Transport process and local thermal reservoirs

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A random walk of N particles on a lattice with M sites is studied under the constraint that each lattice site is coupled to its own mesoscopic heat bath. Such a situation can be conveniently described by using the master equation in a quantized Hamiltonian formulation where the exclusion principle is included by using Pauli operators. If all reservoirs are mutually in contact, giving rise to a temperature gradient, an evolution equation for the particle density with two different currents already results in the mean-field approximation. One is the conventional diffusive current, driven by the density gradient, whereas the other includes a coupling between the local density and the temperature gradient. Due to the competitive currents, the system exhibits a stationary solution, where the local density is determined by the local temperature field and depends on the filling factor M/N. The stability of the solution is related to the eigenvalues of a Schrödinger-like equation. In the case of a fixed temperature gradient the stationary density distribution remains stable. The approach used is totally different from and an alternative to the conventional Onsager ansatz.

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I. INTRODUCTION

Nonequilibrium is far from being on a secure theoretical foundation. Whereas the characteristic feature of equilibrium phenomena is the existence of a probability distribution, such a quantity is missing in nonequilibrium systems [1,2]. Generally, the distribution function depends on the interaction among the particles and on the temperature of a single external source called the heat bath. In nonequilibrium the situation is different. For instance, one needs at least two reservoirs to model heat conductivity. Extending that approach, we study here a system that is characterized by several heat reservoirs. In particular, we model the random walk of particles on a lattice under the constraint that each lattice point is coupled to its own heat reservoir. Because the hopping process of particles can be considered as an annihilation and recreation process, the mapping of the master equation onto a second quantized Hamiltonian formulation due to Doi [3] seems to be an adequate mathematical tool to attack the problem. The inputs required for the master equation [2] are a set of states and a set of transition rates between those states (see [4] for a very recent approach). In general, the transition rates are determined according to the principle of detailed balance, especially if the system is coupled to a single heat bath with a fixed temperature. Typically the hopping rates are assumed to follow an Arrhenius ansatz with an activation energy in terms of the temperature of the underlying heat bath. Otherwise a system might be in contact with several heat baths [5]. Here we study a model with M separate reservoirs, i.e., each of the M lattice points should be coupled to its own bath. If additionally all the reservoirs are mutually connected, there occurs a temperature gradient. To be specific, we analyze a stochastic process where the jump of a particle on a lattice is governed by an individual bath. Consequently, the creation of a particle at, say, lattice site i is triggered by the temperature T_i, whereas the annihilation of the particle at the adjacent lattice site j takes place at the temperature T_j. Clearly, the effective jumping rate between sites i and j depends on both temperatures.

The analysis can be grouped into the current interest in studying systems with different heat reservoirs [6–25] . The analysis is motivated by the search for some generic features of nonequilibrium steady states; in particular, a universal behavior under nonequilibrium conditions. In one of the first papers on this topic [6], the stationary nonequilibrium states in the Ising model with locally competing temperatures were studied. The system reveals a variety of stationary states and phase transitions. A two-temperature, kinetic Ising model is investigated in [8] and extended to a diffusive kinetic system in [10]. The authors found a bicritical point, where two nonequilibrium critical lines meet. The analysis is strongly supported by Monte Carlo simulations in two dimensions. A similar simulation has been performed to study a two-temperature lattice gas model with repulsive interactions [12]. The two-dimensional nonequilibrium Ising model with competing dynamics induced by two heat baths was studied in [7,9,13]. Despite the two reservoirs, the critical exponents belong to the same universality class as in the corresponding equilibrium model. In [7] the authors found a change of the phase transition from second to first order. Alternatively, a two-temperature lattice gas model with repulsive interactions has been studied [12,19]. Hereby, the nonequilibrium transition remains continuous unlike in our approach. Another field of interest is the Carnot engine and Carnot refrigerator [14,22] including a thermally driven ratchet under periodic dichotomous temperature change [8], which can likewise be characterized by two reservoirs. General aspects of a thermodynamic cycle with open flow were considered in [17] and a rectification of the Clausius inequality was recently dis-

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cussed in [25]. Totally different physical situations occur when the flow of complex fluids was analyzed under different heat sources [11], or in the case of a nonlinear oscillator coupled to various heat baths [16]. As pointed out in [18], magnetic systems with annealed degrees of freedom necessarily offer some features of two-temperature systems. An interesting physical explanation for a two-reservoir system was discussed recently [21], where the fast and slow variables of a Hamiltonian system were related to different heat baths. In [21], it is demonstrated that the Onsager relations do not apply if the two baths are not too close. Obviously the transport properties are determined by the heat sources. In [23] the occurrence of anomalous heat conductivity in a one-dimensional non-Markov process was studied, whereas in [24] a hidden heat transfer was observed when nonequilibrium steady states are maintained by two heat reservoirs. Very recently in a series of papers [26] the phase space probability density for steady heat flow was discussed. In that case the two baths were mutually connected, leading to a flow.

As mentioned above, we are interested in hopping processes that can be visualized in terms of creation and annihilation operators obeying the commutation rules of Pauli operators. This guarantees exclusion at a fixed lattice site. An appropriate method to study such a situation is given by the master equation approach formulated in terms of second-quantized operators [3,27–32]. In that approach the flip processes are described by creation and annihilation operators, whereas the temperate dependence of the rates are incorporated in the approach by using a Heisenberg-like picture [33–36]. The approach is generalized in a manner that enables us to consider several different heat baths, where each bath is considered in the sense of hydrodynamics.

II. QUANTUM APPROACH TO NONEQUILIBRIUM SYSTEMS

Let us denote by $P(\vec{n},t)$ the joint probability density for a certain configuration, characterized by a state vector $\vec{n}=(n_1,n_2,\ldots,n_N)$ at time t. Here we use a lattice gas description, where each of the N lattice points is either empty or singly occupied, leading to $n_i=0,1$. Assuming that the evolution process is governed by the Markov property, the probability density satisfies a master equation [1,2] written symbolically in the form

$$\partial_t P(\vec{n},t) = \mathcal{L}P(\vec{n},t). \tag{1}$$

The dynamics of the system is determined by the evolution matrix $\mathcal{L}$ specified for the process. Since the values of n_i can be considered as the eigenvalues of the particle number operator and, due to the similarity of the evolution equation (1) to the Schrödinger equation, one can introduce a quantum formulation of the master equation, which was first realized for a Bose-like system [3]. Later the approach was also generalized for Pauli operators [27–29]; for reviews, see [30–32]. In that case, the restriction of the occupation numbers to empty and singly occupied states is guaranteed. Introducing a state vector $|F(t)\rangle$ according to

$$|F(t)\rangle = \sum_{n_i} P(\vec{n},t)|\vec{n}\rangle. \tag{2}$$

Now $|\vec{n}\rangle$ is a state vector in Fock space represented by creation and annihilation operators $d^\dagger$ and d, which obey the commutation relations

$$[d_i,d_j^\dagger] = \delta_{ij}(1-2d_i^\dagger d_i). \tag{3}$$

Using the expansion (2), the master equation (1) can be rewritten as an equivalent equation in Fock space:

$$\partial_t|F(t)\rangle = L|F(t)\rangle. \tag{4}$$

Here the matrix elements of the operator L correspond to $\mathcal{L}$. It should be emphasized that the procedure is up to now independent of the realization of the basic vectors. As shown by Doi [3], the average of an arbitrary physical quantity $\mathcal{B}(\vec{n})$ can be calculated from the average of the corresponding operator $B(t)$,

$$\langle B(t)\rangle = \sum_{n_i} P(\vec{n},t)\mathcal{B}(\vec{n}) = \langle s|B|F(t)\rangle \quad \text{with } \langle s| = \sum \langle \vec{n}|. \tag{5}$$

The evolution equation for the operator $B(t)$ reads now

$$\partial_t\langle B(t)\rangle = \langle s|[B(t),L]_-|F(t)\rangle. \tag{6}$$

As a result of the procedure, all the dynamical equations governing the classical problem are determined by the structure of the evolution operator L and the commutation rules of the operators.

III. MODELING OF THE TRANSPORT PROCESS

In terms of second-quantized operators the transport of particles through a lattice is described by the following operator:

$$L = \nu\sum_{i\neq j}(d_i^\dagger d_j - d_i d_i^\dagger d_j^\dagger d_j) \equiv \nu\sum_{i\neq j}[(1-d_i d_j^\dagger)d_i^\dagger d_j]. \tag{7}$$

The evolution operator L characterizes the hopping process. A particle at the lattice site j is annihilated and created at the neighboring site i provided there exists a particle at j and the site i is empty. Notice that $d_j^\dagger d_j$ means the particle number operator and $d_i d_i^\dagger = 1-d_i^\dagger d_i$. The two terms in Eq. (7) reflect the gain and loss terms of the underlying master equation, respectively. The operators satisfy the commutation relation of Pauli operators according to Eq. (3), i.e., they anticommute at the same lattice site that manifests the exclusion principle. The hopping process is realized with a rate ν. To be specific, we consider N active, i.e., hopping, particles in a fixed volume V on a simple d-dimensional cubic lattice with M lattice points and lattice spacing l. Due to the exclusion principle, $N\leq M$. The ratio N/M is denoted as the filling factor. Using Eq. (5) the averaged particle number $\langle n_r\rangle \equiv \langle d_r^\dagger d_r\rangle$ obeys

$$\partial_t\langle n_r\rangle = \nu\sum_{j(r)}[\langle n_j\rangle - \langle n_r\rangle]. \tag{8}$$

Here the symbol $j(r)$ means summation over all lattice points j adjacent to lattice point r. Equation (8) is the discrete ver-

sion of the diffusion equation. In the next section we adopt a continuous description, where Eq. (8) appears as the first part in Eq. (15). Normally the hopping rate D is influenced by the temperature of a single heat reservoir. As demonstrated in [33–36], the influence of the heat bath can be incorporated into the quantum formulation by introducing a Heisenberg-like picture for the operators. With this aim the evolution operator L is replaced by

$$L = \nu \sum_{i,j} [(1 - d_i d_j^\dagger) \exp(-\beta H/2) d_i^\dagger d_j \exp(\beta H/2)]. \quad (9)$$

For details we refer to [35], where the procedure was discussed for the Glauber model. Here the global energy functional H is a measure of the activation energy, which may include also the static interaction among the particles. If the system is coupled to a single heat bath, the quantity β is identified with the inverse global temperature (in units of k_B) of the heat bath. The parameter ν is determined by an underlying microscopic time scale, which is defined, for instance, by the hopping rate.

Let us now generalize the model by including individual local heat reservoirs with the local temperature T_i, where i stands for the lattice site. Remark that we adopt here a hydrodynamic point of view, where the discrete lattice site i is identified with a mesoscopic cell, which contains fewer particles than the whole system but enough that the concept of temperature remains reasonable. Note that the quantity T_i does not represent a single degree of freedom. According to the principles of nonequilibrium statistics, the global energy functional H in Eq. (9) should be replaced by local ones denoted as H_i and H_j, respectively. The reason is that the hopping process is realized between adjacent lattice sites i and j. Under these conditions an extension of the evolution operator in Eq. (9) reads

$$L = \nu \sum_{i,j} [(1 - d_i d_j^\dagger) e^{-(H_i/2T_i + H_j/2T_j)} d_i^\dagger d_j e^{H_i/2T_i + H_j/2T_j}]. \quad (10)$$

Here T_i and T_j are the temperatures of the mesoscopic reservoirs coupled to the lattice sites i and j. In general these temperatures are different from each other. For simplicity we assume a single-particle Hamiltonian H_i of the form

$$H_i = \varepsilon d_i^\dagger d_i, \quad (11)$$

where $\varepsilon > 0$ is the activation energy. If necessary, the approach can be extended to interacting particles, as demonstrated for flip processes with two reservoirs [36]. With regard to Eq. (11) we find the nonzero terms of the evolution operator Eq. (10),

$$e^{-H_i/2T_i} d_i e^{H_i/2T_i} = d_i e^{\varepsilon/2T_i}, \quad e^{-H_i/2T_i} d_i^\dagger e^{H_i/2T_i} = d_i^\dagger e^{-\varepsilon/2T_i}. \quad (12)$$

Inserting these results in Eq. (10), it follows that

$$L = \nu \sum_{i,j} [(1 - d_i d_j^\dagger) d_i^\dagger d_j e^{-(\varepsilon/2)(1/T_j - 1/T_i)}]. \quad (13)$$

Let us stress that our system offers a particle-hole-symmetry, where the holes are the empty lattice sites. For this purpose, the annihilation and creation operators of the particles should be replaced by the corresponding ones for the holes according to $d_i = a_i^\dagger$ and $d_i^\dagger = a_i$. For instance, $a_i^\dagger$ is the creation operator for a hole. This substitution leads to $H_i = -\varepsilon a_i^\dagger a_i + \text{const}$, i.e., the activation energy ε is replaced by $-\varepsilon$.

Using Eq. (6) and the algebraic properties of Pauli operators [see Eq. (3)], the evolution equation for the averaged particle density reads

$$\partial_t \langle n_r \rangle = \sum_{j(r)} \{w_{rj} \langle n_j \rangle - w_{jr} \langle n_r \rangle - [w_{rj} - w_{jr}] \langle n_r n_j \rangle\}$$

$$\text{with} \quad w_{rj} = \nu \exp\left[-\frac{\varepsilon}{2} \left(\frac{1}{T_r} - \frac{1}{T_j} \right) \right], \quad w_{jr} = \nu^2 w_{jr}^{-1}. \quad (14)$$

For a single heat bath with $T_r = T_j = T$ it follows that $w_{rj} = 1$. In that case, all the higher-order terms disappear, and Eq. (14) is reduced to the conventional diffusion equation (8). If local reservoirs exist, a whole hierarchy of evolution equations appears, and w_{rj} yields a temperature gradient when the reservoirs are linked. The quantity w_{rj} can be considered as the jumping rate from the occupied site j toward the previously unoccupied site r. With other words, w_{rj} is the frequency with which a particle leaves the site j and jumps over to the site r. Because of the different reservoirs associated with the lattice sites r and j, respectively, the rates w_{rj} and w_{jr} are different. Thus w_{jr} is the frequency with which the occupied site r becomes vacant. To illustrate the situation let us assume, for instance, $T_r > T_j$. From here one concludes that $w_{rj} > w_{jr}$, i.e., jumps from the colder to the hotter bath are more favorable provided the activation energy ε is positive. Within the time evolution the averaged occupation number increases at site r. As a consequence, particles will be concentrated in regions with higher temperatures. The opposite case, $T_j > T_r$, means that the particles prefer to remain at the hotter site.

Whereas the first two terms in Eq. (14) describe a single-site process, the second part is related to the clustering processes manifested by the occurrence of the higher-order term $\langle n_j n_r \rangle$. This quantity is nonzero only if both the site r and at least one of its neighbor sites j are occupied. Moreover, as mentioned above, the rates w_{rj} and w_{jr} are different from each other because of the different local reservoirs. Hence the evolution equation should also offer terms proportional to $w_{rj} - w_{jr}$ as observed in Eq. (14). In the case $w_{rj} - w_{jr} > 0$, discussed already, the frequency of the jumping processes from the colder site j to the hotter one r is larger than the opposite process. However, such a jump is not allowed due to the exclusion principle, because the lattice site r is occupied. As a consequence a nonzero contribution of the nonlinear term in Eq. (14) leads to a decrease of $\langle n_r \rangle$, a behavior that is also suggested by Eq. (14). Let us finish this section with the remark that the particle-hole symmetry is manifest in the interchange of the high- and low-temperature limits. This follows immediately from Eq. (14) combined with Eq. (12), and the interchange of ε and $-\varepsilon$.

IV. STATIONARY SOLUTION

In this section we demonstrate that the evolution equation (14) gives rise to interesting phenomena already in the mean-field approximation, which should reflect the main features of the system. To get a better insight into the behavior let us also take the continuum limit. Using Eq. (14) and introducing the particle density $n(\vec{x},t) \equiv \langle n_r(t) \rangle l^{-d}$, we find in a straightforward manner

$$\partial n(\vec{x},t) = -\vec{\nabla} \cdot [\vec{j}_D(\vec{x},t) + \vec{j}_T(\vec{x},t)]$$

$$\text{with} \quad \vec{j}_D = -D\vec{\nabla}n, \quad \vec{j}_T = \frac{\lambda}{\rho} n(\rho - n)\vec{\nabla}T. \quad (15)$$

Here ρ is the density related to the underlying cubic lattice: $\rho = M/V = l^{-d}$, where M is the number of lattice sites within the volume V. In general, the particle density satisfies the relation $0 \leq n(\vec{x},t) \leq \rho$. The current $\vec{j}_T$ evidently reflects the exclusion principle imposed by using Pauli operators with the commutation relation Eq. (3). When each lattice site is occupied by a particle, i.e., $n=\rho$, the additional current $\vec{j}_T$ disappears. The two independent kinetic coefficients in Eq. (15) are defined by

$$D = \nu l^2, \quad \lambda = \frac{\varepsilon l^2 \nu}{T_e^2}.$$

Here D is the conventional diffusion constant and λ is the coupling parameter between the density and the temperature gradient. This temperature gradient originates from the quantity w_{rj} in (14). In deriving relation (15) the general scheme of nonequilibrium statistics has been taken into account, where $\vec{\nabla}T$ instead of $\vec{\nabla}(1/T)$ is considered as the temperature flux, and T_e stands for the fixed temperature in equilibrium. Let us stress that our approach goes beyond the Onsager theory of nonequilibrium. Here the current is written as

$$\vec{j} = \alpha\vec{\nabla}n + \gamma\vec{\nabla}T,$$

with the phenomenological Onsager coefficients α and γ. In our case the coefficient γ depends on the local density $n(\vec{x},t)$ itself. Notice further that the evolution equation (15) has the form of a Fokker-Planck equation with drift term [1,2], where the driving force is defined by $\vec{F}(\vec{x},t) = -(\lambda/\rho)[\rho - n(\vec{x},t)]\vec{\nabla}T(\vec{x},t)$. If the lattice is fully occupied the driving force disappears.

Due to the competing currents, the system exhibits a stationary solution given by

$$n_s(\vec{x}) = \rho \frac{c \exp[\mu T(\vec{x})]}{1 + c \exp[\mu T(\vec{x})]} \quad \text{with } \mu = \frac{\lambda}{D}. \quad (16)$$

Such an inhomogeneous distribution is realized provided the lattice is not empty ($n \neq 0$) or not fully occupied ($n \neq \rho$). The integration constant c is calculated from the condition

$$\int n_s(\vec{x}) d^d x = N.$$

Owing to the exclusion principle, the total number of active particles should satisfy the relation $N \leq M$. If the filling factor obeys $M/N=1$, i.e., all lattice sites are occupied, the transport of particles through the lattice is impossible. The stationary solution shows that an increasing local temperature field $T(\vec{x})$ leads to an enhanced local density provided that the activation energy is positive $\varepsilon > 0$. As mentioned before, one can also consider $\varepsilon < 0$ leading to $\mu < 0$. In that case, the particle density accumulates in the low-temperature regime. In any case, our approach describes particle aggregation under the influence of a locally different temperature field. If the temperature is everywhere fixed, i.e., $T(\vec{x}) = T_e$, the normalized particle density is likewise fixed, $n_s = N/V$, according to Eq. (16).

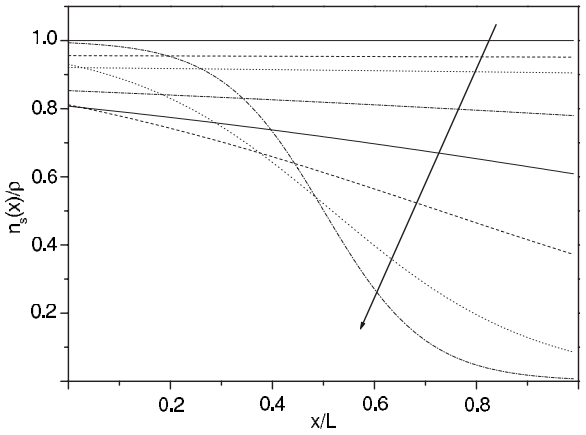

FIG. 1. Reduced particle density n_s/ρ as function of x/L according to Eq. (18) for different temperature gradients $\mu\Delta T = 0$, 0.1, 0.2, 0.5, 1.0, 2.0, 5.0, 10. The arrow points in the direction of increasing temperature gradients.

To illustrate our approach let us discuss a simple one-dimensional system of length L with a constant temperature gradient:

$$T(x) = T_0 - ax, \quad a = \frac{T_0 - T_L}{L} \equiv \frac{\Delta T}{L}. \quad (17)$$

Here T_0 and T_L are the temperatures at the boundaries. Such a constant flow could be reached after a sufficient waiting time when the heat conduction becomes stationary. From Eq. (16) we obtain the inhomogeneous density distribution

$$n_s(x) = \rho \left[\exp(\mu \Delta T x/L) \left(\frac{1 - \exp[-\mu\Delta T(1 - N/M)]}{\exp(\mu \Delta T N/M)} \right) + 1 \right]^{-1}. \quad (18)$$

The stationary particle density depends on the temperature gradient ΔT, the filling factor $M/N \leq 1$, and the parameter ratio $\mu = \lambda/D$. If the number of active particles is low, $N \ll M$, the stationary solution tends to zero, $n_s(x) \to 0$, whereas for $N \simeq M$ one finds $n_s(x) \to \rho$. If $T_0 > T_L$ it follows immediately that $n_s(0) > n_s(L)$. The particles aggregate at the edge with the highest temperature. The behavior of the particle density is crucially influenced by the temperature gradient ΔT, which is shown in Fig. 1. In that figure the dimensionless particle density n_s/ρ is represented versus the reduced spatial coordinate x/L. The decay of the particle

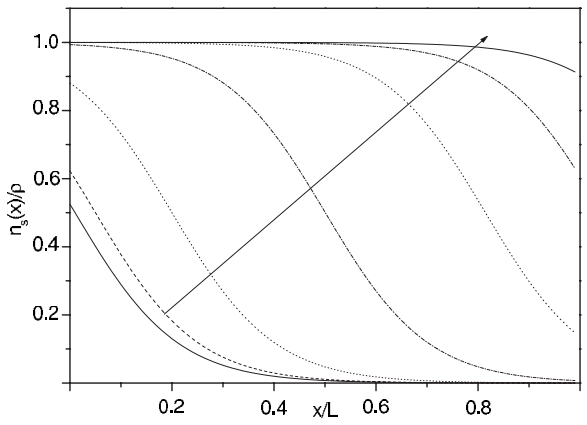

FIG. 2. Reduced particle density n_s/ρ as function of x/L according to Eq. (18) for a fixed temperature gradient $\mu\Delta T=10$, but different filling factors $M/N=0.01, 0.05, 0.2, 0.5, 0.8, 0.95, 0.99$ in the direction of the arrow.

density is stronger the higher the gradient ΔT is.

The behavior of the stationary particle density is also determined by the filling factor M/N, i.e., the ratio of the number of lattice points M and the total number of particles N. In Fig. 2 we show the dependence of the reduced particle density for different ratios of M/N. For small filling factor $M/N \ll 1$, the particles remain localized around the high-temperature region ($x \simeq 0$) and there is a rapid decay of $n_s(x)$. In the other limiting case $M/N \simeq 1$, i.e., almost every lattice site is occupied by a particle, the spreading out of particles is hampered, and the particle density remains nearly constant.

We remark that for a negative energy $\varepsilon < 0$, leading to negative μ, the particles are replaced by holes. As already mentioned, particle-hole exchange is equivalent to interchange of the high- and low-temperature regimes. In that case there is an accumulation at the low-temperature edge of the system.

V. STABILITY OF THE SOLUTION

The stability of the stationary solution $n_s(x)$ can be checked by making the ansatz

$$n(\vec{x},t) = n_s(\vec{x}) + \varphi(\vec{x})\psi(\vec{x},t). \tag{19}$$

Choosing the function $\varphi(\vec{x})$ as

$$\varphi(\vec{x}) = \sqrt{n_s(\vec{x})[\rho - n_s(\vec{x})]},$$

then $\psi(\vec{x},t)$ obeys a Schrödinger-like equation of the form

$$\dot{\psi} = -\hat{H}\psi, \quad \hat{H} = -D\nabla^2 + V(\vec{x},t), \quad V = V_1 + V_2$$

$$\text{with} \quad V_1 = \frac{\lambda^2}{4D\rho^2}[\rho - 2n_s(\vec{x})]^2(\vec{\nabla}T)^2,$$

$$V_2 = \frac{\lambda}{2\rho}\vec{\nabla}\{[\rho - 2n_s(\vec{x})]\vec{\nabla}T\}. \tag{20}$$

Using the stationary solution Eq. (16), it follows that

$$\rho - 2n_S(\vec{x}) = -\rho \tanh[\mu T(\vec{x})/2 + \tilde{c}], \tag{21}$$

where $\tilde{c}$ is related to the normalization constant in Eq. (16) via $\tilde{c} = (1/2)\ln c$. Let us illustrate the approach by considering the one-dimensional realization with a constant temperature gradient according to Eqs. (17) and (18). Equation (20) exhibits solutions of the form $\psi(x,t) = \exp(-Et)\chi(x)$. Using $T(x) = T_0 - ax$ and Eq. (21), the Schrödinger-like equation reads, after the substitution $y = \mu(T_0 - ax)/2$,

$$\left[-\frac{a^2\lambda^2}{4D}\frac{d^2}{dy^2} - \frac{V_0}{\cosh^2 y} - \left(E - \frac{a^2\lambda^2}{4D}\right)\right]\chi(y) = 0, \quad V_0 = \frac{a^2\lambda^2}{2D}. \tag{22}$$

From basic quantum mechanics, the number of bounded discrete states is the largest number Z that satisfies the inequality

$$Z < \frac{1}{2}\sqrt{\frac{16DV_0}{a^2\lambda^2} + 1} - \frac{1}{2}.$$

Inserting V_0, there is no discrete energy level with negative energy. Therefore the stationary solution is stable.

The existence of a stable stationary solution in arbitrary dimensions can be discussed by simple estimations of the potential $V(\vec{x})$. To simplify the problem let us consider as above a constant temperature gradient $\vec{\nabla}T(\vec{x}) = -\vec{a}$. This gives rise to

$$V_1 = \frac{\lambda^2\vec{a}^2}{4D\rho^2}, \quad V_2 = -\frac{\lambda\vec{a}^2}{\rho}n_s'(T).$$

The prime stands for the derivative with respect to T. Whereas V_1 is always positive definite, the second part V_2 may be either positive or negative. From Eq. (16), it is easy to see that the sign of n_s' is determined by the sign of μ. If the particles aggregate in the low-temperature region, then $n_s' < 0$. This case, realized for $\mu < 0$, leads also to a positive definite potential V_2, i.e., the total potential is likewise positive, $V > 0$. As a consequence, the stationary solution remains stable. In the opposite case, when the higher temperature is a basin of attraction, it follows that $n_s' > 0$ and therefore

$$V_2 = -\frac{\lambda\vec{a}^2}{\rho}n_s' < 0.$$

Using the stationary solution, given by Eq. (16), one concludes that the maximum of n_s' is $\mu\rho/4$, i.e.,

$$V_2 > -\frac{\lambda^2\vec{a}^2}{4D}.$$

From here we find that the total potential V is also positive, which leads immediately to a positive definite spectrum of $\hat{H}$. The stationary solution (16) is always stable, independent of the sign of the activation energy ε, provided the temperature gradient is constant. The accumulation process leads to a stationary stable density distribution. If the temperature gradient is not fixed, the situation is more complicated due to the fact that the potential is time dependent.

VI. CONCLUSIONS

We have applied an alternative and more microscopic approach to nonequilibrium problems. In particular, transport processes are considered under the exclusion principle and the influence of a temperature gradient. The last one appears via a coupling to individual heat reservoirs connected with each of the M lattice sites. The situation in mind can be analyzed in a seemingly compact form using a mapping of the master equation into a second-quantized form. As discussed in detail, this quantum formulation of the classical probabilistic problem exhibits the inclusion of local heat baths. In doing this, we have adopted the hydrodynamic point of view for the local temperature. The approach is a generalization of the conventional Onsager ansatz because it allows the inclusion of nonlinear terms originating in the exclusion principle. As a result, we already get in the mean-field approximation a generalized diffusion equation with two competing currents. Additionally to the conventional diffusion current, there is a nonlinear transport current, triggered by the coupling to a temperature gradient. The temperature gradient arises due to the contacts between the local reservoirs. Owing to the two competing currents, the system offers a stationary solution for the relevant particle density $n_s(\vec{x})$. This density is controlled by the local temperature field $T(\vec{x})$. Depending on the sign of the extra current, the particles can aggregate either at high or at low temperatures. The interchange between the high- and low-temperature limits reflects the particle-hole symmetry of our model, where holes correspond to empty lattice sites. The stability analysis leads to a Schrödinger-like equation with a potential that is determined by the exclusion principle and the temperature field. To illustrate our approach we discuss a one-dimensional realization with a constant temperature gradient. The stability is assured by the exact solution of the Schrödinger-like equation. Further, we discuss the stability of the stationary solution under quite general conditions.

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