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Glauber Dynamics of Fluctuations

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We derive the time evolution of the normal fluctuations of a classical lattice spin system induced by a generalized Glauber dynamics. The canonical form of this dynamics is derived. We prove that it is asymptotically (i.e., after the central limit) free. The results are applied to give a rigorous proof of the macroscopic reciprocity relations and the linear theory for small deviations from equilibrium.

KEY WORDS: Central limit theorem; normal fluctuations; reciprocity relations.

1. INTRODUCTION

The static fluctuations for classical lattice spin systems in equilibrium at high temperature are physically well understood. As an illustration, consider $\mu \sim e^{-\beta H}$, β small enough, the unique Gibbs measure at inverse temperature β for an Ising spin system $\{\sigma(x) = \pm 1, x \in \mathbb{Z}^\nu\}$ interacting according to some local translation invariant potential H. Then, the total magnetization $(1/|\Lambda|) \sum_{x \in \Lambda} \sigma(x)$ in a box Λ converges to the average spin $a = \langle \sigma \rangle_\mu$ in the measure μ with Gaussian fluctuations around it. Of course, other quantities, such as the energy density fluctuations, may be equally interesting. If $f(\sigma)$ and $g(\sigma)$ are two local functions of the configuration σ, then their fluctuations

$$\frac{1}{|\Lambda|^{1/2}} \sum_{x \in \Lambda} [\tau_x f(\sigma) - \langle f \rangle_\mu]; \qquad \frac{1}{|\Lambda|^{1/2}} \sum_{x \in \Lambda} [\tau_x g(\sigma) - \langle g \rangle_\mu]$$

with τ_x the translation over lattice vector $x \in \mathbb{Z}^\nu$, become jointly Gaussian white noise as $\Lambda \uparrow \mathbb{Z}^\nu$ with a covariance of strength $\sum_{x \in \mathbb{Z}^\nu} [\langle f \tau_x g \rangle_\mu -$

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$\langle f \rangle_\mu \langle g \rangle_\mu$]. One of the purposes of this paper is in fact to give a precise formulation of such a central limit theorem jointly describing all macroscopic fluctuations.

The main subject is to introduce a dynamics on this large space of macroscopic fluctuations, starting from a given microscopic stochastic time evolution. There is a variety of stochastic dynamics which leave the Gibbs measure μ invariant. Examples of such are the so-called Glauber dynamics, in which the spins flip with rates $c(x, \sigma) > 0$ satisfying the condition of detailed balance:

$$c(x, \sigma) = c(x, \sigma^x) \, e^{\beta \Delta_x H(\sigma)}$$

where $\Delta_x H(\sigma) \equiv H(\sigma^x) - H(\sigma)$ is the energy change due to a spin flip at site $x \in \mathbb{Z}^\nu [\sigma^x(y) = \sigma(y)$ for $y \neq x$ and $\sigma^x(x) = -\sigma(x)]$.

Quite apart from the particular model, the question now arises of how to describe the fluctuations also dynamically. Put differently, how does the induced time evolution look for the coarse-grained quantities as considered above? A very interesting situation occurs in the case where there are locally conserved quantities. For instance, for the Kawasaki-type dynamics in which nearest neighbor spins are exchanged with certain rates, the total spin is a conserved quantity. Dynamically, then, the corresponding fluctuation fields are singled out from all the other fields. One argues (and in some cases proves) that in this case the fluctuation fields of any local function become proportional to the fluctuations of the conserved field. The physical intuition behind this is the occurrence of a natural scale separation: the fluctuations of nonconserved quantities change in time on a much faster scale than those of the conserved quantities. This phenomenon is well studied and sometimes goes under the name of the Boltzmann–Gibbs principle. Detailed discussions and references can be found in refs. 1–5.

Such an effect of establishing a certain hierarchy between the different fluctuation fields is not always present. Consider, for instance the Glauber-type processes introduced above. There, there is no conservation law. Therefore, there is no *a priori* reason to prefer the magnetization fluctuations above any other field, and there is no mechanism by which after an appropriate space-time scaling we can find an autonomous dynamics for the coarse-grained magnetization. Put technically, if the BBGKY hierarchy is not closed at a microscopic level, then it will not close also at a macroscopic scale.

This problem was studied in detail in 1979 by Holley and Stroock.[6] They considered central limit phenomena for various interacting particle systems (for a review on the latter, see ref. 7). They obtain that the time evolution for the limiting fluctuation field corresponding to the magnetization for a Glauber dynamics is Markovian if and only if some rather severe restrictions on the spin flip rates are imposed. Basically, one has to require that the magnetization field satisfies a closed evolution equation, i.e., there is a constant γ such that

$$\frac{d}{dt}\langle\sigma(x)\rangle_t = -2\langle c(x,\sigma)\,\sigma(x)\rangle_t$$

with

$$\lim_{\Lambda}\frac{1}{|\Lambda|}\sum_{x\in\Lambda}[c(x,\sigma)\,\sigma(x)-\gamma(\sigma(x)-a)]=0$$

Here we take up the same problem as in ref. 7, but continue to work consistently with all fluctuations on the same footing. That is, we must consider the induced time evolution on the space of all fluctuations. No extra restrictions on the spin flip rates are then necessary. This requires, however, the more abstract mathematical formulation of the space of fluctuations, but this problem is also present statically. We then show that enlarging the configuration space in this way allows us to find the limiting dynamics as an Ornstein–Uhlenbeck type process on the fluctuation fields. We thus derive quite explicitly the stationary Gaussian Markov process under which the macroscopic fluctuations jointly evolve. Once this structure is clarified (Sections 3 and 4) we are able (in Section 5) to discuss, always in the same context, the linear response of this macroscopic system to small perturbations of equilibrium. We then derive linear relations between the so-called thermodynamic flux and force, which here are the equivalent of what is done for fluctuating hydrodynamics in the corresponding Green–Kubo relations, in the case where there is a conserved quantity.

2. THE MICROSCOPIC SYSTEM

As microscopic system we consider here a classical lattice system endowed with a Glauber dynamics. As usual, $\mathbb{Z}^\nu$ represents the sites of a ν-dimensional lattice, $\mathscr{D}(\mathbb{Z}^\nu)$ the directed set of finite subsets of $\mathbb{Z}^\nu$ with direction the inclusion. With each $x\in\mathbb{Z}^\nu$ we associate a configuration space K_x, a copy of a finite set K. For each $\Lambda\in\mathscr{D}(\mathbb{Z}^\nu)$ consider the tensor product space $K_\Lambda=\bigotimes_{x\in\Lambda}K_x$ and denote by C_Λ the set of real continuous functions on K_Λ. The set $C_L=U_\Lambda C_\Lambda$ is called the set of local observables of our system. Denote also $\mathscr{K}=K_{\mathbb{Z}^\nu}$, which by Tychonov's theorem is a compact Hausdorff space; $\mathscr{K}$ is called the micro configuration space of the system.

States of the system are positive normalized continuous linear forms on C_L and are given by probability regular Borel measures μ on $\mathscr{K}$:

$$\mu(f)=\int_{\mathscr{K}}d\mu(\omega)\,f(\omega);\qquad f\in C_L$$

The group of lattice translations induces a group of transformations $\{\tau_x \mid x \in \mathbb{Z}^\nu\}$ of C_L such that $\tau_x C_\Lambda = C_{\Lambda+x}$, $\Lambda \in \mathscr{D}(\mathbb{Z}^\nu)$.

For this paper we assume that we have given a measure μ which is translation invariant, i.e., $\mu \circ \tau_x = \mu$ for all $x \in \mathbb{Z}^\nu$.

Next we introduce the microdynamics of our system. We consider a generalized Glauber dynamics[7-9] in the following form: suppose we are given a linear map L_0: $C_L \to C_L$

$$(L_0 f)(\omega) = \sum_{K_0} c(\omega, \omega_0)(f({}_{\omega_0}\omega) - f(\omega)) \tag{1}$$

where $c(\omega, \cdot)$ is a positive function on K_0 for all ω, the function $\omega \to c(\omega, \omega_0)$ is a measurable function on $\mathscr{K}$ for all $\omega_0 \in K_0$, and

$$({}_{\omega_0}\omega') = \begin{cases} \omega'_x & \text{if} \quad x \neq 0 \\ \omega_0 & \text{if} \quad x = 0 \end{cases}$$

Assume further that $C_v = \sup_\omega \|c(\omega, \cdot)\|_v < \infty$, where $\|\cdot\|_v$ denotes the total variation norm; then we have the following properties, which are the main tools used in the next section:

$$\text{(a)} \qquad \|L_0 f\| \leqslant 2\, \|C_v\|\; \|f\|$$

$$L_0(f^2) - 2f L_0 f \geqslant 0; \qquad f \in C_L \tag{2}$$

$$\text{(b)} \qquad L_0 f = 0 \quad \text{if} \quad 0 \notin \operatorname{supp} f \tag{3}$$

$$\text{(c)} \qquad L_0(1) = 0 \tag{4}$$

Assume also that L_0 is of finite range, i.e., there exists an $R > 0$ such that for all $i \in \mathbb{Z}^\nu$, $|i| > R$, one has

$$\delta_i c = \sup\{\|c(\omega, \cdot) - c(\omega', \cdot)\|_v; (\omega)_j = (\omega')_j \text{ if } i \neq j\} = 0 \tag{5}$$

and that L_0 is detailed balance (or microreversible) with respect to a basic measure μ:

$$\mu(L_0(f)\, g) = \mu(f L_0(g)); \qquad f, g \in C_L \tag{6}$$

In order to fix the ideas, one can keep in mind the example of the Ising model, where $K = \{0, 1\}$ and μ is the equilibrium state at inverse temperature $\beta = 1/kT$. The dynamics is then determined by the map

$$L_0 = \left\{\exp\left(\beta J \sum_{\langle 0, i\rangle} \sigma_0 \sigma_i\right)\right\} (\eta_0 - 1)$$

where η_0 is the spin-flip operation at the site $0 \in \mathbb{Z}^\nu$.

Define $L_k f = L_0 \tau_{-k} f$ for all $f \in C_L$; then $L = \sum_{k \in \mathbb{Z}^\nu} L_k$ defines a Markov generator which is self-adjoint and negative definite. By the finite range condition (5) the map L is local in the sense that $L: C_L \to C_L$; L is translation invariant by construction and (6) implies

$$\mu \circ L = 0 \tag{7}$$

The Glauber dynamics is then given by the semigroup $\{\gamma_t = \exp tL, t \in \mathbb{R}^+\}$ of contractions of C_L. This finishes the description of the microsystem; it is given, up to technicalities, by the triplet (C_L, μ, γ_t).

3. NORMAL DISTRIBUTION OF FLUCTUATIONS

As indicated above, we are interested in this paper in the derivation of some properties of the theory of fluctuations. For every $f \in C_L$, denote by $\tilde{f}_n$ the local fluctuation of f with respect to the measure μ:

$$\tilde{f}_n = \frac{1}{|\Lambda_n|^{1/2}} \sum_{x \in \Lambda_n} (\tau_x f - \mu(f))$$

where Λ_n is a cube in $\mathbb{Z}^\nu$ centered at the origin with edges of length $2n+1$, $n \in \mathbb{N}$; $|\Lambda_n|$ is the volume of Λ_n or the number of points in Λ_n. In probability, the central limit theorem deals with the limit $\lim_{n \to \infty} \tilde{f}_n$. We will assume that the system has normal fluctuations, i.e., that the central limit exists for all elements of C_L. In the literature there are many different sufficient conditions and strong results for the central limit theorem (see, e.g., ref. 10). The conditions are all of the type of mixing properties of the basic measure μ with respect to the space translations. Here we are not discussing this matter, but we make the assumption that the central limit exists in the sense of Definition 3.1 below.

We define the existence of normal fluctuations for the system (C_L, μ) in terms of the characteristic functions. From now on we assume that the system satisfies:

Definition 3.1. The system (C_L, μ) has *normal fluctuations* if:

(i) For all $f, g \in C_L$:

$$\sum_{x \in \mathbb{Z}^\nu} |\mu(f \tau_x g) - \mu(f)\,\mu(g)| < \infty$$

(ii) For all $f \in C_L$, the central limit holds:

$$\lim_{n \to \infty} \mu(\exp it\tilde{f}_n) = \exp \frac{-t^2}{2} \langle f, f \rangle_\mu, \qquad t \in \mathbb{R}$$

where

$$\langle f, g\rangle_\mu = \lim_{n\to\infty} \mu(\tilde{f}_n \tilde{g}_n) = \sum_{x\in\mathbb{Z}^\nu} [\mu(f\tau_x g) - \mu(f)\,\mu(g)]; \qquad f, g \in C_L$$

We do not discuss here the mixing conditions on the measure μ in order that the system satisfies this definition. For this we refer to the literature on central limits (see, e.g., ref. 10 and also ref. 11).

Consider now C_L equipped with the bilinear form $\langle\cdot,\cdot\rangle_\mu$. Dividing out the kernel of this form, one gets a pre-Hilbert space of elements, denoted by $[f]$, $f\in C_L$. By completion one gets a Hilbert space $\mathscr{K}_\mu$ with scalar product $\langle\cdot,\cdot\rangle_\mu$, where we denote, if no confusion is possible,

$$\langle f, g\rangle_\mu = \langle [f], [g]\rangle_\mu$$

and $f=[f]$, $g=[g]$ for $f, g\in\mathscr{K}_\mu$.

Remark that, e.g., f and all its translates $\tau_x f$, $x\in\mathbb{Z}^\nu$, coincide in $\mathscr{K}_\mu$.

Before formulating the main result of this section, we recall the notion of abstract Wiener spaces.[12]

Let $(H, \langle\cdot,\cdot\rangle)$ be a separable Hilbert space; the Gauss measure $\mu_{\mathscr{G}}$ is the set function from the cylinder sets in H to $\mathbb{R}^+$:

$$\mu_{\mathscr{G}}(E) = \left(\frac{1}{\sqrt{2\pi}}\right)^n \int_E \exp\left\{-\frac{1}{2}\langle f, f\rangle\right\} df$$

where $E=\{f\in H\,|\,P_n f\in\mathscr{F};\ \mathscr{F}$ is a Borel set and P_n an n-dimensional projection$\}$. If $\dim H<\infty$, then $\mu_{\mathscr{G}}$ extends to a measure on H. If $\dim H=\infty$, then $\mu_{\mathscr{G}}$ is not σ-additive. It is, however, possible to construct a σ-additive extension $\tilde{\mu}$ of $\mu_{\mathscr{G}}$ on a Banach space B with H dense in B. The σ-field generated by the cylinder sets of H is the Borel field of B and $\tilde{\mu}(E)=\mu_{\mathscr{G}}(E_{|H})$. Remark that $\tilde{\mu}$ is a Gaussian measure on B, i.e., for all $x^*\in B^*\subset H$, B^* the dual of B, the random variable $x^*(\cdot)$ is normally distributed with mean zero and variance $\langle x^*, x^*\rangle$. This standard construction (H, B) is called a Wiener space and $\tilde{\mu}$ a Wiener measure.

Theorem 3.2. If the system (C_L, μ) has normal fluctuations, then there exists a Wiener space $(B, \mathscr{K}_\mu)$ and a linear map

$$b: C_L \to L^2(B, \tilde{\mu})$$

with $\tilde{\mu}$ the Wiener measure, such that for all $f\in C_L$, the random variable $b(f)$ is $\tilde{\mu}$-normally distributed and

$$\lim_{n\to\infty} \mu(\exp i\tilde{f}_n) = \exp -\tfrac{1}{2}\langle f, f\rangle_\mu = \tilde{\mu}(\exp ib(f))$$

The map b is translation invariant, i.e., for all $x\in\mathbb{Z}^\nu$: $b\circ\tau_x = b$.

Proof. As the space K is finite, the vector space $[C_L] \subseteq C_L/\mathbb{Z}^\nu$ is separable, the above construction yields that $\mathscr{K}_\mu$ is a real, separable Hilbert space.

This guarantees the existence of a Wiener space $(B, \mathscr{K}_\mu)$.

Consider now the map

$$n: \quad B^* \subset \mathscr{K}_\mu \to L^2(B, \tilde{\mu}): \quad h \to n(h)$$

with $n(h): B \to \mathbb{R}: f \to h(f)$.

From ref. 12, Lemma 4.7,

$$\langle h, h \rangle_\mu = \int_B h(f)^2 \, d\tilde{\mu}(f) \equiv \langle n(h), n(h) \rangle_{\tilde{\mu}}$$

where $\langle \cdot, \cdot \rangle_{\tilde{\mu}}$ is the scalar product in $L^2(B, \tilde{\mu})$; i.e., n is isometric. As B^* is dense in H, n has a unique continuous extension, denoted by $\langle h, \cdot \rangle_\mu$, $h \in H$. The random variable $\langle h, \cdot \rangle_\mu$ on B is defined $\tilde{\mu}$ a.e.; it is normally distributed with mean zero and variance $\langle h, h \rangle_\mu$:

$$\int_B e^{it\langle h, f \rangle_\mu} \, d\tilde{\mu}(f) = e^{-(t^2/2)\langle h, h \rangle_\mu}$$

The theorem follows by defining the map b as

$$b: \quad C_L \to L^2(B, \tilde{\mu})$$
$$h \to b(h) = \langle [h], \cdot \rangle_\mu$$

and by the Definition 3.1 of normal fluctuations. ∎

This theorem shows that the central limit

$$\text{“}\lim_{n \to \infty}\text{”} \tilde{f}_n = b(f)$$

yields a map b from the local observables C_L into $L^2(B, \tilde{\mu})$, i.e., we realized an identification of the macroscopic fluctuations with the normally distributed random variables for the Wiener measure on an appropriate Wiener space.

The physical notion of coarse graining consists in the fact that this map b is not injective; it is composed of the maps

$$\mathscr{C}_L \to \mathscr{K}_\mu \to L^2(B, \tilde{\mu})$$
$$f \to [f] \to \langle [f], \cdot] \rangle_\mu$$

The second map being injective, the coarse graining is situated in the first one.

Motivated by this theorem, we consider the elements of $L^2(B, \tilde{\mu})$ as the set of macroscopic fluctuations of our system.

Remark that by construction the set $[\mathscr{C}_L]$ is dense in $\mathscr{H}_\mu$. By ref. 13, Theorem 3 this implies that the set $\{\exp ib(f) \mid f \in \mathscr{C}_L\}$ is total for $L^2(B, \tilde{\mu})$. The above construction is canonical in the sense that this density property holds for all choices of Wiener spaces $(B, \mathscr{H}_\mu)$.

4. GLAUBER DYNAMICS FOR FLUCTUATIONS

As discussed above, in this section we study the dynamics on the fluctuations, i.e., on $L^2(B, \tilde{\mu})$, induced by the microdynamics $\gamma_t = \exp tL$, where L is given in Section 2. First we transport the generator L to the macro phase space, the Hilbert space $\mathscr{H}_\mu$.

Lemma 4.1. The generator L induces a map $\mathscr{L}$ on the Hilbert space $\mathscr{H}_\mu$ such that (i) $\mathscr{L}$ is densely defined, (ii) $\mathscr{L}$ is symmetric, (iii) $\mathscr{L}$ is negative definite.

Proof. For any $[f] \in [C_L] \subseteq \mathscr{H}_\mu$, define

$$\mathscr{L}[f] = [Lf]$$

This definition is independent of the representant; indeed, let $[f] = 0$; then

$$\begin{aligned}\langle [Lf], [Lf] \rangle_\mu &= \lim_{n \to \infty} \mu((\widetilde{Lf})_n^2) \\ &= \lim_n \mu(\tilde{f}_n L^2 \tilde{f}_n) \\ &\leqslant \lim_n \mu(\tilde{f}_n^2)^{1/2} \mu(L^2\tilde{f}_n L^2 \tilde{f}_n)^{1/2} \\ &= \langle [f], [f] \rangle_\mu^{1/2} \langle [L^2 f], [L^2 f] \rangle_\mu^{1/2} = 0\end{aligned}$$

hence $\mathscr{L}[f] = 0$.

Clearly, because of the locality of L and the construction of $\mathscr{H}_\mu$, $\mathscr{L}$ is densely defined.

That $\mathscr{L}$ is symmetric follows immediately from L being microreversible, (6).

Finally, (iii) follows from the dissipativity of L, (2), and the invariance $\mu \circ L = 0$, (7):

$$2\langle [f], \mathscr{L}[f] \rangle_\mu = \lim_n \{2\mu(\tilde{f}_n L \tilde{f}_n) - \mu(L(\tilde{f}_n^2))\} \leqslant 0 \quad ∎$$

In the following theorem we transport the generator to the Wiener measure space level.

Theorem 4.2. If the system (C_L, μ) has normal fluctuations, then for all $f, g \in C_L$

$$\lim_{n \to \infty} \mu(e^{i\tilde{f}_n} L e^{i\tilde{g}_n}) = \langle e^{-ib(f)}, \tilde{L} e^{ib(g)} \rangle_{\tilde{\mu}} \tag{8}$$

where $\tilde{L}$ is a densely defined linear map on $L^2(B, \tilde{\mu})$ explicitly given by

$$\tilde{L} e^{ib(g)} = (ib(\mathscr{L} g) + \langle b(g), b(\mathscr{L} g) \rangle_{\tilde{\mu}})\, e^{ib(g)}$$

where b is defined in Theorem 3.2 and $\mathscr{L}$ in Lemma 4.1.

Proof. First remark that the map $\tilde{L}$ is densely defined by the remark following Theorem 3.2. Using Theorem 3.2 for all $h_1, h_2 \in C_L$, the map

$$s \in \mathbb{R} \to \tilde{\mu}(e^{ib(h_1 + sh_2)})$$

is analytic and one has the formula

$$\tilde{\mu}(e^{ib(h_1)} b(h_2)) = i\tilde{\mu}(e^{ib(h_1)})\, \tilde{\mu}(b(h_1)\, b(h_2))$$

Using this, formula (8) reduces to

$$\lim_n \mu(e^{i\tilde{f}_n} L e^{i\tilde{g}_n}) = -\tilde{\mu}(e^{ib(f+g)})\, \tilde{\mu}(b(f)\, b(\mathscr{L} g))$$

which remains to prove.

For the sake of clarity we work out first in detail the proof in the case that $f, g \in C_{\{0\}}$ and $\mu(f) = \mu(g) = 0$. Using the form of L and the locality (3), one gets

$$\mu(e^{i\tilde{f}_n} L e^{i\tilde{g}_n}) = \sum_{k \in \Lambda_n} \mu\left(\prod_{j \neq k} e^{i(f_j + g_j)/\sqrt{|\Lambda_n|}} e^{if_k/\sqrt{|\Lambda_n|}} L_k e^{ig_k/\sqrt{|\Lambda_n|}} \right)$$

where $f_l = \tau_l f$; $l \in \mathbb{Z}^\nu$.

Then by expansion of exponentials, by (4), and the symmetry of L_0, (6),

$$\begin{aligned}
\mu(e^{i\tilde{f}_n} L e^{i\tilde{g}_n}) &= \sum_{k \in \Lambda_n} \left(\prod_{j \neq k} e^{i(f_j + g_j)/\sqrt{|\Lambda_n|}} \left(1 + \frac{if_k}{\sqrt{|\Lambda_n|}} + \cdots \right) \right. \\
&\qquad \left. \cdot L_k \left(1 + \frac{ig_k}{\sqrt{|\Lambda_n|}} + \cdots \right) \right) \\
&= \sum_{k \in \Lambda_n} i^2 \mu \left(\prod_{j \neq k} e^{i(f_j + g_j)/\sqrt{|\Lambda_n|}} \frac{f_k L_k g_k}{|\Lambda_n|} \right) + O\left(\frac{1}{\sqrt{|\Lambda_n|}} \right)
\end{aligned}$$

where

$$O\left(\frac{1}{\sqrt{|\Lambda_n|}} \right) = \sum_{k \in \Lambda_n} \sum_{l+m \geq 3} \mu \left(\prod_{j \neq k} e^{i(f_j + g_j)/\sqrt{|\Lambda_n|}} \frac{i^{l+m}}{l!\, m!} f_k^l L_k g_k^m \right) \frac{1}{|\Lambda_n|^{(l+m)/2}}$$

which is majorized by

$$\left(\sum_{l+m\geqslant 3}\frac{\|f\|^l\,\|g\|^m\,\|L_0\|}{l!\,m!}\right)\frac{1}{|\Lambda_n|^{1/2}}\xrightarrow[n\to\infty]{}0$$

As

$$\lim_n \|e^{i(f+g)/\sqrt{|\Lambda_n|}}-1\|=0$$

it follows that

$$\begin{aligned}\lim_n \mu(e^{i\tilde{f}_n}Le^{i\tilde{g}_n}) &= \lim_n -\frac{1}{|\Lambda_n|}\sum_{k\in\Lambda_n}\mu(e^{i(\tilde{f}_n+\tilde{g}_n)}\tau_k(f\,L_0\,g))\\ &= \lim_n -\left\{\frac{1}{\sqrt{|\Lambda_n|}}\mu(e^{i(\tilde{f}_n+\tilde{g}_n)}(\widetilde{fL_0\,g})_n)+\mu(e^{i(\tilde{f}_n+\tilde{g}_n)})\,\mu(fLg)\right\}\\ &= -\tilde{\mu}(e^{ib(f+g)})\,\tilde{\mu}(b(f)\,b(\mathscr{L}g))\end{aligned}$$

where we used the existence of the limit $n\to\infty$ as a consequence of Definition 3.1. The last equality is based on the symmetry of L and the translation invariance of μ, yielding

$$\begin{aligned}\tilde{\mu}(b(f)\,b(\mathscr{L}g)) &= \lim_n \frac{1}{|\Lambda_n|}\sum_{i,j\in\Lambda_n}\mu(f_i(Lg)_j)\\ &= \lim_n \frac{1}{|\Lambda_n|}\sum_{i,j\in\Lambda_n}\mu(L_j(f_i)\,g_j)\\ &= \lim_n \frac{1}{|\Lambda_n|}\sum_{i\in\Lambda_n}\mu(L_i(f_i)\,g_i)\\ &= \mu(fL_0\,g)\end{aligned}$$

This finishes the proof for the case f, $g\in C_{\{0\}}$. For general functions f, $g\in C_{\Lambda_d}$, denote $\Lambda_d^k=\tau_k\Lambda_d$; then one has $L_kf_i\neq 0$ implies $k\in\Lambda_d^i$ or $i\in\Lambda_d^k$.

Analogously as above,

$$\begin{aligned}\lim_n \mu(e^{i\tilde{f}_n}Le^{i\tilde{g}_n}) &= \lim_n -\frac{1}{|\Lambda_n|}\sum_{k\in\Lambda_{n+d}}\mu\left(e^{i(\tilde{f}_n+\tilde{g}_n)}\sum_{i,j\in\Lambda_d^k}f_iL_k\,g_j\right)\\ &= -\tilde{\mu}(e^{ib(f+g)})\lim_n\frac{1}{|\Lambda_n|}\sum_{k\in\Lambda_{n+d}}\mu\left(\tau_k\sum_{i,j\in\Lambda_d}f_iL_0\,g_j\right)\\ &= -\tilde{\mu}(e^{ib(f+g)})\,\tilde{\mu}(b(f)\,b(\mathscr{L}g))\end{aligned}$$

yielding a complete proof of the theorem. ∎

In Lemma 4.1 we proved that the map $\mathscr{L}$ on $\mathscr{K}_\mu$ is symmetric and negative; hence it has a self-adjoint Friedrich extension, which we continue to denote by $\mathscr{L}$. It follows that $\mathscr{L}$ is exponentiable to a semigroup $\{\gamma_t = \exp t\mathscr{L}, t \geqslant 0\}$ of linear positive contractions, strongly continuous in the parameter t.

Theorem 4.3. The semigroup of contractions $(\gamma_t)_{t\geqslant 0}$ on $\mathscr{K}_\mu$ induces a semigroup of contractions $(\tilde{\gamma}_t)_{t\geqslant 0}$ on $L^2(B, \tilde{\mu})$ explicitly given by: for all $f \in \mathscr{K}_\mu$,

$$\tilde{\gamma}_t(\exp ib(f)) = \exp\{ib(\gamma_t f) - \tfrac{1}{2}\langle f, (1-\gamma_t^2) f\rangle_\mu\} \tag{9}$$

It satisfies the *reciprocity relations*: for all $\varphi, \psi \in L^2(B, \tilde{\mu})$,

$$\langle \tilde{\gamma}_t \psi, \varphi\rangle_{\tilde{\mu}} = \langle \psi, \tilde{\gamma}_t \varphi\rangle_{\tilde{\mu}} \tag{10}$$

The semigroup $(\tilde{\gamma}_t)_{t\geqslant 0}$ is strongly continuous in t with generator a self-adjoint extension of the map $\tilde{L}$ of Theorem 4.2.

Proof. Clearly, by (9), $\tilde{\gamma}_t$ is a densely defined linear map of $L^2(B, \tilde{\mu})$. The semigroup property of $\tilde{\gamma}_t$ is an immediate consequence from its definition and the semigroup property of $(\gamma_t)_{t\geqslant 0}$ on $\mathscr{K}_\mu$.

Now we show that the $\tilde{\gamma}_t$ are contractions.

Let

$$\psi = \sum_{j=1}^{n} \lambda_j e^{ib(f_j)}, \qquad \lambda_j \in \mathbb{C}, \quad f_j \in \mathscr{K}_\mu$$

Then one computes with the Wiener measure $\tilde{\mu}$

$$\langle \psi, \psi\rangle_{\tilde{\mu}} - \langle \tilde{\gamma}_t \psi, \tilde{\gamma}_t \psi\rangle_{\tilde{\mu}} = \sum_{i,j=1}^{n} \bar{\rho}_i \rho_j \{e^{\langle f_i, f_j\rangle_\mu} - e^{\langle f_i, \gamma_t^2 f_j\rangle_\mu}\} \tag{$*$}$$

where $\rho_i = \lambda_i e^{\langle f_i, f_i\rangle_\mu/2}$.

Using the contraction property of γ_t,

$$(g, g) \geqslant (\gamma_t g, \gamma_t g), \qquad g \in \mathscr{K}_\mu, \quad t \geqslant 0$$

one gets

$$\sum_{i,j=1}^{n} \bar{\rho}_i \rho_j \{\langle f_i, f_j\rangle_\mu - \langle f_i, \gamma_t^2 f_j\rangle_\mu\} \geqslant 0 \tag{$**$}$$

for all $\rho_i \in \mathbb{C}$ and $f_i \in \mathscr{K}_\mu$.

Using the well-known matrix property that if $A=(a_{ij})\geqslant 0$ and $B=(b_{ij})\geqslant 0$ then $(a_{ij}b_{ij})\geqslant 0$, one derives immediately by iteration the positivity of the matrix

$$(a_{ij}^n - b_{ij}^n) = \left((a_{ij}-b_{ij}) \sum_{l=1}^{n} a_{ij}^{l-1} b_{ij}^{n-l} \right), \qquad n \in \mathbb{N}$$

if the matrix $(a_{ij}-b_{ij})\geqslant 0$, and straightforwardly for the exponential function

$$(e^{a_{ij}} - e^{b_{ij}}) \geqslant 0$$

Hence, take $a_{ij} = \langle f_i, f_j \rangle_\mu$, $b_{ij} = \langle f_i, \gamma_t^2 f_j \rangle_\mu$; then (**) implies the positivity of formula (*), proving the contraction property. In order to prove the reciprocity relation, it is now sufficient to check the equality

$$\langle \tilde{\gamma}_t e^{ib(f)}, e^{ib(g)} \rangle_{\tilde{\mu}} = \langle e^{ib(f)}, \tilde{\gamma}_t e^{ib(g)} \rangle_{\tilde{\mu}}$$

for $f, g \in \mathscr{K}_\mu$.

But this follows from the symmetry of γ_t on $\mathscr{K}_\mu$ and an explicit and easy computation using the definition formula (9). The strong continuity $t \to \tilde{\gamma}_t$: because of the group property and the boundedness of the maps $\tilde{\gamma}_t$, it is sufficient to prove the continuity at $t=0$. As the maps are contractions, it is sufficient to prove

$$\lim_{t\to 0} \|\psi - \tilde{\gamma}_t \psi\|_{\tilde{\mu}} = 0$$

for all $\psi \in L^2(B, \tilde{\mu})$ of the form

$$\psi = \sum_{j=1}^{n} \lambda_j e^{ib(f_j)}, \qquad \lambda_j \in \mathbb{C}, \quad f_j \in \mathscr{K}_\mu$$

As

$$\|\psi - \tilde{\gamma}_t \psi\|_{\tilde{\mu}} \leqslant \sum_{j=1}^{n} |\lambda_j| \; \|e^{ib(f_j)} - \tilde{\gamma}_t e^{ib(f_j)}\|_{\tilde{\mu}}$$

it is sufficient to prove

$$\lim_{t\to 0} \|e^{ib(g)} - \tilde{\gamma}_t e^{ib(g)}\|_{\tilde{\mu}} = 0; \qquad g \in \mathscr{K}_\mu$$

But

$$\begin{aligned} &\|e^{ib(g)} - \tilde{\gamma}_t e^{ib(g)}\|_{\tilde{\mu}}^2 \\ &\quad = 1 + \exp\{-\langle g, (1-\gamma_t^2)\, g\rangle_\mu\} - 2\exp\{-\langle g - \gamma_t g, g - \gamma_t g\rangle_\mu \\ &\qquad - \tfrac{1}{2}\langle g, (1-\gamma_t^2)\, g\rangle_\mu\} \end{aligned}$$

tends to zero if $t \to 0$, because $t \to \gamma_t$ is strongly continuous on $\mathscr{K}_\mu$.

Finally, one computes the generator of $(\tilde{\gamma}_t)_{t \geq 0}$ on a dense set of $L^2(B, \tilde{\mu})$, again using formula (9):

$$\left.\frac{d}{dt} \tilde{\gamma}_t e^{ib(g)}\right|_{t=0} = \{ib(\mathscr{L}g) + \langle g, \mathscr{L}g \rangle_\mu\} e^{ib(g)}$$

Using the equality (see proof of Theorem 4.2)

$$\langle g, \mathscr{L}g \rangle_\mu = \tilde{\mu}(b(g)\, b(\mathscr{L}g))$$

one completes the proof of the theorem. ∎

This result completes the description of the macrodynamics $\tilde{\gamma}_t = \exp t\tilde{L}$ acting on the normal fluctuations of the system and induced by the Glauber dynamics acting on the microsystem. It is interesting to remark that the map $\tilde{L}$ and hence also the dynamics $\tilde{\gamma}_t$ depend on the basic measure μ (see the limit Theorem 4.2). The map $\tilde{L}$ has the important property that it maps polynomials in the Wiener random variables $b(f)$, $f \in \mathscr{K}_\mu$, into polynomials in these variables of the same order. Such kinds of maps are called generalized free because they describe a free evolution on the level of the random variables $b(f)$. As an illustration we give the map $\tilde{L}$ explicitly on the monomials of order one and two:

$$\tilde{L}b(f) = b(\mathscr{L}f)$$
$$\tilde{L}(b(f)^2) = 2b(\mathscr{L}f)\, b(f) - 2\langle b(f), b(\mathscr{L}f) \rangle_{\tilde{\mu}}$$

In fact, one checks easily that these are sufficient to characterize completely $\tilde{L}$ and hence $\tilde{\gamma}_t$ on $L^2(B, \tilde{\mu})$.

So far we have given a rigorous mathematical model description of the basic ingredients of the phenomenological theory of fluctuations. In order to make the connection with this theory somewhat more explicit, we make a small digression into this physical theory.

One assumes[14] that the macroscopic behavior of a system is describable by the points of a finite-dimensional space $\Gamma \subseteq \mathbb{R}^n$. The space Γ is assumed to be obtained by a coarse-graining procedure from a microscopic (infinite-dimensional) phase space. The macro states are taken to be probability measures on Γ.

One assumes that, due to the coarse graining, the equilibrium measure is a Gaussian measure on $\mathbb{R}^n$:

$$d\mu_{\mathscr{G}}(\alpha) = e^{-(1/2k)(\alpha, S\alpha)}\, d\alpha$$

where S is a positive-definite, symmetric $n \times n$ matrix, $(\cdot, \cdot)$ is the Euclidean scalar product, and k is Boltzmann's constant, which we put $k=1$. Denote the random variables

$$b(x) = \langle x, \cdot \rangle \equiv (x, S\,\cdot), \qquad x \in \Gamma$$

They have a Gaussian distribution:

$$\mu_{\mathscr{G}}(e^{ib(x)}) = \int_{\mathbb{R}^n} e^{i\langle x, \alpha \rangle}\, d\mu_{\mathscr{G}}(\alpha) = e^{\quad \langle x, x \rangle/2}$$

The time evolution is assumed to be a flow on the phase space determined by a linear differential equation

$$\frac{d\alpha(t)}{dt} = \mathscr{L}\alpha(t), \qquad \alpha \in \Gamma$$

where $\mathscr{L}$ is a linear map on Γ. The property of microreversibility implies $\langle \alpha, \mathscr{L}\beta \rangle = \langle \mathscr{L}\alpha, \beta \rangle$; α, $\beta \in \Gamma$.

The reciprocity relations are nothing but this symmetry expressed by duality on the Gaussian random variables: if

$$\tilde{L}b(x) = b(\mathscr{L}x)$$

the symmetry of $\mathscr{L}$ becomes now for $\tilde{L}$

$$\mu_{\mathscr{G}}(b(y)\, \tilde{L}b(x)) = \mu_{\mathscr{G}}(\tilde{L}(b(y))\, b(x)), \qquad x, y \in \Gamma$$

In the physics literature this relation is usually written in terms of the matrix elements of $\tilde{L}$. Take $\{e_i\}_{i=1,\dots,n}$ an orthonormal basis of $(\mathbb{R}^n, \langle \cdot, \cdot \rangle)$; then it becomes

$$\tilde{L}_{ij} = \tilde{L}_{ji}$$

where $\tilde{L}_{ij} = \mu_{\mathscr{G}}(b(e_i)\, \tilde{L}b(e_j))$. These are the well-known forms of the reciprocity relations.

It is clear that we realized above a rigorous mathematical model for this theory. For infinite lattice systems the Gaussian measure space Γ becomes the Wiener measure space $(B, \mathscr{K}_\mu)$ introduced in Section 2; the phase space Γ should be identified to the infinite-dimensional real Hilbert space $\mathscr{K}_\mu$. As dynamics we have chosen the generalized Glauber dynamics satisfying the symmetry (6), yielding finally the reciprocity relations for L in Theorem 4.3. Apart from the rigorous description of all this, the new item we added to the field is the explicit formula for the generator $\tilde{L}$ as given in Theorem 3.2. All this was proved on the only condition of the measure μ having normal fluctuations as formulated in Definition 3.1.

5. SMALL DEVIATIONS AND LINEAR RESPONSE

Here we have in mind that the basic measure μ is an equilibrium state of the lattice system for a local Hamiltonian H_Λ, $\Lambda \subset \mathscr{D}(\mathbb{Z}^\nu)$, and at inverse temperature, say $\beta = 1$.

The corresponding Wiener measure $\tilde{\mu}$ constructed in Section 2 represents the equilibrium measure for the coarse-grained system, i.e., for the fluctuations of the system, in mathematical terms for the elements of $L^2(B, \mu)$.

Now we are interested in small perturbations of the equilibrium measure μ, yielding perturbations for the measure $\tilde{\mu}$.

Consider the perturbed Hamiltonian

$$H_\Lambda + \tilde{f}_n; \qquad f \in C_L$$

with a local fluctuation $\tilde{f}_n$. Clearly, the locally perturbed equilibrium measure is given by

$$\mu(e^{-\tilde{f}_n} \cdot)/\mu(e^{-\tilde{f}_n})$$

In a separate paper[11] we prove that under the supplementary condition that there exists a constant $c \in \mathbb{R}^+$ such that

$$|\mu(\tilde{f}_n^k)| \leqslant c^k k!$$

for all $k \in \mathbb{N}$, the limit measure

$$\lim_{n \to \infty} [\mu(e^{-\tilde{f}_n} \cdot)/\mu(e^{-\tilde{f}_n})]$$

exists as a measure $\tilde{\mu}_f$ on the Wiener space $(B, \mathscr{K}_\mu)$, which is absolutely continuous with respect to the measure $\tilde{\mu}$ and explicitly given by

$$\tilde{\mu}_f(\cdot) = \tilde{\mu}(e^{-b(f)} \cdot)/\tilde{\mu}(e^{-b(f)})$$

where b is the map given in Theorem 3.2.

We are not discussing here further in detail the microscopic construction of these measures, but motivated by the above discussion, we define the following set of perturbed measures:

$$\mathscr{E}_\mu = \left\{ \tilde{\mu}_f = \frac{\tilde{\mu}(e^{-b(f)} \cdot)}{\tilde{\mu}(e^{-b(f)})}; f \in \mathscr{K}_\mu \right\}$$

The measures $\tilde{\mu}_f$ are also Gaussian on the Hilbert space $\mathscr{K}_\mu$ with the same variance as $\tilde{\mu}$, but with a mean generally different from zero. Hence $\mathscr{E}_\mu$ is a set of macroscopic states labeled by $\mathscr{K}_\mu$, i.e., there is a one-to-one correspondence between $\mathscr{E}_\mu$ and $\mathscr{K}_\mu$. Moreover, the elements are equal as functionals on the set of macroscopic quantities $\mathscr{K}_b = \{b(f), f \in \mathscr{K}_\mu\}$, namely the evaluation map $\hat{f}$, $f \in \mathscr{K}_\mu$:

$$\hat{f}: \quad \mathscr{K}_b \to \mathbb{R}: \quad \hat{f}(b(g)) = b(g)(f)$$

coincides with the linear functional $\tilde{\mu}_f$:

$$\tilde{\mu}_f(b(g)) = \hat{f}(b(g)) = \langle g, f \rangle_\mu$$

As usual, the *thermodynamic potential* of a perturbed state $\tilde{\mu}_f$ is given by the *relative entropy*:

$$S(\tilde{\mu}_f \mid \tilde{\mu}) = -\tilde{\mu}_f \left(\log \frac{d\tilde{\mu}_f}{d\tilde{\mu}} \right)$$

A straightforward computation yields

$$S(\tilde{\mu}_f \mid \tilde{\mu}) = -\tfrac{1}{2}\langle f, f \rangle_\mu = -\tfrac{1}{2}\langle b(f), b(f) \rangle_{\tilde{\mu}} \tag{11}$$

Notice that the thermodynamic potential is quadratic in the perturbation variable $f \in \mathscr{K}_\mu$, i.e., we constructed a model such that the so-called harmonic approximation becomes exact.

Furthermore, the map

$$f \in \mathscr{K}_\mu \to S(\tilde{\mu}_f \mid \tilde{\mu})$$

is Fréchet differentiable and we are able to define for our model the *thermodynamic forces* as the Fréchet derivatives of the thermodynamic potential: the force F_f in the f direction is given by

$$F_f = \frac{\partial}{\partial f} S(\tilde{\mu}_f \mid \tilde{\mu}) = -\langle f, \cdot \rangle_\mu = -b(f) \tag{12}$$

The force is linear in the perturbation.

Now we discuss the dynamics on the set of macroscopic states $\mathscr{E}_\mu$. Through the central limit we obtained a dynamics on the macroscopic phase space, yielding an evolution $\tilde{\gamma}_t$ on the macroscopic fluctuations. In the following theorem we show that as an immediate consequence of the reciprocity relations (10), the state space is globally invariant under the dynamics; i.e., the time evolution $\tilde{\gamma}_t^*$ on $\mathscr{E}_\mu$ defined by $\tilde{\gamma}_t^* \mu_f = \mu_f \circ \tilde{\gamma}_t$ for all $f \in \mathscr{K}_\mu$ maps $\mathscr{E}_\mu$ into $\mathscr{E}_\mu$:

Theorem 5.1. For all $t \in \mathbb{R}^+$: $\tilde{\gamma}_t: \mathscr{E}_\mu \to \mathscr{E}_\mu$ in particular

$$\tilde{\gamma}_t \tilde{\mu}_f \equiv \tilde{\mu}_f \circ \tilde{\gamma}_t = \tilde{\mu}_{\gamma_t f} \equiv \gamma_t f; \quad f \in \mathscr{K}_\mu$$

Proof. From the reciprocity relations (10) and the time invariance of $\tilde{\mu}$, for all $g \in \mathscr{K}_\mu$,

$$\tilde{\mu}_f(\tilde{\gamma}_t e^{ib(g)}) = \frac{\tilde{\mu}(e^{-b(f)}\tilde{\gamma}_t e^{ib(g)})}{\tilde{\mu}(e^{-b(f)})}$$
$$= \frac{\tilde{\mu}(\tilde{\gamma}_t(e^{-b(f)})\, e^{ib(g)})}{\tilde{\mu}(\tilde{\gamma}_t(e^{-b(f)}))}$$

Using (9), we obtain

$$\tilde{\mu}_f(\tilde{\gamma}_t e^{ib(g)}) = \frac{\tilde{\mu}(e^{-b(\gamma_t f)} e^{ib(g)})}{\tilde{\mu}(e^{-b(\gamma_t f)})} = \tilde{\mu}_{\gamma_t f}(e^{ib(g)}) \quad \blacksquare$$

It is also interesting to remark that by this theorem the flow on the phase space $\mathscr{K}_\mu$ coincides with the dynamics on the set of perturbed states $\mathscr{E}_\mu$, i.e., the identification state space–phase space is dynamically invariant. In the physics literature (see, e.g., ref. 14) the *thermodynamic flux* is the time derivative of the macroscopic quantities: J_f, the flux in the f direction (at $t = 0$), is given by

$$J_f(\cdot) = \frac{d}{dt}\tilde{\gamma}_t(b(f))\bigg|_{t=0}$$

The linear relations well known in fluctuation theory between the flux and the force in a particular direction immediately follow from (12). Furthermore, by Lemma 4.1 we have:

Corollary 5.2. If the system (C_L, μ) shows normal fluctuations, then for all $f \in \mathscr{K}_\mu$,

$$J_f = -\tilde{L}F_f$$

By the equivalence of $\mathscr{K}_\mu$ and $\mathscr{E}_\mu$ one can also define the flux on the macroscopic state space by

$$\hat{g}(J_f) = \tilde{\mu}_g(J_f) = \frac{d}{dt}\tilde{\mu}_g\tilde{\gamma}_t(b(f))$$
$$= \frac{d}{dt}\tilde{\mu}_{\gamma_t g}(b(f))$$

This gives a direction for the generalization of the thermodynamic functionals to the quantum-mechanical situation, where the notion of phase space is no longer present.

Finally, for the sake of completeness one can consider the quantity of *entropy production* of the perturbed measures:

$$\sigma(\tilde{\mu}_f) = \frac{d}{dt} S(\tilde{\mu}_{\gamma_t f} \mid \tilde{\mu})|_{t=0}; \qquad \tilde{\mu}_f \in \mathscr{E}_\mu$$

A straightforward computation, using (11), yields

$$\sigma(\mu_f) = -\langle f, \mathscr{L} f \rangle_\mu; \qquad f \in \mathscr{K}_\mu$$

and

$$\sigma(\tilde{\mu}_f) = \langle J_f, F_f \rangle_{\tilde{\mu}}$$

By the negativity of the operator $\mathscr{L}$ (Lemma 4.1), one gets a rigorous proof of the positivity of the entropy production for all perturbations:

$$\sigma(\mu_f) \geqslant 0, \qquad \forall \tilde{\mu}_f \in \mathscr{E}_\mu$$

As in the quantum mechanical case,[15] one shows, under very mild conditions on the generator L, that the equilibrium measure $\tilde{\mu}$ is characterized as the measure of minimal entropy production.

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