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Finite size effects in quantum field theory

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1. Introduction

Quantum field theory is the most accurate theory available at the moment that has passed validation through a variety of experimental checks. Within the framework of quantum field theory it was possible to incorporate three of the known forces (the electro-magnetic, the weak and the strong) into the so-called Standard Model of Particle Physics. Much of the success came through the framework of Yang-Mills theory which provided a systematic way of describing weak and strong interactions.

Quantum field theory has proved very fruitful also in many other fields of physics, such as solid state physics (superconductivity, superfluidity), atomic physics, cosmology and astrophysics. Nevertheless some questions are still unanswered and the last building block of the Standard Model is yet to be discovered. The Higgs boson, first theoretically predicted in the 60's and incorporated in the Standard Model through the Weinberg-Glashow-Salam theory of electroweak interactions, is the particle through which all other massive elementary particles acquire their mass.

Even if the Higgs boson will be discovered, there is nowadays still a general belief that the Standard Model of Particle Physics is only an effective theory of a more general one, that incorporates also gravity.

Despite the fact that both the theory and the tools to calculate quantities of interest are in principle known, applying them to the known world involves lots of difficulties and many calculations are far from being under control. Throughout the years different directions have emerged in order to surpass computational difficulties.

Analytical methods use approximations, symmetries of the underlying theories, empirical and experimental evidence in order to simplify the calculations. The computational lattice Monte Carlo approach on the other hand also makes approximations in practice, one of them being the reduced size of physical systems that can be numerically managed. Since both methods contain approximations, considerable effort is put into estimating the errors and the accuracy of the two approaches.

The following thesis treats the effects occurring in a scalar field theory due to the finite volume it lives in. By calculating the partition function, the contributions due to the finite volume are determined for the free energy density in both the massive and the massless case. The results for the massive scalar field can be used on one hand for estimations on finite size effects in the low temperature and large volume limit of chiral perturbation theory and on the other hand for a Yang-Mills theory at very high temperature.

The thesis is structured as follows. The second chapter gives a short introduction to quantum field theory and thermal field theory. The correspondence between the partition function of statistical mechanics and the path integral method of quantum field theory is discussed in some detail. This chapter provides also the starting point for the calculations in chapter 4.

The third chapter presents the effective theory approach for two different regimes of interest in the theory of strong interactions. The physics of low energy hadrons is described within the framework of chiral perturbation theory. The symmetries of the QCD Lagrangian in the chiral (massless quarks) limit and the phenomenon of spontaneous symmetry breaking are used in order to develop a theory in terms of the physical degrees of freedom occurring in the low energy regime of the underlying theory. Effective thermal field theory provides an approach to the deconfined quark-gluon plasma at very high temperatures. The static limit of the QCD Lagrangian is used and the different scales appearing in the thermal field theory are separated in such a way that the remaining Lagrange density contains only the non-perturbative scale.

Finally, the forth chapter provides the calculation of the partition function of a scalar field theory in a finite volume. The results are used to estimate the contributions of finite size effects in perturbative thermal field theory and in theories with spontaneous symmetry breaking, applicable to low energy hadronic physics. The two physical limits of massless and massive scalar fields will exhibit qualitatively different finite size corrections.

2. Theoretical framework

In this chapter the main ideas of quantum field theory and thermal field theory that will be used throughout the thesis are introduced. First, elementary notions of quantum field theory are defined. Afterwards the connection between quantum field theory and statistical mechanics is made through the path integral formalism as a mathematical link. For a detailed treatment on this subject for instance Ref. [1] is recommended. Natural units will be used throughout the thesis, $\hbar = c = k_B = 1$.

2.1. Quantum field theory and statistical mechanics

Quantum field theory (QFT) provides a theoretical framework in which both the concepts of quantum mechanics and special relativity are put together. Within this framework particles and fundamental interactions are treated as physical fields and are quantized. Mathematically this is done by transforming the fields entering the Lagrange density into field operators. This leads also to the possibility of describing physical systems of a varying number of degrees of freedom, in terms of the so called creation and annihilation operators. With these 4 operators (2 for fermions and 2 for bosons) and their (anti-)commutation relation,

$$\begin{aligned} &[a_{\mathbf{p}}, a_{\mathbf{q}}^\dagger] = (2\pi)^3 \delta^{(3)}(\mathbf{p}-\mathbf{q}),\ [a_{\mathbf{p}}, a_{\mathbf{q}}] = [a_{\mathbf{p}}^\dagger, a_{\mathbf{q}}^\dagger] = 0 \text{ for bosons,} \\ &\{a_{\mathbf{p}}, a_{\mathbf{q}}^\dagger\} = (2\pi)^3 \delta^{(3)}(\mathbf{p}-\mathbf{q}),\ \{a_{\mathbf{p}}, a_{\mathbf{q}}\} = \{a_{\mathbf{p}}^\dagger, a_{\mathbf{q}}^\dagger\} = 0 \text{ for fermions,} \end{aligned} \tag{2.1}$$

field operators describing all types of particles can be constructed.

The principles of special relativity are integrated into quantum field theory through the equal time commutation relations of the field operators. The simplest example of how special relativity is integrated into quantum field theory is given through a free real scalar field. First the scalar field is written in terms of its Fourier modes and is required to be the solution of the Klein-Gordon equation, $(\partial_t^2 + \mathbf{p}^2 + m^2)\tilde{\phi}(\mathbf{p}, t) = 0$. By substituting the field amplitudes with the creation and annihilation operators for bosons (thus quantizing the field), it finally can be written as:

$$\phi(x) = \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^3} \frac{1}{\sqrt{2E_{\mathbf{p}}}} \left(a_{\mathbf{p}} e^{-ipx} + a_{\mathbf{p}}^\dagger e^{ipx} \right) \Big|_{p^0 = E_{\mathbf{p}}} \quad \text{with } E_{\mathbf{p}} = \sqrt{\mathbf{p}^2 + m^2}. \tag{2.2}$$

Its commutator is

$$[\phi(x), \phi(y)] = \int \frac{\mathrm{d}^3p}{(2\pi)^3} \frac{1}{2E_{\mathbf{p}}} \left(e^{-ip(x-y)} - e^{ip(x-y)}\right) \begin{cases} = 0, & (x-y)^2 < 0 \\ \neq 0, & (x-y)^2 > 0. \end{cases} \tag{2.3}$$

This commutation relation is interpreted as follows: provided two fields are separated by a time-like interval (are causally connected), operators do not commute ($\neq 0$), that is, they cannot be determined simultaneously with an arbitrary precision. As soon as they are separated by a space-like interval they will commute ($= 0$)[1], meaning they are no longer causally connected and can be simultaneously measured with an arbitrary precision.

The time ordered product of two fields projected on the ground state in the free theory describes the propagation of particles through space and is a Green's function for the differential equation that describes this field (Klein-Gordon equation for scalar fields, Dirac equation for spinor fields, Maxwell equation for vector fields). It is called the Feynman propagator and for a real scalar field it looks like:

$$\langle 0|T\phi(x)\phi(y)|0\rangle = D_F(x-y) = \int \frac{\mathrm{d}^4p}{(2\pi)^4} \frac{ie^{-ip(x-y)}}{p^2 + m^2 - i\epsilon}. \tag{2.4}$$

In an interacting theory the field propagator cannot be calculated in the same way, due to the fact that it is not known a priory how field operators act on the vacuum state of an interacting theory. However, it can be expressed in terms of the vacuum state of the free theory and the interaction part of the Hamiltonian expressed in the interaction picture.

$$\langle \Omega|T\{\phi(x)\phi(y)\}|\Omega\rangle = \lim_{t\to\infty(1-i\epsilon)} \frac{\langle 0|T\{\phi_I(x)\phi_I(y)\exp\left[-i\int_{-t}^{t}\mathrm{d}t'\, H_I(t')\right]\}|0\rangle}{\langle 0|T\{\exp\left[-i\int_{-t}^{t}\mathrm{d}t'\, H_I(t')\right]\}|0\rangle} \tag{2.5}$$

By expanding the exponential into a Taylor series in the coupling constant and using Wick's theorem [2], the right hand side of the equation can be expressed as an infinite sum of products of Feynman propagators. Each term in the expansion can be diagrammatically represented as a Feynman diagram. Through the LSZ reduction formula the scattering matrix can be expressed in terms of a series of such Feynman diagrams. In this way physical quantities such as scattering cross sections or particle decay rates may be calculated explicitly.

The path integral formalism is an alternative approach to quantum field theory. It generalizes the action principle of classical mechanics for fields. Its physical interpretation is that the evolution of a system from one state to another is the sum of all different (in principle infinitely many) paths the system can take in the phase space.

[1] For a space-like interval a Lorentz transformation can be performed, $(x-y)^2 \to -(x-y)^2$, so that the integrand vanishes, whereas for time-like intervals no such transformation exists.

The details of this approach can be found in every QFT book. Here, only the result from Ref. [3][2] is shown:

$$\langle\Omega|T\{\phi(x_1)\cdot ... \cdot\phi(x_n)\}|\Omega\rangle = \lim_{t\to\infty(1-i\epsilon)} \frac{\int \mathcal{D}\phi\, \phi(x_1)\cdot ... \cdot \phi(x_n) \exp\left[i\int_{-t}^{t} \mathrm{d}t \int \mathrm{d}^3\mathbf{x}\mathcal{L}\right]}{\int \mathcal{D}\phi \exp\left[i\int_{-t}^{t} \mathrm{d}t \int \mathrm{d}^3\mathbf{x}\mathcal{L}\right]} \tag{2.6}$$

An essential difference between these two approaches is that classical fields enter the path integral rather than field operators. Second, due to the fact that the exponent of the integrand contains the Lagrange density and not the Hamiltonian, the n-point function is manifestly Lorentz invariant.

A systematic way of obtaining n-point functions in the path integral formulation is by defining the generating functional as:

$$Z[J] = \int \mathcal{D}\phi \exp\left[i\int \mathrm{d}^4x(\mathcal{L} - J\phi)\right]. \tag{2.7}$$

The J field of the integrand is called source term. Through functional derivatives with respect to this source term, n-point functions can be generated as:

$$\langle\Omega|T\{\phi(x_1)...\phi(x_n)\}|\Omega\rangle = Z[J]^{-1}\left(-i\frac{\delta}{\delta J(x_1)}\right)...\left(-i\frac{\delta}{\delta J(x_n)}\right)Z[J]\Big|_{J=0}. \tag{2.8}$$

The generating functional (2.7) is similar to the partition function from statistical mechanics; it has the same structure of a sum over all possible configurations of a statistical weight. The only difference is that the exponent is purely imaginary and not real and negative as in statistical mechanics. To construct the link between them a procedure similar to the Wick rotation is used, in which the time coordinate is defined as purely imaginary.

$$x_4 = ix_0,\ \vec{x}_E = \vec{x} \tag{2.9}$$

This leads to:

$$\int \mathcal{D}\phi \exp\left[i\cdot(-i)\int \mathrm{d}^4x_E(\mathcal{L}_E - J\phi)\right] \tag{2.10}$$

with

$$\begin{aligned} -\mathcal{L}_E &= \frac{1}{2}(\partial_0\phi\partial_0\phi - \nabla\phi\cdot\nabla\phi) - V(\phi) \\ &= -\left[\frac{1}{2}\left(\partial_4\phi\partial_4\phi + \nabla\phi\cdot\nabla\phi\right) + V(\phi)\right] \\ &= -\left[\frac{1}{2}\partial_\mu\phi\partial_\mu\phi + V(\phi)\right]. \end{aligned} \tag{2.11}$$

The exponent is now real and negative, and it also seems that the euclidean Lagrangian is the sum of the kinetic part and the potential energy $V(\phi)$, which is just the total energy of the system. Summing up, the generating functional in the imaginary time formalism becomes:

$$Z[J=0] = C\int \mathcal{D}\phi \exp\left[-\int \mathrm{d}^4x\mathcal{L}_E\right]. \tag{2.12}$$

[2] The difference to the free theory is that here the projection is realized on the vacuum state of the interacting theory, $|\Omega\rangle$ and that the Lagrangian contains also the interacting part.

Trying now to express the partition function for a real scalar field (appendix A), one obtains

$$\begin{aligned} Z &= \mathrm{Tr}[e^{-\beta\hat{H}}] \\ &= \int_{\phi(\beta,\mathbf{x})=\phi(0,\mathbf{x})} \prod_{\mathbf{x}} [C\mathcal{D}\phi(\tau,\mathbf{x})] \exp\left[-\int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3\mathbf{x}\mathcal{L}_E\right]. \end{aligned} \tag{2.13}$$

The partition function of statistical mechanics has the same structure as the generating functional of quantum field theory. The difference lies only in the integration limits of the time integral in the exponent. For the partition function, the "time" integral spans from 0 to the inverse temperature with the additional requirement of periodicity of the fields in the time variable.

2.2. Partition function in thermal field theory

This section provides an introduction to the main ideas of quantum field theory at finite temperature in the non-interacting case. The interacting case will be presented in section 3.2 within the framework of effective thermal field theories.

The main object in statistical mechanics is the partition function of the system, calculated in the last section. Starting with the partition function, all thermodynamic quantities can be determined. Some examples are the free energy, the entropy and the average energy:

$$\begin{aligned} F &= -T \ln Z, \\ S &= -\frac{\partial F}{\partial T}, \\ E &= \frac{1}{Z}\mathrm{Tr}(\hat{H}\mathrm{e}^{\beta\hat{H}}). \end{aligned} \tag{2.14}$$

In the following, the partition function for a scalar field will be explicitly calculated and this will be the starting point of the calculations in chapter 4 in determining the finite size effects. In order to keep the calculation as general as possible, d spatial dimensions are considered. Some results will then be calculated for $d = 3$.

The starting point is Eq. (2.13) [4]. The strategy is to express the fields through their Fourier representation as

$$\phi(\tau,\mathbf{x}) = T \sum_{n=-\infty}^{\infty} \tilde{\phi}(\omega_n,\mathbf{x}) e^{i\omega_n\tau},\ \omega_n = 2\pi T n. \tag{2.15}$$

For bosons periodic boundary conditions in the τ-direction are required whereas for fermions anti-periodic ones. The spatial volume will be regarded as finite as well, since finite size effects will be calculated later on. Having now a function with one spatial coordinate, it will be represented as

$$f(x) = \frac{1}{L} \sum_{n=-\infty}^{\infty} \tilde{f}(n) e^{ikx} \text{ with } k = \frac{2\pi n}{L},\ n \in \mathbb{Z}. \tag{2.16}$$

Here $1/L$ plays the same role as T. Now the Fourier representation of ϕ becomes:

$$\phi(\tau, \mathbf{x}) = T \sum_n \frac{1}{V} \sum_{\mathbf{k}} \tilde{\phi}(\omega_n, \mathbf{k}) e^{i\omega_n \tau + i\mathbf{k}\cdot\mathbf{x}} \text{ with } V = L_1 ... L_d. \tag{2.17}$$

The requirement that ϕ is a real scalar field reads in the reciprocal space as:

$$\left[\tilde{\phi}(\omega_n, \mathbf{k})\right]^* = \tilde{\phi}(-\omega_n, -\mathbf{k}). \tag{2.18}$$

Therefore only half of the Fourier modes are independent.

In order to express the integrand of (2.13) in terms of the Fourier representation, first express quadratic forms in the fields as:

$$\begin{aligned}\int_0^\beta \mathrm{d}\tau \int \mathrm{d}^d\mathbf{x} \phi_1(\tau, \mathbf{x}) \phi_2(\tau, \mathbf{x}) &= \frac{T^2}{V^2} \sum_{n,m} \sum_{\mathbf{k},\mathbf{p}} \tilde{\phi}_1(\omega_n, \mathbf{k}) \tilde{\phi}_2(\omega_m, \mathbf{p}) \cdot \\ &\cdot \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^d x e^{i\tau(\omega_n + \omega_m) + i\mathbf{x}\cdot(\mathbf{k}+\mathbf{p})} \\ &= T \sum_n \frac{1}{V} \sum_{\mathbf{k}} \tilde{\phi}_1(-\omega_n, -\mathbf{k}) \tilde{\phi}_2(\omega_n, \mathbf{k}).\end{aligned} \tag{2.19}$$

The euclidean Lagrangian for a scalar field is (2.11). In the free case $V(\phi) = \frac{1}{2}m^2\phi^2$. The exponent can be written as:

$$\begin{aligned}\exp(-S_E) &= \exp\left[-\int_0^\beta \mathrm{d}\tau \int \mathrm{d}^d x \mathcal{L}_E\right] \\ &= \exp\left[-\frac{1}{2} T \sum_n \frac{1}{V} \sum_{\mathbf{k}} (\omega_n^2 + \mathbf{k}^2 + m^2) |\tilde{\phi}(\omega_n, \mathbf{k})|^2\right] \\ &= \prod_{\mathbf{k}} \left\{\exp\left[-\frac{T}{2V} \sum_n (\omega_n^2 + \mathbf{k}^2 + m^2) |\tilde{\phi}(\omega_n, \mathbf{k})|^2\right]\right\}.\end{aligned} \tag{2.20}$$

Turning now to the calculation of the path integral one could first try to solve the integral directly. This turns out to be rather difficult because one has to keep track of the degrees of freedom one chooses for the integration. Therefore it is useful instead to recall the calculation of the partition function for a harmonic oscillator and transfer the result to the case of a scalar field. Using Eq. (A.16) the exponential can be rewritten as

$$\exp\left[-\frac{1}{2} mT\omega^2 a_0^2 - mT \sum_{n\geq 1} (\omega_n^2 + \omega^2)(a_n^2 + b_n^2)\right] = \exp\left[-\frac{1}{2} T \sum_{n=-\infty}^{\infty} m(\omega_n^2 + \omega^2) |x_n|^2\right]. \tag{2.21}$$

Now the exponential has the same structure as that in Eq. (2.20) with the difference of an overall d-dimensional product over $\mathbf{k}$ suggesting again that the scalar field is described as coupled harmonic oscillators in all spatial dimensions. Through the replacements

$$m \to \frac{1}{V},\ \omega_{HO}^2 \to \mathbf{k}^2 + m^2 \equiv E_{\mathbf{k}}^2,\ |x_n^2| \to |\tilde{\phi}(\omega_n, \mathbf{k})|^2 \tag{2.22}$$

the final result is (cf Eq. A.18)

$$Z = \prod_{\mathbf{k}} \left[T \prod_{n} (\omega_n^2 + E_{\mathbf{k}}^2)^{-\frac{1}{2}} \prod_{n'} (\omega_n^2)^{\frac{1}{2}} \right]. \tag{2.23}$$

This equation will be the starting point for the finite size calculations in chapter 4.

Making now use of the relation $\sum_{k=-\infty}^{\infty} 1/(k^2+x^2) = \pi/x\tanh(\pi x)$, the expression in brackets can be rewritten so that the free energy density in infinite volume becomes:

$$\lim_{V\to\infty} \frac{F}{V} = \int \frac{\mathrm{d}^d\mathbf{k}}{(2\pi)^d} \left[\frac{E_{\mathbf{k}}}{2} + T\ln\left(1 - e^{-\beta E_{\mathbf{k}}}\right) \right] \equiv J(m,T). \tag{2.24}$$

The first term in Eq. (2.24) is the vacuum energy density, independent of temperature. Its evaluation is possible in terms of a more general function by using dimensional regularization,

$$\int \frac{\mathrm{d}^d\mathbf{k}}{(2\pi)^d} \frac{1}{(\mathbf{k}^2+m^2)^A} = \frac{1}{(4\pi)^{d/2}} \frac{\Gamma(A-d/2)}{\Gamma(A)} \frac{1}{(m^2)^{A-d/2}}, \tag{2.25}$$

which, unlike the vacuum integral, is finite. Inserting $A = -1/2$, the vacuum energy density becomes in four space-time dimensions:

$$J_0(m) = -\frac{m^4}{64\pi^2}\mu^{-2\epsilon} \left[\frac{1}{\epsilon} + \ln\frac{\mu^2}{m^2} + \ln 4\pi - \gamma_E + \frac{3}{2} \right], \tag{2.26}$$

where μ is an arbitrary scale parameter.

The expression contains a divergence $(1/\epsilon)$ due to the regularization scheme used. The divergence is expected to appear, since the expression represents the vacuum energy density in the infinite volume limit.

The thermal part cannot be calculated exactly. In the low temperature region, i.e. for $m/T \gg 1$, its expression is:

$$J_T(m) = T\int \frac{\mathrm{d}^d\mathbf{k}}{(2\pi)^d} \ln\left(1 - e^{-\beta E_{\mathbf{k}}}\right) = -T^4 \left(\frac{m}{2\pi T}\right)^{\frac{3}{2}} e^{-\frac{m}{T}} \left[1 + \mathcal{O}\left(\frac{m}{T}\right) + \mathcal{O}\left(e^{-m/T}\right) \right]. \tag{2.27}$$

Eq. (2.27) shows that in the low temperature regime the thermal effects are suppressed by an exponential factor.

In the high temperature limit $(T \gg m)$, the integral can be evaluated by first calculating

$$\begin{aligned} I(m,T) &= \frac{1}{m}\frac{\mathrm{d}}{\mathrm{d}m} J(m,T) \\ &= T\sum_n \int \frac{\mathrm{d}^d\mathbf{k}}{(2\pi)^d} \frac{1}{\omega_n^2 + E_{\mathbf{k}}^2} \end{aligned} \tag{2.28}$$

in the high temperature limit and then performing the integration over m. The integration constant is an m-independent quantity, namely $J(0,T) = -\pi^2 T^4/90$. Therefore, the first few terms of the free energy density are:

$$J_T(m) = -\frac{\pi^2 T^4}{90} + \frac{m^2 T^2}{24} - \frac{m^3 T}{12\pi} - \frac{m^4}{32\pi^2} \left[\ln\left(\frac{m e^{\gamma_E}}{4\pi T}\right) - \frac{3}{4} \right] + \mathcal{O}\left(\frac{m^6}{T^2}\right) + \mathcal{O}(\epsilon). \tag{2.29}$$

The first term (the integration constant) is just the free energy density of a massless gas with one degree of freedom. The following corrections come with increasing powers of m but are suppressed by increasing powers of T in the denominator. In addition, the expansion shows that $J_T(m)$ is not analytic in m^2 containing an odd power in m. This is the reflection of the so-called infrared (IR) problem of thermal field theory and will lead in the interacting case to the necessity of doing a resummation of diagrams to all orders in the coupling constant in order to keep the perturbation expansion finite.

3. Effective field theories

Having the basic mathematical tools to perform calculations in quantum field theory and thermal field theory as well, the physical model of strong interactions can be approached, Quantum Chromodynamics (QCD). This non-abelian gauge theory is used in the following chapter do work out effective theories that are applicable for low energies and for high temperatures. The physical systems described range from low energy hadronic physics and scattering processes to high temperature plasma of quarks and gluons.

In the first section the symmetries of the fermionic part of the Lagrangian are used in order to construct a low energy effective theory, whereas in the second section the different energy scales appearing in the gluonic part of the Lagrangian are exploited in order to develop an effective theory for strong interactions at temperatures far above that of the deconfinement transition.

3.1. Chiral perturbation theory

Starting with the mid 50's experiments revealed an increasing number of new particles, with masses ranging within several nucleon masses. Without an exact theory describing the interactions between these new particles, several attempts were made to describe the underlying physics. Using the known hadron spectrum by that time, Gell-Mann organised them into octets and decuplets according to their masses approaching therefore a group theoretical description of the hadrons (Ref. [5]).

Further experiments (deep inelastic scattering) lead to the conclusion that hadrons do have a substructure. The parton model (Refs. [6] and [7]) with the Bjorken scaling was a success as it managed to reproduce several properties of hadrons in agreement with experiment. In addition it revealed the property of quarks to manifest themselves as almost free particles in the limit of large momentum transfer and therefore to be considered as asymptotically free (Refs. [8], [9], [10], [11]). The scepticism of physicists regarding these fictitious constituents of hadrons was diminished once a theoretical framework of strong interactions was put into place and in terms of which it was argued that particles subject to strong interactions appear freely only as color singlets. This was later on known as confinement and explained why quarks cannot be seen as free particles.

Even if the theory of strong interactions was successfully described in terms of a Yang-Mills theory (non-abelian gauge theory), it was the large coupling constant of strong interactions that lead to considerable difficulties. Due to the strong coupling regular perturbation theory (proved very successful in QED) failed to work at energies of most interest, namely those of the hadron physics.

At a closer look one observes that the quarks account in average only for $\approx 1\%$[1] of the hadron's mass. The remaining mass originates in the dynamics of the quarks within the hadron and obviously cannot be treated as a perturbative correction.

There are however analytical methods for describing such systems perturbatively where the expansion is performed in terms of the momentum rather then the coupling constant. Yet there is a qualitative difference between the two classes of hadrons. In the case of mesons the approximate chiral symmetry and its breaking are exploited in the formalism such that mesons are treated as Goldstone bosons. Baryons on the other hand cannot be treated as Goldstone bosons since they are massive even in the chiral limit. The treatment of both types of hadrons is analogous but the asymptotic states (physical degrees of freedom) that enter the calculations are different.

The method for describing such systems in a perturbative way is chiral perturbation theory. This effective theory does not describe the system in terms of its elementary constituents (quarks) but only in terms of the physical degrees of freedom, namely baryons and mesons. The perturbative treatment is realised as a momentum and not a coupling constant expansion. In the case of a mesonic system the explanation comes from the fact that the physical degrees of freedom (the mesons) are Goldstone bosons and their interaction vanishes at 0 momentum.

It is useful to first determine the symmetries of the underlying full theory, in order to construct an effective theory with the same symmetries built in. Now, inspecting the range of the quark masses, one observes that they differ by 6 orders of magnitude from each other, the up-quark being the lightest one ($1.5 - 3.3$ MeV) and the top-quark the heaviest (171.2 ± 2.1 GeV) [12]. For describing the physics of low energy hadronic matter it is sufficient to account for the physical degrees of freedom of the system by allowing only the lightest quarks to enter the Lagrangian. This is formalized through the statement that heavier virtual quarks (c,b,t) can be integrated out. Furthermore, the energies involved can still be considered much higher then the masses of the remaining 3 quarks, such that one can treat the mass term in the Lagrangian as a perturbation[2]. In this way the Lagrangian exhibits new symmetries.

[1]For instance the proton has a mass of 938 MeV/c^2, whereas the sum of the masses of its constituents, (uud) is between 6 and 12 MeV.

[2]In fact, the mass term in the QCD Lagrangian will be at first dropped completely in order to determine all the symmetries of the Chiral Lagrangian. In the end, when the effective Lagrangian will be determined to a give order, the mass term will be included.

In the following, the symmetries of the QCD Lagrangian in the chiral limit, as well as for small quark masses will be determined. A short introduction to spontaneous symmetry breaking and its application in QCD follows. In the last part, the method for constructing effective Lagrangians is described. This section employs the notation and the line of argument of Ref. [13].

3.1.1. Properties of the chiral Lagrangian

The QCD Lagrangian in the massless limit[3] is:

$$\mathcal{L}_{QCD} = \sum_{l=u,d,s} (\overline{q_{Rl}} \not{D} q_{Rl} + \overline{q_{Ll}} \not{D} q_{Ll}). \tag{3.1}$$

For a short introduction to the QCD Lagrangian and its properties, see appendix B.

The quarks can be also written as a triplet $(u\ d\ s)^T$ and be split into right and left handed parts. The Lagrangian exhibits two global symmetries (each acting separately on the left and right handed components of the triplet):

$$\begin{aligned} \begin{pmatrix} u_L \\ d_L \\ s_L \end{pmatrix} &\rightarrow U_L \begin{pmatrix} u_L \\ d_L \\ s_L \end{pmatrix} = \exp\left(-i\sum_{a=1}^{8}\theta_a^L \frac{\lambda^a}{2}\right) \mathrm{e}^{-i\theta^L} \begin{pmatrix} u_L \\ d_L \\ s_L \end{pmatrix}, \\ \begin{pmatrix} u_R \\ d_R \\ s_R \end{pmatrix} &\rightarrow U_R \begin{pmatrix} u_R \\ d_R \\ s_R \end{pmatrix} = \exp\left(-i\sum_{a=1}^{8}\theta_a^R \frac{\lambda^a}{2}\right) \mathrm{e}^{-i\theta^R} \begin{pmatrix} u_R \\ d_R \\ s_R \end{pmatrix}. \end{aligned} \tag{3.2}$$

The transformation matrices belong to the $SU(3)$ group and are written in terms of the 8 generators of this group[4]. Besides the $SU(3)_L \times SU(3)_R$ symmetry, the QCD Lagrangian has also a global $U(1)_V$ symmetry, whose physical significance is related to the conservation of total baryon number: it is parametrized by

$$\theta_V \equiv \frac{\theta^R + \theta^L}{2}. \tag{3.3}$$

This is a singlet vector current (relative to the $SU(3)_L \times SU(3)_R$ group) of the form: $V^\mu = \overline{q}\gamma^\mu \mathbb{1} q$. So $\mathbb{1}$ is a 3 matrix acting in the flavour space. At the classical level there is also a so called axial $U(1)_A$ symmetry which is parametrized by

$$\theta_A = \frac{\theta^R - \theta^L}{2}. \tag{3.4}$$

[3]The kinetic part of the gluons is not shown.

[4]It is important to specify that the new symmetries of the QCD Lagrangian in the chiral limit are the same as for the gauge symmetry of the strong force. The difference is that the gauge symmetry is a local one, whereas this symmetry is global. Physically, the gauge symmetry acts in the color space where the new $SU(3)$ global symmetry in the flavour space of the massless fermions. If one would have considered only two flavours, the global symmetry would have been $SU(2)$.

However at quantum level it is explicitly broken due to anomalies (Ref. [14]): the corresponding axial current is not conserved: $\partial_\mu A^\mu = \frac{N_f g_s^2}{32\pi^2}\epsilon_{\mu\nu\rho\sigma}\mathrm{Tr}(F^{\mu\nu}F_{\rho\sigma})$. Here, the trace is taken in the flavour space.

The non-singlet global symmetry currents that can be constructed from the Lagrangian with respect to its $SU(3)_L \times SU(3)_R$ symmetries are:

$$\begin{aligned} L^{\mu a} &= \overline{q_L}\gamma^\mu \frac{\lambda^a}{2} q_L, \\ R^{\mu a} &= \overline{q_R}\gamma^\mu \frac{\lambda^a}{2} q_R. \end{aligned} \tag{3.5}$$

They satisfy $\partial_\mu L^{\mu,a} = 0$, $\partial_\mu R^{\mu,a} = 0$.

Often used quantities are linear combinations of these two currents,

$$\begin{aligned} V^{\mu,a} &= R^{\mu,a} + L^{\mu,a}, \\ A^{\mu,a} &= R^{\mu,a} - L^{\mu,a}, \end{aligned} \tag{3.6}$$

because they are parity eigenstates with positive and negative parity, respectively.

Since the chiral Lagrangian exhibits new symmetries, the corresponding charges have to be time independent and therefore to commute with the Hamilton operator. The charges are the zero components of the underlying symmetry currents:

$$\begin{aligned} Q^a_{R/L} &= \int \mathrm{d}^3x \overline{q_{R/L}}\gamma^0(\vec{x},t)\frac{\lambda^a}{2} q_{R/L}(\vec{x},t), \\ Q_V &= \int \mathrm{d}^3x \left[\overline{q_L}(\vec{x},t)\gamma^0 q_L(\vec{x},t) + \overline{q_R}(\vec{x},t)\gamma^0 q_R(\vec{x},t)\right], \end{aligned} \tag{3.7}$$

and obey the following commutation relations:

$$[Q^a_{R/L}, H_{QCD}] = [Q_V, H_{QCD}] = 0. \tag{3.8}$$

Now, using the standard equal time commutation relation of fermionic field operators,

$$\{q_\alpha(\vec{x},t), q^\dagger_\beta(\vec{y},t)\} = \delta^3(\vec{x}-\vec{y})\delta_{\alpha\beta}, \text{ everything else } 0, \tag{3.9}$$

where α and β are spinor indices, it is possible to establish the following commutation relations for the charge operators:

$$\begin{aligned} [Q^a_{L/R}, Q^b_{L/R}] &= i f_{abc} Q^c_{L/R} \\ [Q^a_L, Q^b_R] &= [Q^a_{L/R}, Q^b_V] = 0. \end{aligned} \tag{3.10}$$

The charges Q^a_L and Q^a_R form separately Lie algebras. They act as generators of the respective symmetry transformations.

3.1.2. Explicit symmetry breaking

So far the symmetries of the chiral Lagrangian in the limit of vanishing quark masses have been determined. The non-zero masses of the u, d and s quarks however, produce a term in the QCD Lagrangian which explicitly breaks its invariance under the $SU(3)_L \times SU(3)_R$ group and therefore generates non-vanishing terms for the divergences of the previously introduced currents.

The symmetry breaking term in the Lagrangian is:

$$-\overline{q}Mq = -(\overline{q_L}Mq_R + \overline{q_R}M^\dagger q_L) \tag{3.11}$$

with:

$$M = \begin{pmatrix} m_u & 0 & 0 \\ 0 & m_d & 0 \\ 0 & 0 & m_s \end{pmatrix}. \tag{3.12}$$

The terms in Eq. (3.11) transform non-trivially under $SU(3)_L \times SU(3)_R$,

$$\overline{q_R}Mq_L \to \overline{q_R}U_R^\dagger MU_Lq_L. \tag{3.13}$$

The divergences of the symmetry currents are now:

$$\begin{aligned} &\partial_\mu V^{\mu,a} = i\overline{q}[M, \frac{\lambda^a}{2}]q \\ &\partial_\mu A^{\mu,a} = i\overline{q}\{\frac{\lambda^a}{2}, M\}\gamma_5 q \\ &\partial_\mu V^\mu = 0 \\ &\partial_\mu A^\mu = 2i\overline{q}M\gamma_5 q + \frac{3g_s^2}{32\pi^2}\epsilon_{\mu\nu\rho\sigma}F_a^{\mu\nu}F_a^{\rho\sigma}. \end{aligned} \tag{3.14}$$

The only conserved current corresponds to the $U(1)_V$ symmetry and its physical significance is the baryon number conservation (which is obviously not dependent on the numerical value of the quark masses). The axial current contains also the anomaly term. Furthermore, if the quark masses would be equal, the vector multiplet current would be conserved since the mass matrix would be proportional to the unit matrix and $[\mathbb{1}, \frac{\lambda^a}{2}] = 0$.

3.1.3. Spontaneous symmetry breaking

An important property of the strong interaction is that the ground state of the theory does not exhibit all the symmetries of the (chiral) Lagrangian. However, the theoretical aspects are not well understood and evidence for this phenomenon in strong interactions come rather from experimental data and empirical considerations. Therefore it is useful to start with a simple model that illustrates the underlying dynamics.

Generally, the breaking of a symmetry is said to be spontaneous if the ground state of the Lagrangian describing the physical system does not exhibit the same symmetry as the Lagrangian i.e. the symmetry group under which the ground state is invariant is a subgroup of the symmetry group of the Lagrangian. Every spontaneously broken global continuous symmetry generates massless bosons [15].

The Linear Sigma Model is a toy model of such a theory. In the following section the main ingredients are taken from Peskin and Schröder [1]. The starting point is a Lagrange density composed of N real scalar fields and with $O(N)$ symmetry.

$$\mathcal{L} = \frac{1}{2}(\partial_\mu \phi^i)(\partial^\mu \phi^i) + \frac{1}{2}\mu^2(\phi^i \phi^i) - \frac{\lambda}{4}(\phi^i \phi^i)^2. \tag{3.15}$$

The Lagrangian is invariant under the symmetry transformations of the fields $\phi^i = R_{ij}\phi^j$, R_{ij} being an $N \times N$ orthogonal matrix. An important property of this Lagrangian is that the mass term has the wrong sign (usually $\mathcal{L} = ... - m^2\phi^2$), suggesting that the fields have no physical meaning (their mass would be purely imaginary). The reason for this is that in this form, the Lagrange density does not manifestly describe the ground state, but some unstable state.

The ground state is described by the fields ϕ_0^i that minimise the potential $V(\phi^i) = -\frac{1}{2}\mu^2(\phi^i\phi^i) + \frac{\lambda}{4}(\phi^i\phi^i)^2$:

$$\frac{\partial V(\phi^i)}{\partial \phi_j} = 0 \Rightarrow \phi_0^i \phi_0^i = \frac{\mu^2}{\lambda}. \tag{3.16}$$

This result only determines the length of the vector ϕ_0^i but does not provide any information about the distinct ϕ^i's, so the direction of the vector is arbitrary. The ground state is said to be degenerate.

The fields can be redefined by choosing a preferred direction of the field that minimises the potential:

$$\begin{aligned} &\phi_0^i = (0, ..., 0, v), \text{ where } v = \frac{\mu}{\sqrt{\lambda}} \\ &\phi^i = \left(\pi^k(x), v + \sigma(x)\right), \ k = 1, ..., N-1. \end{aligned} \tag{3.17}$$

By introducing the new field into the Lagrange density the original $O(N)$ symmetry disappears and new types of interaction terms appear:

$$\begin{aligned} \mathcal{L} =& \frac{1}{2}(\partial_\mu \pi^k)(\partial^\mu \pi^k) + \frac{1}{2}(\partial_\mu \sigma)(\partial^\mu \sigma) - \frac{1}{2}(2\mu^2)\sigma^2 \\ &- \sqrt{\lambda}\mu\sigma^3 - \sqrt{\lambda}\mu\sigma(\pi^k\pi^k) - \frac{\lambda}{4}\sigma^4 - \frac{\lambda}{2}(\pi^k\pi^k)\sigma^2 - \frac{\lambda}{4}(\pi^k\pi^k)^2. \end{aligned} \tag{3.18}$$

The Lagrangian describes now $N-1$ massless fields and one massive field $\sigma(x)$ with $m = 2\mu^2$.[5] Besides the kinetic and the mass terms, new types of interactions emerge that couple the σ fields to the π^k 's and simultaneously break the original $O(N)$ symmetry into an $O(N-1)$ symmetry.

[5] Note the correct sign of $2\mu^2$

The $O(N)$ symmetry contains $\frac{N(N-1)}{2}$ independent parameters[6]. After redefinition of the fields, the Lagrangian exhibits an $O(N-1)$ symmetry with only $\frac{(N-1)(N-2)}{2}$ parameters. The difference of independent parameters is the number of broken symmetries and at the same time the number of massless bosons that emerge (Goldstone bosons).

The proof of the Goldstone theorem is as follows: consider a Lagrangian with an arbitrary potential

$$\mathcal{L} = \mathcal{L}_{kin} - V(\phi). \tag{3.19}$$

Let ϕ_0^a be a constant field that minimises the potential. The potential is expanded now about this minimum and one obtains:

$$V(\phi) = V(\phi_0) + \frac{1}{2}(\phi-\phi_0)^a(\phi-\phi_0)^b \left.\frac{\partial^2 V(\phi)}{\partial\phi^a\partial\phi^b}\right|_{\phi_0} + \dots \,. \tag{3.20}$$

The coefficient of the quadratic term can be interpreted as a mass matrix, so its eigenvalues have to be positive.

$$\left.\frac{\partial^2 V}{\partial\phi^a\partial\phi^b}\right|_{\phi_0} = m_{ab}^2. \tag{3.21}$$

Considering now a general continuous transformation of the form

$$\phi^a \to \phi^a + \alpha\Delta^a(\phi) \tag{3.22}$$

the condition that $V(\phi)$ be invariant under this transformation reads:

$$V(\phi^a) = V(\phi^a + \alpha\Delta^a(\phi)) \approx V(\phi^a) + \alpha\Delta^a(\phi)\frac{\partial}{\partial\phi^a}V(\phi). \tag{3.23}$$

Differentiating with respect to ϕ^b at $\phi = \phi_0$, the following equation is obtained:

$$\left(\frac{\partial\Delta^a}{\partial\phi^b}\right)_{\phi_0}\underbrace{\left(\frac{\partial V}{\partial\phi^a}\right)_{\phi_0}}_{=0} + \Delta^a(\phi_0)\left(\frac{\partial^2 V}{\partial\phi^a\partial\phi^b}\right)_{\phi_0} = 0. \tag{3.24}$$

The interpretation of this equation is the following: If the transformation leaves the ground state unchanged ($\Delta^a(\phi_0) = 0$), the equation is satisfied trivially. On the other hand, if the transformation of the field is not a symmetry of the ground state, so $\Delta^a(\phi_0) \neq 0$, then the m_{ab}^2 component of the mass matrix has to vanish and the field corresponding to the eigenvector Δ^a is massless.

3.1.4. Spontaneous symmetry breaking in QCD

The toy model introduced in section 3.1.3 provides a simple picture of the mechanism of spontaneous symmetry breaking and its physical implications. Nevertheless, when trying to investigate the properties of the chiral QCD Lagrangian and the ground state of this theory, several problems occur.

[6]The independent parameters can be determined as follows: A matrix O, belonging to the $O(N)$ group has N^2 elements. The condition $O^T O = 1$ represents $\frac{N(N-1)}{2}$ (off diagonal) and N (diagonal) equations that relate these N^2 elements. The number of independent parameters (degrees of freedom) is finally $N^2 - \frac{N(N-1)}{2} - N = \frac{N(N-1)}{2}$.

There is indirect evidence from experimental data (mainly through the hadron spectrum) and numerical evidence from lattice QCD that suggest spontaneous symmetry breaking. The exact mechanism and the underlying physics of this phenomenon is not well understood since it is not known how the ground state of QCD looks like.

The first indication of spontaneous symmetry breaking (SSB) is the so called parity doubling. Since the left and right handed charge operators (3.7) commute with the Hamiltonian (3.8) and have opposite parity, the occurrence of a state with a positive parity suggests the existence of a degenerate state of negative parity. The measured hadron spectrum on the other hand does not confirm the existence of degenerate states with opposite parities. This indicates that the ground state of the theory is not, as expected, symmetric under the full $SU(3)_L \times SU(3)_R \times U(1)_V$ group.

Another empirical evidence is the organisation of baryons of spin 1/2 and 3/2 into an octet and a decuplet respectively, suggesting $SU(3)$ rather then $SU(3)_L \times SU(3)_R$ as the underlying symmetry. In addition, the octet of the pseudoscalar mesons are viable candidates for Goldstone bosons, due to their relatively small masses in comparison to the baryons.

The theoretical indication for spontaneous symmetry breaking comes from Ref.[16] where it is shown that in the chiral limit the ground state is necessarily invariant under $SU(3)_V \times U(1)_V$ transformation, i.e. the charge operators annihilate the ground state:

$$Q_V^a|0\rangle = Q_V|0\rangle = 0. \tag{3.25}$$

If we draw the attention to the vector and axial vector charge operators and their commutation relation, it is clear that the former do form a closed Lie algebra while the latter do not. Defining

$$Q_{V/A}^a = Q_R^a \pm Q_L^a, \tag{3.26}$$

one has

$$\begin{aligned} [Q_V^a, Q_V^b] &= i f_{abc} Q_V^c, \\ [Q_A^a, Q_A^b] &= i f_{abc} Q_V^c, \\ [Q_V^a, Q_A^b] &= i f_{abc} Q_A^c. \end{aligned} \tag{3.27}$$

Now, since parity doubling does not occur in the hadron spectrum and due to the properties of the vector and axial vector charge operator one is lead to the conclusion that the axial vector charge operator does indeed not annihilate the ground state:

$$Q_A^a|0\rangle \neq 0. \tag{3.28}$$

Another aspect that should be mentioned is that a non-vanishing chiral condensate, $\langle \overline{q} q \rangle$ is a sufficient (but not necessary) condition for spontaneous symmetry breaking to occur in the QCD Lagrangian in the chiral limit. The following proof is rather schematic. For a detailed argumentation see Ref. [13].

First define the following nine scalar and pseudoscalar quark densities:

$$\begin{aligned} S_a(x) &= \overline{q}(x)\lambda^a q(x),\ a = 0, ..., 8 \\ P_a(x) &= \overline{q}(x)\gamma_5\lambda^a q(x),\ a = 0, ..., 8 \end{aligned} \tag{3.29}$$

with $\lambda^0 = \mathbb{1}_{3\times3}$. Knowing the definition of the vector charge operator $Q_V^a(t)$ (Eq. (3.26)) and using the commutation relations of the γ and λ matrices, one can express the eight scalar quark densities as

$$S_a(x) = -\frac{i}{3}\sum_{b,c=1}^{8} f_{abc}[Q_V^b(t), S_c(x)] \tag{3.30}$$

and show that (Eq. (3.25))

$$\langle 0|S_a(x)|0\rangle = 0 \text{ for } a = 1, ..., 8. \tag{3.31}$$

By choosing $a = 3$ and $a = 8$, one obtains through a linear combination:

$$\langle \overline{u}u\rangle = \langle \overline{d}d\rangle = \langle \overline{s}s\rangle. \tag{3.32}$$

Evaluating now the commutator of the axial charge operator with the pseudoscalar quark density for the ground state and using the following commutation relation:

$$i^2[\gamma_5\frac{\lambda_a}{2}, \gamma_0\gamma_5\lambda_a] = \lambda_a^2\gamma_0, \tag{3.33}$$

one obtains:

$$i[Q_a^A(t), P_a(x)] = \begin{cases} \overline{u}u + \overline{d}d, & a = 1, 2, 3 \\ \overline{u}u + \overline{s}s, & a = 4, 5 \\ \overline{d}d + \overline{s}s, & a = 6, 7 \\ \frac{1}{3}(\overline{u}u + \overline{d}d + 4\overline{s}s), & a = 8 \end{cases} \tag{3.34}$$

or generally:

$$\langle 0|i[Q_A^a, P_a(x)]|0\rangle = \frac{2}{3}\langle \overline{q}q\rangle,\ a = 1, ..., 8 \tag{3.35}$$

with $\langle \overline{q}q\rangle = 3\langle \overline{u}u\rangle = 3\langle \overline{d}d\rangle = 3\langle \overline{s}s\rangle$.

Therefore a non-vanishing scalar quark condensate is a sufficient condition for spontaneous symmetry breaking to occur, that is, for the axial charge operator not to annihilate the ground state.

3.1.5. Effective Lagrangians

After determining the properties of the QCD Lagrangian in the chiral limit, and knowing the symmetries that the ground state of QCD should exhibit, the goal is to construct the most general Lagrangian that satisfies the $SU(3)_L \times SU(3)_R \times U(1)_V$ symmetry and that describes the dynamics of the Goldstone bosons associated with the spontaneous symmetry breaking in QCD. Having only this restriction, the Lagrangian would in principle contain an infinity of terms of arbitrarily high order in the fields and as many free parameters. Such theories are not renormalizable. The task that arises from this fact is to organize the Lagrangian in such a way as to determine the importance of diagrams generated by the interaction terms. The free parameters are redefined order by order so that infinities (arising from loop integrals) can be hidden in the following higher orders. This technique of construction of effective theories was proposed by Weinberg [17].

The starting point is a non-linear redefinition of the Goldstone boson fields,

$$U(x) = \exp\left(i\frac{\phi(x)}{F_0}\right) \tag{3.36}$$

where $U(x)$ is a group element of $SU(3)$ and

$$\begin{aligned}\phi(x) = \sum_{a=1}^{8}\lambda_a\phi_a(x) &= \begin{pmatrix} \phi_3 + \frac{1}{\sqrt{3}}\phi_8 & \phi_1 - i\phi_2 & \phi_4 - i\phi_5 \\ \phi_1 + i\phi_2 & -\phi_3 + \frac{1}{\sqrt{3}}\phi_8 & \phi_6 - i\phi_7 \\ \phi_4 + i\phi_5 & \phi_6 + i\phi_7 & -\frac{2}{\sqrt{3}}\phi_8 \end{pmatrix} \\ &= \begin{pmatrix} \pi^0 + \frac{1}{\sqrt{3}}\eta & \sqrt{2}\pi^+ & \sqrt{2}K \\ \sqrt{2}\pi^- & -\pi^0 + \frac{1}{\sqrt{3}}\eta & \sqrt{2}K^0 \\ \sqrt{2}K^- & \sqrt{2}\bar{K}^0 & -\frac{2}{\sqrt{3}}\eta \end{pmatrix}.\end{aligned} \tag{3.37}$$

F_0 is a parameter which is related to the pion decay $\pi^+ \to \mu^+\nu_\mu$ and is known from experimental data ($F_0 \approx 93$ MeV).

Through group theoretical arguments (Ref. [13] Sec. 4.2.2), it is possible to show how $U(x)$ transforms under the action of a group element $g = (L, R)$ of the $SU(3) \times SU(3) = \{(L, R)|L \in SU(3), R \in SU(3)\}$ [7] group, namely

$$U \to U^{'} = R\,U\,L^\dagger. \tag{3.38}$$

The most general Lagrangian that satisfies the required symmetries and with the minimal number of derivatives is:

$$\mathcal{L}_{\text{eff}} = \frac{F_0^2}{4}\text{Tr}(\partial_\mu U\partial^\mu U^\dagger). \tag{3.39}$$

This is easy to check:

$$\mathcal{L}_{\text{eff}}^{'} = \frac{F_0^2}{4}\text{Tr}(R\partial_\mu U\underbrace{L^\dagger L}_{1}\partial^\mu U^\dagger R^\dagger) = \frac{F_0^2}{4}\text{Tr}(\underbrace{R^\dagger R}_{1}\partial_\mu U\partial^\mu U^\dagger) = \mathcal{L}_{\text{eff}}. \tag{3.40}$$

The pre-factor is chosen such that by expanding U in a Taylor series the lowest order terms (so the kinetic part) should be $\frac{1}{2}\partial_\mu\phi_a\partial^\mu\phi_a$. The $U(1)_V$ symmetry is satisfied trivially since Goldstone bosons have baryon number 0 and therefore do not transform.

[7] $L/R = \exp\left(-i\sum_{a=1}^{8}\Theta_a^{L/R}\frac{\lambda^a}{2}\right)$

This is not the entire picture. Given that quark masses are not zero, a mass term has to be included in the lowest order Lagrangian. Since the mass matrix contains only constant values, such a term in the Lagrangian would break the symmetry. If one however, motivated by Eq. (3.11), assigns a transformation law

$$M \to RML^\dagger \tag{3.41}$$

to M, then the QCD Lagrangian is invariant. Therefore a term of the form

$$\mathcal{L}_{SB} = \frac{F_0^2 B_0}{4}\mathrm{Tr}(MU^\dagger + UM^\dagger) \tag{3.42}$$

can be added on the chiral theory side as well. B_0 is related to the chiral quark condensate as $B_0 = -\frac{\langle \overline{q}q\rangle}{3F_0^2}$.

Writing the term quadratic in the ϕ fields explicitly, in the limit that $m_u = m_d = m$, the masses of the mesons can be determined [18]:

$$\begin{aligned} M_\pi^2 &= 2B_0 m, \\ M_K^2 &= B_0(m + m_s), \\ M_\eta^2 &= \frac{2}{3}B_0(m + 2m_s). \end{aligned} \tag{3.43}$$

In order to generalize now Weinberg's procedure, one organises the effective Lagrangian in terms of an increasing order of derivatives and mass terms because the derivatives of the fields are related to the momenta of the respective fields:

$$\mathcal{L}_{\text{eff}} = \mathcal{L}_2 + \mathcal{L}_4 + ... \tag{3.44}$$

For instance, the 2 stands for the second power in the momenta or the first power in the mass matrix, because the meson masses are related to the mass matrix through Eq. (3.43).

The next step in determining the importance of diagrams in calculations is the power counting scheme which is based on the behaviour of diagrams under rescaling of momenta and mass like $p_i \to tp_i$ and $m_q \to t^2 m_q$. Accordingly, diagrams are organized by transformation of their amplitude as:

$$\mathcal{M}(tp_i, t^2 m_q) = t^D \mathcal{M}(p_i, m_q) \tag{3.45}$$

with

$$D = 2 + \sum_{n=1}^{\infty} 2(n-1)N_{2n} + 2N_L, \tag{3.46}$$

N_L being the number of independent loops and N_{2n} stands for the number of vertices coming from $\mathcal{L}_{2n}$.

Before determining the higher order terms in the effective Lagrangian it is important to establish what quantities are of interest, in order to make measurable predictions. The most important object is the S-matrix (scattering matrix), which is related through the LSZ formula to Green's functions or time ordered products of fields evaluated between the vacuum states.

An elegant procedure is to obtain the Green's functions from the generating functional through its functional derivatives with respect to some external fields (see Chap. 2). By introducing these fields the original global symmetry of the theory should be promoted to a local one. The procedure is actually the same used by Gasser and Leutwyler in Refs. [19] and [20] where they introduced in the QCD Lagrangian eight vector and axial vector currents as well as the scalar and pseudoscalar quark densities, $v^{\mu}(x)$, $a^{\mu}(x)$, $s(x)$ and $p(x)$ with the following definition:

$$v^{\mu}(x) = \sum_{a=1}^{8} \frac{\lambda_a}{2} v_a^{\mu},\ a^{\mu}(x) = \sum_{a=1}^{8} \frac{\lambda_a}{2} a_a^{\mu},\ s(x) = \sum_{a=0}^{8} \lambda_a s_a,\ p(x) = \sum_{a=0}^{8} \lambda_a p_a. \tag{3.47}$$

In order for the Lagrangian to have the same (now local) symmetries, the external fields have to be subject to the following transformations:

$$\begin{aligned} r_{\mu} &\to V_R r_{\mu} V_R^{\dagger} + i V_R \partial_{\mu} V_R^{\dagger}, \\ l_{\mu} &\to V_L l_{\mu} V_L^{\dagger} + i V_L \partial_{\mu} V_L^{\dagger}, \\ \chi &\to V_R \chi V_L^{\dagger}. \end{aligned} \tag{3.48}$$

Here the vector and axial vector current have been redefined in terms of the left and right handed vector currents l_{μ} and r_{μ} as:

$$v_{\mu}(x) = \frac{1}{2}(r_{\mu}(x) + l_{\mu}(x)),\ a_{\mu}(x) = \frac{1}{2}(r_{\mu}(x) - l_{\mu}(x)) \tag{3.49}$$

and χ is:

$$\chi = 2B_0(s + ip). \tag{3.50}$$

The derivative terms in Eq. (3.48) have the same role as those in the covariant derivative, namely to compensate for term arising from the kinetic part of the Lagrangian. In addition, the transformation matrices are independent members of the $SU(3)$ group but depend now on the space-time-coordinate x through $\Theta_a^R(x)$ and $\Theta_a^L(x)$ respectively, since we have promoted the original global symmetry to a local one.

Having all the ingredients for writing a Lagrangian with the required symmetries the next step is to express the generating functional as a sequence of effective functionals, each containing an effective Lagrangian of a certain order in momenta:

$$\ln Z_{QCD}[v, a, s, p] = \ln Z_{\text{eff}}^{(2)}[v, a, s, p] + \ln Z_{\text{eff}}^{(4)}[v, a, s, p] + ... \tag{3.51}$$

Now we can sum up the orders of momenta each field contains and try to construct the most general effective Lagrangian of a given order:

$$\begin{aligned} &U = \mathcal{O}(p^0) \\ &D_\mu U,\, r_\mu,\, l_\mu = \mathcal{O}(p^1) \\ &f_{\mu\nu}^{L/R},\, \chi = \mathcal{O}(p^2), \end{aligned} \tag{3.52}$$

where $f_{\mu\nu}^{L/R}$ is the field strength tensor of r_μ and l_μ respectively:

$$\begin{aligned} f_{\mu\nu}^R &= \partial_\mu r_\nu - \partial_\nu r_\mu - i[r_\mu, r_\nu], \\ f_{\mu\nu}^L &= \partial_\mu l_\nu - \partial_\nu l_\mu - i[l_\mu, l_\nu]. \end{aligned} \tag{3.53}$$

Given two objects, A and B, that transform as $A^{'} = V_R A V_L^\dagger$ (and B in a similar way), the simplest invariant object to form is $\mathrm{Tr}(AB^\dagger)$ since

$$\mathrm{Tr}(AB^\dagger) \to \mathrm{Tr}[V_R A V_L^\dagger (V_R B V_L^\dagger)^\dagger] = \mathrm{Tr}(V_R A V_L^\dagger V_L B^\dagger V_R^\dagger) = \mathrm{Tr}(AB^\dagger). \tag{3.54}$$

The only candidates for such invariant objects up to $\mathcal{O}(p^2)$ are: U, $D_\mu U$, $D_\mu D_\nu U$, χ, $U f_{\mu\nu}^L$, $f_{\mu\nu}^R U$. In addition, by imposing Lorentz invariance, the most general Lagrangian to $\mathcal{O}(p^2)$ is:

$$\mathcal{L}_2 = \frac{F_0^2}{4}\mathrm{Tr}[D_\mu U (D^\mu U)^\dagger] + \frac{F_0^2}{4}\mathrm{Tr}(\chi U^\dagger + U\chi^\dagger). \tag{3.55}$$

From this Lagrangian one obtains the generating functional $Z_{\mathrm{eff}}^{(2)}[v, a, s, p]$, from which it is possible to calculate the desired Green functions.

The free parameters of higher order Lagrangians contain information about the dynamics and can in principle be calculated by other techniques like empirical data, or lattice QCD calculations [21]. They encode the dynamics of QCD in the non-perturbative regime.

3.1.6. Conclusions

It has been shown that it is possible to exploit the approximate chiral symmetry of the QCD Lagrangian as well as the observed, but not yet well understood spontaneous symmetry breaking of this symmetry in order to construct an effective theory that is applicable at low energies, far beyond the reach of the perturbative approach with the full (physical) QCD Lagrangian.

Of course, the issues presented here are not the whole picture. As for the mesons, there is a similar approach for the heavier degrees of freedom, the baryons. This however, would be beyond the scope of this thesis since only the light degrees of freedom, the mesons (pseudo Goldstone bosons) are important in accounting for finite size effects.

3.2. Effective thermal field theory

Not only low energy particle physics has gained importance in the past decades but also hot and dense hadronic matter. This is due to the fact that hadronic matter under these conditions is relevant for many different areas of physics. First of all, the theoretical understanding of hot matter is important for describing the early universe as it is believed that this was the initial state of matter right after the Big Bang [22]. Also different properties of quantum fields at extreme temperatures such as the electro-weak phase transition may account for the electro-weak baryogenesis. Closely related to cosmology is astrophysics within which neutron stars and other massive objects are constituted of elementary matter under extreme conditions and therefore describable with this theory. Equally important is the study of heavy ion collisions. Collision experiments of gold ions and lead ions (RHIC at BNL New York, CERN in Geneva, GSI in Darmstadt) try to reveal the theoretically predicted but not yet observed and well understood quark gluon plasma. This plasma (QGP) is a new phase occurring above temperatures of $T_c \approx 175$ MeV and is believed to arise due to the asymptotic freedom of QCD.

Difficulties arise however when trying to push calculations beyond the leading order. First it is the large coupling of the strong force that renders a perturbative weak coupling expansion applicable only beyond huge temperatures $\approx 10^5$ GeV. However, different techniques that will be treated in this section to some extent can push the applicability of perturbation theory to lower temperatures.

Secondly, as seen in Chapter 2, the finite dimension of the imaginary time direction (the finite temperature) leads to a sum over Matsubara modes, which in the case of bosons include the $n = 0$ mode. It turns out that this mode is most sensible to thermal effects and leads to infrared divergences.

Different techniques have been developed to deal with these problems. The most straightforward is to use effective theories that separate the degrees of freedom most sensitive to infrared problems from those that are of ultraviolet type and can be handled perturbatively. In this manner the theory becomes simpler and still exhibits the correct temperature dependence.

Since the correspondence of finite temperature field theory and field theory at $T = 0$ is straight-forward, lattice calculations can be carried out also for hot matter. Actually through numerical calculations a possible phase transition from ordinary hadronic matter to quark gluon plasma was established at temperatures of $T_c \approx 175$ MeV.

Just how in chiral perturbation theory the light pseudo-Goldstone bosons account for most of the finite size effects in numerical calculations, finite size effects appear also in thermal field theory. They depend not only on the mass gap of the theory but also on the temperature.

In the following sections difficulties that arise in thermal field theories are briefly exposed and the main ingredients for writing an effective theory of QCD are presented. Notation and the line of argument are partially used from Ref. [4]. Having the effective theory it is possible to carry out lattice calculations and numerically determine quantities of interest.

3.2.1. Thermal masses and resummation

In order to proceed to the effective theory approach it is important to understand the main features of an interacting thermal field theory [4]. As seen in Chapter 2 it is not possible to obtain an exact result of the free energy of a system and a power expansion is always necessary.

Going now to the interacting theory an expansion in terms of the coupling constant of the respective theory is desired. However, at next to leading order divergences occur and some resummation technique has to be used in order to get rid of these divergences. Closely related to this problem is the occurrence of a new scale in the problem generated by a so-called thermal mass. All these new features render the perturbative expansion non-trivial.

Using a real scalar field with ϕ^4 interaction, the interaction action is

$$S_I = \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3\mathbf{x}\mathcal{L}_I = \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^3\mathbf{x}\frac{\lambda}{4}\phi^4. \tag{3.56}$$

Therefore, the partition function reads:

$$Z(T) = C\int \mathcal{D}\phi e^{-S_0 - S_I} = C\int \mathcal{D}\phi e^{-S_0}\left[1 - \langle S_I\rangle_0 + \frac{1}{2}\langle S_I^2\rangle_0 - ...\right], \tag{3.57}$$

where the exponential factor e^{-S_I} has been expanded in Taylor series. The thermal average in the free theory is defined as:

$$\langle ...\rangle_0 = \frac{C\int \mathcal{D}\phi[...]\mathrm{exp}(-S_0)}{C\int \mathcal{D}\phi\,\mathrm{exp}(-S_0)}. \tag{3.58}$$

The free energy density can then be calculated as follows:

$$\begin{aligned} f(T) &= -\frac{T}{V}\mathrm{ln}Z = \frac{F_{(0)}}{V} - \frac{T}{V}\mathrm{ln}\left[1 - \langle S_I\rangle_0 + \frac{1}{2}\langle S_I^2\rangle_0 - ...\right] \\ &= \frac{F_{(0)}}{V} - \frac{T}{V}\left\{-\langle S_I\rangle_0 + \frac{1}{2}\underbrace{\left[\langle S_I^2\rangle_0 - \langle S_I\rangle_0^2\right]}_{=\langle S_I^2\rangle_{0,c}} - ...\right\}. \end{aligned} \tag{3.59}$$

By expanding $\ln(1-x) = -x - x^2/2 - ...$ only the connected diagrams remain at each order in λ. For instance, terms of the form: $\bigcirc \cdot \bigcirc$ are cancelled. The first term in Eq. (3.59) is just the free energy density determined in Chapter 2:

$$f_{(0)} = J(m,T). \tag{3.60}$$

The next term, of order $\mathcal{O}(\lambda^1)$, is calculated in terms of the scalar field propagator in the free theory.

$$\langle\phi(x)\phi(y)\rangle_0 \equiv G_0(x-y) = T\sum_n \int \frac{\mathrm{d}^3\mathbf{k}}{(2\pi)^3}e^{iP(x-y)}\frac{1}{P^2+m^2}. \tag{3.61}$$

The integration variable P is defined as $P \equiv (\omega_n, \mathbf{p})$. Evaluated at $x = y$, the field propagator becomes just (cf. Eq. (2.28)):

$$G_0(0) = T \sum_n \int \frac{\mathrm{d}^3\mathbf{p}}{(2\pi)^3} \frac{1}{P^2 + m^2}. \tag{3.62}$$

With these notations, the next term in the expansion of the free energy density can finally be written as:

$$\begin{aligned} f_{(1)}(T) = \lim_{V\to\infty} \frac{T}{V} \langle S_I \rangle_0 &= \lim_{V\to\infty} \frac{T}{V} \int_0^\beta \mathrm{d}\tau \int_V \mathrm{d}^3\mathbf{x} \frac{\lambda}{4} \langle \phi(x)\phi(x)\phi(x)\phi(x)\rangle_0 \\ &= \frac{3}{4}\lambda \langle \phi(0)\phi(0)\rangle_0 \langle \phi(0)\phi(0)\rangle_0 \\ &= \frac{3}{4}\lambda [I(m,T)]^2. \end{aligned} \tag{3.63}$$

In the last relation Wick's theorem and the translational invariance of $\langle \phi(x)\phi(y)\rangle_0$ was used and therefore the integrals became trivial. The factor 3 is a combinatorial factor arising from all the possibilities of combining 4 identical fields.

In the same manner $f_{(2)}$ of $\mathcal{O}(\lambda^2)$ can be determined:

$$\begin{aligned} f_{(2)}(T) &= \lim_{V\to\infty} \left[-\frac{T}{2V} \left(\langle S_I^2 \rangle_0 - \langle S_I \rangle_0^2 \right) \right] \\ &= -\frac{\lambda^2}{16} \left[12 \int_0^\beta \mathrm{d}\tau \int_V \mathrm{d}^3\mathbf{x} \langle \phi(x)\phi(0)\rangle_0^4 + 36 \langle \phi(0)\phi(0)\rangle_0^2 \int_0^\beta \mathrm{d}\tau \int_V \mathrm{d}^3\mathbf{x} \langle \phi(x)\phi(0)\rangle_0^2 \right]. \end{aligned} \tag{3.64}$$

Again $f_{(2)}$ can be rewritten as

$$f_{(2)}(T) = -\frac{3}{4}\lambda^2 \int_0^\beta \mathrm{d}\tau \int_V \mathrm{d}^3\mathbf{x} [G_0(x)]^4 - \frac{9}{4}\lambda^2 [I(m,T)]^2 \int_0^\beta \mathrm{d}\tau \int_V \mathrm{d}^3\mathbf{x} [G_0(x)]^2. \tag{3.65}$$

However, these three terms (Eqs. (3.60), (3.63) and (3.65)) cannot be simply added together because they are functions of the bare parameters $m \equiv m_B$ and $\lambda \equiv \lambda_B$. First, the bare parameters have to be expressed in terms of the renormalized ones[8], $m_B = m_B(m_R, \lambda_R)$, $\lambda_B = \lambda_B(m_R, \lambda_R)$. The renormalized parameters should be chosen in such a way that in the weak interaction limit, $\lambda_R \ll 1$, these relations can be written as an expansion in terms of λ_R:

$$\begin{aligned} m_B^2 &= m_R^2 + \lambda_R f(m_R^2) + \mathcal{O}(\lambda_R^2) \\ \lambda_B &= \lambda_R + \lambda_R^2 g(m_R^2) + \mathcal{O}(\lambda_R^3). \end{aligned} \tag{3.66}$$

The function f is determined by choosing a specific scheme, in which for instance the physical mass corresponds to the exponential fall-off factor of the propagator for a particle at rest, $\exp(-m_R\tau)$. Calculating the propagator $\langle \phi(x)\phi(0)(1 - S_I)\rangle_{0,c}$ in the 0 temperature limit up to $\mathcal{O}(\lambda_B)$, the physical mass can be read off from the pole of the propagator:

$$m_R^2 = m_B^2 + 3\lambda_B I_0(m_B) \text{ for } T = 0. \tag{3.67}$$

[8]The renormalization of parameters is performed at $T = 0$ since thermal effects do not modify short-distance (ultraviolet) divergences (cf. Ref. [23]).

Here, $I_0(m)$ denotes the $n = 0$ part of $I(m,T)$. The 0 mass limit is interesting through the way the soft modes that become increasingly important, change the qualitative behaviour of $f(T)$. For the particular case of vanishing mass, the bare mass can be directly replaced with the renormalized one, since $I_0(0) = 0$.

In the limit of small masses the high temperature expansion can be used to express the 3 leading terms of the free energy density:[9]

$$f_{(0)}(T) = J(m_B, T) = -\frac{\pi^2 T^4}{90} + \frac{m_B^2 T^2}{24} - \frac{m_B^3 T}{12\pi} + \mathcal{O}(m_B^4), \tag{3.68}$$

$$\begin{aligned} f_{(1)}(T) &= \frac{3}{4}\lambda_B [I(m_B, T)]^2 \\ &= \frac{3}{4}\lambda_B \left[\frac{T^4}{144} - \frac{m_B T^3}{24\pi} + \mathcal{O}(m_B^2 T^2)\right], \end{aligned} \tag{3.69}$$

$$f_{(2)}(T) = -\frac{9}{4}\lambda_B^2 \frac{T^4}{144}\frac{T}{8\pi m_B} + \mathcal{O}(m_B^0). \tag{3.70}$$

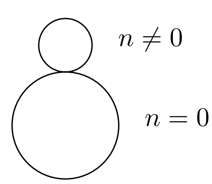
All the odd powers of m_B are associated with the zero Matsubara modes, either they come directly from these modes, as in the case of $f_{(0)}$ or they are some products of zero Matsubara modes with leading non-zero modes, as in $f_{(1)}$ and $f_{(2)}$.

Taking the fractions of the odd terms in m_B to each order, one obtains

$$\frac{\delta_{\mathrm{odd}} f_{(1)}}{\delta_{\mathrm{odd}} f_{(0)}} \sim \frac{\delta_{\mathrm{odd}} f_{(2)}}{\delta_{\mathrm{odd}} f_{(1)}} \sim \frac{\lambda_B T^2}{8 m_B^2}. \tag{3.71}$$

It is obvious that in the limit $m_B \to 0$ odd terms of higher order in λ_B become increasingly important, leading to a breakdown of the perturbative series. To solve this problem one can try to sum up every first odd term in m_B to all orders and hope that by taking afterwards the limit $m_B \to 0$ the result will be finite.

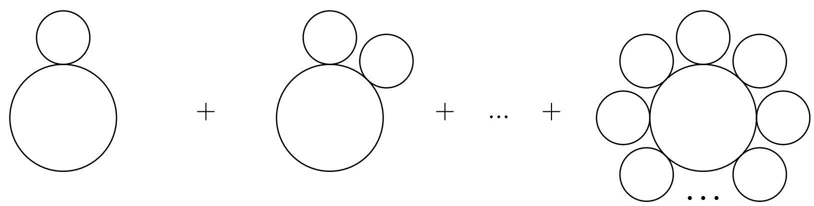
Inspecting the structure of the odd terms, one observes that they are produced by a product of one 0 Matsubara mode contribution and, to a given order, the corresponding number of non-zero mode contributions. Diagrammatically, the odd terms are given by ring diagrams of the form:



[9]The bare quantities are used throughout the calculation and only in the end they will be replaced by the renormalized quantities.

The larger circle is to be seen as only the $n = 0$ mode contribution of the loop while the smaller (outer) one contains only the non-zero modes.

The purpose is to sum these diagrams to all orders:



At order N the first odd term in m_B is

$$\frac{(-1)^{N+1}}{N!}\left(\frac{\lambda_B}{4}\right)^N 6^N 2^{N-1}(N-1)!\left[\underbrace{\frac{T^2}{12}}_{=I'(0,T)}\right]\underbrace{T\int\frac{\mathrm{d}^d\mathbf{p}}{(2\pi)^d}\left(\frac{1}{\mathbf{p}^2+m_B^2}\right)^N}_{\text{zero-mode ring}}, \tag{3.72}$$

where $I^{'}(0,T)$ denote the non-zero-mode ring. The zero-mode contribution can generally be expressed as:

$$\int\frac{\mathrm{d}^{3-2\epsilon}\mathbf{p}}{(2\pi)^{3-2\epsilon}}\frac{1}{(\mathbf{p}^2+m_B^2)^N} = \frac{(-1)^{N+1}}{(N-1)!}\left(\frac{\mathrm{d}}{\mathrm{d}m_B^2}\right)^N\left(\frac{m_B^3}{6\pi}\right) \tag{3.73}$$

so that the odd term at order N is

$$\delta_{\text{odd}}f_{(N)} = -\frac{T}{2}\frac{1}{N!}\left(\frac{\lambda_B T^2}{4}\right)^N\left(\frac{\mathrm{d}}{\mathrm{d}m_B^2}\right)^N\left(\frac{m_B^3}{6\pi}\right). \tag{3.74}$$

This term looks just as the Nth term of a Taylor expansion. So summing the odd terms to all orders in λ_B, one gets

$$\sum_{N=0}^{\infty}\delta_{\text{odd}}f_{(N)} = -\frac{T}{12\pi}\left(m_B^2+\frac{\lambda_B T^2}{4}\right)^{\frac{3}{2}}. \tag{3.75}$$

Collecting all remaining terms of $f_{(0)}$, $f_{(1)}$ and $f_{(2)}$ after sending m_B (and implicitly m_R) to 0, the free energy density becomes:

$$f(T) = -\frac{\pi T^4}{90}\left[1-\frac{15}{32}\frac{\lambda_R}{\pi^2}+\frac{15}{16}\left(\frac{\lambda_R}{\pi^2}\right)^{\frac{3}{2}}+\mathcal{O}(\lambda_R^2)\right], \tag{3.76}$$

with $\lambda_B = \lambda_R + \mathcal{O}(\lambda_R^2)$.

The zero mode contribution of the Matsubara sums gives rise to infrared divergences that can be eliminated only through resummation. Furthermore the resummation procedure accounts for the non-analyticity of the loop expansion. At increasing order in the coupling parameter, the non-analytical structure of the expansion remains due to the fact that at each order zero Matsubara modes give rise to infrared divergences.

Closely related to the infrared divergences occurring from the soft modes is the thermal mass. The procedure of resummation can be avoided by introducing in the free Lagrange density an effective mass for the $n = 0$ field, $(1/2)m_{\text{eff}}^2\phi_{n=0}^2$ and substracting the same quantity from the interacting part of the Lagrange density. Following the procedure of mass renormalization, the effective mass can be read again from the pole of the field propagator:

$$m_{\text{eff}}^2 \underset{m_B \to 0}{=} \frac{\lambda_R T^2}{4} + \mathcal{O}(\lambda_R^2) \tag{3.77}$$

Due to the small coupling constant this effective mass plays a role only for the Matsubara zero mode, and prevents it from exhibiting the typical divergent behaviour as one would normally expect. Therefore the free energy density can be rewritten up to the term $f_{(1)}$ as:

$$f(T) = -\frac{\pi^2 T^4}{90} + \frac{3}{4}\lambda_R \frac{T^4}{144} - \frac{m_{\text{eff}}^3 T}{12\pi} + \mathcal{O}(\lambda_R^2). \tag{3.78}$$

So the last term in Eq. (3.78) is nothing else but the leading order contribution, $\mathcal{O}(\lambda_R^0)$ of the Matsubara zero-mode to the free energy density arising from thermal effects.

In the case of QCD, the calculations are similar, merely the result differs partially. Since QCD is a non-abelian gauge theory, the gauge bosons (gluons) are subject also to self-coupling, which in terms of the QCD coupling constant is of the order $\mathcal{O}(g^2)$.

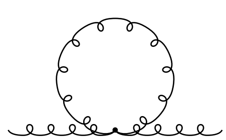
The procedure works as follows. The full gluon propagator $\langle \tilde{A}_\mu^a(P)\tilde{A}_\nu^b(Q)\rangle$ [10] will be calculated to $\mathcal{O}(g^2)$ and will be expressed for small momenta as

$$\delta_{A,B} \cdot \frac{1}{P^2 + m_{\text{eff}}^2}, \tag{3.79}$$

where A and B stand for all indices of the gauge fields A_μ^a. The propagator to $\mathcal{O}(g^2)$ is

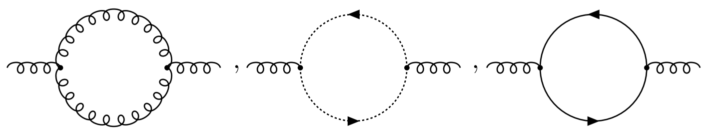
$$\langle \tilde{A}_\mu^a(P)\tilde{A}_\nu^b(P)(1 - S_I + \frac{1}{2}S_I^2)\rangle_{0,c}. \tag{3.80}$$

The $-S_I$ term contributes with the self-energy of the gluon:



The $\frac{1}{2}S_I^2$ term contributes with the 3-vertex diagrams: gluon-fermion, gluon-ghost and gluon self-interaction.

[10]The tilde over A denotes the vector field in the Fourier space.



After calculating the contributions of all these terms, the propagator reads:

$$
\begin{aligned}
&\langle \tilde{A}^a_\mu(P)\tilde{A}^b_\nu(Q)(-S_I+\frac{1}{2}S_I^2)\rangle_{0,c} \\
&= -g^2\frac{\delta^{ab}\delta(P+Q)}{(P^2)^2}\left\{\left[\left(3+\frac{3}{2}-\frac{1}{2}\right)N_c+2N_f\right]\delta_{\mu 0}\delta_{\nu 0}+\left[\left(3-\frac{7}{2}+\frac{1}{2}\right)N_c\right]\delta_{\mu i}\delta_{\nu i}\right\}\frac{T^2}{12}+\mathcal{O}(g^4) \\
&= -\frac{\delta^{ab}\delta(P+Q)}{(P^2)^2}\delta_{\mu 0}\delta_{\nu 0}\cdot g^2T^2\left(\frac{N_c}{3}+\frac{N_f}{6}\right)+\mathcal{O}(g^4),
\end{aligned}
\tag{3.81}
$$

where N_c denotes the number of colors of the gauge fields and N_f the number of flavours of the fermions. The contribution is of order $1/(P^2)^2$ and does not have the structure of a propagator as (3.79) but it can be considered as the second term of a Taylor expansion. Tracing the expansion back, one obtains

$$
\langle \tilde{A}^2_\mu(P)\tilde{A}^b_\nu(Q)\rangle \approx \frac{\delta^{ab}\delta(P+P)}{\tilde{P}+\delta_{\mu 0}\delta_{\nu 0}m_{\mathrm{E}}^2}
\tag{3.82}
$$

with

$$
m_{\mathrm{E}}^2 = g^2T^2\left(\frac{N_c}{3}+\frac{N_f}{6}\right).
\tag{3.83}
$$

Several conclusions can be drawn. First of all m_{E} is of order $\mathcal{O}(g)$ indicating non-analyticity of $f(T)$ (cf. Eq. (3.78)) in the weak coupling expansion. Secondly, it only affects the "time" component of the A_μ field due to the prefactor $\delta_{\mu 0}\delta_{\nu 0}$. Therefore it is said that at next to leading order only color-electric fields are screened in a QCD plasma. The occurrence of an electrostatic screening mass introduces also an additional scale in the problem of order $\sim gT$.

The calculation of the magnetic screening mass raises however more problems. As seen previously it vanishes at the gT scale. It is generally believed that the contribution from the magnetic mass is of order g^2T ([24], [25], [26]). Also in Refs. [27] and [28], based on dimensionally reduced QCD, it is stated that the magnetic screening mass should be of order g^2T. This fact has two implications. Starting from this premise, the contribution to the free energy involving only four-gluon couplings is

$$
\delta f_N(T) = g^6T^4\left(\frac{g^2T}{m(T)}\right)^{N-3},
\tag{3.84}
$$

N being the number of vertices. Replacing now $m(T)$ with $\# \cdot g^2T$ the contribution from individual diagrams becomes of order g^6T^4 and their sum cannot be estimated in a loop expansion. Second, through similar arguments it is shown that the magnetic screening mass cannot be calculated or even defined unambiguously, being purely non-perturbative.

This is the famous infrared problem of QCD which shows that perturbation theory loses its predictive power at higher order even if renormalization group arguments state that the coupling becomes small at high energies.

So far the only way to overpass this difficulty is through lattice calculations. These can be carried out using effective theories where the coupling constants are determined analytically through perturbative calculations from the full theory.

3.2.2. Effective thermal field theory approach

As seen in chapter 2, zero Matsubara modes are the most infrared sensitive degrees of freedom. Due to these modes, theories often exhibit infrared divergences (see massless scalar fields) and give rise to the necessity of using resummation in order to render physical quantities finite.

Generally, in order to predict whether different effects are perturbative or non-perturbative ones, it is useful to determine the magnitude of the expansion parameter. For that the most general dimensionless expansion parameter is determined for both bosons and fermions. Here, only that for bosons is of interest.

With increasing order in the expansion, an additional vertex factor appears which is denoted as g^2. Since summation over Matsubara modes involve a factor T, a preliminary expansion parameter is g^2T. In order to generate a dimensionless expansion parameter, the mass has to be used also:

$$\epsilon_b \sim \frac{g^2 T}{m}. \tag{3.85}$$

Thus, closely related to the discussion of the previous section, it seems that due to the mass dependence of the expansion parameter the perturbation expansion may break down in different regimes. For instance the zero Matsubara mode appears to be non-perturbative in the limit of vanishing mass. Furthermore, due to resummation of ring diagrams an effective mass (colour electrical screening) occurs and is of the order $m_{\text{eff}}^2 \sim g^2T^2$ so that the bosonic expansion parameter becomes $\epsilon_b \sim \frac{g^2T}{gT} = g$. This shows that the expansion is still valid and the terms are finite but the structure of the expansion becomes peculiar (Eq. (3.76)). As the magnetic screening mass is of order g^2T, colour magnetic screening is expected to be a purely non-perturbative effect since $\epsilon_b \sim 1$.

Generally speaking the system seems to posses a so-called scale hierarchy, not only common to thermal field theories but also to effective theories at vanishing temperature. The scale is expressed as $g^2T/\pi \ll gT \ll \pi T$. The first scale refers to non-perturbative effects such as screening of color magnetic fields in a QCD plasma. The second scale refers to the perturbative scale where resummation is required and the last scale refers to the purely perturbative scale.

The breakdown of perturbation theory at high temperatures can be understood physically in the following way [29]. At low temperatures perturbation theory is applied for processes where only a small number of particles participate in. At high temperatures the number of particles that participate in collisions increases, especially for the bosonic degrees of freedom for which the amplification factor is the bosonic distribution function,

$$n_B(E) = \frac{1}{\exp(\frac{E}{T}) - 1},\ E \equiv \sqrt{k^2 + M^2}, \tag{3.86}$$

and the expansion parameter becomes $g^2 n_B(E)$. In the small momentum limit, through expansion of the distribution function into a Taylor series, one obtains the previous result:

$$g^2 n_B(E) \approx \frac{g^2 T}{m}. \tag{3.87}$$

For dealing with non-perturbative effects and infrared divergences, effective field theory is used, in which the strongly coupled soft modes (the ones that generate infrared divergences) are factorized from the weakly coupled high-momentum modes into a simple Lagrangian.

Knowing the structure of the partition function, one can expand the field into a Fourier sum for the time coordinate as shown in Eq. (2.15):

$$\phi(x, \tau) = \sum_{n=-\infty}^{\infty} \phi_n(x) \exp(i\omega_n^b \tau),\ \omega_n^b = 2\pi n T. \tag{3.88}$$

Placing now the expansion into the action, it is possible to carry out the integration over the time variable and obtain a 3-dimensional action corresponding to a 3-dimensional Lagrange density composed of an infinity of fields. Schematically the procedure is

$$S_E = \int \mathrm{d}^4 x \mathcal{L} \to \sum \int \mathrm{d}^3 x \mathcal{L}^{3d}. \tag{3.89}$$

The masses of the new fields depend now on ω_n^b.

Now the heavy modes (with masses $\sim \pi T$) of the 3d theory interact only weakly with each other and can be integrated out

$$\exp(-S_{\text{eff}}) \simeq \int \mathcal{D}\psi \mathcal{D}\phi_{n\neq 0} \exp(-S_E). \tag{3.90}$$

The effective action can be written as

$$S_{\text{eff}} \simeq cVT^3 + \int \mathrm{d}^3 x \left[L_b(T) + \sum_{n=0}^{\infty} \frac{O_n}{T^n} \right]. \tag{3.91}$$

Here $L_b(T)$ is a 3d super-renormalizable effective Lagrangian containing temperature dependent constants. O_n are higher order operators and are suppressed by powers of temperature.

Once a 3-dimensional Lagrangian has been determined all the parameters entering the 3d Lagrangian have to be determined also. This is done by constructing Green's functions with the effective

Lagrangian and requiring that the they match with a certain accuracy to the static 4-dimensional Green's functions:

$$G^{3d}(k_1, ..., k_n) = G^{4d}_{\omega=0}(k_1, ..., k_n)(1 + \mathcal{O}(g^m)). \tag{3.92}$$

The number of higher order operators O_n that are included in the effective Lagrangian depends on the desired accuracy.

As a consistency check the scales that enter the new effective Lagrangian should be smaller than scale that has been integrated out

$$\frac{m_{\text{eff}}}{2\pi T} \ll 1 \tag{3.93}$$

With the effective action the partition function can be calculated and other quantities of interest. Non-perturbative methods can also be used such as numerical simulations on the lattice.

3.2.3. Dimensionally reduced QCD

As outlined in the introductory chapter, finite temperature QCD is of particular interest in high energy physics due to its theoretical relevance for heavy ion collisions, as well as cosmological problems and effects related to these topics such as the quark gluon plasma and phase transitions.

The goal is to write an effective $SU(3)$ gauge theory that describes only the soft modes, those that are most sensitive to IR effects. Since fermions are not affected by IR effects due to the lack of the Matsubara zero mode, only the gluonic part of the QCD Lagrangian [11] will be written

$$\mathcal{L} = -\frac{1}{4}F^{a\mu\nu}F^a_{\mu\nu} \tag{3.94}$$

with

$$F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + gf^{abc}A^b_\mu A^c_\nu. \tag{3.95}$$

For the properties of the QCD Lagrangian recall appendix B.

Since the vector fields A^a are bosons, the infrared sensitive modes are the zero Matsubara modes that do not depend on the τ coordinate. Therefore the effective theory will be $d = 3 - 2\epsilon$ dimensional (Refs. [28], [30]). In addition, the effective Lagrangian has to inherit the symmetries of the original theory. The heat bath breaks Lorentz invariance but since the effective theory is a 3 dimensional it needs to be symmetric only in the spatial directions.

The underlying gauge symmetry

$$A^{'}_\mu = UA_\mu U^{-1} + \frac{i}{g}U\partial_\mu U^{-1} \tag{3.96}$$

[11] The folowing derivation of the effective QCD Lagrangian is taken from Ref. [4]. Originally, these calculations were performed in Refs. [27] and [28].

reads now [12]

$$\begin{aligned} A_i^{'} &= UA_iU^{-1} + \frac{i}{g}U\partial_i U^{-1}, \\ A_0^{'} &= UA_0U^{-1}, \end{aligned} \tag{3.97}$$

where U does not depend on τ since the static limit is considered. The effective theory is described in the static limit by a d-dimensional bosonic vector field and a scalar field A_0 in the adjoint representation.

With these ingredients note that Eq. (B.17) becomes:

$$F_{i0}^a = \mathcal{D}_i^{ab} A_0^b \tag{3.98}$$

and the Lagrangian can be written as

$$\mathcal{L} = \frac{1}{4} F_{ij}^a F_{ij}^a + \frac{1}{2} (\mathcal{D}_i^{ab} A_0^b)(\mathcal{D}_i^{ac} A_0^c). \tag{3.99}$$

By rewriting

$$\frac{\lambda^a}{2} \mathcal{D}_i^{ab} A_0^b = \partial_i A_0 + g f^{acb} \frac{\lambda^a}{2} A_i^c A_0^b = \partial_i A_0 - ig[A_i, A_0] = [D_i, A_0], \tag{3.100}$$

where D_i is the covariant derivative in the fundamental representation (see appendix B), the effective Lagrangian reads

$$\mathcal{L}_{\text{eff}}^{(0)} = \frac{1}{4} F_{ij}^a F_{ij}^a + \text{Tr}\{[D_i, A_0][D_i, A_0]\}. \tag{3.101}$$

As a next step, one can add terms of increasing order built up of the vector fields A_i^a and the scalars A_0^a. Operators of the lowest dimensionalities are

$$\begin{aligned} &\text{dim=2: } \text{Tr}[A_0^2]; \\ &\text{dim=4: } \text{Tr}[A_0^4],\ (\text{Tr}[A_0^2])^2; \\ &\text{dim=6: } \text{Tr}\{[D_i, F_{ij}][D_k, F_{kj}]\},\ \text{Tr}[A_0^6], ... \end{aligned} \tag{3.102}$$

The effective action thus becomes

$$\begin{aligned} S_{\text{eff}} = &\frac{1}{T} \int \mathrm{d}^d \mathbf{x} \left\{ \frac{1}{4} F_{ij}^a F_{ij}^a + \text{Tr}([D_i, A_0][D_i, A_0]) + m_E^2 \text{Tr}[A_0^2] \right. \\ &\left. + \lambda^{(1)} (\text{Tr}[A_0^2])^2 + \lambda^{(2)} \text{Tr}[A_0^4] + ... \right\}. \end{aligned} \tag{3.103}$$

The prefactor $1/T$ comes from the integration over τ. Since no field depends on τ the integration is trivial and generates only this prefactor.

Instead of going further with the simplification of the effective theory down to the scale of g^2T, the concrete procedure of calculating the free energy of a gluon gas is sketched as done in Ref. [31].

[12] The same notation as for A_μ^a was used for the new fields A_i^a and A_0^a.

The procedure is as follows: first, the momentum scale πT is integrated out, generating the EQCD effective theory that describes the system at length scales of $1/(gT)$. Next, the gT scale is integrated out from the EQCD Lagrangian generating thus a Lagrangian which contains the lowest scale, g^2T/π. This Lagrangian describes the physics at length scales of $\pi/(g^2T)$ and is purely non-perturbative. After having separated all existing scales from each other the coefficients of effective Lagrangians have to be calculated by matching with the Lagrangian of full QCD. Having determined the coefficients to the desired precision, lattice calculations can be performed with the MQCD Lagrangian.

The free energy density can be written as a sum of contributions coming from these three scales:

$$f(T) = f_{\mathrm{QCD}}(\pi T, \Lambda) + f_{\mathrm{EQCD}}(gT, \Lambda, \Lambda^{'}) + f_{\mathrm{MQCD}}(g^2T/\pi, \Lambda^{'}). \tag{3.104}$$

There are two ultraviolet cutoff scales Λ and $\Lambda^{'}$. They appear in the individual contributions to the free energy density but cancel against each other in the final result. This is expected since $f(T)$ is a physical quantity independent of ultraviolet cutoffs.

After the first step of the scale separation, the partition function can be factorized as:

$$Z_{\mathrm{QCD}}(T) = e^{-f_{\mathrm{QCD}}(\pi T,\Lambda)T^3V} \int^{(\Lambda)} \mathcal{D}A_0^a \mathcal{D}A_i^a \exp\left[-\int \mathrm{d}^3x \mathcal{L}_{\mathrm{EQCD}}\right], \tag{3.105}$$

where $\mathcal{L}_{\mathrm{EQCD}}$ is the Lagrangian of Eq. (3.103).

Practically, at this step there are at least two matching coefficients that have to be expressed as functions of g^2 and T. These are f_{QCD} and g_E. The latter stems from the covariant derivative D_i. Since we want to go to the next scale of g^2T also the term of m_E has to be included in the effective Lagrangian. For instance in Ref. [32], where the pressure was calculated at $\mathcal{O}(g^6\ln(1/g))$, five coefficients had to be determined coming from operators up to dimension 4.

Generally, these coefficients are determined by calculating static quantities in both EQCD and QCD (or EQCD and MQCD) and matching the results up to the desired order in the parameters of the underlying theory.

The f_{QCD} term can be calculated from the full theory without any resummation since all the infrared effects are considered to be in $\mathcal{L}_{\mathrm{EQCD}}$. For instance, using the $\overline{MS}$ scheme with Λ as the scale and renormalizing the coupling g at the scale $4\pi T$ one obtains

$$\begin{aligned} f_{\mathrm{QCD}} = \frac{(N_c^2-1)\pi^2}{9} \Bigg\{ &-\frac{1}{5} + \frac{N_c g^2(4\pi T)}{16\pi^2} + \\ &+ \left(\frac{N_c g^2(4\pi T)}{16\pi^2}\right)^2 \left[-\frac{12}{\epsilon} - 72\ln\frac{\Lambda}{4\pi T} - 4\gamma - \frac{116}{5} - \frac{220}{3}\frac{\zeta^{'}(-1)}{\zeta(-1)} + \frac{38}{3}\frac{\zeta^{'}(-3)}{\zeta{-3}}\right]\Bigg\}. \end{aligned} \tag{3.106}$$

By simply reading the coupling from the full theory, the coupling constant g_E is at leading order in g simply:

$$g_E = \sqrt{T} g \tag{3.107}$$

The parameter m_E can be considered the color electric screening mass with higher order corrections. Therefore, it can be calculated by matching the perturbative expansion in g^2 from both QCD and EQCD. To leading order it is [31]:

$$m_E^2 = \frac{N_c g^2 T^2}{3}\left[1+\epsilon\left(2\ln\frac{\Lambda}{2\pi T}+2\frac{\zeta^{'}(-1)}{\zeta(-1)}\right)\right]. \tag{3.108}$$

Next, the massive field A_0^a can also be integrated out simplifying the theory even further. The new Lagrangian looks like:

$$\mathcal{L}_{\rm MQCD} = \frac{1}{4}F_{ij}^a F_{ij}^a + \delta\mathcal{L}_{\rm MQCD}, \tag{3.109}$$

where the same notation was used for the F_{ij}^a fields as in the EQCD Lagrangian. The second term on the rhs of Eq. (3.109) stands for higher order operators of the A_i^a fields that respect the symmetries of the original Lagrangian. Now it is possible to make the identification

$$\begin{aligned}&\int^{(\Lambda)}\mathcal{D}A_0^a\mathcal{D}A_i^a \exp\left[-\int \mathrm{d}^3\mathbf{x}\mathcal{L}_{\rm EQCD}\right] = \\ &= e^{-f_{\rm EQCD}(gT,\Lambda,\Lambda^{'})(gT)^3 V}\int^{(\Lambda^{'})}\mathcal{D}A_i^a \exp\left[-\int \mathrm{d}^3\mathbf{x}\mathcal{L}_{\rm MQCD}\right].\end{aligned} \tag{3.110}$$

This relation comes from Eq. (3.104) with:

$$f_{\rm MQCD}(g^2T/\pi,\Lambda^{'}) = -\frac{T}{V}\ln\left[\int^{(\Lambda^{'})}\mathcal{D}A_i^a \exp\left(-\int \mathrm{d}^3\mathbf{x}\mathcal{L}_{\rm MQCD}\right)\right]. \tag{3.111}$$

In the MQCD Lagrangian (3.109) the only scale is g^2T. It enters the Lagrangian through the coupling constant in the covariant derivative D_i [32]:

$$g_M^2 = g_E^2\left(1+\mathcal{O}(g_E^2/m_E)\right). \tag{3.112}$$

The term $f_{\rm EQCD}$ can be determined by calculating the logarithm of the partition function in both EQCD and MQCD. The result is:

$$f_{\rm EQCD}\cdot(gT)^3 = \frac{N_c-1}{4\pi}m_E^3\left\{-\frac{1}{3}+\frac{N_c g_E}{16\pi m_E}\left[\frac{1}{\epsilon}+4\ln\frac{\Lambda}{2m_E}+4\right]\right\}. \tag{3.113}$$

The term $f_{\rm MQCD}$ is non-perturbative. In principle, it can be estimated via lattice simulations using the parameters determined perturbatively as shown before. However, the conversion of the results from $3d$ lattice regularization to $3d$ continuum regularization and than to the $4d$ original theory necessitates some perturbative matchings.

In Ref. [32] higher order computation were performed in determining the pressure up to $\mathcal{O}(g^6\ln(1/g))$. Beyond this order perturbation theory is expected to break down. In order to determine the parameters of the effective Lagrangians to that precision higher order operators were needed. Their coefficients have been determined by matching 4-point functions calculated in both theories.

Even if high order corrections are known for static quantities such as pressure or the free energy, their convergence is still poor even for large temperatures. The next section is devoted to this aspect.

3.2.4. Convergence issues

In the final result of $f(T)$ all Λ and $\Lambda^{'}$ dependences should cancel since f describes a physical quantity. However there remains a scale dependence from the running coupling constant $g(\mu)$.

The result can be written as a sum of terms with increasing power in the coupling g (or $\alpha_S^{1/2}$). In this way the relative contribution of each term can be observed and by successively adding these terms together the convergence of the perturbative series can be studied.

The following plot is from Ref. [33] and shows the pressure calculated to different orders normalized to the non-interacting value p_{SB}.

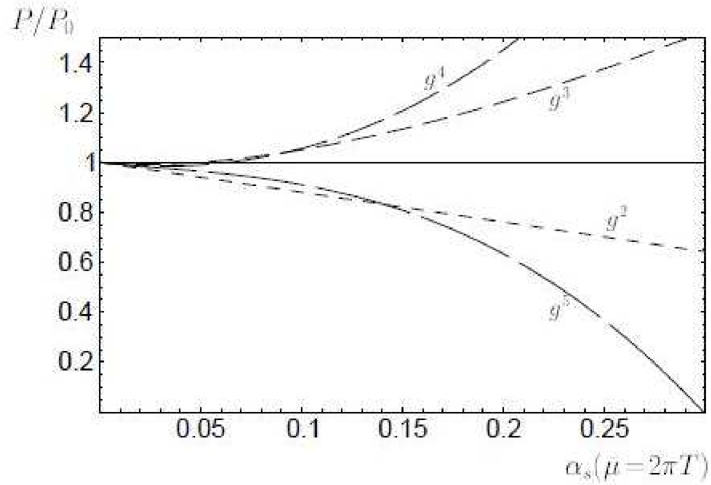


Figure 3.1.: Perturbative results for the thermal pressure of pure glue QCD normalized to the ideal-gas value as a function of $\alpha_S(\overline{\mu} = 2\pi T)$. Ref. [33]

Convergence of the perturbative series seems to appear only for $\alpha_S < 0.05$. Additionally it seems that in different regions higher order terms yield a larger contribution than lower order terms. This raises the question of how much higher order (and not yet calculated) terms contribute to the final result.

Another aspect that should be mentioned is the dependence of the result on the renormalization scale. As seen from Fig. 3.2, taken from [33] the numerical dependence on the renormalization scale grows with increasing order. So it seems perturbation theory loses its predictive power at temperatures of interest.

In conclusion, a significant progress has been made in the last years to push perturbative calculations

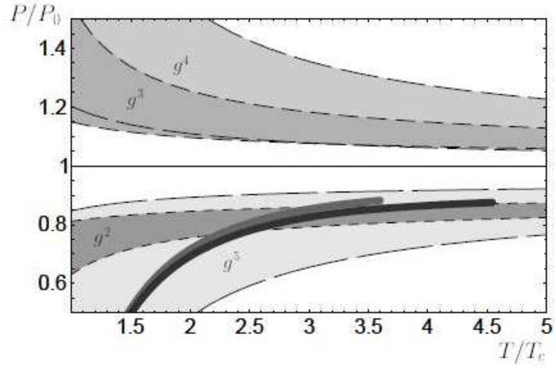


Figure 3.2.: Perturbative results for the thermal pressure of pure glue QCD as a function of T/T_c ($T/\Lambda_{\overline{MS}} = 1.14$). The various grey bands bounded by differently dashed lines show the perturbative results from order g^2 to order g^5, using a 2-loop running coupling with $\overline{\mathrm{MS}}$ renormalization point $\overline{\mu}$ varied between πT and $4\pi T$. The thick grey lines show the continuum extrapolated lattice results. Ref [33].

as far as possible. Still, due to the non-perturbative nature of the color-magnetic sector of QCD, lattice calculations are so far the only reliable approach.

4. Finite size effects

Even if QCD is in general not susceptible to an analytic treatment, it has been shown in the previous chapter that under special circumstances such as very low temperature (and momenta) or very high temperature effective field theory methods allow to simplify the problem considerably. In this chapter these frameworks are used in order to address a particular phenomenon, namely the appearance of finite volume effects in physical observables.

For the regime of low temperatures and momenta, where hadrons are the physical states, an effective theory described in terms of these states has been constructed. At high temperatures, another theory appears where degrees of freedom related to gluons play a dominant role.

In both regimes an alternative approach is to treat the entire problem numerically through lattice Monte Carlo simulations. However, extrapolation of numerical data is often difficult due to the finite lattice spacing and due to the effects of using a finite volume instead of doing calculations in an infinite volume.

In this chapter I concentrate on the effects due to a finite volume in a scalar field theory. This is done by calculating the free energy density and comparing it with the result in the infinite volume limit. It is useful to look at scalar fields since they have similar infrared properties as QCD. In fact, in order to obtain the free energy density for a gluon gas in the non-interacting limit, one has only to multiply the massless scalar field result with the degrees of freedom of the gluons. On the other hand an $O(N)$ symmetric field theory, describing QCD at low momenta, contains $N-1$ weakly interacting scalar fields.

For theories with spontaneous symmetry breaking two regimes are investigated. The first one is the case in which the inverse dimension of the box is smaller than the temperature and than any mass scale in the theory. In the second case the inverse dimension of the box is larger then the light Goldstone modes. In both cases the light Goldstone modes dominate the effects of finite volume.

Massless fields are investigated in the limit of high temperature. It turns however out that the naïve model of non-interacting massless fields is not applicable to a physical situation since thermal masses, however small, change the finite size contributions qualitatively.

4.1. Massive scalar field

In this section the free energy for a massive scalar field in a volume $V = L_1 ... L_d$ and at temperature $T = 1/L_0 \equiv 1/\beta$ will be derived. Here, d denotes, as in chapter 2 the spatial dimension whereas $D = d + 1$ will be the space-time dimension. Dimensional regularization is recommended as it keeps the Lorentz invariance intact by not imposing cutoffs in the sums (integrals in the infinite volume limit).

The starting point is the partition function in Eq. (2.23). Its logarithm can be expressed as:

$$\ln Z = \sum_{\mathbf{k}} \left[\ln T + \frac{1}{2} \sum_{n'} \ln \omega_n^2 - \frac{1}{2} \sum_{n} \ln \left(\omega_n^2 + E_{\mathbf{k}}^2 \right) \right] \tag{4.1}$$

with

$$E_{\mathbf{k}}^2 = \mathbf{k}^2 + m^2 \tag{4.2}$$

Taking the last term in Eq. (4.1) and denoting $k \equiv (\omega_n, \mathbf{k})$[1], the logarithm can be expressed as:

$$\ln \left(k^2 + m^2 \right) = \left[-\frac{\mathrm{d}}{\mathrm{d}r} \left(k^2 + m^2 \right)^{-r} \right]_{r=0}. \tag{4.3}$$

Using the Poisson summation formula,

$$\frac{1}{\beta V} \sum_{k} H(k) = \sum_{l} \int \frac{\mathrm{d}^D k}{(2\pi)^D} H(k) e^{ikl},\, l \equiv (\beta l_0, L_i l_i) \tag{4.4}$$

with $kl = \sum_{\mu=0}^{d} k_\mu l_\mu$, the sum can be expressed as:

$$-\beta V \sum_{l} \left[\frac{\mathrm{d}}{\mathrm{d}r} \int \frac{\mathrm{d}^D k}{(2\pi)^D} \left(k^2 + m^2 \right)^{-r} e^{ikl} \right]_{r=0}. \tag{4.5}$$

In order perform the D-dimensional integral over k, the integrand should be modified such that it becomes Gaussian. Rewriting

$$\left(k^2 + m^2 \right)^{-r} = \frac{1}{\Gamma(r)} \int_0^\infty \mathrm{d}\lambda \lambda^{r-1} e^{-\lambda(k^2+m^2)}, \tag{4.6}$$

the sum becomes:

$$\begin{aligned} S(m) = \sum_{k} \ln \left(k^2 + m^2 \right) = \\ - \beta V \sum_{l} \left\{ \frac{\mathrm{d}}{\mathrm{d}r} \int \frac{\mathrm{d}^d k}{(2\pi)^d} \frac{1}{\Gamma(r)} \int_0^\infty \mathrm{d}\lambda \lambda^{r-1} \exp \left[-\lambda \left(k - i \frac{kl}{2\lambda} \right)^2 - \lambda m^2 - \frac{l^2}{4\lambda} \right] \right\}_{r=0}, \end{aligned} \tag{4.7}$$

where $\Gamma(r)$ is the Gamma function. After integration over k and differentiation with respect to r, by setting $r = 0$, the sum can be written as

$$S(m) = -\beta V \frac{1}{(4\pi)^{d/2}} \sum_{l} \int_0^\infty \mathrm{d}\lambda \lambda^{-1-\frac{d}{2}} e^{-\lambda m^2 - \frac{l^2}{4\lambda}}. \tag{4.8}$$

[1] $k_i = \frac{2\pi n}{L_i}$.

The zero-mode contribution, $l = (0,0,0,0)$ corresponds to the zero temperature and infinite volume limit. Separating this mode from the others and performing the integral, we obtain

$$S(m) = -\beta V \frac{1}{(4\pi)^{D/2}} (m^2)^{\frac{D}{2}} \Gamma\left(-\frac{D}{2}\right) - \beta V \frac{2}{(2\pi)^{\frac{D}{2}}} \sum_{l}{}' \left(\frac{m^2}{l^2}\right)^{\frac{D}{4}} K_{\frac{D}{2}}\left(\sqrt{m^2 l^2}\right). \tag{4.9}$$

The function $K_d(x)$ is the modified Bessel function of the second kind and the prime in the previous sum denotes omission of the zero mode.

For the moment let us concentrate on the first term in Eq. (4.9). For that express the free energy density as

$$f = -\frac{T}{V} \ln Z \tag{4.10}$$

so that the infinite volume and zero temperature part of the free energy density is

$$f_{V\to\infty, T\to 0} = -\frac{1}{2}\left(\frac{m^2}{4\pi}\right)^{\frac{D}{2}} \Gamma\left(-\frac{D}{2}\right). \tag{4.11}$$

Inserting now $D = 4 - 2\epsilon$ we get the same result as in Chapter 2, Eq. (2.26):

$$S(m)|_{T=0,V=\infty} = -\frac{m^4}{64\pi^2}\mu^{-2\epsilon}\left(\frac{1}{\epsilon} + \ln\frac{\mu^2}{m^2} + \ln 4\pi - \gamma_E + \frac{3}{2}\right). \tag{4.12}$$

The second term in Eq. (4.9) contains the thermal part of infinite volume and the finite volume corrections:

$$\sum_{l}{}' = \underbrace{2\sum_{l_0=1}^{\infty}}_{\substack{T\neq 0 \\ V\to\infty}} + \underbrace{\sum_{\mathbf{l}}{}'}_{\substack{T=0 \\ V\neq\infty}} + \underbrace{2\sum_{l_0=1}^{\infty}\sum_{\mathbf{l}}{}'}_{\substack{T\neq 0 \\ V\neq\infty}}. \tag{4.13}$$

The first term in Eq. (4.13) is just the finite temperature term from chapter 2:

$$J_T(m) \equiv f_{T,\infty} = -\frac{1}{2\pi^2}(mT)^2 \sum_{l_0=1}^{\infty} l_0^{-2} K_2(m\beta l_0), \tag{4.14}$$

whereas the remaining part is denoted as:

$$\begin{aligned} f_L = &-\frac{1}{(2\pi)^2}\left(\frac{m}{L}\right)^2 \sum_{\mathbf{l}}{}' \mathbf{l}^{-2} K_2(mL|\mathbf{l}|) \\ &-\frac{1}{2\pi^2}(mT)^2 \sum_{l_0=1}^{\infty}\sum_{\mathbf{l}}{}' \left(l_0^2 + (LT)^2\mathbf{l}^2\right)^{-1} K_2\left(m\beta\sqrt{l_0^2 + (LT)^2\mathbf{l}^2}\right). \end{aligned} \tag{4.15}$$

The remaining terms in Eq. (4.1) appear to be infinite since they are 3-dimensional sums over constant factors. It turns out however that, as we now demonstrate, they can be calculated explicitly after suitable regularization and the temperature dependence drops out always. So these sums can contribute to the free energy density at most with a constant term.

The second sum in Eq. (4.1) can be written as:

$$\begin{aligned}\sum_{\mathbf{k}}\sum_{n'}\ln\omega_n^2 =& -2\sum_{\mathbf{k}}\sum_{n=1}^{\infty}\frac{\mathrm{d}}{\mathrm{d}r}\left.\frac{1}{(2\pi nT)^{2r}}\right|_{r=0} \\ =& -2\sum_{\mathbf{k}}\left(-2\ln(2\pi T)\zeta(0)+\zeta^{'}(0)\right).\end{aligned} \tag{4.16}$$

Evaluating the Zeta function and its derivative at 0, $\zeta(0) = -1/2$, $\zeta^{'}(0) = -(1/2)\ln(2\pi)$, the T dependent part cancels against the first sum and the remaining term is:

$$-\frac{1}{2}\ln 2\pi\sum_{\mathbf{k}} = -\frac{1}{2}\ln 2\pi\left(\mathcal{Z}_d(1,...,1;0)+1\right). \tag{4.17}$$

The sum is expressed in terms of the Epstein Zeta function whose definition is:

$$\mathcal{Z}_d(a_1,...a_d;s) \equiv \sum_{n_1=-\infty}^{\infty}...\sum_{n_d=-\infty}^{\infty}{}'\left[(a_1n_1)^2+...+(a_dn_d)^2\right]^{-s}. \tag{4.18}$$

Useful relations concerning the Epstein Zeta functions are found in Refs. [34] and [35]. It is not possible to establish an analytic expression for this function in every dimension. For even dimensions ($d = 2, 4, ...$) it can be expressed in terms of Γ (Gamma) and ζ (Riemann Zeta) functions. For odd dimension usually it can be expressed as a sum of a dominating term and a small remainder truncated at a given order. Details on the calculation of the Epstein Zeta function are given in appendix C. For the particular case of $d = 3 - 2\epsilon$,

$$\mathcal{Z}_3(1,1,1;0) = -1. \tag{4.19}$$

This result is convenient because it means that the first two sums in Eq. (4.1) are exactly 0 after proper regularization.

4.2. Massless scalar field

The massless case of a scalar field can be applied to a non-interacting photon or gluon gas subject to boundary conditions. It exhibits a non-trivial contribution due to the presence of the massless mode.

The starting point in calculating the free energy density of the massless scalar field is the last sum of Eq. (4.1). For consistency and for keeping dimensions correct, the mass is replaced by an infinitesimally small mass, which is smaller than any other scale in the problem, $m \equiv \epsilon$. Therefore, the sum can be written as:

$$\begin{aligned}\sum_{\mathbf{k}}\sum_{n}\ln\left(\mathbf{k}^2+\omega_n^2+\epsilon^2\right) \overset{\epsilon\to 0}{=}& \ln(\epsilon^2)+\sum_{\mathbf{k}}\sum_{n}{}'\ln\left(\mathbf{k}^2+\omega_n^2\right) \\ =& \ln(\epsilon^2)+\sum_{k}{}'\ln k^2.\end{aligned} \tag{4.20}$$

In order to calculate the second sum in Eq. (4.20) the definition from Ref. [36] for the massless propagator is used:

$$\sum_k{}' \mathrm{ln} k^2 = -\frac{\mathrm{d}}{\mathrm{d}r}\left(\frac{V_d}{\Gamma(r)}\lim_{m\to 0}\left(G_r - \frac{\Gamma(r)}{m^{2r}V_D}\right)\right). \tag{4.21}$$

The definition of G_r is given in appendix C.

Using now the expansion for small masses, the sum becomes:

$$\begin{aligned}
\sum_k{}' \mathrm{ln} k^2 =& -\frac{\mathrm{d}}{\mathrm{d}r}\lim_{m\to 0}\left(\frac{V_D}{\Gamma(r)}\left(\frac{\Gamma\left(r-\frac{D}{2}\right)}{(4\pi)^{D/2}}m^{D-2r}+\right.\right.\\
&\left.\left.+\ \frac{1}{V_D}\left(\frac{\bar{L}^2}{4\pi}\right)^r\left(a_r+b_r-b_{r-\frac{D}{2}}\right)-\frac{\Gamma(r)}{V_D m^{2r}}\right)\right)_{r=0}\\
=& -\frac{\mathrm{d}}{\mathrm{d}r}\lim_{m\to 0}\left[\frac{V_D}{\Gamma(r)}\frac{\Gamma\left(r-\frac{D}{2}\right)}{(4\pi)^{D/2}}m^{D-2r}+\right.\\
&+\left(\frac{\bar{L}^2}{4\pi}\right)^r\frac{1}{\Gamma(r)}\left(\sum_{n=0}^{\infty}\left(-\frac{m^2\bar{L}^2}{4\pi}\right)^n\frac{1}{n!}\alpha_{r+n}+\left(\frac{m^2\bar{L}^2}{4\pi}\right)^{-r}\Gamma(r)-\right.\\
&-\sum_{n=0}^{\infty}\frac{1}{n!}\left(-\frac{m^2\bar{L}^2}{4\pi}\right)^n\frac{1}{n+r}-\\
&-\frac{(-1)^{\frac{D}{2}-r-1}}{\Gamma\left(\frac{D}{2}-r+1\right)}\left(\frac{m^2\bar{L}^2}{4\pi}\right)^{\frac{D}{2}-r}\left(\mathrm{ln}\frac{m^2\bar{L}^2}{4\pi}+\gamma_E-\sum_{n=1}^{\frac{D}{2}-r}\frac{1}{n}\right)-\\
&\left.\left.-\sum_{n\neq\frac{D}{2}-r}^{\infty}\frac{1}{n!}\left(-\frac{m^2\bar{L}^2}{4\pi}\right)^n\frac{1}{\frac{D}{2}-r-n}\right)-\frac{1}{m^{2r}}\right]_{r=0}\\
=&\mathrm{ln}\bar{L}^2-\alpha_0+\frac{2}{D}+\gamma_E-\mathrm{ln}4\pi,
\end{aligned} \tag{4.22}$$

where $\bar{L}$ is the average dimension of the D-dimensional system, $\bar{L} \equiv (L_0 \cdot ... \cdot L_d)^{1/D}$ and V_D is the D-dimensional volume, $V_D \equiv L_0 \cdot ... \cdot L_d$. An exact derivation of the a_r, the b_r as well as the α_r function is given in appendix C.

Turning now to Eq. (4.1) for a massless field, we have:

$$\mathrm{ln}Z = \sum_{\mathbf{k}}\mathrm{ln}T + \frac{1}{2}\sum_{\mathbf{k}}\sum_{n'}\mathrm{ln}\omega_n^2 - \mathrm{ln}\epsilon - \frac{1}{2}\sum_{\mathbf{k}}\sum_{n}{}'\mathrm{ln}\left(\omega_n^2+\mathbf{k}^2\right). \tag{4.23}$$

As was shown at the end of the previous section, the first two terms cancel against each other. The last sum in Eq. (4.23) is split into the $n = 0$ and the $n \neq 0$ modes:

$$\sum_{\mathbf{k}}{}'\mathrm{ln}\mathbf{k}^2 + 2\sum_{n=1}^{\infty}\sum_{\mathbf{k}}\mathrm{ln}\left(\omega_n^2+\mathbf{k}^2\right). \tag{4.24}$$

The first sum of Eq. (4.24) is just the massless sum of a d-dimensional system, evaluated in Eq. 4.22:

$$\sum_{\mathbf{k}}{}'\mathrm{ln}\mathbf{k}^2 = \mathrm{ln}\frac{\bar{L}^2}{4\pi} - \alpha_0 + \frac{2}{d} + \gamma_E. \tag{4.25}$$

Here the logarithm contains L instead of $\bar{L}$ since all spatial dimensions are considered equal.

In the second term of Eq. (4.24), the ω_n term can be considered an n-dependent mass. Therefore, from Eq. 4.7 we have:

$$\begin{aligned} 2\sum_{n=1}^{\infty}\sum_{\mathbf{k}}\ln\left(\omega_n^2+\mathbf{k}^2\right) &= -2\pi^{\frac{d}{2}}\left(\frac{L}{\beta}\right)^d\Gamma\left(-\frac{d}{2}\right)\zeta(-d) \\ &- \frac{L^d}{(4\pi)^{d/2}}\sum_{n=1}^{\infty}\int_0^{\infty}\mathrm{d}\lambda\lambda^{-1-\frac{d}{2}}\mathrm{e}^{-\lambda(2\pi Tn)^2}\sum_{\mathbf{l}}{}'\exp\left[-\sum_{\mu=1}^{d-1}\frac{(l_\mu L)^2}{4\lambda}\right]. \end{aligned} \tag{4.26}$$

The first term on the rhs of Eq. (4.26) stems from the vacuum energy density through:

$$2\sum_{n=1}^{\infty}\left[-\frac{L^d}{(4\pi)^{\frac{d}{2}}}(\omega_n^2)^{\frac{d}{2}}\Gamma\left(-\frac{d}{2}\right)\right] \tag{4.27}$$

Since the only term depending on n is ω_n, the sum becomes:

$$\sum_{n=1}^{\infty}(\omega_n^2)^{\frac{d}{2}} = (2\pi T)^d\zeta(-d), \tag{4.28}$$

where $\zeta(s)=\sum_{n=1}^{\infty}n^{-s}$ is the Riemann Zeta function.

Gathering all terms of Eq. (4.23), we get:

$$\begin{aligned} \ln Z =&(LT)^d\frac{\Gamma\left(\frac{D}{2}\right)}{\pi^{\frac{D}{2}}}\zeta(D)-\ln LT \\ &+2(LT)^{\frac{d}{2}}\sum_{n=1}^{\infty}\sum_{\mathbf{l}}{}'\left(\frac{n}{|\mathbf{l}|}\right)^{\frac{d}{2}}K_{\frac{d}{2}}(2\pi LT|\mathbf{l}|n)-\ln\frac{\epsilon}{T} \\ &+\frac{1}{2}\alpha_0+\frac{1}{2}\ln 4\pi-\frac{1}{d}-\frac{\gamma_E}{2}-\ln 2\pi(Z_d(1,...,1;0)+1), \end{aligned} \tag{4.29}$$

where the following relation has been used:

$$\pi^{-\frac{s}{2}}\Gamma\left(\frac{s}{2}\right)\zeta(s)=\pi^{\frac{s-1}{2}}\Gamma\left(\frac{1-s}{2}\right)\zeta(1-s). \tag{4.30}$$

Inserting $D = 4$ and $d = 3$, along with the numerical evaluation of α_0 from Ref. [36] and $\mathcal{Z}_3(1,1,1;0) = -1$ from Eq. 4.19, the partition function for the massless scalar field in 4 dimensions becomes:

$$\ln Z = \frac{\pi^2}{90}(LT)^3-\ln LT+\frac{1}{2\pi}\sum_{\mathbf{l}}{}'\frac{1}{|\mathbf{l}|^3}\frac{e^{2\pi LT|\mathbf{l}|}(1+2\pi LT|\mathbf{l}|)-1}{(e^{2\pi LT|\mathbf{l}|}-1)^2}+0.72. \tag{4.31}$$

The constant factor is not important in determining thermodynamic quantities and can be left out. It partially stems from the α_0 function evaluated in 3 dimensions and with equal box dimensions.

4.3. Theories with spontaneous symmetry breaking

As discussed in section 3.1, chiral perturbation theory provides a useful tool to describe low energy systems of hadronic matter. When the system is evaluated on the lattice, light Goldstone modes can feel the boundaries and finite size effects can be important. Effects of higher modes are expected to be suppressed.

Scalar field theory provides an useful tool to analyse the effects of finite volume and temperature for low energy QCD for two reasons. First of all, this is due to the isomorphic relation between the $O(4)$ group used to describe spontaneous symmetry breaking in scalar field theory and the $SU(2)_L \times SU(2)_R$ symmetry of the chiral Lagrangian. The subgroups of the two systems are also isomorphic after symmetry breakdown, $O(3) \sim SU(2)_V$. So an effective theory of a broken $O(N)$ symmetry is merely $N-1$ interacting scalar fields. Secondly, it is shown in section 3.1 that interaction occurs only at next-to-leading order and that it is weak (of $\mathcal{O}(p)$). Therefore the dominant finite size effects appear due to free Goldstone modes.

It is useful to distinguish between two cases. In the first case the linear size of the box is large. A reference scale could be the pion mass ($L^{-1} \gg M_\pi$). This limit implies that even for the lightest Goldstone modes the Compton wavelength does not extend beyond the size of the box. The other limit is when the Compton wavelengths of the lightest Goldstone modes do extend beyond the box ($L^{-1} \lesssim M_\pi$). In this regime regular chiral perturbation theory breaks down and a different expansion scheme has to be used.

In Refs. [37],[38] and [39] the first regime was inspected and it was found that in the limit of large volumes (that extend beyond any m^{-1} scale) and low temperatures the chiral Lagrangian does not change and it corresponds to the zero temperature and infinite volume limit. Moreover it is shown that the expansion parameters do not depend on either the temperature or the linear dimension of the box provided the fields are subject to the standard boundary conditions, periodic for bosons and anti-periodic for fermions. This can be seen also in Fig. 4.1 where the finite volume effects on the partition function of the scalar field is shown. Indeed, in the regime of large volume ($M_\pi L \simeq 5$) and not too low temperatures the effects vary between approximately 1% and 10%.

Even for higher temperatures ($T \simeq M_\pi$) finite size effects are still small. This confirms the statement that in the large volume limit no significant effects appear in the partition function of the scalar field.

However, in the small volume limit, $mL \lesssim 1$ finite size corrections are orders of magnitude higher then the free energy density in the thermodynamical limit, suggesting that in this region the simple picture of a non-interacting scalar field is no longer applicable. This case is discussed in the following.

The other regime occurs if m tends to 0 at fixed L. The perturbation series in terms of the effective Lagrangian breaks down and a reorganization of the perturbative series has to be performed [39]. In order to control the effects due to the finite volume, an expansion in terms of $1/L$ is used, called the large volume expansion. In Ref. [36] such an expansion is performed for a theory with an $O(N)$ symmetry. "Magnetic" language is used in order to keep the approach general. Therefore the

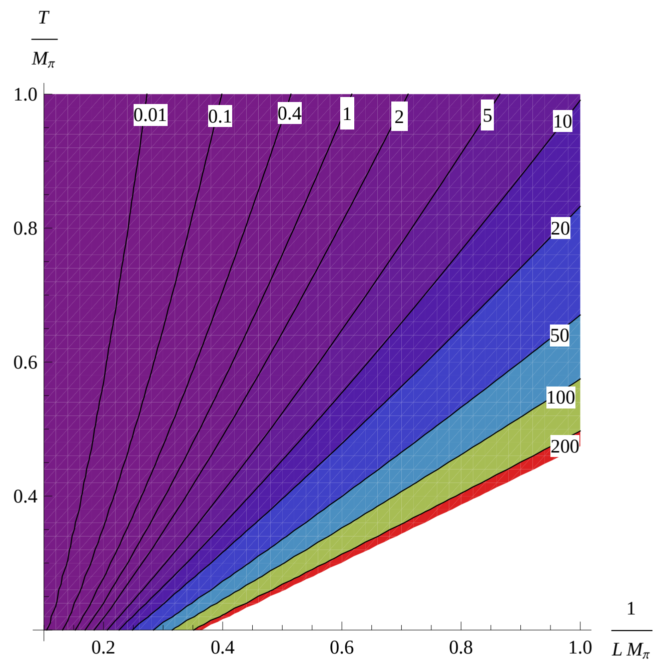


Figure 4.1.: Finite size effects for a scalar field in the large volume limit $m, T \gg L^{-1}$ by plotting $f_L/f_{T,\infty}$ from Eqs. 4.14 and 4.15. No absolute scale is set since the partition function depends only on dimensionless quantities mL and LT. In the region of $m, T \simeq L$, in which the finite size corrections are orders of magnitude larger than the free energy density in the thermodynamic limit, the scalar field approach loses its predictive power.

symmetry breaking field, $\chi(x)$ is reinterpreted as the magnetic field $\mathbf{H}(x)$ and the Goldstone boson fields are rather $\mathbf{S}(x)$ then $U(x)$ [2].

An important difference to the infinite volume limit is the fact that in a finite volume the Goldstone modes have a net magnetization of

$$\mathbf{m} = \frac{1}{V}\int \mathrm{d}x \mathbf{S}(x), \tag{4.32}$$

that appears in the action as

$$-\mathbf{m} \cdot \mathbf{H} V. \tag{4.33}$$

At vanishing magnetic field ($\mathbf{H} = 0$), the magnetization rotates freely in the group space rendering the partition function divergent[3]. In order to keep the integral finite, the magnetization has to be treated as a collective variable by using the Fadeev-Popov procedure. A factor

$$\int \mathrm{d}\mathbf{m}\, \delta\left(\mathbf{m} - \frac{1}{V}\int \mathrm{d}x \mathbf{S}(s)\right) \equiv \mathbb{1} \tag{4.34}$$

[2]Bold letters are used to remind that they are multi-component scalar fields, $\mathbf{S}(x) = (S^1(x), ..., S^n(x))$.

[3]It is the analogous situation of defining a path integral for a gauge field, when attention has to be paid not to integrate over physically identical fields.

is introduced in the partition function. The integral over $\mathbf{m}$ is split into its magnitude and its direction

$$\mathrm{d}\mathbf{m} = m^{N-1}\mathrm{d}m\mathrm{d}\mathbf{e}, \text{ with } \mathrm{e} = \Omega^T(1,0,...0) \tag{4.35}$$

and where Ω^T is an $O(N)$ rotation.

By rotating the Goldstone fields, $\mathrm{S}(x) = \Omega^T \mathrm{R}(x)$, the factor becomes

$$\int \mathrm{d}\Omega \mathrm{d}m m^{N-1}\delta\left(m\cdot(1,0,...,0) - \frac{1}{V}\int \mathrm{d}x\mathbf{R}(x)\right). \tag{4.36}$$

The collective variable, Ω is associated with the zero mode $\mathrm{S}(x) = \text{const}$, while $\mathrm{R}(x)$ is the non-zero mode and enters the effective Lagrangian. It is expressed through $\Pi = (\pi^1, ..., \pi^{N-1})$ as

$$\begin{aligned} R^i(x) &= \pi^i(x) \\ R^0(x) &= \sqrt{1-\Pi^2(x)} = 1 - \frac{1}{2}\Pi^2(x) + ... \end{aligned} \tag{4.37}$$

Physically, the contribution from the dominant (light) mode has been separated from heavier modes that are treated perturbatively.

Establishing now counting rules for the fields in terms of $1/L$ (just as in Sec. 3.1.5),

$$\Pi \sim L^{1-d/2},\ \partial_\mu \sim L^{-1},\ \mathrm{H} \sim L^{-d}, \tag{4.38}$$

the first contribution to the effective action, taking $\mathrm{H} = (H, 0, ..0)$, is:

$$\int \mathrm{d}x \frac{1}{2}F_\pi^2 \partial_\mu \Pi \partial_\mu \Pi - \Sigma H V \Omega^{00}, \tag{4.39}$$

with F_π being the pion decay constant and $\Sigma \equiv \lim_{H\to 0}\langle\phi^0\rangle$ being in chiral language the negative quark condensate.

With all these ingredients the partition function can be calculated to the desired order in $1/L$ and with it, correlation functions and other quantities of interest. An important consequence of treating the zero Goldstone mode as a collective variable is the behaviour of the magnetization or, in the chiral language, the quark condensate in a finite volume. Its value is in the limiting case $H \to 0$:

$$\langle\phi^0\rangle = \frac{1}{V}\frac{\partial}{\partial H}\ln Z \propto \frac{1}{N}VH. \tag{4.40}$$

This means that, when H tends to 0, the magnetization will also drop linearly with H to zero. In chiral perturbation theory this means that, in the chiral limit of vanishing quark masses and a finite fixed volume the chiral condensate will vanish. This is the reason why in lattice simulations the chiral condensate cand be calculated only for non-vanishing quark masses and needs to be extrapolated to the chiral limit. In Ref. [39] the behaviour of the chiral condensate was in detail examined.

It is now clear that familiar physics and exponentially small finite-volume effects are found only if $L \gg M_\pi^{-1}$; nevertheless, the chiral effective theory itself is valid also for $L \lesssim M_\pi^{-1}$ as long as L is still larger then the QCD scale[4].

[4]The QCD scale is roughly speaking the scale below which a perturbative expansion in terms of the strong coupling

4.4. Yang-Mills theory at very high temperatures

The partition function of the massless field contains only one scale, the dimensionless parameter LT. Due to the lack of any other intrinsic scale, the thermodynamic quantities are expected to be very sensitive to the geometric shape of the box. Indeed, this is obvious from the logarithmic correction of the free energy density in the non-interacting case (cf. Eq. (4.31)).

$$f(T) = -\frac{\pi}{90}T^4 + \frac{T}{L^3}\ln LT - \frac{T^2}{L^2}\sum_{\mathbf{l}'}\frac{1}{\mathbf{l}^2}e^{-2\pi LT|\mathbf{l}|}. \tag{4.41}$$

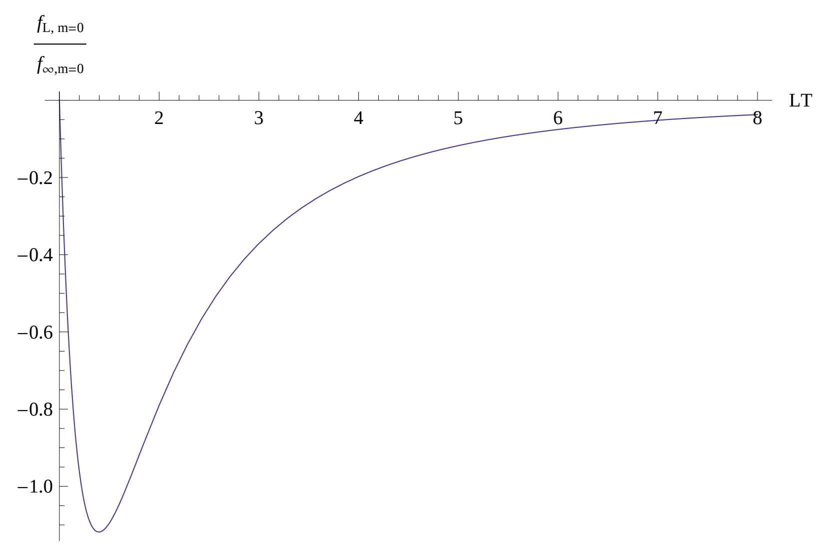


Figure 4.2.: Contribution of the zero mode finite volume correction to the free energy density. The sum in Eq. 4.41 is negligible with respect to the zero mode contribution. The definitions for $f_{L,m=0}$ and $f_{\infty,m=0}$ are given in Eqs. (4.42) and (4.43).

The last term in Eq. (4.41) is an approximation of the sum in Eq. (4.31) in the limit of large LT and is negligible. The second term however is a non-trivial correction to the thermodynamic limit. It stems from the Matsubara zero mode evaluated in a finite volume. In Fig. (4.2) its importance is illustrated by plotting the ratio between the zero mode contribution due to finite size effects,

$$f_{L,m=0} = \frac{T}{L^3}\ln LT, \tag{4.42}$$

and the free energy density of the massless scalar field in the infinite volume limit,

$$f_{\infty,m=0} = -\frac{\pi^2}{90}T^4. \tag{4.43}$$

constant, $\alpha_s(Q)$ is no longer possible due to its large value. This scale is about $\Lambda_{\mathrm{QCD}} \approx 200$ MeV for which $\alpha_s(\Lambda_{\mathrm{QCD}}) \approx 0.4$.

The plot shows an extremum at the value

$$T = \frac{e^{\frac{1}{d-1}}}{L}, \tag{4.44}$$

so at $LT = 1.39$ finite volume corrections seem to exceed the quantity in infinite volume. In addition, the shape varies slowly with increasing LT, requiring $LT = 7$ in order to get contributions of only 5%, or $LT = 13$ in order to reduce them to under 1%.

We note that the expression in Eq. (4.41) is not in agreement with the calculations performed in Ref. [40]. The method used there to calculate the partition function of a non-interacting massless gas is based on the Zeta function renormalization. It is the requirement for modular invariance and the vanishing dimensionality of the partition function which ultimately leads for the finite size effects to be d times smaller than in this case; indeed Gliozzi obtains a term of

$$-\frac{1}{d}\ln LT. \tag{4.45}$$

Naively, omitting interactions, this results can be compared to lattice simulations. In Ref. [41] the $SU(3)$ gauge theory has been simulated with different improved actions of $\mathcal{O}(a^2)$ and $\mathcal{O}(a^4)$. The energy density has been calculated with these actions for $N_s/N_t = 4$ and $N_s/N_t = 6$ with increasing number of N_t.

In order to compare the results, the partition function for a gluon gas has to be determined. In the non-interacting case, this is just the partition function of the scalar field multiplied by the polarization states of the gluon (2) and the dimension of the adjoint representation of the $SU(3)$ group. Therefore:

$$\frac{Z}{N^2-1} = \frac{\pi^2}{45}(LT)^3 - 2\ln LT + \mathcal{O}(e^{-2\pi LT}). \tag{4.46}$$

The energy density in a finite box is:

$$\epsilon \equiv \frac{T^2}{V}\left(\frac{\partial \ln Z}{\partial T}\right)_V = (N^2-1)\left(\frac{\pi^2 T^4}{15} - \frac{2T}{V}\right). \tag{4.47}$$

Calculating the ratio of this expression and the energy density in the thermodynamic limit, the factor

$$1 - \frac{30}{\pi^2}\frac{1}{(LT)^3} \tag{4.48}$$

is obtained. Interpolating now the numerical results for $LT = 4, 6$ with a function of $a - b(LT)^{-3}$ the result for b is 0.62 which clearly is smaller than $30/\pi^2 \approx 3.03$.

On the other hand, the analytic result obtained by Gliozzi, $15/2\pi^2 \approx 0.76$ differs after all with about 20% from the numerical result. However, obviously the functional form cannot be tested on two data points, and many other simulations have indicated very small volume dependence. In fact, as will be discussed below, in an interacting theory the volume dependence is expected to be exponentially small.

In conclusion, the partition function calculated within the framework of Ref. [36] fails to provide quantitative results but gives a qualitative picture on the behaviour of non-interacting massless fields subject to boundary conditions.

Still the obtained result shows that the relation $p = -f$ valid in infinite volume limit cannot be used in finite volumes. Calculating

$$\begin{aligned} p &= T \left(\frac{\partial \mathrm{ln} Z}{\partial V} \right)_T , \\ f &= -\frac{T}{V} \mathrm{ln} Z, \end{aligned} \tag{4.49}$$

one obtains

$$\frac{p+f}{T^4} = \frac{2}{3} \frac{(N^2-1)}{(LT)^3} \left(\ln(LT)^3 - 1 \right), \tag{4.50}$$

which is only in the $LT \to \infty$ limit small.

As already mentioned, this model of a massless scalar field can however not be regarded as a good approximation for the physical case of a gas of non-abelian gauge bosons. It is known from the previous chapter that a non-abelian plasma exhibits a screening of order $g(T)T$ for the electric sector and of order $g^2(T)T$ for the magnetic sector. Even in the low temperature limit, the existence of a small thermal mass changes the picture qualitatively.

A detailed picture is given in Ref. [42] where the finite size effects of a relativistic Yang-Mills theory were analysed by using the symmetries of the Euclidean partition function. The thermodynamical observables where interpreted in terms of the energy-momentum tensor living in a $\beta \times L^3$ volume.

By using the properties of the traceless part of the energy-momentum tensor, coordinate axes could be interchanged such that the energy density, expressed in terms of the energy levels of the system would depend explicitly on temperature. In this manner, by using QCD sum rules the thermodynamic observables could be related to the expectation values of the energy-momentum tensor.

By making use of the empirical fact that the theory exhibits a mass gap denoted as the difference between the first excited state and the ground state, the finite size effects can be determined in terms of the product mL, the inverse temperature β and the mass derivative $\partial_\beta m(\beta)$.

The corrections to the pressure hold only up to energies that do not exceed the second excited state. Writing the pressure in a finite volume as the sum of the pressure in the thermodynamic limit and the correction,

$$\frac{p(T,L)}{T} = \frac{p(T,L=\infty)}{T} + \delta, \tag{4.51}$$

the leading order correction to the pressure is:

$$-\frac{m^2}{T^2} \frac{e^{-mL}}{2\pi LT}. \tag{4.52}$$

In conclusion the finite size effects on the pressure[5] were found to fall off exponentially with increasing linear dimension of the box. Moreover, the corrections are negative denoting a dropping of pressure with decreasing volume.

A similar conclusion can now be drawn for the scalar field theory *with mass*. The leading finite size corrections to the scaled free energy density, f_L/T^4 is in the large mL limit (cf. Eq. 4.15):

$$-\frac{3}{\pi^2}\sqrt{\frac{\pi}{2}}e^{-mL}\left(\frac{(mL)^{3/2}}{2(LT)^4}+\frac{1}{mL}\right). \tag{4.53}$$

As in Ref. [42], the correction are negative and exhibit the same exponential falling.

In the following, the corrections of the free energy density due to the finite volume have been calculated in different regimes for massive scalar fields.

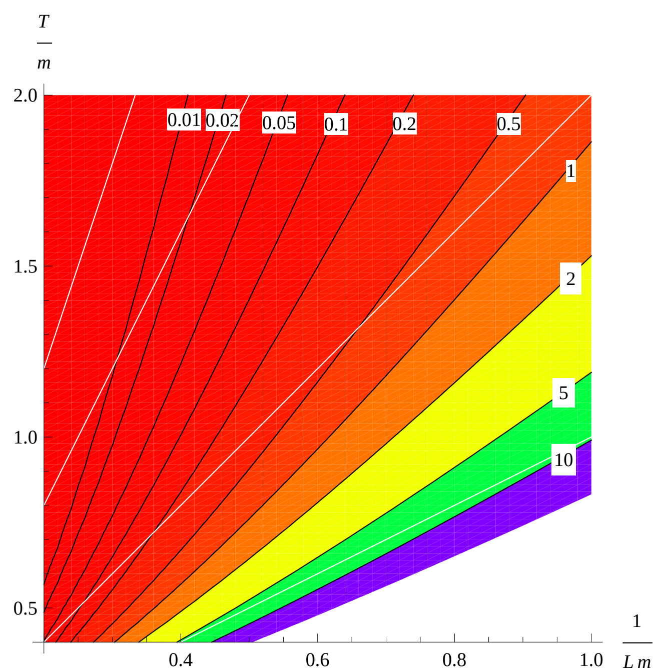


Figure 4.3.: Finite size corrections of the free energy, $f_L/f_{T,\infty}$ (cf. Eqs. (4.14) and (4.15)) as function of T and L^{-1}. The three light lines are (from left to right) the lines of constant parameter $LT = 6, 4, 2$.

The free energy density is a function of 3 parameters, T, L and m. They are expressed in terms of dimensionless parameters that are usually used also in lattice calculations. These parameters are $N_s/N_t = LT$ and mL. The former parameter characterises the geometric shape of the of the system whereas the latter parameter gives a clue on the spectrum of the theory, whether there is a mass gap and how large it is. So, the scales can be set through a proper choice of these parameters.

[5]Or free energy, since $p = -f$ in the thermodynamic limit.

Figure 4.3 illustrates the contribution to the free energy due to finite volume effects. No absolute values are set here, since the ratio $f_L/f_{t,\infty}$ is a function of only the dimensionless parameters LT, mL and $m/T = mL/LT$. Nevertheless, several properties can be drawn.

In Ref. [43] the numerical value of the lightest screening mass is given in terms of m/T for high temperatures above the deconfining temperature T_c. The mass grows for temperatures between approximately $1.2T_c$ and $2.2T_c$ and ranges typically from $m/T \approx 2.6$ to $m/T \approx 2.9$. With these numerical values and for $LT = 4$, it was found in Ref. [42] that the corrections to the pressure due to finite volume are negligible small, namely of the order of 10^{-5}. Calculating the finite volume correction for the massive scalar field, $f_L/f_{T,\infty}$ (cf. Eqs. (4.14) and (4.15)) with the same values for m/T and LT respectively, it turns out to be of the same order, $\approx 1.7 \cdot 10^{-5}$. Fig. 4.3 contains also the lines of constant $LT = 6, 4, 2$. Having a theory with the given mass spectrum, the corrections due to finite volume with constant LT down to 4 is only of $\approx 1\%$ for high enough temperatures. This confirms the empirical rule that finite size corrections are small for $LT \geq 4$. Below this ratio finite size corrections become important or even dominant. Therefore, it is expected that in this region the simple model of a scalar field loses its predictive power and its applicability.

Fig. 4.3 also shows that with increasing temperature the effects of finite volume increase for any given constant LT. This is expected since, by only keeping LT constant, the product mL decreases with increasing temperature, meaning that the Compton wavelength of the particle expands beyond the linear length of the box. This can be seen more in detail in Fig. 4.4 where finite size corrections of the free energy are plotted for constant $LT = 4, 6$. Indeed, for increasing temperature, that is for decreasing m/T, finite size corrections increase.

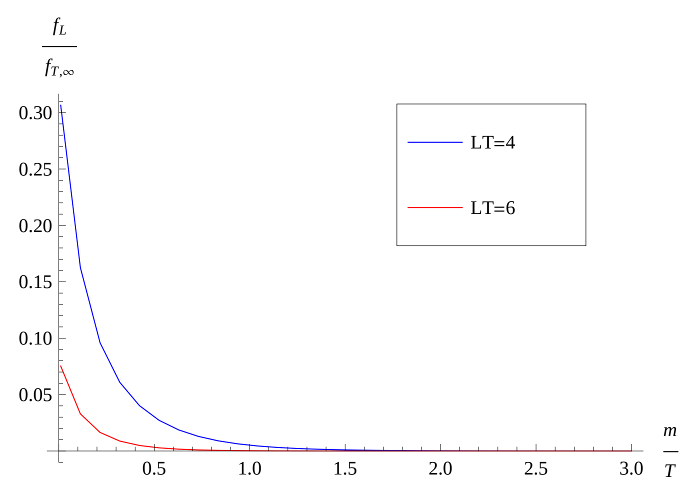


Figure 4.4.: Variation of finite volume contribution to the free energy density (cf. Eqs. (4.14) and (4.15)) with constant $LT = 4, 6$ as function of m/T. The contributions increase with decreasing m/T.

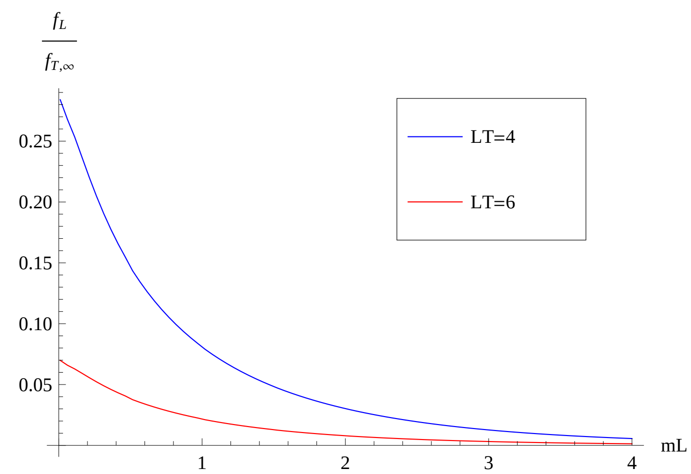


Figure 4.5.: Contribution of finite volume effects to the free energy density (cf. Eqs. (4.14) and (4.15)) with variation of the mL parameter for two cases, $LT = 4$, $LT = 6$.

In addition, as seen from Fig. 4.5, the contribution of finite volume corrections decreases with increasing mass. This comes due to the correlation of the field that varies as

$$\propto e^{-\frac{|x-y|}{m}}. \tag{4.54}$$

Therefore, with increasing mass, the correlation of the field decreases over long distances and thermal effects do not "feel" the sides of the box any more. By ensuring small finite size effects for light masses, all other heavier fields will have negligible contributions to these effects.

In conclusion Ref. [42] showed that even in the high temperature limit, ($T_c \ll T \ll 10^5$ GeV) finite size effects should be suppressed by a Boltzmann factor coming from dynamically generated masses rather then being a non-negligible function of LT. While the model proposed in Ref. [40] generates qualitatively different results then those in Ref. [42] it is not applicable to thermodynamic systems with dynamically generated masses.

5. Conclusion

I have calculated the partition function of a scalar field in a finite box and analysed the effects of finite volume on the free energy density in different regimes. The formulas can be used to make estimates on thermodynamical quantities calculated on the lattice.

If in theories with spontaneous symmetry breaking the inverse volume is beyond any mass scale, the effects are negligible and ordinary chiral perturbation theory can be used. Finite size effects are only relevant if the dimension of the box is of the order of the lightest Goldstone boson Compton wavelengths. They become dominant, and change the behaviour of various observables qualitatively, if the box size is smaller than the pion wavelength. The effects manifest themselves in the partition function through the lightest Goldstone boson modes that rotate freely in group space unless the explicit symmetry breaking term is large enough. By using the Fadeev-Popov procedure, the quasi-zero modes are treated as collective variables and the heavier modes are treated as higher order terms. However in both regimes only the lightest Goldstone modes (the π-mesons) contribute to the finite size effects.

For the case of a massless scalar field the partition function features a non-negligible contribution of a logarithmic term. This term stems from the Matsubara zero mode contribution of the momentum sum. However, the technique used was not able to reproduce quantitatively other results in the literature, it turns out that the factor of the logarithmic term is 3 times larger than that in Ref. [40]. However, several conclusion can be drawn. The translational invariance of the energy-momentum tensor remains intact and $e - 3p = 0$ remains an exact identity. On the other hand, the relation of pressure and free energy density, that exists in the thermodynamical limit $f = -p$ is not fulfilled and the pressure can be traded for the free energy density only in the large LT limit.

In Ref. [40] it is expected that even in the interacting case of a boson gas with dinamically generated masses the logarithmic behaviour of finite size effects is maintained. However, it turns out that the finite size corrections are exponentially small provided the theory exhibits a mass gap in its spectrum whose Compton wave length does not extend beyond the dimension of the box [42]. In addition if a lattice with a ratio $N_s/N_t = LT \geq 4$ is used, effects can be reduced to below 1%. This contradicts the previous statement, since thermal masses are always generated in a plasma and the finite size corrections are thus expected to fall off exponentially with increasing volume and not to grow logarithmically.

A. Partition function in quantum mechanics

The starting point is the spatial coordinate and its canonical momentum with their respective operators obeying the commutation relation ($\hbar \equiv 1$)

$$[\hat{q}, \hat{p}] = -i, \tag{A.1}$$

the completeness relation

$$\int \mathrm{d}q |q\rangle\langle q| = \mathbb{1}, \int \frac{\mathrm{d}p}{2\pi} |p\rangle\langle p| = \mathbb{1} \tag{A.2}$$

and the projection on each other:

$$\langle q|p\rangle = \mathrm{e}^{ipq} \tag{A.3}$$

The partition function can be expressed in the spatial representation as follows:

$$Z = \mathrm{Tr}[e^{-\beta \hat{H}}] = \int \mathrm{d}q \langle q|e^{-\beta \hat{H}}|q\rangle. \tag{A.4}$$

Now β is split into N intervals so that $\beta = N\epsilon$ and for each slice a completeness relation for the position operator on the right side and for the conjugated momentum on the left side of the exponential (A.2) is introduce:

$$\begin{aligned} Z = &\int \frac{\mathrm{d}p_N}{2\pi} ... \int \frac{\mathrm{d}p_1}{2\pi} \int \mathrm{d}q_N ... \int \mathrm{d}q_1 \int \mathrm{d}q \langle q|p_N\rangle\langle p_N|e^{-\epsilon \hat{H}}|q_N\rangle \cdot \\ &\cdot \langle q_N|p_{N-1}\rangle ... \langle p_1|e^{-\epsilon \hat{H}}|q_1\rangle\langle q_1|q\rangle. \end{aligned} \tag{A.5}$$

By expanding the exponential in Taylor series, one obtains:

$$Z \approx \int \prod_{i=1}^{N} \frac{\mathrm{d}p_i \mathrm{d}q_i}{2\pi} e^{ip_i(q_{i+1}-q_i)} \left(1 - \epsilon H(q_i, p_i) + \mathcal{O}(\epsilon^2)\right)\Big|_{x_{N+1}=x_1}. \tag{A.6}$$

Now using $\lim_{N\to\infty}(1 + \frac{x}{N})^N = \mathrm{e}^x$ and $\lim_{N\to\infty} \prod_{n=1}^{N}(1 + \frac{x_n}{N}) = \exp[\lim_{N\to\infty} \frac{1}{N} \sum_{n=1}^{N} x_n]$, the partition function:

$$Z = \lim_{N\to\infty} \int \left[\prod_{i=1}^{N} \frac{\mathrm{d}q_i \mathrm{d}p_i}{2\pi}\right] \exp\left\{-\sum_{j=1}^{N} \epsilon \left[\frac{p_j^2}{2m} - ip_j \frac{q_{j+1} - q_j}{\epsilon} + V(q_j)\right]\right\}\Bigg|_{x_{N+1}=x_1}. \tag{A.7}$$

With the following identifications:

$$\int \prod_{i=1}^{N} \mathrm{d}q_i \to \int \mathcal{D}q \text{ and } \int \prod_{i=1}^{N} \frac{\mathrm{d}p_i}{2\pi} \to \int \mathcal{D}p \tag{A.8}$$

and

$$\frac{q_{i+1}-q_i}{\epsilon} \to \dot{q}(t_i),$$
$$\epsilon \sum_{n=0}^{N-1} f(t_n) \to \int_0^\beta \mathrm{d}\tau f(\tau), \tag{A.9}$$

the final result is:

$$\mathcal{Z} = \int_{q(\beta)=q(0)} \frac{\mathcal{D}q\mathcal{D}p}{2\pi} \exp\left\{-\int_0^\beta \mathrm{d}\tau \left[\frac{p(\tau)^2}{2m} - ip(\tau)\dot{q}(\tau) + V(q(\tau))\right]\right\}. \tag{A.10}$$

The path integral is gaussian in the conjugated momenta, so that, without loss of generality, the integration over all momenta can be carried out:

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}p_i}{2\pi} \exp\left\{-\epsilon\left[\frac{p_i^2}{2m} - ip_i \frac{q_{i+1}-q_i}{\epsilon}\right]\right\} = \sqrt{\frac{m}{2\pi\epsilon}} \exp\left[-\frac{m(q_{i+1}-q_i)^2}{2\epsilon}\right], \tag{A.11}$$

obtaining

$$\mathcal{Z} = C \int_{q(\beta)=q(0)} \mathcal{D}q \exp\left\{-\int_0^\beta \mathrm{d}\tau \left[\frac{m}{2}\left(\frac{\mathrm{d}q(\tau)}{\mathrm{d}\tau}\right)^2 + V(q(\tau))\right]\right\} \tag{A.12}$$

with

$$C \equiv \left(\frac{m}{2\pi\epsilon}\right)^{N/2}. \tag{A.13}$$

The factor C does not contain any information about the dynamics of the system since it does not depend on $V(q)$. It is divergent in the limit $\epsilon \to 0$ and $N \to \infty$ but still is important in determining the correct partition function in the continuum limit. In combination with the remaining path integral the partition function will be finite. It can be easily determined for the simple case of an harmonic oscillator. Its partition function has the following structure:

$$Z = C \int_{q(\beta)=q(0)} \mathcal{D}q \exp\left\{-\int_0^\beta \mathrm{d}\tau \left[\frac{m}{2}\left(\frac{\mathrm{d}q(\tau)}{\mathrm{d}\tau}\right)^2 + \frac{m\omega^2}{2} q(\tau)^2\right]\right\}. \tag{A.14}$$

Using the Fourier representation for $q(\tau)$:

$$q(\tau) = T \sum_{n=-\infty}^{\infty} (a_n + ib_n) e^{i\omega_n \tau}, \tag{A.15}$$

and dropping half of the non-zero Matsubara modes (due to reality of the $q(\tau)$ coordinate) one obtains:

$$\begin{aligned} Z &= C^{'} \int_{-\infty}^{\infty} \mathrm{d}a_0 \int_{-\infty}^{\infty} \prod_{n\geq 1} \mathrm{d}a_n \mathrm{d}b_n \exp\left[-\frac{1}{2} mT\omega^2 a_0^2 - mT \sum_{n\geq 1} (\omega_n^2 + \omega^2)(a_n^2 + b_n^2)\right] \\ &= C^{'} \sqrt{\frac{2\pi}{mT\omega^2}} \prod_{n=1}^{\infty} \frac{\pi}{mT(\omega_n^2+\omega^2)}, \quad C^{'} = C \left|\det\left[\frac{\delta x(\tau)}{\delta x_n}\right]\right|. \end{aligned} \tag{A.16}$$

Since the prefactor, $C^{'}$ is independent of ω it can be calculated in the limit $\omega \to 0$. Moreover, because the integral over the $n = 0$ Matsubara mode is divergent, it will be regulated for the moment by evaluating it on a finite interval. Using Eq. (A.4) and making the calculations again in a finite volume, it is possible to extract $C^{'}$ by matching the sides of both calculations:

$$C^{'} = \frac{T}{2\pi}\sqrt{2\pi mT}\prod_{n=1}^{\infty}\frac{mT\omega_n^2}{\pi} \tag{A.17}$$

and thus, for the harmonic oscillator the partition function reads:

$$Z = \frac{T}{\omega}\prod_{n=1}^{\infty}\frac{\omega_n^2}{\omega_n^2+\omega^2}. \tag{A.18}$$

Turning now to the partition function of a scalar field the difference to "ordinary" statistical mechanics is that the trace is to be understood as an integration over all (in principle infinitely many) degrees of freedom of the fields. This provides also the link to quantum field theory at zero temperature. It is possible to transfer the result obtained previously by making the following observations. First, consider now the spatial coordinate q as an internal variable of the scalar field $\phi(t,q)$. Therefore the field taken at a certain position, let us say $\phi(t,0)$ behaves like $q(t)$. So the simplest way to determine the partition function of a scalar field is to take the Lagrange density for a scalar field as a replacement for the previous Lagrangian. Second, if we do not fix the number of spatial coordinates yet, an additional d-dimensional integration has to be performed. The Lagrangian for a scalar field now contains an additional term namely the derivative term with respect to the spatial coordinates $\partial_i\phi\partial_i\phi$. This term originates from a nearest neighbour interaction but does not affect the calculation of the partition function[1]. Third, the path integral has to be performed not only in the time direction, but also in the additional d dimensions ($q \to \mathbf{x}$). Therefore the result is:

$$\mathcal{Z} = \int_{\phi(\beta,\mathbf{x})=\phi(0,\mathbf{x})}\prod_{\mathbf{x}}\left[C\mathcal{D}\phi(\tau,\mathbf{x})\right]\exp\left[-\int_0^{\beta}\mathrm{d}\tau\int\mathrm{d}^d\mathbf{x}\mathcal{L}_E\right]. \tag{A.19}$$

with

$$\mathcal{L}_E = -\mathcal{L}_M(t\to -i\tau) = \frac{1}{2}\left(\frac{\partial\phi}{\partial\tau}\right)^2 + \sum_{i=1}^{d}\frac{1}{2}\left(\frac{\partial\phi}{\partial x^i}\right)^2 + V(\phi). \tag{A.20}$$

[1]The term that is important in calculating the partition function is the one that is quadratic in the time derivative of the field, $\partial_t\phi\partial_t\phi$.

B. The QCD Lagrangian

Quantum Chromodynamics is the theory of strong interactions. It relies on the property of quarks not to be only electrically charged but to have also a so-called color charge of either "red", "blue" or "green". Therefore the fermionic fields describing the quarks are written as triplets in color space:

$$\psi(x) \equiv \begin{pmatrix} \psi_r(x) \\ \psi_b(x) \\ \psi_g(x) \end{pmatrix}. \tag{B.1}$$

A term of the form $\overline{\psi}\psi$ is to be understood as $\overline{\psi}\mathbb{1}\psi$.

The principle of gauge invariance in Quantum Electrodynamics proved very fruitful as it introduced the photon as an interaction particle between charged fermions in a natural way.

For determining the QCD Lagrangian the same procedure as in the case of Quantum Electrodynamics is followed. It is expected that the interaction particles of QCD, the gluons, emerge from the same requirement of gauge invariance as in QED. The difference lies merely in the symmetry group of the Lagrangian.

The free Lagrangian of massive fermions,

$$\overline{\psi}(x)(i\partial\!\!\!/ - m)\psi, \tag{B.2}$$

exhibits a global $SU(3)$ symmetry because of Eq. (B.1). It is invariant under the following transformation of the fields:

$$\psi(x) \to U\psi(x) = \exp\left(i\alpha^a \frac{\lambda^a}{2}\right) \text{ with } a = 1, ..., 3^2 - 1 = 8. \tag{B.3}$$

The λ^a matrices are the generators of the fundamental representation of the $SU(3)$ group. They obey the following commutation relations:

$$\left[\frac{\lambda^a}{2}, \frac{\lambda^b}{2}\right] = i f^{abc} \frac{\lambda^c}{2}, \tag{B.4}$$

and are normalized as:

$$\mathrm{Tr}(\lambda^a \lambda^b) = 2\delta_{ab}. \tag{B.5}$$

The set of real numbers f^{abc} are called the structure constants.

A second irreducible representation is called the adjoint representation and the generators are defined in terms of the structure constants as follows:

$$(\lambda_G^b)_{ac} = if^{abc}. \tag{B.6}$$

When trying to promote the global symmetry of the Lagrangian to a local one,

$$U \to U(x) \equiv \exp\left(i\alpha^a(x)\frac{\lambda^a}{2}\right), \tag{B.7}$$

the derivative term $\partial_\mu\psi$ generates the difficulty. A detailed treatment of this problem can be found in Ref. [1]. Here, merely the result is stated by formally adding to the partial derivative a term in the following way:

$$\partial_\mu \to D_\mu = \partial_\mu - igA_\mu^a\frac{\lambda^a}{2}. \tag{B.8}$$

Additionally, the $A_\mu^a(x)$ vector fields are required to transform in the following way under a local $SU(3)$ group:

$$A_\mu^a(x)\frac{\lambda^a}{2} \to U(x)\left(A_\mu^a(x)\frac{\lambda^a}{2} + \frac{i}{g}\partial_\mu\right)U^\dagger(x). \tag{B.9}$$

For small α this reads:

$$A_\mu^a\frac{\lambda^a}{2} \to A_\mu^a\frac{\lambda^a}{2} + \frac{1}{g}(\partial_\mu\alpha^a)\frac{\lambda^a}{2} + i\left[\alpha^a\frac{\lambda^a}{2}, A_\mu^b\frac{\lambda^b}{2}\right] + ... \tag{B.10}$$

All these modifications finally ensure that the derivative term behaves like:

$$D_\mu\psi \to D_\mu^{'}\psi^{'} = U(x)D_\mu\psi, \tag{B.11}$$

making thus the new Lagrangian invariant under local $SU(3)$ transformations.

The A_μ^a fields are thus the 8 gluons which act as interaction particles between the matter fields. Now, an additional term involving only the gluon fields is needed in the Lagrangian in order to describe their propagation. Noting that the transformation law of the covariant derivative implies that:

$$[D_\mu, D_\nu]\psi(x) \to U(x)[D_\mu, D_\nu]\psi, \tag{B.12}$$

one concludes that $[D_\mu, D_\nu]$ transforms as:

$$[D_\mu, D_\nu] \to U(x)[D_\mu, D_\nu]U^\dagger(x). \tag{B.13}$$

By calculating explicitly $[D_\mu, D_\nu]$ one obtains:

$$[D_\mu, D_\nu] = -igF_{\mu\nu}^a\frac{\lambda^a}{2} \tag{B.14}$$

with

$$F^a_{\mu\nu} = \partial_\mu A^a_\nu - \partial_\nu A^a_\mu + g f^{abc} A^b_\mu A^c_\nu. \tag{B.15}$$

called the field strength tensor.

By defining the covariant derivative in the adjoint representation,

$$\mathcal{D}^{ac}_\mu = \delta^{ac}\partial_\mu + g f^{abc} A^b_\mu, \tag{B.16}$$

The field strength tensor can be also written as:

$$F^a_{\mu\nu} = \partial_\mu A^a_\nu - \mathcal{D}^{ac}_\nu A^c_\mu. \tag{B.17}$$

The field strength tensor is not a gauge-invariant quantity. Since it involves only the gluon field it is a candidate for the kinetic term in the Lagrangian. The simplest gauge invariant quantity that can be constructed and regarded as the kinetic term of the A^a_μ fields is:

$$-\frac{1}{2}\mathrm{tr}\left[(F^a_{\mu\nu}\frac{\lambda^a}{2})^2\right] = -\frac{1}{4}(F^a_{\mu\nu})^2. \tag{B.18}$$

The trace is to be understood of acting in color space.

Summing the terms up, the Lagrangian that is now invariant under local $SU(3)$ transformations reads:

$$\mathcal{L} = \overline{\psi}(i\not{D} - m)\psi - \frac{1}{4}F^a_{\mu\nu}F^{a\mu\nu}. \tag{B.19}$$

One can perform a sum over all quark flavours in order to get the full Lagrangian of QCD.

C. Momentum sum for massless case

In this appendix the functions used in section 4.2 are defined.

The derivation of Ref. [36] is used. For simplicity D denotes the dimensionality of the space-time as was the case in section 4.2 whereas d stands again only for the spatial dimensions.

By denoting:

$$G_r = \frac{\Gamma(r)}{V} \sum_p \frac{1}{(p^2+m^2)^r}, \tag{C.1}$$

with $V_D \equiv L_0 ... L_d$, one obtains the following identity:

$$\sum_p \ln(p^2+m^2) = \frac{\mathrm{d}}{\mathrm{d}r} \frac{V}{\Gamma(r)} G_r \bigg|_{r=0}. \tag{C.2}$$

The sum in Eq. (C.1) can be evaluated, obtaining:

$$G_r = \frac{\Gamma(r-D/2)}{(4\pi)^{D/2}} (m^2)^{d/2-r} + \sum_l{}' \int_0^\infty \mathrm{d}t\, t^{r-1} (4\pi t)^{-D/2} e^{-tm^2 - \frac{l^2}{4t}}, \tag{C.3}$$

where $l \equiv (l_0 L_0, ..., l_d L_d)$ and the prime in the sum denotes omission of the zero mode again. In order to use this function in the calculation of the partition function for the massless case, a low mass expansion is performed. Having this expansion, the limit $m \to 0$ can than be taken. Given the theta function

$$S(x) \equiv \sum_{n=-\infty}^{\infty} e^{-\pi n^2 x}, \tag{C.4}$$

the second term in Eq. (C.3) can be written as:

$$g_r = \frac{1}{V_D} \left(\frac{\bar{L}^2}{2\pi}\right)^r \int_0^\infty \mathrm{d}t\, t^{r-D/2-1} \exp\left(-\frac{m^2 \bar{L}^2 t}{4\pi}\right) \left[\prod_{i=0}^{d} S\left(\frac{L_i^2}{t\bar{L}^2}\right) - 1\right], \tag{C.5}$$

with $\bar{L} \equiv V^{1/D}$ the mean size of the box.

By splitting now the integral into 2 pieces, $0 \le t \le 1$ and $1 \le t \le \infty$ the identity

$$S(x) = \frac{1}{\sqrt{x}} S\left(\frac{1}{x}\right) \tag{C.6}$$

is used for the second interval. After substituting in the second interval the variable of integration,

$t \to 1/t$, the entire integral can be written as:

$$
\begin{aligned}
g_r &= \frac{1}{V_D}\left(\frac{\bar{L}^2}{4\pi}\right)^r \left(a_r + b_r - b_{r-D/2}\right), \\
a_r &= \int_0^1 \mathrm{d}t\, t^{r-D/2-1} \exp\left(-\frac{m^2\bar{L}^2 t}{4\pi}\right)\left[\prod_{i=0}^{d} S\left(\frac{L_i^2}{t\bar{L}^2}\right) - 1\right] \\
&+ \int_0^1 \mathrm{d}t\, t^{-r-1} \exp\left(-\frac{m^2\bar{L}^2 t}{4\pi}\right)\left[\prod_{i=0}^{d} S\left(\frac{\bar{L}^2}{tL_i^2}\right) - 1\right], \\
b_r &= \int_1^\infty \mathrm{d}t\, t^{r-1} \exp\left(-\frac{m^2 L^2 t}{4\pi}\right).
\end{aligned}
\tag{C.7}
$$

Now the only quantity that contains infrared divergences in the limit $m \to 0$ is b_r. Therefore, the a_r function can be expanded in powers of m^2 without problems, yielding:

$$
a_r = \sum_{n=0}^{\infty}\left(-\frac{m^2\bar{L}^2 t}{4\pi}\right)^n \frac{1}{n!}\alpha_{r+n}. \tag{C.8}
$$

The expansion coefficient is:

$$
\alpha_s = \hat{\alpha}_{s-D/2}\left(\frac{L_i}{\bar{L}}\right) + \hat{\alpha}_{-s}\left(\frac{\bar{L}}{L_i}\right) \tag{C.9}
$$

with

$$
\hat{\alpha}_p(l_i) = \int_0^1 \mathrm{d}t\, t^{p-1}\left[\prod_{i=0}^{d} S(l_i^2/t) - 1\right]. \tag{C.10}
$$

The infrared divergence in b_r comes in the form of a fractional power of m, namely m^{-2r}. This contribution stems from the $p = 0$ mode in the momentum sum (C.1):

$$
b_r = \left(\frac{m^2\bar{L}^2}{4\pi}\right)^{-r}\Gamma(r) - \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{m^2\bar{L}^2}{4\pi}\right)^n \frac{1}{n+s}. \tag{C.11}
$$

The function b_r may be evaluated also for negative r because the singularities occurring in the power expansion at $n = 0, -1, ...$ are compensated for by the divergences of the Gamma function. Thus, for negative $r \equiv -N$ one obtains:

$$
b_{-N} = \frac{(-1)^{N+1}}{N!}\left(\frac{m^2\bar{L}^2}{4\pi}\right)^N\left(\ln\frac{m^2\bar{L}^2}{4\pi} + \gamma_E - \sum_{n=1}^{N}\frac{1}{n}\right) + \sum_{n\neq N}\frac{1}{n!}\left(-\frac{m^2 L^2}{4\pi}\right)^n \frac{1}{N-n}. \tag{C.12}
$$

Having now expressed the integral in Eq. (C.3) as a power expansion in m^2 and having separated the infrared singularities from the finite part, it is possible to calculate the sum in Eq. (C.1) in the massless case by noticing that one has to subtract first the zero mode contribution $p = (0, ..., 0)$ before taking the limit $m \to 0$.

The Epstein Zeta function is defined as:

$$
\mathcal{Z}_{d-1}(a_1, ...a_d; s) \equiv \sum_{n_1=-\infty}^{\infty} ... \sum_{n_d=-\infty}^{\infty}{}' \left[(a_1 n_1)^2 + ... + (a_d n_d)^2\right]^{-s}, \tag{C.13}
$$

and is called homogeneous if all the coefficients a_i are equal to 1. It can be expressed in terms of sums over the arithmetical function $r_d(n)$ that is the number of representations of an integer n as a sum of d squares disregarded to sign or order:

$$\mathcal{Z}_d(s) = \sum_{n=1}^{\infty} \frac{r_d(n)}{n}^s . \tag{C.14}$$

The formulas for $r_d(n)$ are known exactly in even dimensions $d = 2, 4, 6, 8$ in terms of one-dimensional sums. In odd dimensions however the function is difficult to obtain and is expressed as a sum of a dominant term and a small reminder.

For $d = 1$, $\mathcal{Z}$ is by definition related to the Riemann Zeta function:

$$\mathcal{Z}_1(s) = 2\zeta(2s). \tag{C.15}$$

In the calculations of chapter 4 $d = 3$ was needed. Its expression is:

$$\mathcal{Z}_3(s) = 4\frac{\sqrt{\pi}\Gamma(s-\frac{1}{2})}{\Gamma(s)}\zeta(s-\frac{1}{2})\beta(s-\frac{1}{2})-4\frac{\sqrt{\pi}\Gamma(s-\frac{1}{2})}{\Gamma(s)}\zeta(2s-1)+8\zeta(s)\beta(s)-2\zeta(2s)+8R_3(s), \tag{C.16}$$

where

$$\beta(s) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)^s} \tag{C.17}$$

is the Dirichlet Beta function.

The reminder in d dimensions is:

$$\begin{aligned} R_d(s) = &\sum_{n_1=1}^{\infty} ... \sum_{n_{d-1}=1}^{\infty} \sum_{l=1}^{\infty} \frac{2}{\sqrt{\pi}}\Gamma(1-s)\sin(\pi s)\left(\frac{\pi l}{\sqrt{n_1^2+...+n_{d-1}^2}}\right)^{s-\frac{1}{2}} \\ &\cdot K_{s-1/2}\left(2\pi l\sqrt{n_1^2+...+n_{d-1}^2}\right), \end{aligned} \tag{C.18}$$

where $K_d(x)$ is the modified Bessel function of the second kind. It should be noted that for $s = 0$, the reminder is identical zero leading to an expression for the Epstein Zeta function in terms of only one-dimensional sums.

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Eidesstattliche Erklärung

Hiermit versichere ich, dass ich die vorliegende Masterarbeit selbstständig verfasst und keine anderen als die angegebenen Quellen und Hilfsmittel benutzt habe.

Ioan Ghişoiu

October 7, 2010
