High-Temperature Expansion for Nonequilibrium Steady States in Driven Lattice Gases

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We develop a controlled high-temperature expansion for nonequilibrium steady states of the driven lattice gas, the "Ising model" for nonequilibrium physics. We represent the steady state as $P(\eta) \propto e^{-\beta H(\eta) - \Psi(\eta)}$ and evaluate the lowest order contribution to the nonequilibrium effective interaction $\Psi(\eta)$. We see that, in dimensions $d \geq 2$, all models with nonsingular transition rates yield the same summable $\Psi(\eta)$, suggesting the possibility of describing the state as a Gibbs state similar to equilibrium. The models with the Metropolis rule show exceptional behavior.

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The issue of constructing a statistical mechanics that applies to nonequilibrium states has been among the most challenging open problems in theoretical physics. By statistical mechanics, we mean a universal theoretical framework which would enable one to compute arbitrary macroscopic quantities of a given macroscopic state, starting from its microscopic description. Even for (hopefully) the simplest problem of characterizing nonequilibrium steady states, we still do not know of any general principles.

One of the most essential questions is whether a nonequilibrium steady state in general is a Gibbs state [1], i.e., whether the corresponding probability measure $P(\eta)$ can be written (as in equilibrium) as $P(\eta) \propto \exp[-\beta \tilde{H}(\eta)]$ with a summable "effective Hamiltonian" $\tilde{H}$. If such a description is possible, then there is a chance that one can find a corresponding variational principle and a statistical mechanics somewhat similar to those for equilibrium states. If it turns out that the description in terms of Gibbs states is not appropriate, then we must look for a completely new theoretical framework.

Since there are no general theories, a natural strategy is to examine the effective Hamiltonian $\tilde{H}$ in various concrete models. Here we make a first step by studying in detail the $\tilde{H}$ for the simplest possible but still highly nontrivial model for nonequilibrium steady states, namely, the driven lattice gas [2–4]. It is an idealized model of interacting particles in a thermal medium which perform random motion influenced by an external driving field. This model was originally designed to play a role analogous to the Ising model in equilibrium statistical mechanics. It has been widely studied both numerically and theoretically over recent years and is believed to exhibit important features of nonequilibrium phenomena.

In this Letter, we develop a high-temperature expansion for the nonequilibrium steady state of the driven lattice gas. Expressing the above effective Hamiltonian as $\tilde{H} = H + \Psi/\beta$, where H is the equilibrium Hamiltonian and Ψ may be called the nonequilibrium effective interaction, we explicitly compute Ψ in the lowest order of the expansion. Although some attempts to develop expansions in the driven lattice gas [4–6] have been made, our approach to evaluate the effective interaction explicitly is novel. Recently, a field theoretic perturbation method has been developed for the one-dimensional lattice gas models with soft potential driven by boundary conditions [7].

Our finding is partly encouraging and partly puzzling. In the lowest order [$O(\beta^2)$ for $d \geq 2$, and $O(\beta^2)$ or $O(\beta^3)$ for $d = 1$] of the expansion, the nonequilibrium effective interaction contains only two-body and three-body contributions as in (16). Interestingly, these effective interactions are generally nonlocal and exhibit a power law decay even though the Hamiltonian is short ranged.

When the transition rate function $\phi(h)$ [see (1) below] is nonsingular and the dimension is higher than one, the result of our expansion is rather encouraging, suggesting a universal behavior of the nonequilibrium steady states. We see that, in the lowest order, the nonequilibrium effective interaction $\Psi(\eta)$ consists only of an effective three-body interaction and is completely independent of the transition rule and the density. The effective interaction decays as in (17) and is summable, suggesting that a description in terms of a Gibbs state is possible.

The models with the Metropolis update rule, on the other hand, display a quantitatively different behavior, which denies the possibility of a Gibbsian description [8]. This suggests that the choice of transition rules might be a serious issue in driven nonequilibrium systems, as was pointed out in [7,9]. Note that the Metropolis rule has been widely used in numerical computations of the driven lattice gases.

Model.—Let $\Lambda \subset \mathbf{Z}^d$ be the d-dimensional $L \times \cdots \times L$ hypercubic lattice with periodic boundary conditions. We denote the sites as $x = (x_1, \ldots, x_d) \in \Lambda$. A configuration of the system is described by $\eta = (\eta_x)_{x \in \Lambda}$, which is a collection of occupation variables $\eta_x = 0, 1$. We set $\eta_x = 1$ if x is occupied by a particle and $\eta_x = 0$ if x is empty. Throughout this Letter, we fix the lattice size L and the particle number $N = \sum_{x \in \Lambda} \eta_x$. The interaction between the particles is described by the Ising Hamiltonian

$H(\eta) = -(J/2)\Sigma_{\langle x,y\rangle}\eta_x\eta_y$. When we write $\Sigma_{\langle x,y\rangle}$, we sum over all pairs of sites with $|x-y|=1$, double counting x, y and y, x.

The stochastic dynamics of the driven lattice gas is determined by specifying the transition rates. For neighboring x, y, we set (as usual)

$$c(x \to y; \eta) = \delta^{(\eta)}_{x\to y}\phi(\beta\{H(\eta^{x,y}) - H(\eta) + E(x_1 - y_1)\}), \tag{1}$$

which is the rate for the particle to hop from x to y in the configuration η. Here, β is the inverse temperature, E is the electric field in the x_1 direction, $\delta^{(\eta)}_{x\to y} = \eta_x(1-\eta_y)$ is 1 only when the hop is possible, and $\eta^{x,y}$ is the configuration obtained by switching η_x and η_y in the original configuration η. We use periodic boundary conditions so as to have $x_1 - y_1 = 0, \pm 1$ for any neighboring pair x, y. The function $\phi(h)$ satisfies $\phi(h) = e^{-h}\phi(-h)$ so that the local detailed balance condition

$$c(x \to y; \eta) = e^{\beta\{H(\eta)-H(\eta^{x,y})-E(x_1-y_1)\}}c(y \to x; \eta^{x,y}) \tag{2}$$

holds. We also require continuity, and set $\phi(h) = 1 + O(h)$. When $\phi(h)$ is differentiable at $h = 0$, the above condition implies $\phi'(0) = -1/2$. The standard choices are (i) the exponential rule with $\phi(h) = e^{-h/2}$, (ii) the heat-bath (or Kawasaki) rule with $\phi(h) = 2/(1+e^h)$, and (iii) the Metropolis rule with $\phi(h) = 1$ for $h \le 0$ and $\phi(h) = e^{-h}$ for $h \ge 0$.

Steady state.—Let $P_t(\eta)$ be the probability of configuration η at time t. It satisfies the master equation

$$\dot{P}_t(\eta) = \sum_{\langle x,y\rangle} - P_t(\eta)c(x\to y;\eta) + P_t(\eta^{x,y})c(y\to x;\eta^{x,y}). \tag{3}$$

The steady state distribution $P(\eta)$ is obtained by setting $\dot{P}_t(\eta) = 0$ in (3). Thus, it is the unique solution of

$$\sum_{\langle x,y\rangle} c(x \to y; \eta) - \frac{P(\eta^{x,y})}{P(\eta)}c(y \to x; \eta^{x,y}) = 0 \tag{4}$$

for any η (with the fixed $N = \Sigma_x \eta_x$). Let us write an ansatz for the steady state distribution as

$$P(\eta) = \frac{1}{Z(J,E)}e^{-\beta H(\eta) - \Psi(\eta)}, \tag{5}$$

where $\Psi(\eta)$ is the "effective interaction" which represents a nonequilibrium correction. Then (4) becomes

$$\sum_{\langle x,y\rangle} c(y\to x;\eta^{x,y})e^{\beta\{H(\eta)-H(\eta^{x,y})\}}\{1 - e^{\Psi(\eta)-\Psi(\eta^{x,y})}\} = \sum_{\langle x,y\rangle} c(y\to x;\eta^{x,y})e^{\beta\{H(\eta)-H(\eta^{x,y})\}} - c(x\to y;\eta), \tag{6}$$

which is the starting point of our perturbation theory.

Since $\Psi(\eta)$ is vanishing when $\beta = 0$, we expand $\Psi(\eta)$ in a power series of β and explicitly evaluate the lowest order contribution. We first note that the left-hand side of (6) may be written as $\{1 + O(\beta)\}\Delta\Psi(\eta)$, where

$$\Delta\Psi(\eta) = \sum_{\langle x,y\rangle} \delta^{(\eta)}_{x\to y}\{\Psi(\eta^{x,y}) - \Psi(\eta)\}. \tag{7}$$

Let us denote the right-hand side of (6) as $-\tilde{Q}(\eta)$. From (2), we have

$$\tilde{Q}(\eta) = \sum_{\langle x,y\rangle}(1 - e^{\beta E(x_1-y_1)})c(x\to y;\eta). \tag{8}$$

We first assume that $\phi(h)$ is differentiable at $h = 0$. By substituting (1) into (8) and expanding in β to the second order, we get $\tilde{Q}(\eta) \simeq Q_{\rm gen}(\eta)$ with

$$Q_{\rm gen}(\eta) = \frac{\beta^2 E}{2}\sum_{\langle x,y\rangle}\delta^{(\eta)}_{x\to y}(y_1 - x_1)\{H(\eta) - H(\eta^{x,y})\}, \tag{9}$$

where the result is independent of the choice of $\phi(h)$. For the Metropolis rule, which has a nondifferentiable $\phi(h)$, the result is different. We get $\tilde{Q}(\eta) \simeq Q_{\rm MP}(\eta)$ with

$$Q_{\rm MP}(\eta) = -\beta^2 E \sum_{\substack{\langle x,y\rangle \\ x_1 > y_1}}\delta^{(\eta)}_{x\to y}\{H(\eta) - H(\eta^{x,y})\}, \tag{10}$$

provided that $E > (2d-1)|J|$. The formula is much more complicated for $|E| \le 2(d-1)|J|$.

We have thus found that the lowest order contribution to the effective interaction $\Psi(\eta)$ is determined by the Poisson-like equation

$$\Delta\Psi(\eta) = -Q(\eta), \tag{11}$$

where we set $Q(\eta) = Q_{\rm gen}(\eta)$ or $Q(\eta) = Q_{\rm MP}(\eta)$, depending on the transition rules.

Decomposition.—Equation (11) looks intractable since it is formulated in the huge space of all possible configurations η. Fortunately, there are beautiful decomposition properties that enable us to determine the solution.

We start from the Laplacian (7). For $A \subset \Lambda$, let $\eta^A = \prod_{x\in A}\eta_x$. We expand $\Psi(\eta)$ as $\Psi(\eta) = \Sigma_{A\subset\Lambda}\psi_A\eta^A$ with real coefficients ψ_A. Note that an arbitrary function of η can be expanded in this way. From the translation invariance and the particle number conservation, we can set $\psi_A = 0$ when $|A| = 1$. (We denote by $|A|$ the number of sites in A.) Now note that $(\eta^{x,y})^A = \eta^{A_{x,y}}$ for any η and $A \subset \Lambda$, where $A_{x,y}$ is obtained from A by switching the occupation status at x and y. (If, for example, $x \in A$ and $y \notin A$, then $A_{x,y} = A\backslash\{x\}\cup\{y\}$.) Then from the linearity of the Laplacian (7), we see that

$$\Delta\Psi(\eta) = \sum_{\langle x,y\rangle}\sum_A \psi_A\delta^{(\eta)}_{x\to y}(\eta^{A_{x,y}} - \eta^A) = \sum_{\langle x,y\rangle}\sum_A(\psi_{A_{x,y}} - \psi_A)\delta^{(\eta)}_{x\to y}\eta^A = \sum_A(\Delta\psi_A)\eta^A, \tag{12}$$

where

$$\Delta\psi_A = \sum_{\substack{\langle x,y\rangle\\ x\in A, y\notin A}} \{\psi_{A\setminus\{x\}\cup\{y\}} - \psi_A\}. \quad (13)$$

We then treat the lowest order charges (9) and (10). Note that $\delta^{(\eta)}_{x\to y}\{H(\eta) - H(\eta^{x,y})\} = \eta_x(1-\eta_y) \times J\{\Sigma_{z(|z-x|=1,z\neq y)}\eta_z - \Sigma_{z(|z-y|=1,z\neq x)}\eta_z\}$. Since the charge $Q(\eta)$ is a linear combination of these terms, it can be expanded as

$$Q(\eta) = \sum_{x,y\in\Lambda} q^{(2)}_{x,y}\eta_x\eta_y + \sum_{x,y,z\in\Lambda} q^{(3)}_{x,y,z}\eta_x\eta_y\eta_z, \quad (14)$$

with suitable coefficients $q^{(2)}_{x,y}$ and $q^{(3)}_{x,y,z}$. Note that when evaluating the "charges" $q^{(2)}_{x,y}$, $q^{(3)}_{x,y,z}$, we need to consider only configurations η with two or three particles. This means that the calculations are (in principle) elementary. In what follows we present only the results of charge calculations, leaving details to [10].

We now substitute these decompositions into the Poisson equation (11) to get $\Delta\psi_A = -q_A$. Then we find that $\psi_A = 0$ unless $|A| = 2$ or 3, and ψ_A with $|A| = 2, 3$ are determined by the (tractable) Poisson equations

$$\Delta\psi^{(2)}_{x,y} = -q^{(2)}_{x,y}, \qquad \Delta\psi^{(3)}_{x,y,z} = -q^{(3)}_{x,y,z}. \quad (15)$$

Here Laplacian Δ is defined by (13) by identifying $\{x, y\}$ or $\{x, y, z\}$ as the subset A. Equivalently they may be regarded as the standard Laplacian [11] on the lattices $\Lambda_2 = \{(x, y)| x, y \in \Lambda, x \neq y\} \subset \mathbf{Z}^{2d}$ or $\Lambda_3 = \{(x, y, z)| x, y, z \in \Lambda, x \neq y, y \neq z, z \neq x\} \subset \mathbf{Z}^{3d}$. Two sites in Λ_2 (Λ_3) are regarded to be neighboring when their Euclidean distance in $\mathbf{Z}^{2d}$ ($\mathbf{Z}^{3d}$) is equal to 1.

The effective interaction $\Psi(\eta)$ is exactly written as

$$\Psi(\eta) = \sum_{x,y\in\Lambda} \psi^{(2)}_{x,y}\eta_x\eta_y + \sum_{x,y,z\in\Lambda} \psi^{(3)}_{x,y,z}\eta_x\eta_y\eta_z, \quad (16)$$

in the lowest order. It is remarkable that the effective interaction (at least in this order) is independent of the particle number. We stress that we are not expanding in the density. We now determine $\psi^{(2)}_{x,y}$ and $\psi^{(3)}_{x,y,z}$ by solving the Poisson equations (15).

General models in $d \geq 2$.—We first concentrate on general models with $\phi(h)$ being differentiable at $h = 0$. As for the two-body charge, we find that $q^{(2)}_{x,y} = 0$ for all x, y. This means $\psi^{(2)}_{x,y} = 0$. There are no two-body contributions to the effective nonequilibrium interaction of the measure in the lowest order.

The three-body charge $q^{(3)}_{x,y,z}$, on the other hand, is nonvanishing. Let $e_1 = (1, 0, \ldots, 0)$, and $\mathcal{U}'$ be the set of the $2(d-1)$ unit vectors of $\mathbf{Z}^d$ other than $\pm e_1$. One has $q^{(3)}_{x,x\pm e_1,x+\delta} = \pm\beta^2 JE$ for any $x \in \Lambda$ and any $\delta \in \mathcal{U}'$. Other nonvanishing $q^{(3)}_{x,y,z}$ are determined by requiring $q^{(3)}_{x,y,z}$ to be symmetric in x, y, and z. The rest are vanishing. To get a feeling for the behavior of the solution $\psi^{(3)}_{x,y,z}$ of the Poisson equation (15), we make an orthogonal transformation and introduce a new coordinate by $X = (2x - y - z)/\sqrt{6}$, $Y = (y - z)/\sqrt{2}$, and $Z = (x + y + z)/\sqrt{3}$ with $x, y, z \in \Lambda$. Apparently the charge distribution depends only on X and Y, and so does the solution $\psi^{(3)}_{x,y,z}$. By denoting $\psi^{(3)}_{x,y,z} = \varphi^{(3)}_{X,Y}$, we get $\Delta\varphi^{(3)}_{X,Y} = -\tilde{q}^{(3)}_{X,Y}$, which is the Poisson equation in the $2d$-dimensional space. Here the charge distribution $\tilde{q}^{(3)}_{X,Y}$ is still complicated, but when projected onto the (X_1, Y_1) plane (where X_1 and Y_1 are the first coordinates of X and Y, respectively), we see that the plus charges are located at $(\sqrt{2/3}, 0)$, $(-1/\sqrt{6}, \pm 1/\sqrt{2})$, and the minus charges at $(-\sqrt{2/3}, 0)$, $(1/\sqrt{6}, \pm 1/\sqrt{2})$. Close to the origin of the $2d$-dimensional space, there is a hexapole parallel to the (X_1, Y_1) plane. Roughly speaking, the corresponding solution $\varphi^{(3)}_{X,Y}$ behaves like $\{1/r^{2d-2}\}''' \sim 1/r^{2d+1}$ with $r = (X^2 + Y^2)^{1/2}$. This estimate can be made into a reliable asymptotic estimate [10] by going back to the original $3d$-dimensional lattice, and treating properly the "mirror charge" induced at the defect sites. The result is

$$\psi^{(3)}_{x,y,z} \sim c\beta^2 JE \frac{U_1 V_1 W_1}{(|U|^2 + |V|^2 + |W|^2)^{d+2}}, \quad (17)$$

where c is a constant depending only on the dimension, and we have set $U = 2x - y - z$, $V = 2y - z - x$, and $W = 2z - x - y$. We note that the quantity in the denominator can be written as $|U|^2 + |V|^2 + |W|^2 = 2\{|x - y|^2 + |y - z|^2 + |z - x|^2\}$. It is notable that the $1/r^{2d+1}$ decay of (17) implies $\Sigma_{y,z}|\psi^{(3)}_{x,y,z}| \leq$ const with an L independent constant. We stress that such a summable (effective) interaction is a sign that the steady state is a Gibbs state [1].

To summarize, the lowest order contribution to the effective interaction $\Psi(\eta)$ is independent of the transition rule provided that $d \geq 2$ and $\phi'(0)$ exists. Moreover, $\Psi(\eta)$ in this order consists only of the summable three-body interaction with the asymptotic behavior (17). The robustness of the result may suggest that we have captured a universal aspect of the nonequilibrium steady state.

It should be noted, however, that the higher order contributions to $\Psi(\eta)$ may be more complicated and may become rule dependent. In particular, the results in [9] suggest that the two-body effective interaction $\psi^{(2)}_{x,y}$ is nonvanishing and exhibits a $1/r^d$ power law decay as in (18) in $O(\beta^3)$ for the heat-bath rule, while there is no $1/r^d$ decay for the exponential rule.

Metropolis rule in $d \geq 2$.—In models with the Metropolis rule [with $E > (2d-1)|J|$], the situation becomes completely different. By the translation invariance, we have $q^{(2)}_{x,y} = \tilde{q}^{(2)}_{x-y}$, where $\tilde{q}^{(2)}_z = \beta^2 EJ$ if $z = \pm e_1$, $\tilde{q}^{(2)}_z = -\beta^2 EJ$ if $z = \pm 2e_1$, or $z = \pm e_1 + \delta$, $\tilde{q}^{(2)}_z = 2\beta^2 EJ$ if $z = \delta$, for any $\delta \in \mathcal{U}'$, and $\tilde{q}^{(2)}_z = 0$ otherwise. Again, by the translation invariance the corresponding effective interaction can be written as $\psi^{(2)}_{x,y} = \varphi^{(2)}_{x-y}$, where $\varphi^{(2)}_z$ is determined by $\Delta\varphi^{(2)}_z = -\tilde{q}^{(2)}_z$. (Here Δ is the

Laplacian [11] on $\Lambda\backslash\{(0,\ldots,0)\}$.) Since $\tilde{q}_z^{(2)}$ corresponds to the charge distribution of a quadrupole in d dimension, the resulting field $\varphi_z^{(2)}$ is expected to decay like $1/|z|^d$ for large $|z|$. Again, this can be made into a precise estimate [10], and we have

$$\varphi_z^{(2)} \simeq c'\beta^2 EJ|z|^{-(d+2)}\left\{(d-1){z_1}^2 - \sum_{j=2}^{d}{z_j}^2\right\}, \qquad (18)$$

for any $d \geq 2$ where c' is a constant that depends only on the dimension. This power law decaying effective interaction can be regarded as the origin of the $1/r^d$ long range two-point correlation [3–6,9] known to exist in the driven lattice gas and related models. Note that the interaction decays so slowly that the sum $\sum_{y\in\Lambda}|\psi_{x,y}^{(2)}|$ is divergent as $L\to\infty$, which implies (and, indeed, proves [10]) that the infinite volume limit of the steady state is not Gibbsian. Thus, in a stark contrast with general models with nonsingular $\phi(h)$, the steady state measure for Metropolis dynamics has a significant nonequilibrium correction in the two-body sector already in the lowest order.

Curiously enough, in the lowest order of the perturbation, the behavior of the three-body effective interaction $\psi_{x,y,z}^{(3)}$ is exactly the same as the general models that we have discussed. We still do not know if this is a mere coincidence or an indication of a deeper universality in the structure of nonequilibrium steady states.

Models in $d=1$.—The models in $d=1$ show exceptional behavior, which requires extra estimates [10].

Suppose that $\phi(h)$ is twice differentiable at $h=0$. In this case a nonvanishing contribution to $\Psi(\eta)$ is found only in the third order. Formula (9) for the charge is thus no longer useful. By going back to the original definition (8), we get the following results. In the two-body effective interaction $\psi_{x,y}^{(2)}$, there is a short-range correction proportional to $\{2\phi''(0)-(1/2)\}\beta^3E^2J$. The three-body effective interaction $\psi_{x,y,z}^{(3)}$ exhibits a $1/r^3$ long range correlation as in (17), and its magnitude is proportional to $\phi''(0)\beta^3EJ^2$. Unlike in the models with $d\geq 2$, the lowest order correction is already very much rule dependent. Note, in particular, that $\phi''(0)=0$ in the heat bath rule.

In Appendix 4 of [2], one-dimensional exactly solvable models of driven lattice gases are introduced, where the nonequilibrium steady states coincide with the corresponding equilibrium states. In the language of the present work, these models turn out to possess vanishing charges (8). We therefore recover the known results that the models have no nonequilibrium corrections.

As for the one-dimensional model with the Metropolis rule, there is a nonvanishing contribution to $\Psi(\eta)$ from $O(\beta^2)$. We find a short-range correction to $\psi_{x,y}^{(2)}$ and no contribution to $\psi_{x,y,z}^{(3)}$.

Discussions.—We still do not know how to evaluate higher order contributions in a systematic manner (although a brute force calculation always seems possible). We expect to get higher body effective interactions as we go to the higher orders in the perturbation. We note that the expansion is much easier in the models with soft-core interactions, where we can take into account the effect of the field E without expanding it [10].

We found that $\Psi(\eta)$ in $d\geq 2$ is independent of the rule provided that $\phi(h)$ is differentiable. This strongly suggests that the results thus obtained are universal and physically meaningful [12]. As we go to the higher orders in the expansion, however, even the models with differentiable $\phi(h)$ are expected to show strong rule dependence [9,10]. We still do not know of any way to determine the "right" transition rule. It is our conjecture [9,10] that the models with the exponential transition rule are free from the $1/r^d$ long range correlation, and have a chance of possessing Gibbsian infinite volume steady states. Although there seems to be no physical reasons to prefer models with Gibbsian steady state, it would be quite interesting if such a criterion plays a role in the future development of nonequilibrium statistical mechanics.

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[11] Let G be an arbitrary discrete set and $B\subset G\times G$ be the set of "neighboring" sites. Then the Laplacian Δ on G is defined as $\Delta f_x = \sum_{y;(x,y)\in B}(f_y - f_x)$.
[12] This, in turn, suggests that results and conclusions obtained using the Metropolis rule should be reconsidered.