\gamma(\Delta_\mathrm{d}+\lambda V_\omega)}\mathrm{d}\gamma \right\|_{\mathrm{op}} \leq D\beta\lambda |t| \ . \tag{4.186}$$

Meanwhile, note that

$$\int_0^1 \mathrm{e}^{-it(1-\gamma)\Delta_\mathrm{d}} it\lambda V_\omega \mathrm{e}^{-it\gamma(\Delta_\mathrm{d}+\lambda V_\omega)}\mathrm{d}\gamma = it\lambda V_\omega + \frac{t^2\lambda}{2}\left(V_\omega\Delta_\mathrm{d} + \Delta_\mathrm{d} V_\omega + \lambda V_\omega^2\right) + \mathcal{O}(\lambda |t|^3) \tag{4.187}$$

uniformly for $\lambda \in (0,1)$ and $\omega \in \Omega$. Therefore, by combining (4.183) and (4.185) with (4.184), (4.186) and (4.187), we arrive at the equality

$$\begin{aligned}\Gamma_{1,1}(t) \ = \ & \lim_{l\to\infty} \frac{1}{|\Lambda_l|}\sum_{x,y\in\Lambda_l} \mathbb{E}\left(\int_0^\beta \widehat{\mathfrak{C}}_{t+i\alpha}^{(\omega)}(x, x-e_1, y, y-e_1)\mathrm{d}\alpha\right) \\ & +\mathcal{O}(\beta^2\lambda) + \mathcal{O}(\beta\lambda|t|^3)\end{aligned} \tag{4.188}$$

for sufficiently small $|t|$, where

$$\widehat{\mathfrak{C}}_{t+i\alpha}^{(\omega)}(\mathbf{x},\mathbf{y}) := \frac{1}{4}\sum_{\pi,\pi'\in S_2} \varepsilon_\pi\varepsilon_{\pi'} \hat{C}_{t+i\alpha}^{(\omega)}(y^{\pi'(1)}, x^{\pi(1)}) \hat{C}_{-t+i(\beta-\alpha)}^{(\omega)}(x^{\pi(2)}, y^{\pi'(2)})$$

for all $\mathbf{x} := (x^{(1)}, x^{(2)}) \in \mathfrak{L}^2$ and $\mathbf{y} := (y^{(1)}, y^{(2)}) \in \mathfrak{L}^2$.

We use now that V_ω is an i.i.d. potential satisfying $\mathbb{E}(V_\omega(x)) = 0$ for all $x \in \mathfrak{L}$ to compute that, for any $\mathbf{x} := (x^{(1)}, x^{(2)})$ and $\mathbf{y} := (y^{(1)}, y^{(2)}) \in \mathfrak{L}^2$, $x^{(1)} \neq x^{(2)}$, $y^{(1)} \neq y^{(2)}$,

$$\begin{aligned}&\mathbb{E}\left(\int_0^\beta \widehat{\mathfrak{C}}_{t+i\alpha}^{(\omega)}(\mathbf{x},\mathbf{y})\mathrm{d}\alpha\right) - \int_0^\beta \mathfrak{C}_{t+i\alpha}^{(0)}(\mathbf{x},\mathbf{y})\mathrm{d}\alpha \\ &= -\frac{\lambda^2 t^2}{16}\mathbb{E}\left(V_\omega^2\right)\sum_{\pi,\pi'\in S_2}\varepsilon_\pi\varepsilon_{\pi'}\left\{\left(\int_0^\beta \langle \mathfrak{e}_{x^{\pi(1)}}, \mathrm{e}^{-it\Delta_\mathrm{d}} F_\alpha^\beta(\Delta_\mathrm{d})\, \mathfrak{e}_{y^{\pi'(1)}}\rangle \mathrm{d}\alpha\right)\delta_{x^{\pi(2)},y^{\pi'(2)}}\right. \\ &\quad + \left.\left(\int_0^\beta \langle \mathfrak{e}_{y^{\pi'(2)}}, \mathrm{e}^{it\Delta_\mathrm{d}} F_{\beta-\alpha}^\beta(\Delta_\mathrm{d})\, \mathfrak{e}_{x^{\pi(2)}}\rangle \mathrm{d}\alpha\right)\delta_{y^{\pi'(1)},x^{\pi(1)}}\right\} + \frac{\beta\lambda^2 t^4}{64}\mathbf{D}(\mathbf{x},\mathbf{y}) \ ,\end{aligned} \tag{4.189}$$

where, for any $\mathbf{x} = (x^{(1)}, x^{(2)}), \mathbf{y} = (y^{(1)}, y^{(2)}) \in \mathfrak{L}^2$, $x^{(1)} \neq x^{(2)}$, $y^{(1)} \neq y^{(2)}$,

$$\begin{aligned}\mathbf{D}(\mathbf{x}, \mathbf{y}) := \sum_{\pi,\pi' \in S_2} \varepsilon_\pi \varepsilon_{\pi'} \Big\{ & \lambda^2 \left(\mathbb{E}\left(V_\omega^2\right)\right)^2 \delta_{y^{\pi'(1)}, x^{\pi(1)}} \delta_{x^{\pi(2)}, y^{\pi'(2)}} \\ & + \mathbb{E}\left(\langle \mathfrak{e}_{x^{\pi(1)}}, (V_\omega \Delta_{\mathrm{d}} + \Delta_{\mathrm{d}} V_\omega) \mathfrak{e}_{y^{\pi'(1)}} \rangle \langle \mathfrak{e}_{y^{\pi'(2)}}, (V_\omega \Delta_{\mathrm{d}} + \Delta_{\mathrm{d}} V_\omega) \mathfrak{e}_{x^{\pi(2)}} \rangle \right) \Big\} \ .\end{aligned}$$

Note that, for each $\lambda \in \mathbb{R}_0^+$ and $t \in \mathbb{R}$, $\mathbf{D} \equiv \mathbf{D}^{(\lambda)}$ can be seen as the kernel (w.r.t. the canonical basis $\{\mathfrak{e}_x \otimes \mathfrak{e}_{x'}\}_{x,x' \in \mathfrak{L}}$) of a bounded operator on $\ell^2(\mathfrak{L}) \otimes \ell^2(\mathfrak{L})$ with operator norm uniformly bounded w.r.t. λ on compact sets. Similar to (4.130), it follows that

$$\lim_{l \to \infty} \frac{1}{|\Lambda_l|} \sum_{x,y \in \Lambda_l} \mathbf{D}(x, x - e_1, y, y - e_1) = \mathcal{O}(1) \tag{4.190}$$

uniformly for λ in compact sets.

Because of Lemma 4.6.9 and (4.179), note that

$$\begin{aligned}&\lim_{l \to \infty} \frac{1}{|\Lambda_l|} \sum_{x,y \in \Lambda_l} \int_0^\beta \mathfrak{C}_{t+i\alpha}^{(0)}(x, x - e_1, y, y - e_1) \mathrm{d}\alpha \\ &\qquad = \lim_{l \to \infty} \frac{1}{|\Lambda_l|} \sum_{x,y \in \Lambda_l} \int_0^\beta \mathfrak{C}_{i\alpha}^{(0)}(x, x - e_1, y, y - e_1) \mathrm{d}\alpha\end{aligned}$$

does not depend on $t \in \mathbb{R}$. Using this we infer from (4.179) and (4.188)-(4.190) the existence of a constant $D \in \mathbb{R}^+$ such that the AC-conductivity σ is of the form

$$\sigma(t) = -D\lambda^2 \beta t^2 + \mathcal{O}(\beta^2 \lambda) + \mathcal{O}(\beta\lambda |t|^3) \tag{4.191}$$

for sufficiently small $\beta, \lambda, |t|$.

Now we choose sufficiently small $\lambda_0, \beta_0, T_0 > 0$ and estimate the energy increment caused by the time-rescaled potential $\mathbf{A}^{(T)} \in \mathbf{C}_0^\infty \backslash \{0\}$ for $T \in (T_0/2, T_0)$, $\lambda \in (\lambda_0/2, \lambda_0)$, $\beta \in (0, \beta_0)$. We assume w.l.o.g. that $E_{\mathbf{A}}$ is zero in all but the first component which equals a function $\mathcal{E}_t \in C_0^\infty\left(\mathbb{R}^d; \mathbb{R}\right)$ for any $t \in \mathbb{R}$. Then, by (4.191) and Fubini's theorem, we have

$$\begin{aligned}&\int_{t_0}^t \int_{t_0}^{s_1} \left[\sigma(s_2 - s_1) \int_{\mathbb{R}^d} \langle E_{\mathbf{A}^{(T)}}(s_1, x), E_{\mathbf{A}^{(T)}}(s_2, x) \rangle \, \mathrm{d}^d x \right] \mathrm{d}s_1 \mathrm{d}s_2 \\ &\qquad = -\frac{D\lambda^2 \beta T^2}{2} \int_{\mathbb{R}^d} \left[\int_{\mathbb{R}} \int_{\mathbb{R}} (s_2 - s_1)^2 \mathcal{E}_{s_1}(x) \mathcal{E}_{s_2}(x) \mathrm{d}s_1 \mathrm{d}s_2 \right] \mathrm{d}^d x \\ &\qquad\quad + \mathcal{O}(\beta^2 \lambda) + \mathcal{O}(\beta\lambda T^3) \ .\end{aligned} \tag{4.192}$$

Because of the AC-condition (4.16), observe that, for all $x \in \mathbb{R}^d$,

$$-\int_{\mathbb{R}} \int_{\mathbb{R}} (s_2 - s_1)^2 \mathcal{E}_{s_1}(x) \mathcal{E}_{s_2}(x) \mathrm{d}s_1 \mathrm{d}s_2 = 2 \left(\int_{\mathbb{R}} s \mathcal{E}_s(x) \mathrm{d}s \right)^2 . \tag{4.193}$$

As a consequence, if

$$\int_{\mathbb{R}} \left(\int_{\mathbb{R}} s \mathcal{E}_s(x) \mathrm{d}s \right)^2 \mathrm{d}^d x > 0 ,$$

then (4.192)-(4.193) yield the lemma, provided $\lambda_0 T_0^2 \gg \beta_0, \lambda_0 T_0^2 \gg T_0^3$. □

Note that Lemma 4.6.11 implies that, for sufficiently small $\lambda, \beta > 0$, the AC-conductivity measure μ_σ on $\mathbb{R} \backslash \{0\}$ is non-zero. This property implies the following result:

Lemma 4.6.12.
Assume that the AC-conductivity measure μ_σ on $\mathbb{R} \backslash \{0\}$ is non-zero. Then the set

$$\mathcal{Z} := \left\{ \varphi \in \mathcal{S}(\mathbb{R}; \mathbb{R}) : \int_{\mathbb{R}} \int_{\mathbb{R}} \sigma(s_2 - s_1) \varphi(s_1) \varphi(s_2) \mathrm{d}s_1 \mathrm{d}s_2 = 0 \right\}$$

is meager in the (Fréchet) space $\mathcal{S}(\mathbb{R}; \mathbb{R})$ of Schwartz functions equipped with the usual locally convex topology.

Proof. Since μ_σ is by assumption non-zero, there is at least one point $\nu_0 \in \mathbb{R} \backslash \{0\}$ such that $\mu_\sigma(\mathcal{V}) \neq 0$ for all open neighborhoods $\mathcal{V}$ of ν_0. To see this, observe that

$$\mathbb{R} \backslash \{0\} = \bigcup_{n \in \mathbb{N}} \left[\frac{1}{n}, n \right] \cup \left[-n, -\frac{1}{n} \right] ,$$

and thus there is $n \in \mathbb{N}$ such that

$$\mu_\sigma \left(\left[\frac{1}{n}, n \right] \cup \left[-n, -\frac{1}{n} \right] \right) > 0 .$$

Then, by compactness, there is $\nu_0 \in \left[\frac{1}{n}, n \right] \cup \left[-n, -\frac{1}{n} \right]$ such that

$$\mu_\sigma \left(\mathcal{V} \cap \left(\left[\frac{1}{n}, n \right] \cup \left[-n, -\frac{1}{n} \right] \right) \right) \neq 0$$

for all open neighborhoods $\mathcal{V}$ of ν_0.

Take now any non-zero function $\varphi \in C_0^\infty(\mathbb{R};\mathbb{R}) \subset \mathcal{S}(\mathbb{R};\mathbb{R})$. Its Fourier transform $\hat{\varphi}$ obeys

$$\left|\frac{d^n\hat{\varphi}}{d\nu^n}(\nu)\right| \leq D_1 D_2^n \ , \qquad n \in \mathbb{N} \ , \ \nu \in \mathbb{R} \ ,$$

for some constants $D_1, D_2 \in \mathbb{R}^+$. In particular, there is a unique continuation of $\hat{\varphi} : \mathbb{R} \to \mathbb{C}$ to an entire function, again denoted by $\hat{\varphi} : \mathbb{C} \to \mathbb{C}$. Hence, the set of zeros of $\hat{\varphi}$ has no accumulation points.

If $\hat{\varphi}(\nu_0) \neq 0$ then, by continuity of $\hat{\varphi}$,

$$\int_{\mathbb{R}} \int_{\mathbb{R}} \sigma(s_2 - s_1)\varphi(s_1)\varphi(s_2)\mathrm{d}s_1\mathrm{d}s_2 = \int_{\mathbb{R}\backslash\{0\}} |\hat{\varphi}(\nu)|^2 \,\mathrm{d}\mu_\sigma(\nu) > 0 \ . \qquad (4.194)$$

If $\hat{\varphi}(\nu_0) = 0$ then, for all $\alpha \in (0,1)$, we define the rescaled function $\hat{\varphi}_\alpha(\nu)$ by $\hat{\varphi}(\alpha\nu)$, which is the Fourier transform of $\alpha^{-1}\varphi(\alpha^{-1}x)$. For sufficiently small $\varepsilon \in \mathbb{R}^+$ and all $\alpha \in (1-\varepsilon, 1)$,

$$\int_{\mathbb{R}\backslash\{0\}} |\hat{\varphi}_\alpha(\nu)|^2 \,\mathrm{d}\mu_\sigma(\nu) > 0 \ ,$$

because the set of zeros of $\hat{\varphi}$ has no accumulation points. On the other hand, $\alpha^{-1}\varphi(\alpha^{-1}x)$ converges in $\mathcal{S}(\mathbb{R};\mathbb{R})$ to $\varphi(x)$, as $\alpha \to 1$. Thus, the complement of $\mathcal{Z}$ is dense in $\mathcal{S}(\mathbb{R};\mathbb{R})$, by density of the set $C_0^\infty(\mathbb{R};\mathbb{R})$ in $\mathcal{S}(\mathbb{R};\mathbb{R})$. Since μ_σ is bounded (see Section 4.6), note that the map

$$\hat{\varphi} \mapsto \int_{\mathbb{R}\backslash\{0\}} |\hat{\varphi}(\nu)|^2 \,\mathrm{d}\mu_\sigma(\nu)$$

is continuous on $\mathcal{S}(\mathbb{R};\mathbb{R})$. Because the Fourier transform is a homeomorphism of $\mathcal{S}(\mathbb{R};\mathbb{R})$, by the first equation in (4.194), the map

$$\varphi \mapsto \int_{\mathbb{R}} \int_{\mathbb{R}} \sigma(s_2 - s_1)\varphi(s_1)\varphi(s_2)\mathrm{d}s_1\mathrm{d}s_2$$

is also continuous on $\mathcal{S}(\mathbb{R};\mathbb{R})$ and the complement of $\mathcal{Z}$ is hence an open set. □

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