RESULTS AND PROBLEMS IN IRREVERSIBLE STATISTICAL MECHANICS OF OPEN SYSTEMS

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§ 1. Introduction

Rigorous results about the foundations of equilibrium statistical mechanics are extremely difficult to obtain. The beautiful proof of the Bernoulli property of billiards with smooth convex scatterers [S1] , the geometry of the energy surface for large closed systems [R3], and the justification of the Boltzmann equation for hard spheres in the Grad limit [L1] are illustrative examples, which will caution us from expecting rapid progress in this difficult field.

The study of open systems does not really help to overcome these technical problems. It does, however, open new possibilities which are in a sense complementary to collision mixing in closed systems. One can rather easily prove that small quantum systems coupled to suitable reservoirs of a diffusive type (e.g. an ideal gas in thermal equilibrium) via suitable interactions strongly approach equilibrium. Conceptually, however, open systems are important for describing stationary nonequilibrium situations. Here the proof of the Onsager relations [O1] is more natural than in linear response theory, and the main input is the KMS property [H1] of the reservoir rather than time reversal invariance. Most interesting are open systems far from thermal equilibrium with the possibility of a wide range of non-equilibrium phase transitions (see [G2]) .

In my review I shall not treat the classical case and deal only with a very special class of models, which have come up frequently in my joint work with E.H. Lieb, but which belong to the folklore of the yet unwritten general theory of irreversible statistical mechanics.

§ 2. Open Systems of Finitely Many Degrees of Freedom

Small quantum systems of finitely many degrees of freedom (for instance any number of particles in a box) coupled to suitable (but not very physical) infinite quantum systems, called reservoirs, can show a very strong approach to equilibrium.

The small system S has a Hilbert space $\mathcal{H}^S$ with the C^*-algebra $\mathfrak{A}^S$ of all bounded operators on $\mathcal{H}^S$ as observables. The states of S are all positive normalized trace class operators ω^S on $\mathcal{H}^S$, and the time evolution α_t^S is generated by a self-adjoint Hamiltonian $H^S = H^{S*}$ with $\operatorname{Tr} \exp -\beta H^S < \infty$ for all inverse temperatures $\beta > 0$. For simplicity of exposition we shall make the inessential assumption that $\dim \mathcal{H}^S < \infty$. The reservoir R is composed of r parts $R^1, .. R^r$, each with a C^*-algebra of observables $\mathfrak{A}^\varrho$, and a continuous 1-parameter group of time evolutions $\alpha_t^\varrho \in \operatorname{Aut} \mathfrak{A}^\varrho$. We set $\mathfrak{A}^R = \mathfrak{A}^1 \otimes \cdots \otimes \mathfrak{A}^r$ and $\alpha_t^R = \alpha_t^1 \otimes \cdots \otimes \alpha_t^r$.

The combined system has then the algebra $\mathfrak{A} = \mathfrak{A}^R \otimes \mathfrak{A}^S$. An interaction is any $V = V^* \in \mathfrak{A}$, and this gives rise to a time evolution α_t of $\mathfrak{A}$ [A1], [R2], which is the perturbation of $\alpha_t^R \otimes \alpha_t^S$. In an equilibrium state ω^R for α_t^R, where one has a GNS Hamiltonian H^R, the generator of α_t is $H^S + H^R + V$.

The reservoir (R, α^R) drives the system (S, α^S) strongly into equilibrium through the interaction V, if for a dense set of $A \in \mathfrak{A}$ in the strong topology of $\mathfrak{A}$

$$\underset{t \to \pm\infty}{\text{n-lim}} \; \alpha_{-t}^R \circ \alpha_t(A) = \alpha_\pm(A) \tag{2.1}$$

exists and $\alpha_\pm(A) \in \mathfrak{A}^R$.

Wave epimorphisms $\alpha_\pm$ have been studied by Robinson in the return to equilibrium of closed systems [R2]. It is not necessary that $\alpha_+ = \alpha_-$, as we shall see in theorem 2.4. The $\alpha_\pm$ intertwine between α_t and α_t^R : $\alpha_\pm \circ \alpha_t = \alpha_t^R \circ \alpha_\pm$. For many purposes, the following weaker property is sufficient: The reservoir (R, α^R, ω^R) in the α^R equilibrium state ω^R drives (S, α^S) weakly into equilibrium via V, if for a dense set of $A \in \mathfrak{A}$

$$\underset{t \to \pm\infty}{\text{s-lim}} \; \pi \circ \alpha_{-t}^R \circ \alpha_t(A) = A_\pm \tag{2.2}$$

exists in the strong topology in the GNS representation space $\mathcal{H}^R \otimes \mathcal{H}^S$ for ω^R, and if $A_\pm \in \pi(\mathfrak{A}^R)''$. The following obvious result motivates our definition:

<u>Theorem 2.1:</u> If (R, α^R, ω^R) drives (S, α^S) weakly via V, then for every initial state ω^S of S

$$\lim_{t \to \pm\infty} \omega^R \otimes \omega^S(\alpha_t(A)) = \omega_\pm(A) \tag{2.3}$$

exists on $\mathfrak{A}$ and is an equilibrium state with respect to α_t. If ω^R is a thermal equilibrium (KMS) state w.r.t. α^R with inverse temperature β, then $\omega_\pm$ are KMS states w.r.t. α for the same β.

We are interested in reservoirs $R^1, \ldots R^r$ which are in KMS states $\omega^{\beta_1}, \ldots \omega^{\beta_r}$ at different temperatures $\beta_1, \ldots \beta_r$ and which are coupled to S by $V = \sum_{\varrho=1}^r V^\varrho$, where $V^\varrho = V^{\varrho *} \in \mathfrak{A}^\varrho \otimes \mathfrak{A}^S$. For such a coupling, there is still some ambiguity in defining energy flux observables J^ϱ from R^ϱ to S. We require $J^\varrho = J^{\varrho *} \in \mathfrak{A}^\varrho \otimes \mathfrak{A}^S$ and

$$\frac{d}{dt} \alpha_t(H^S) \Big|_{t=0} = \dot{H}^S = \sum_{\varrho=1}^r J^\varrho . \tag{2.4}$$

Obviously, $J^\varrho = i[V^\varrho, H^S] + J^\varrho_o$, where $J^\varrho_o = J^{\varrho *}_o \in \mathfrak{A}^S$ and $\sum J^\varrho_o = o$.

<u>Problem:</u> Suppose that $(R, \alpha^R, \omega^{\beta_1} \ldots \omega^{\beta_r})$ drives (S, α^S) weakly via $\sum V^\varrho$ for an open neighborhood of $\beta_1 = \ldots \beta_r = \beta$. When do there exist energy fluxes $J^1, \ldots J^r$ (independent of $\beta_1 \ldots \beta_r$) such that the <u>Onsager relations</u> hold:

$$\omega_\pm(J^\varrho)\big|_\beta = 0 \tag{2.5}$$

$$\frac{\partial}{\partial \beta_\sigma} \omega_\pm(J^\varrho)\big|_\beta = \frac{\partial}{\partial \beta_\varrho} \omega_\pm(J^\sigma)\big|_\beta$$

for $\beta_1 = \ldots \beta_r = \beta$ and all $1 \leq \varrho, \sigma \leq r$?

<u>Problem:</u> Suppose that (R, α^R, ω^R) drives (S, α^S_λ) weakly via V for all $-\lambda_o \leq \lambda \leq \lambda_o > 0$, where α^S_λ is generated by $H^S + \lambda A$ with $A = A^* \in \mathfrak{A}^S$. Under what conditions is the equilibrium stable under the "mechanical perturbation" A, and when does it define a <u>linear response</u> to A by

$$\omega^\lambda_\pm(B) = \omega_\pm(B) + i\lambda \int_{\mp\infty}^{0} ds\, \omega_\pm([\alpha_s(A), B]) + o(\lambda)$$

$$\text{for } \lambda \to 0 \text{ and all } B \in \mathfrak{A} \text{ ?} \tag{2.6}$$

Up to now the most satisfactory results on the drive to equilibrium are known in the weak coupling (van Hove [H11]) limit. Let $\{\phi_1, \dots \phi_n\}$ be an orthonormal basis of $\mathcal{H}^S$ with $H^S \phi_i = \varepsilon_i \phi_i$ and $H^S \neq \varepsilon \mathbb{1}$. The reservoirs $R^1, \dots R^r$ are taken in KMS states $\omega^{\beta_1}, \dots \omega^{\beta_r}$, defining a representation π of $\mathfrak{A}$ and a Hamiltonian H^R. We take $V = \sum V^\varrho$, $V^\varrho = V^{\varrho *} \in \mathfrak{A}^\varrho \otimes \mathfrak{A}^S$ and set $H_o = H^R + H^S$ and (suppressing π)

$$H_\lambda = H_o + \lambda V \tag{2.7}$$

In this framework, the following result by Davies [D2] and Pulè [P1] is relevant:

<u>Theorem 2.2:</u> Assume that for all $1 \leq \varrho \leq r$

$$\omega^R(V^\varrho) = o \qquad \text{and} \tag{2.8}$$

$$\sup_t \| \omega^R(V^\varrho e^{iH_o t} V^\varrho e^{-iH_o t}) \| (1 + |t|)^{1+\varepsilon} < \infty \tag{2.9}$$

for some $\varepsilon > o$, and let either ω^R be quasifree, or assume bounds of type (2.9) for all truncated multi-time correlation functions of k V-operators, with rapid decrease of the suprema in k. Then for every $B \in \mathfrak{A}^S$ and every ω^S

$$\lim_{\substack{\lambda \to o \\ \lambda^2 t = \tau}} \omega^R \otimes \omega^S (e^{-iH_o t} e^{iH_\lambda t} B e^{-iH_\lambda t} e^{iH_o t}) = \omega^S(\tau)(B) =$$
$$= \lim_{\substack{\lambda \to o \\ \lambda^2 t = \tau}} \omega^R \otimes \omega^S (e^{iH_\lambda t} e^{-iH_o t} B e^{iH_o t} e^{-iH_\lambda t}) \tag{2.10}$$

exists and defines a density matrix in $\mathcal{H}^S$. For many interactions the non-diagonal elements $\omega^S_{ij}(\tau)$ of $\omega^S(\tau)$ in the energy basis decrease purely exponentially for $\tau \geq o$, $\omega^S_{ij}(\tau) = \exp \lambda_{ij} \, \omega^S_{ij}$, $\operatorname{Re} \lambda_{ij} < o$, while the weak coupling time evolution defines on the diagonal elements a strongly continuous Markov semigroup with the <u>master equation</u>

$$\frac{d}{d\tau} \omega^S_{ii}(\tau) = \sum_{j=1}^{n} K_{ij}(\beta_1, \dots \beta_r) \, \omega^S_{jj}(\tau) \tag{2.11}$$

$$K_{ij}(\beta_1, \dots \beta_r) = \sum_{\varrho=1}^{r} \{ W^\varrho_{ij} - \delta_{ij} \sum_{k=1}^{n} W^\varrho_{ki} \} ,$$

where the W^ϱ_{ij} satisfy <u>detailed balance</u>

$$W^\varrho_{ij} \exp - \beta_\varrho \varepsilon_j = W^\varrho_{ji} \exp - \beta_\varrho \varepsilon_i \quad . \tag{2.12}$$

Generically for H^S, this Markov process is ergodic. Then the unique equilibrium state $\overline{\omega}^S(\beta_1,\dots\beta_r)$ is for $\beta_1 = \dots = \beta_r = \beta$ the Gibbs state

$$\overline{\omega}^S_{ij}(\beta,\dots\beta) = Z^{-1}\exp(-\beta\varepsilon_i)\,\delta_{ij}\;,\; Z = \sum \exp-\beta\varepsilon_i\,. \tag{2.13}$$

In thermal equilibrium the only manifestation of the reservoir is its temperature. There exists a large class of interactions, where $\overline{\omega}^S(\beta_1,\dots\beta_r)$ for small deviations $|\beta_\varrho - \beta|$ from thermal equilibrium can be computed by a convergent perturbation expansion. This gives a microscopic model for the stochastic approach to open systems by Bergmann, Lebowitz et al. [B2]. Obviously, the energy H^S of S satisfies

$$\lim_{\substack{\lambda\to 0\\ \lambda^2 t=\tau}} \omega^R\otimes\omega^S\left(e^{iH_\lambda t} H^S e^{-iH_\lambda t}\right) = \omega^S(\tau)\,(H^S) \tag{2.14}$$

and the time evolution of $\omega^S(\tau)(H^S)$ is completely determined by (2.9). We take the simplest choice for the energy flux in the weak coupling limit:

$$\frac{d}{d\tau}\,\omega^S(\tau)(H^S) = \sum_{\varrho=1}^{r}\omega^S(\tau)(J^\varrho)\,, \tag{2.15}$$

$$J^\varrho = \sum_{i,j=1}^{n} W^\varrho_{ji}(\beta_\varrho)(\varepsilon_j - \varepsilon_i)\,|\phi_i\rangle\langle\phi_i|\,.$$

Then the entropy production in $\omega^S(\tau)$

$$\sigma(\omega^S(\tau)) = -\frac{d}{d\tau}\,k\sum_{i=1}^{n}\omega^S_{ii}(\tau)\ln\omega^S_{ii}(\tau) - k\sum_{\varrho=1}^{r}\beta_\varrho\,\omega^S(\tau)\,(J^\varrho) \tag{2.16}$$

is ≥ 0 with equality only for $\beta_1 = \dots = \beta_r = \beta$ and $\omega^S_{ii}(\tau) = \overline{\omega}^S_{ii}(\beta,\dots\beta)$ [B2]. An easy calculation [H8] leads to

<u>Theorem 2.3:</u> For the energy flows (2.15) through S weakly coupled to $R^1, \dots R^r$ in KMS states $\omega^{\beta_1},\dots\omega^{\beta_r}$, the Onsager relations hold in the stationary state $\overline{\omega}^S(\beta_1,\dots\beta_r)$ of (2.11):

$$\overline{\omega}^S(\beta_1,\dots\beta_r)\,(J^\varrho)\Big|_\beta = 0 \tag{2.17}$$

$$L_{\varrho\sigma} = \frac{\partial}{\partial\beta_\sigma}\overline{\omega}^S(\beta_1,\dots\beta_r)\,(J^\varrho)\Big|_\beta = \frac{\partial}{\partial\beta_\varrho}\overline{\omega}^S(\beta_1,\dots\beta_r)\,(J^\sigma)\Big|_\beta = L_{\sigma\varrho}$$

for $\beta_1 = \dots \beta_r = \beta$ and all $1 \leq \varrho, \sigma \leq r$. The assumptions about $\dim \mathcal{H}^S$ can be relaxed for suitable V, retaining only $\mathrm{Tr}\exp-\beta H^S < \infty$ for $\beta > o$. For interacting particles in an external magnetic field $\underline{B}$, our model leads to the symmetry

$$L_{\varrho\sigma}(\underline{B}) = L_{\sigma\varrho}(\underline{B}) \tag{2.18}$$

<u>without assuming time reversal invariance</u>. If in addition the latter holds for H^S and H_λ, then one obtains the standard form

$$L_{\varrho\sigma}(\underline{B}) = L_{\sigma\varrho}(-\underline{B}) . \tag{2.19}$$

Not very much is known about the drive to equilibrium without taking the weak coupling limit. It is <u>not</u> true that closed infinite systems with a strong return to equilibrium can always serve as reservoirs for driving even very simple open systems to equilibrium. Let e.g. S be one fermion with creation and annihilation operators $a^\#$ ($\{a,a^*\} = 1$, $\{a,a\} = o$) and

$$\mathcal{H}^S = \mathbb{C}^2 \quad , \quad H^S = \varepsilon a^* a \quad , \ \varepsilon \geq o . \tag{2.20}$$

Let $\mathfrak{A}$ be the C^*-algebra generated by $a^\#$ and a Fermi field $A^\#(\underline{k})$, $\underline{k} \in \mathbb{R}^3$, with $\{A(\underline{k}), A^*(\underline{k}')\} = \delta(\underline{k}-\underline{k}')$ and $\alpha_t^R(A(\underline{k})) = \exp(-i|\underline{k}|^2 t)A(\underline{k})$. Take the interaction $V = a^* A(v) + A(v)^* a$, where $A(v) = \int d\underline{k}\; v(\underline{k})\, A(\underline{k})$ and $v = v^* \in \mathcal{S}(\mathbb{R}^3)$ and $\int d\underline{k}\; v(\underline{k})^2 / |\underline{k}|^2 > \varepsilon$. The full time evolution α_t acts in the test function space $\mathcal{K} = \mathbb{C} \oplus L^2(\mathbb{R}^3)$: For $\mathcal{A}(F) = \varphi a + A(f)$, $F = (\varphi, f) \in \mathcal{K}$, $\alpha_t(\mathcal{A}(F)) = \mathcal{A}(e^{-iHt}F)$, where $HF = (\varepsilon\varphi + \int d\underline{k} v(\underline{k})\, f(\underline{k})$, $v(\underline{k})\varphi + |\underline{k}|^2 f(\underline{k}))$. The existence of an eigenstate $F_d = (\varphi_d, f_d)$ of H with $\varphi_d \neq o$ is responsible for the memory on the initial state ω^S in the approach to equilibrium: For $A \in \mathfrak{A}$, $\omega^R \otimes \omega^S\,(\alpha_t(A))$ converges for $t \to \pm\infty$, but the limit depends on ω^S.

A good case for drive to equilibrium is found in a class of small Fermi systems coupled to Fermi field reservoirs, which we shall call <u>elementary open systems</u> (EOS) and which one can couple to <u>interacting open systems</u> (IOS).

An <u>EOS</u> is one fermion $a^\#$ with $\mathcal{H}^S = \mathbb{C}^2$, $H^S = \varepsilon a^* a$, coupled to r Fermi fields $A_\varrho^\#(\omega)$, $\omega \in \mathbb{R}^1$, $1 \leq \varrho \leq r$, with $\alpha_t^R(A_\varrho(\omega)) = e^{-i\omega t} A_\varrho(\omega)$ and $\mathfrak{A}$ the CAR algebra generated by $\{a^\#, A_\varrho^\#(\omega)\}$. A family of <u>regular</u> interactions is given by $V^\tau = \sum_{\varrho=1}^{r} V_\varrho^\tau$, where $g_\varrho = g_\varrho^* \neq o$, $1 \leq \tau < \infty$ and

$$V_\varrho^\tau = g_\varrho \int (1 + \omega^2/\tau^2)^{-1/2} (A_\varrho^*(\omega)\, a + a^*\, A_\varrho(\omega))\, d\omega \tag{2.21}$$

The interacting time evolution α_t^τ leads to a stochastic differential equation for $a^\tau(t) = \alpha_t^\tau(a)$:

$$\dot{a}^\tau(t) = -i\varepsilon a^\tau(t) - \sum_{\varrho=1}^{r} \gamma_\varrho \tau \int_0^t ds\; e^{-\tau(t-s)} a^\tau(s)$$
$$- i\sum_{\varrho=1}^{r} g_\varrho A_\varrho^\tau(t) \quad , \quad a^\tau(o) = a \;, \tag{2.22}$$

where $\pi g_\varrho^2 = \gamma_\varrho$ and $A_\varrho^\tau(t) = \int d\omega\, A_\varrho(\omega)\, e^{-i\omega t}\,(1+\omega^2/\tau^2)^{-1/2} \in \mathfrak{A}^R$. From $a^\tau(t)$, $A_\varrho^\tau(\omega,t) = \alpha_t^\tau(A_\varrho(\omega))$ can be computed: $A_\varrho^\tau(\omega,t) = e^{-i\omega t} A_\varrho(\omega) - ig_\varrho \int_0^t ds\,(1+\omega^2/\tau^2)^{-1/2} e^{-i\omega(t-s)} a^\tau(s)$. One differentiation removes the retardation in (2.22), and the elementary solution shows exponential approach to equilibrium uniformly in $1 \leq \tau \leq \infty$. This property is not restricted to the Lorentzian kernel in (2.21). The <u>singular interaction</u> limit $\tau \to \infty$ is particularly simple: α_t^∞ is still an automorphism of $\mathfrak{A}$, derived from the 1st order stochastic differential equation

$$\dot{a}^\infty(t) = -(i\varepsilon + \sum \gamma_\varrho)\, a^\infty(t) - i\sum g_\varrho A_\varrho^\infty(t) \;, \tag{2.23}$$

with fermion "white noise" $A_\varrho^\infty(t) = \int d\omega e^{-i\omega t} A_\varrho(\omega)$ as input. For $t < o$, the γ_ϱ change to $-\gamma_\varrho$.

An <u>IOS</u> consists of N EOS with uncoupled identical reservoirs, $a_n^\#$, $A_{\varrho n}^\#(\omega)$ $(1 \leq n \leq N$, $1 \leq \varrho \leq r)$, and any nonlinear interaction $H_I^S = H_I^{S*} \in \mathfrak{A}^S$:

$$H^S = \sum_{n=1}^{N} \varepsilon_n a_n^* a_n + H_I^S$$

$$V^\tau = \sum_{n=1}^{N} \sum_{\varrho=1}^{r} V_{\varrho n}^\tau$$

where $V_{\varrho n}^\tau$ has the form (2.21) with $g_{\varrho n} = g_\varrho$ n-independent. In the singular limit, this system is a Hamiltonian model for the following non-linear dissipative stochastic differential equation $(t \geq o)$

$$\dot{a}_n^\infty(t) = -(i\varepsilon + \sum \gamma_\varrho)\, a_n^\infty(t) - i\sum g_\varrho A_{\varrho n}^\infty(t) \tag{2.24}$$
$$+ i[H_I^S, a_n]^\infty(t) \quad , \quad a_n^\infty(o) = a_n \;.$$

As energy flow we take

$$J_{\varrho}^{\tau}(t) = i\left[V_{\varrho}^{\tau}, H^{S}\right]^{\tau}(t) \quad . \tag{2.25}$$

For $\tau<\infty$, $J_{\varrho}^{\tau}(t)\in\mathfrak{A}$, while $J_{\tau}^{\infty}(t)$ is an operator-valued distribution which in Theorem 2.4 has continuous expectation values in $\omega^{R}\otimes\omega^{S}$:

Theorem 2.4: In every EOS and in every IOS with small non-linearity, $\| H_{1}^{S}\|<C_{N}\sum\gamma_{\varrho}$, the reservoirs (R, α^{R}) and interaction V^{τ} drive (S,α^{S}) strongly to equilibrium and uniformly for $1\leq\tau\leq\infty$. In general $\alpha_{+}\neq\alpha_{-}$. If the reservoirs R^{ϱ} are in KMS states with respect to α^{ϱ} with temperatures β_{ϱ} , then in the equilibrium state $\omega_{\pm}^{\tau}$ of the open driven system the Onsager relations (2.5) hold and $\omega_{\pm}^{\tau}$ is stable in the sense of (2.6).

One proves this proposition for an IOS by an analysis of the time dependent perturbation expansion, which converges uniformly for $-\infty\leq t\leq +\infty$, if $\| H_{1}^{S}\| < C_{N}\sum\gamma_{\varrho}$ holds [H9]. In the weak coupling limit one recovers Theorem 2.3. Again, instead of assuming time reversal invariance, one uses the KMS property of the reservoir states $\omega^{\beta_{\varrho}}$.

§ 3. The Limit of ∞-Many Degrees of Freedom

Nothing dramatic happens in the weak coupling limit, if the temperatures of the reservoirs are far apart. If the generator $P(\tau)$ of the positive transition semigroup (2.11) on ℓ is (quasi)compact for some $\tau > 0$, then there exist a projection Π with finite dimensional range and strictly positive constants $\varkappa$ and γ , such that $\|P(\tau) - \Pi\| < \varkappa \exp -\gamma\tau$. Then zero is an isolated point of $\sigma(K)$, and the remainder of $\sigma(K)$ lies in the half-plane $\{\mathrm{Re}\,\lambda\leq -\gamma\}$ [W1]. In particular there exist <u>no oscillatory stationary states</u> for these continuous time Markov chains even far from thermal equilibrium.

Similarly, the non-linear Langevin equations of the type (2.24) for finitely many degrees of freedom should not lead to sharp "dissipative structures"[G1] even for strong nonlinearities. A general theory is lacking, but the example of the classical equation

$$\dot{z}(t) = (i\omega+\mu)\, z(t) - |z(t)|^{2}\, z(t) + f(t) \tag{3.1}$$

with $z\in\mathbb{C}$, $\omega,\mu\in\mathbb{R}$ and $f(t)$ Gaussian white noise, should be typical.

Without f one has a Hopf bifurcation [H10] at $\mu = o$ from a stationary to aperiodic attractor, while the stochastic equation has a unique equilibrium state which is analytic in μ across $\mu = o$ [R1].

Hence, as in the case of closed systems, one has to pass to the thermodynamic limit in order to obtain phase transitions. In this section we study the limit $N \to \infty$ for IOS of the type (2.24). With the present technology, only mean field non-linearities can be analysed in a conclusive way, and this has been done by Lieb and myself in a series of papers [H4-6], [L2], guided from the findings in quantum optics [H3].

Mean field interactions between EOS are introduced by grouping the local fermion degrees of freedom into a large number N of groups each having M elements. The fermions with a_n^m, $a_{n'}^{m'}$ ($1 \leq m,m' \leq M$, $1 \leq n,n' \leq N$) interact for fixed m,m' with the same strength, irrespective of whether n and n' are close together or far apart. Such nonlinearities occur in qualitatively successful models for lasers [H3] and superconductors [B1] and lead to H^S of the type

$$H^S_{(N)} = N\ P(\underline{\sigma}_{(N)})\ , \tag{3.2}$$

where P is a hermitean polynomial in the <u>intensive observables</u>

$$\underline{\sigma}_{(N)} = (\sigma^{ij}_{(N)} = N^{-1} \sum_{n=1}^{N} a_n^{i*} a_n^j\ )\ . \tag{3.3}$$

It is helpful, but not necessary, to restrict oneself to Hamiltonians of the type (3.2). The advantage is algebraic: the $\sigma^{ij}_{(N)}$ are closed under commutation. Hence under the combined action of $H^S_{(N)}$ and $H^R_{(N)}$ (see (3.5)) one obtains the Heisenberg equations of motion for $t \geq o$:

$$\dot{\sigma}^{ij}_{(N)}(t) = -\gamma^{ij}(\sigma^{ij}_{(N)}(t) - \eta^{ij}) + i[H^S_{(N)}, \sigma^{ij}_{(N)}](t) + \varphi^{ij}_{(N)}(t)\ . \tag{3.4}$$

Hence $i[H^S_{(N)}, \sigma^{ij}_{(N)}] = Q^{ij}(\underline{\sigma}_{(N)})$ is again a polynomial in the components of $\underline{\sigma}_N = \underline{\sigma}_N(0)$. We have taken singular reservoirs and have suppressed $\tau = \infty$. For finite τ one needs a larger set of intensive observables for closure [H6]. We further choose ω^R to be a Fock state and double the number of reservoirs in order to obtain sufficiently many parameters:

$$\begin{aligned} H^R_{(N)} = & \sum_{m,n} \int_{-\infty}^{+\infty} d\omega\ \omega (A_n^m(\omega)^* A_n^m(\omega) + B_n^m(\omega)^* B_n^m(\omega)\ ) \\ & + \sum_{m,n} \int_{-\infty}^{+\infty} d\omega\ \{ f^m A_n^m(\omega)^* a_n^m + g^m B_n^m(\omega)^* a_n^m + \text{h.c.} \} \end{aligned} \tag{3.5}$$

$$A_n^m(\omega)\Omega^R = B_n^m(\omega)^* \Omega^R = o \quad . \tag{3.6}$$

Then the damping and pumping constants in (3.4) become

$$\gamma^{ij} = \gamma^i + \gamma^j, \; \pi(|f^i|^2 + |g^i|^2) = \gamma^i \; , \tag{3.7}$$
$$\eta^{ij} = \delta^{ij} \; |g^i|^2 (\,|f^i|^2 + |g^i|^2)^{-1}.$$

The remarkable feature of (3.4) is that the influence of the reservoir in the Heisenberg equation of motion for the intensive observables splits into a friction and a pumping term and a <u>fluctuation force</u>

$$\varphi^{ij}_{(N)} = \varphi^{ij}_{+(N)} + \varphi^{ij}_{-(N)} \; , \; \varphi^{ij\,*}_{-(N)} = \varphi^{ji}_{+(N)} \tag{3.8}$$

$$\varphi^{ij}_{\pm(N)}(t) = \frac{i}{N} \sum_{n=1}^{N} \{ f^i A_n^i(t)^* a_n^j(t) + g^{j*} B_n^j(t) \; a_n^i(t)^* \} \, . \tag{3.9}$$

Due to (3.9) one has, quite independent of the solutions $a_n^m(t)$ of the microscopic system observables, for all $t \geq o$

$$\varphi^{ij}_{-(N)}(t)\Omega_R = \varphi^{ji}_{+(N)}(t)^* \Omega_R = o \quad . \tag{3.10}$$

Furthermore, the $\varphi^{ij}_{\pm(N)}(t)$ are averages over the contributions of the individual degrees of freedom. At $t = o$ they are all independent, and the $A_n^m(t)^{\#}$, $B_n^m(t)^{\#}$ anticommute for all times. If the $a_n^m(t)^{\#}$ are only weakly dependent due to their mean field interaction, then one expects some kind of "law of large number" to make $\varphi^{ij}_{(N)}(t)$ vanish for $N \to \infty$. The $\sigma^{ij}_{(N)}(t)$ should become c-numbers, because of $[\sigma^{ij}_{(N)}(t) \; , \sigma^{k\ell}_{(N)}(t)] = N^{-1}\{\delta^{jk} \, \sigma^{i\ell}_{(N)}(t) - \delta^{i\ell} \, \sigma^{kj}_{(N)}(t)\}$, and this is in fact true in sufficiently homogeneous states $\omega^S_{(N)}$, where the $\sigma^{ij}_{(N)}$ converge weakly for $N \to \infty$. $\omega^S_{(N)}$ is called <u>classical</u> w.r.t. $\underline{\sigma}_{(N)}$, if there exists a probability measure μ on phase space

$$\mathbb{P} = \{ \; \underline{\sigma} \in \mathbb{C}^{M^2} \mid \sigma^{ij} = \sigma^{ji*} \; , \; \sum |\sigma^{ij}|^2 \leq M \; \} \tag{3.11}$$

such that for all monomials

$$\lim_{N\to\infty} \omega^S_{(N)} \; (\sigma^{ij}_{(N)} \; \ldots \; \sigma^{pq}_{(N)}) = \int \mu(d\underline{\sigma}) \; \sigma^{ij} \ldots \sigma^{pq} \, . \tag{3.12}$$

<u>Theorem 3.1:</u> If $\omega^S_{(N)}$ is classical and $\omega^R_{(N)}$ satisfies (3.6), then for all monomials and positive times

$$\lim_{N\to\infty} \omega^R_{(N)}\otimes\omega^S_{(N)} \, (\sigma^{ij}_{(N)}(r) \ldots \sigma^{pq}_{(N)}(t))$$
$$= \int \mu(d\underline{\alpha})\,\sigma^{ij}(r,\underline{\alpha})\ldots\sigma^{pq}(t,\underline{\alpha}) \ , \tag{3.13}$$

where $\underline{\sigma}(t,\underline{\alpha})$ is the unique solution of

$$\dot{\sigma}^{ij}(t,\underline{\alpha}) = -\gamma^{ij}\,(\sigma^{ij}(t,\underline{\alpha})-\eta^{ij}) + Q^{ij}(\underline{\sigma}(t,\underline{\alpha})), \tag{3.14}$$

$$\sigma^{ij}(0,\underline{\alpha}) = \alpha^{ij} \ .$$

The proof of this theorem as well as finer results on the fluctuations of the quantum observables $\sigma^{ij}_{(N)}(t)$ around the classical orbit $\sigma^{ij}(t)$ can be found in [H4]. In [H5] a different topology is used to deal with the unbounded boson observables, which occur in the laser. KMS reservoirs are studied in [D1].

One sees that in the limit $N\to\infty$ open systems built up from EOS with a strong mean field non-linearity can show very dramatic non-equilibrium phase transitions, which manifest themselves in the non-analytic change of the attractors of the corresponding classical "mean motion" equations when varying the parameters η^{ij} and γ^{ij} of the reservoirs. In the 1-mode laser the threshold can be explained by a Hopf bifurcation, which is a second-order phase transition from a time-independent to a periodic attractor [H4]. There exists a model for a Josephson oscillator with a first order non-equilibrium phase transition [H7]. In this framework we expect most of the "catastrophies" of classical dynamical systems as non-equilibrium phase transitions.

The next difficult and unsolved problem is the investigation of the thermodynamic limit of EOS with a local nonlinear interaction. The physically most interesting example is macroscopic quantum electrodynamics, e.g. the interaction of a continuum of modes of the radiation field with localized "pumped" M-level atoms. The semiclassical theory, where the electromagnetic field is treated classically, shows interesting nonlinear wave propagation phenomena [C2]. W. Braun and myself [B3] have studied the model of a nerve membrane built from EOS ("pores" for Na- and K-conductivity) and interacting through a classical potential. The resulting non-linear diffusion equation has a propagating pulse solution [C1] under conditions which are typical in real life (necessity of two ion species with different time constants and opposite concentration gradients).

§ 4.) Conclusions

The beauty of our approach to irreversible statistical mechanics lies in the possibility of building microscopic models for dynamical systems with considerable structure. One of the many unsatisfactory aspects of the present state of the art is the very special class of quasifree reservoirs and interactions (weak coupling limit or IOS), for which a drive to equilibrium can be established. The validity of many conclusions about the nature of non-equilibrium phase transitions will remain doubtful, as long as non-markovian reservoirs and local interactions cannot be treated rigorously. Open systems close to thermal equilibrium, however, might soon be understood from first principles, and the Onsager relations for heat flows be related to the intrinsic stability properties of the KMS state [H2].

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