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Non-equilibrium Statistical Mechanics of a Driven Lattice Gas Model: Probability Function, FDT-violation, and Monte Carlo Simulations

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***Abstract*—**The study of non-equilibrium systems has attracted increasing interest in recent years, mainly due to the lack of theoretical frameworks, unlike their equilibrium counterparts. Studying the steady state and/or simple systems is thus one of the main interests. Hence in this work we have focused our attention on the driven lattice gas model (DLG model) consisting of interacting particles subject to an external field E. The dynamics of the system are given by hopping of particles to nearby empty sites with rates biased for jumps in the direction of E. Having used small two dimensional systems of DLG model, the stochastic properties at non-equilibrium steady state were analytically studied. To understand the non-equilibrium phenomena, we have applied the analytic approach via master equation to calculate probability function and analyze violation of detailed balance in term of the fluctuation-dissipation theorem. Monte Carlo simulations have been performed to validate the analytic results.

***Keywords*—**Non-equilibrium, lattice gas, stochastic process

I. Introduction

IN nature, an equilibrium state is an exception. In both real physical and biological systems, non-equilibrium situations are far more common in nature than equilibrium ones [1-3]. The development of a comprehensive theoretical characterization of non-equilibrium behavior is thus one of the key challenges of modern condensed matter and statistical physics. Undisputedly, it has grown rapidly in the past decades, mainly due to non-equilibrium extensions and applications to dynamical systems [4], molecular biology and bioinformatics [5], materials science [6], complex systems and networks [7-8], digital communication and information theory [9-10], econophysics and other social sciences [11].

Unlike its equilibrium counterpart, dealing with the task of predicting macroscopic behaviors from microscopic information for these non-equilibrium systems (NES), the familiar Gibbs-Boltzmann framework fails. Specifically, when studying systems in thermal equilibrium from statistical mechanics viewpoint, one utilizes the framework established by Gibbs, i.e., firstly specify the microscopic Hamiltonian of the system and then express the time-independent or stationary distribution over the configuration space in terms of the Boltzmann factor. The observable averages are then applied to calculate investigated quantities using this distribution provided. As a result, it allowed equilibrium statistical mechanics to reach a rather mature status and was applied to various problems and applications. In contrast, there is no sound foundation for studying non-equilibrium phenomena like equilibrium version, so these phenomena are far less understood and are generally much more difficult to study. In other words, up to now even there are large number of works concerning non-equilibrium phenomena [1-18], there is however no well-established systematic framework for investigating non-equilibrium systems.

Part of the difficulty with NES is that the distributions associated with these systems are generally time dependent. To attack this kind of problem, one typically can start with a master equation [19]. In other words, the time evolution of such systems in configuration space is governed by a master equation. However, the master equation(s) derived for the real world system is (are) normally complicated and contains a large degree of freedom. It is consequently difficult to solve both analytically and numerically. From a theoretical point of view, instead, one can apply computational methods or analytic methods containing approximations such as mean-field theory [20], renormalization group [21, 22], and so on. However, these methods are not suitable for the problem that needs the high accuracy as well as the quantity, the probability distribution that is too difficult to obtain from these methods. To have exact solutions for the problem via modeling, one could study very simplified models such as interaction-free or infinitely high temperature models. Due to the fact that an exact solution cannot be obtained by using a master equation approach since the many-particle system has too many degrees of freedom to allow for exact solution, one thus takes the

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system size to be small enough, yet still describe the essential governing physics. Hence it would open up the way to attack the problem analytically. Especially, non-equilibrium steady state (NESS) models have been the cases of interest for research [23]. In our opinion, keeping the model simple to begin with seems to be one of the most important approaches to establish the framework of non-equilibrium research.

Among the simple models studied, major focuses are on the driven lattice gas model (DLG model) introduced by Katz, Lebowitz, and Spohn [24]. The study of the DLG model has attracted growing attention due to its interesting far-from-equilibrium behavior. The dynamics of the system are given by hopping of particles to nearby empty sites with rates biased for jumps in the direction of E (see Fig. 1). This interacting DLG, driven into NESS mainly by an external field, exhibits remarkable properties such as its non-Hamiltonian nature, the violation of the fluctuation-dissipation theorem (FDT-violation), and the occurrence of anisotropic critical behavior [25-27]. In term of application, DLG model is often used to model fast ionic conductors [28-30].

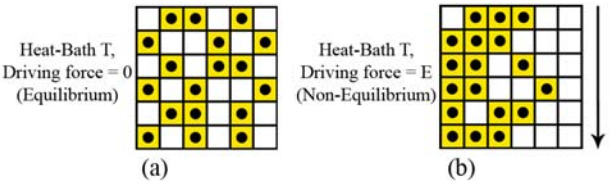

Fig. 1 A half-filled 6x6 lattice system based on the periodic boundary condition in the heat-bath of constant temperature T. (a) If there is no driving force, then the system is in an equilibrium state. On the other hand, (b) if there is a driving force, then the system is driven into a non-equilibrium state.

Motivated by the above mentioned details, we study the very small system sized DLG model to understand non-equilibrium phenomena and their stochastic properties. Our aim is to obtain analytic exact solutions of the model as well as find out what the possible patterns and non-equilibrium dynamic behavior are in stationary states of the system. In addition, Monte Carlo simulations are used to generate results of the same model but of large system size to compare the results and make connections between physical properties of small and large systems.

II. Model and Formulation

In this section, we aim to formulate the model dynamics of the DLG model [24] by setting up the master equation. We consider a very small system (2x4) with four particles (half-filled configuration). Each lattice site consists of two states (n_i): $n_i = 1$ (occupied cell or particle), and $n_i = 0$ (unoccupied cell or vacancy). The external field results in a biased hopping of the particles along one of the lattice directions. For a particle, the field favors jumps along its direction, and suppresses jumps in the opposite direction. Imposing periodic boundary conditions (PBC) in both directions, translational invariance is obtained. Conservation of particle numbers and the hard-core constraints (multiple occupancy being forbidden) are also imposed (see Fig. 1).

Based on the Ising model for lattice gas analogy, without an external field, the Harmiltonian can be given by

$$H[C] = -J\sum_{\langle ij\rangle} n_i n_j \qquad (1),$$

where the constant J is the interaction energy having dimensions of energy. Positive and negative J corresponds to attracting and repelling particles, respectively. C represents the configuration of the system specified by a set of occupation numbers $\{n_i\}$. The symbol $<ij>$ denotes a nearest-neighbor pair of spins. There is no difference between $<ij>$ and $<ij>$.

Typically, an exact solution of the model would correspond to the knowledge of the full time-dependent distributions $P(C,t)$, the probability of finding configuration C at time t, for given initial condition. The dynamics is described by a master equation:

$$\partial_t P(C,t) = \sum_{\{C'\}} \{W[C' \to C]P(C',t) - W[C \to C']P(C,t)\} \qquad (2)$$

where $W[C \to C']$ is the transition rate from one configuration C to other configurations C'. In the absence of the field, One can assume that this process satisfies detailed-balance condition and results in (3):

$$W[C' \to C]/W[C \to C'] = P^*_{eq}(C)/P^*_{eq}(C') \qquad (3)$$

Here, P^*_{eq} represents the probability distribution at equilibrium state. The transition rates depending only on the difference between the energy of configurations, i.e., $W[C \to C'] = w(\beta\Delta H)$, where $\Delta H = H[C'] - H[C]$. One of solutions of $w(\beta\Delta H)$ is well-known in most simulations of statistical physics and called "the Metropolis rate" [31]. It can be illustrated that $w(\beta\Delta H) = e^{-\beta\Delta H}$ when $e^{-\beta\Delta H} < 1$ and $w(\beta\Delta H) = 1$ when $e^{-\beta\Delta H} > 1$. With the driving force, it will create the work done on the particles when they move through the distance L and the work done is $\vec{E} \cdot \vec{L}$. This yields the transition rate:

$$\begin{aligned} W[C \to C'] &= w(\beta[\Delta H - \vec{E}.\vec{L}]) \\ &= Min(1, \exp[\beta(\Delta H - \vec{E}.\vec{L})]) \end{aligned} \qquad (4)$$

Because the particle moves one time step per site, we define $\vec{L}$ to represent a unit vector pointing from the particles to the hole in configurations. In our particular model, the direction of the driving force is assumed to be downward along the vertical axis of the rectangular lattice. The particles favor to hop along the direction of the external field and restrained to hop against it. The external field does not affect those in the transverse direction. From the master equations, at least in principle one can find P^* by solving the system of linear master equations at steady state. In practice, this task is insurmountable, with two exceptions. The first is the system with $J = 0$, i.e., biased diffusion of particles with no interactions other than excluded volume, then $P^* \propto 1$ [32], though there are some non-trivial time-dependent effects. For $J>0$ models, the other solvable case involves very small

systems, e.g. 2x3 and 2x4 [33-34]. While it is difficult to bring together reliable information on collective behavior and singularities in thermodynamic functions (without thermodynamic limit satisfaction), exact solutions to such systems do provide insight into some of the remarkable differences between equilibrium and non-equilibrium steady states.

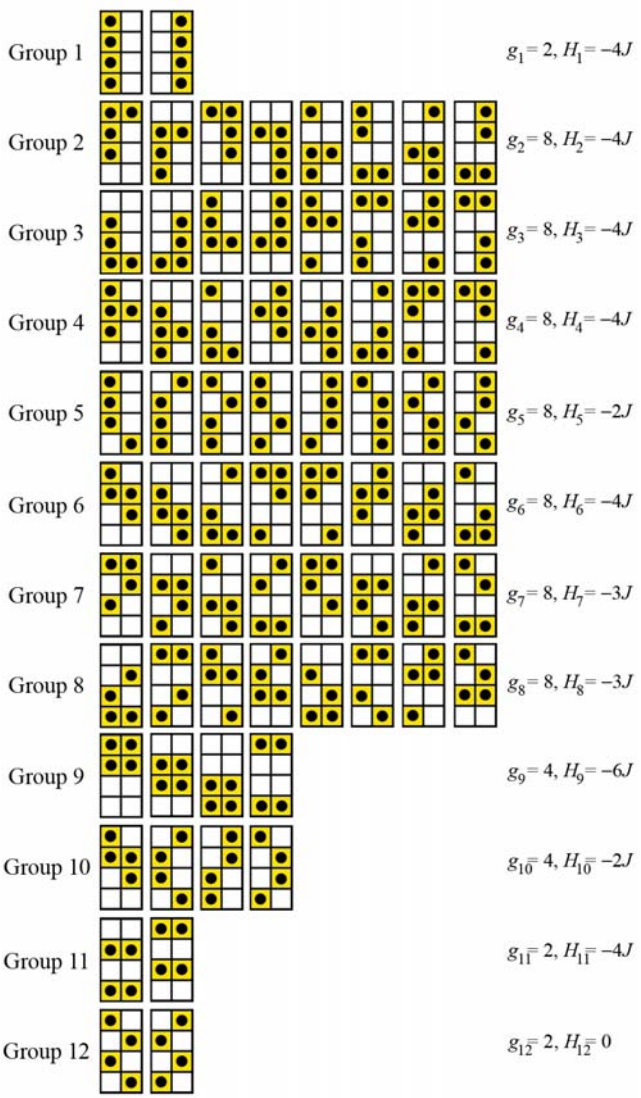

Fig. 2 Mapping nonlinear data to a higher dimensional feature space
All possible configurations of a 2×4 system. The yellow cells are the particles and the white cells are the vacant states. g_i represents the number of members in the i^{th} group and $H_i$represents the internal energy of the i^{th} group.

To meet our goal of building a better understanding about non-equilibrium, we choose to consider a suitable 2x4 driven diffusive system. Since there are 4 particles of 8 lattice sites, we will have altogether ${}^8P_4 = 70$ possible configurations. If the translational invariance condition due to periodic boundary condition (PBC) is applied, the 70 possible configurations fall into 12 groups. The members and energy of each group without the external field can be obtained from each other by a translation as shown in Fig.2. Next, we derive the master equations describing the dynamics of this system. To set up a set of master PDEs of a time-dependent distribution $P(C,t)$, a set of transition rates between the configurations will need to be specified. This chosen rate is constrained to drive $P(C,t)$ asymptotically toward the desired equilibrium. To do so, we begin by drawing the diagrams of the probability flow where the gain is represented by incoming arrows and the loss is represented by outgoing arrows as shown in Fig. 3-4.

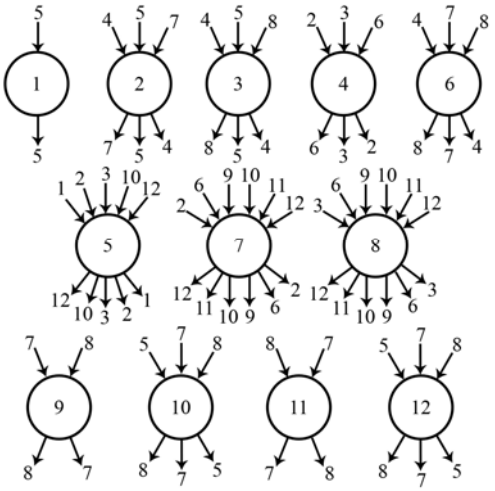

Fig. 3 Schematics of the configuration probability flowing into or out of each configuration of the 2×4 system. The number inside a circle is the group number. The direction of the arrow represents direction of probability flow, the "gain" and "loss" terms. Each configuration can change alternately with a couple configurations, e.g. the configuration of group 1 can exchange the probabilities with the configuration of group 5. Sometimes, the net probability flow is called "the net probability current" where they are zero at equilibrium state and non-zero at non-equilibrium state.

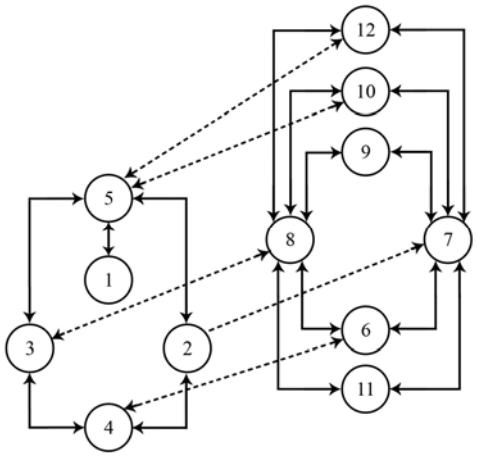

Fig. 4 The flow pattern of the configuration probability. The notations are the same as in Fig. 2-3. The dash-line represents the interchange of the probabilities between two circles. The probability flow can be determined by the effect of the direction of the external filed, i.e. for our system with external field, the direction of

probability flow prefers to change into the configurations that a particle hops along the direction of the external field.

We next calculate the transition rate $W[C\to C']$ by using (4). With the convention: where $a = e^{-\beta J}$, $b = e^{-2\beta J}$, $c = e^{-3\beta J}$, $x = e^{-\beta|\vec{E}|}$, $d = \text{Min}\{1, e^{-\beta J+\beta|\vec{E}|}\}$, $q = \text{Min}\{1, e^{\beta J-\beta|\vec{E}|}\}$, $r = \text{Min}\{1, e^{-2\beta J+\beta|\vec{E}|}\}$, $s = \text{Min}\{1, e^{2\beta J-\beta|\vec{E}|}\}$, $t = \text{Min}\{1, e^{-3\beta J+\beta|\vec{E}|}\}$, and $u = \text{Min}\{1, e^{-3\beta J-\beta|\vec{E}|}\}$.

From (2) and the transition rates $W[C\to C']$, we now write down the system of partial differential equations (PDEs) for the probability of the group i (P_i). We have

$$
\begin{aligned}
\partial_t P_1 &= P_8 \\
\partial_t P_2 &= -(6 + 8a + 6bx)P_2 + 6xP_4 + 6P_5 + 8P_7 \\
\partial_t P_3 &= -(6x + 6r + 8a)P_3 + 6P_4 + 6sP_5 + 8P_8 \\
\partial_t P_4 &= -(6x + 6r + 8a)P_3 + 6P_4 + 6sP_5 + 8P_8 \\
\partial_t P_5 &= 4bP_1 + 6bxP_2 + 6rP_3 - (18 + 4b + 6s) + 8P_{10} + 4P_{12} \\
\partial_t P_6 &= 8P_4 - (8 + 6d + 6ax)P_6 + 6P_7 + 6qP_8 \\
\partial_t P_7 &= 8aP_2 + 6axP_6 - (17 + 3u + 3ax + 3ac)P_7 + 3tP_9 + 3P_{10} \\
&\quad 3axP_{11} + 3P_{12} \\
\partial_t P_8 &= 8aP_3 + 6dP_6 - (11 + 3d + 3t + 3q)P_8 + 3cxP_9 + 3qP_{10} \\
&\quad 3dP_{11} + 3uP_{12} \\
\partial_t P_9 &= 3uP_7 + 3P_8 - (3t + 3ax)P_9 \\
\partial_t P_{10} &= 8P_5 + 3axP_7 + 3dP_8 - (11 + 3q)P_{10} \\
\partial_t P_{11} &= 8P_5 + 3axP_7 + 3dP_8 - (11 + 3q)P_{10} \\
\partial_t P_{12} &= 4bP_5 + 3cxP_7 + 3tP_8 - (7 + 3u)P_{12} \qquad (5)
\end{aligned}
$$

This is the system of 12 linear first-order homogeneous PDEs. We can also view this system as an eigenvalue problem. It may be convenient to write (5) in matrix form $\partial_t P = WP$ where W is the stochastic transition matrix and P is the evolutionary eigenvector (data not show).

III. Exact Analytic Results

First of all we consider (5) that has a unique stationary solution, $P_i^* \equiv \lim_{t\to\infty} P_i(t)$ or $\partial_t P_i = 0$ if $P_i \to P_i^*$. We thus set the left-hand side of (5) to zero independent of the initial conditions. This implies that P_i^* is a *right* eigenvector of W matrix with eigenvalue zero. This eigenvalue is non-degenerate so that P_i^* spans the null space of the matrix W. In general, P_i^* depends on the chosen rates. When simulating systems in thermal equilibrium, the challenge is to specify a set of rates such that the resulting stationary state equals the desired equilibrium distribution, P_i^{eq}. Since the analytic solutions for symbolic problem solving) for general case is very complicated even though it is straightforward (with the help of Mathematica software [http://support. wolfram.com/mathematica]. Thus we analyze the solution to gain insight into non-equilibrium properties of the model under various conditions. The controlled parameters to the steady state: (1) the external field E, (2) Temperature $T = 1/\beta$, and (3) spin interaction J. However, for the sake of brevity, we only show some results which are enough to explain the non-equilibrium phenomena.

Firstly, we consider the steady state total probability distribution functions. Having known from the base line Ising-like model, at an infinitely high temperature ($\beta = 0$), the energy of particles is then very large. Both the interaction from external field and the nearest-neighbors interaction are defeated by the energy of particles. Hence the interaction J no longer plays a role. The configurations of ensembles of the systems will be formed with the same probability. They are equally likely to occur. When the temperature is sufficiently decreased or the system is cooled down ($\beta > 0$), both the interaction from external field and the particle interaction will start to affect to the system. Now, the correlation is finite which implies that the particle can "communicate" with each other throughout the system. Therefore, the probability distribution of possible configurations is controlled by the parameters, β, J, and E.

We firstly focus on two specific extreme steady state cases, i.e. $E = 0$ (equilibrium) and $E\to\infty$ (non-equilibrium). In equilibrium state: $E = 0$, then $x = 1$. It is found that $P_1^* = P_2^* = P_3^* = P_4^* = P_6^* = P_{11}^*$, $P_7^* = P_8^* = aP_1^*$, $P_5^* = P_{10}^* = a^2P_1^*$, $a^2P_9^* = P_1^*$ and $P_{12}^* = a^4P_1^*$, while, when $E\to\infty$, then $x = 0$. It gives

$$
\begin{aligned}
P_2^* &= \frac{a^2\left(64299 + 37620a + 8228a^2 + 5808a^3\right)}{50683 + 52072a + 13200a^2}P_1^*, \\
P_3^* &= \frac{a^2\left(61095 + 35280a + 12188a^2 + 7392a^3\right)}{50683 + 52072a + 13200a^2}P_1^*, \\
P_4^* &= \frac{a^2\left(44631 + 43380a + 17560a^2 + 8272a^3 + 2112a^4\right)}{50683 + 52072a + 13200a^2}P_1^*, \\
P_5^* &= a^2P_1^*, \\
P_6^* &= \frac{a^2\left(29880 + 47700a + 24559a^2 + 10120a^3 + 3696a^4\right)}{50683 + 52072a + 13200a^2}P_1^*, \\
P_7^* = P_{11}^* &= \frac{a^2\left(10212 + 53460a + 33891a^2 + 12584a^3 + 5808a^4\right)}{50683 + 52072a + 13200a^2}P_1^*, \\
P_8^* = P_9^* &= \frac{a^2\left(12348 + 55020a + 31251a^2 + 11528a^3 + 5808a^4\right)}{50683 + 52072a + 13200a^2}P_1^*, \\
P_{10}^* &= \frac{a^2\left(40228 + 52876a + 18123a^2 + 3144a^3 + 1584a^4\right)}{50683 + 52072a + 13200a^2}P_1^*, \text{ and} \\
P_{12}^* &= \frac{a^2\left(5292 + 23580a + 42355a^2 + 34696a^3 + 10032a^4\right)}{50683 + 52072a + 13200a^2}P_1^*. \qquad (6)
\end{aligned}
$$

From the statistical viewpoint, it is common question to ask what the most likely configuration is for given circumstances. To answer this question and gain more insight into this probability function, we present the histogram of how an event occurs configuration-wise as shown in Fig. 5-Fig. 8.

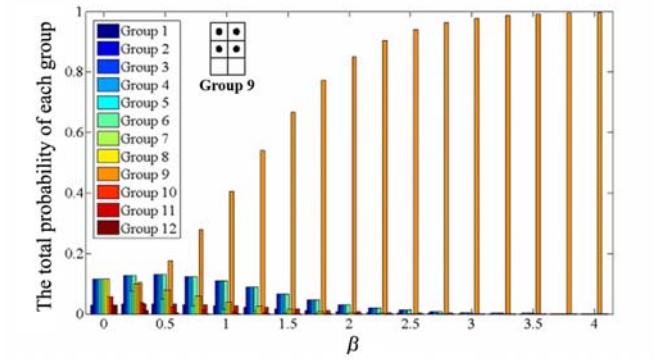

Fig. 5 The histograms of the total probability ($g_iP_i^*$) of each group in equilibrium state $E = 0$ and $J = 1$. It is dominated by group 9. The typical configuration of group 9 is also shown on the graph. At infinite temperature ($\beta = 0$) the probability (P_i^*) is the same for all groups so that the total probability of each group depends on the number of members (g_i) of each group or the degeneracy of each group.

In Fig 5, $E = 0$ for the selected interaction energy $J = 1$, we show a chart of the total probability of each group ($g_iP_i^*$), hereafter referred to as P_i^*, where g_i represents the number of members of the group i, versus β for $E = 0$, $J = 1$. It is found that as β increases or temperature decreases, the total probability of group 9 (P_9^*) becomes more and more dominated and finally reaches the highest value among others. While the total probabilities of groups 5, 7, 8, 10, and 12 monotonically decrease to zero, it appears that the total probabilities of groups 1, 2, 3, 4, 6, and 11 do not change monotonically. They instead increase at relative low β until they reach the maximum value and then decrease to zero eventually. These behaviors can be explained as follows. With $E = 0$, i.e. diffusion without biased or driven force, the dynamics is under the influence of particle interactions and the excluded volume. Hence, we recover the "standard model" which is in the absence of the field. We should expect the usual Ising lattice gas like behavior, but using particle language in stead of spin language. It is noted that the conservation law is a crucial factor responsible for a number of exciting phenomena. The interactions of the particle system with its surroundings are represented by a coupling to a heat bath at the given temperature. As a result, all steady states which are in equilibrium can be computed by weighting with the canonical distribution: $P_{eq}^* = \exp(-\beta H)/Z$ where Z is the partition function. It is commonly known that for a large enough system (thermodynamic limit) in two dimensional cases, the Ising lattice gas exhibits the second order phase transition at about $0.5673J/k_B$ [35]. As seen once again in Fig. 5 that the most likely dominated group is shifted to group 9 in which the particles organize in cluster or aggregate like form as temperature is lowered. It is quite to be expected because all critical properties are universal, belonging to the "Ising universality class" [36]. This phenomenon corresponds to the phase transition from the high temperature disordered phase to the low temperature ordered phase,

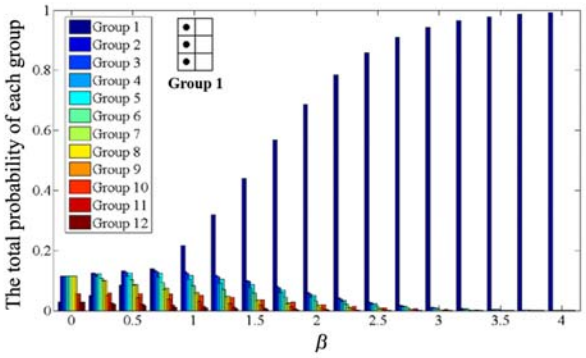

Fig. 6 The special case of non-equilibrium state $E \to \infty$ and $J = 1$. It is completely dominated by group 1. The typical configuration of group 1 is also shown on the graph.

Fig. 6, presents the similar data histogram of the above case for $E \to \infty$ which is now in the case of typical non-equilibrium steady state corresponding to $x = 0$. It is found that initially at infinitely high temperature, the probabilities of all groups are equal. Indeed the "random walk drive" out-performs the bias drive. As we lower the temperature the total probability of the group 1 increases to about one when β increases and it becomes the most dominated configuration, while the total probabilities of other groups decrease to zero. This quite makes sense because the field tends to line up the particles in the field direction. Specifically, the field biases the jump rates, favoring jumps along its direction while leaving jumps in the transverse directions unaffected. Due the PBC used, it does not permit the global energy flux to become zero resulting in non-equilibrium steady state. When the particles "feel" each other's interaction or non-zero β, the correlation then plays the role of correlating all particles to lower the energy. In this case, since the field is so large, it thus becomes dominated quite rapidly as long as the particles are interacting with each other.

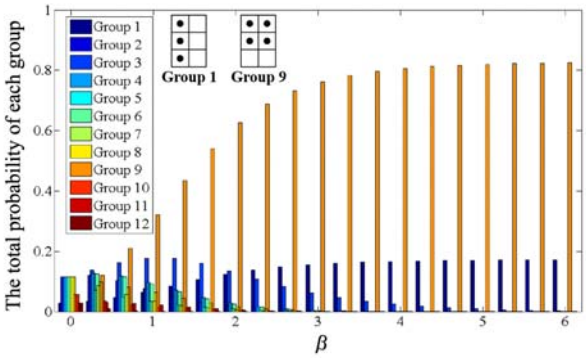

Fig. 7 The result of interest in case of $E = J = 1$ that has two dominations. The first is group 9 and the second is group 1. It can be seen that the system starts to change its main configuration from group 9 to 1 at this point.

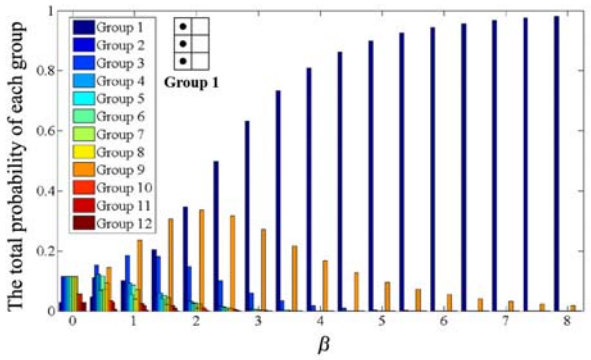

Fig. 8 For E = 1.5, the configuration of the group 1 replaces the configuration of group 9 to become the most dominant one at large β while group 9 and others descents to zero probability after reaching the maximum value.

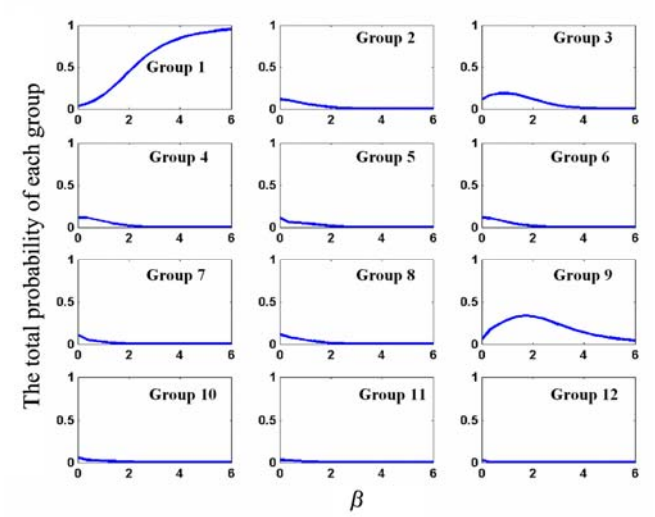

Fig. 9 The distinct plots of the total probability of each group in non-equilibrium state condition E = 1.5 and J = 1.

In Fig. 7, the distribution functions for finite temperature are plotted for each group of configurations. We consider an intermediate value of E, $0 < E = 1 < \infty$ (the rest has also been done, but the data are not shown). The interesting result is that this condition gives two most likely groups, namely the most dominant group 9 and the second most dominant group 1. As E is increased further, for example E = 1.5 as in Fig. 8 and Fig. 9, the configuration group 9 becomes less dominant and in turn is replaced by group 1 that takes over and becomes solely dominant as group 9's probability decays to zero at larger β. It should be pointed out that for the finite field especially at low β or large T, other groups like groups 2, 3, and 4 also contribute to the collective behavior of the whole system. It should be noted that the net probability flow ($K_{C'\to C}$): $K_{C'\to C} \equiv W[C'\to C]P(C') - W[C\to C']P(C)$, such that at steady state $\sum_{C'\neq C} K^*_{C'\to C} = 0$.

For our problem the total probability of all groups will be according to the assumption of net probability flows at steady state $\sum_{C'\neq C} K^*_{C'\to C} = 0$. Hence, in any condition, the probability flows are a constant, i.e., if $W[C'\to C]$ is large, $W[C\to C']$ then is small.

Next we turn to the violation of fluctuation-dissipation theorem (FDT-violation) of non-equilibrium system. Known in statistical physics, the fluctuation dissipation theorem is a powerful tool for predicting the non-equilibrium behavior of a system from its reversible fluctuations in thermal equilibrium. The fluctuation dissipation theorem relies on the assumption that the response of a system in thermodynamic equilibrium to a small applied force is the same as its response to a spontaneous fluctuation. Therefore, there is a direct relation between the fluctuation properties of the thermodynamic system and its linear response properties. In other words, in non-equilibrium system FDT is violated, the so called "FDT-violation". We thus here aim to illustrate how our analytic results of the small system could be used to distinguish between equilibrium and non-equilibrium.

From the results on section 3.1 of probability functions, we calculate an internal and associated fluctuations (1st and 2nd moments): To calculate the energy fluctuation $\Delta U \equiv \langle U^2\rangle - \langle U\rangle^2$, we first calculate the average internal energy according to

$$\langle U\rangle = \frac{\sum_{i=1}^{n} u_n P_n}{\sum_{i=1}^{n} P_n} \tag{7}$$

Explicit calculation of $\langle U\rangle$ for E = 0and $E\to\infty$ are given by

$$\langle U\rangle = \frac{-12\left(1+6a^2+2a^3+a^4\right)}{\left(2+18a^2+8a^3+6a^4+a^6\right)}J, \text{ when } E=0,$$

$$\langle U\rangle = -\frac{4(50683+52072a+1069350a^2+1356900a^3+\ldots}{50683+52072a+1226448a^2+1590960a^3+\ldots}$$
$$= \frac{\ldots+617733a^4+249016a^5+82896a^6)}{\ldots+738502a^4+299440a^5+100320a^6}J, \text{ when } E\to\infty.$$

Naturally, one can also find the second moment of the energy, it gives the corresponding $\langle U^2\rangle$:

$$\langle U^2\rangle = \frac{4\left(3+12a^2+3a^3+a^4\right)}{\left(2+18a^2+8a^3+6a^4+a^6\right)}J^2, \text{ when } E=0,$$

$$\langle U^2\rangle = -\frac{8(101336+104144a+2000310a^2+2559120a^3+\ldots}{50683+52072a+1226448a^2+1590960a^3+\ldots}$$
$$= \frac{\ldots+1186983a^4+493304a^5+164208a^6)}{\ldots+738502a^4+299440a^5+100320a^6}J^2, \text{ when } |\bar{E}|\to\infty.$$

Hence, the explicit form of energy fluctuations for E = 0 and $|\bar{E}|\to\infty$ are

$$\Delta U = \begin{cases} \dfrac{24a^2(6+6a+8a^2+6a^3+21a^4+\ldots}{(2+18a^2+8a^3+\ldots} \\ \dfrac{\ldots+2a^5+12a^6+3a^7+a^8)}{\ldots+6a^4+a^6)^2}J^2, \quad when\ E=0, \\ 8a^2(8910375498+25040649552a \\ +192363408125a^2+531961153280a^3 \\ +686508142956a^4+56612596320a^5 \\ +360456105912a^6+172487525696a^7 \\ +59212705152a^8+16088979456a^9 \\ +2729852928a^{10})J^2/(50683+52072a \\ +1226448a^2+1590960a^3+738502a^4+299440a^5 \\ +100320a^6), \qquad when\ |\vec{E}| \to \infty \end{cases} \tag{9}$$

At this point we can gain more understanding about <U> and <U^2> by plotting the 3d profile of U–E–β (see Fig. 10) and ΔU–E–β diagram (see Fig. 11). There is a phase transition at $E = J = 1$. At low temperature the system tends to keep the ordered configuration. Thus, it is seen that the internal energy for (β>2) is stable at any external field. However, at very high temperature ($\beta \to 0$) the internal energy will be the same in any external field again because the energy of particles as a function of temperature can absolutely overcome both interactions, i.e. the particles interaction and the external field. For the intermediate temperature (0<β<2) the influence of the temperature is not sufficient to break the interactions. In Fig. 11, it is clearly seen that there is no fluctuation of energy except at $E = J = 1$ because at $E = 1$ there are two main possible configurations which are groups1 and 9.

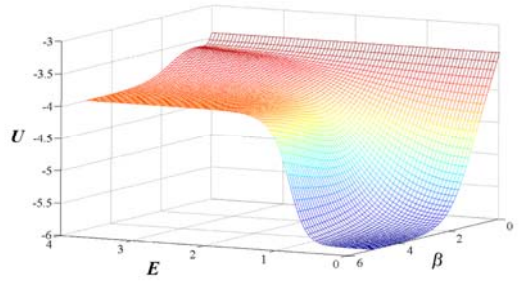

Fig. 10 Phase diagram of U–E–β.

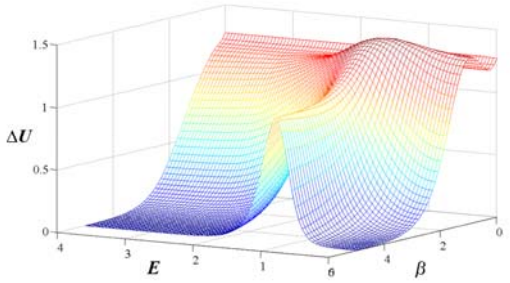

Fig. 11 Phase diagram of ΔU–E–β.

To investigate the FDT-violation phenomenon of non-equilibrium, we calculate the quantity corresponding to how a system in thermodynamic equilibrium responds to a small applied force. To calculate $-\partial U/\partial\beta$, one obtains

$$-\frac{\partial\langle U\rangle}{\partial\beta} = \begin{cases} \dfrac{24a^2(6+6a+8a^2+6a^3+21a^4+\ldots}{(2+18a^2+8a^3+\ldots} \\ \dfrac{\ldots+2a^5+12a^6+3a^7+a^8)}{\ldots+6a^4+a^6)^2}J^2, \quad when\ E=0, \\ 16a^2(3981098967+10942248999a \\ +12214921387a^2+17192508216a^3 \\ +20000185074a^4+17056087314a^5 \\ +10677378912a^6+3448779752a^7 \\ +376056384a^8+39726720a^9)J^2/(50683 \\ +52072a+1226448a^2+1590960a^3 \\ +738502a^4+299440a^5+100320a^6), \quad when\ \vec{E} \to \infty \end{cases}$$

It is found that $\Delta U = -\partial U/\partial\beta$, when $E = 0$, and $\Delta U \neq -\partial U/\partial\beta$, when $E \to \infty$.Therefore, without a driving field present ($E = 0$), i.e. in the equilibrium case, the FDT is satisfied, but in the presence of a driving field ($E \to \infty$), FDT is violated. In fact the FDT-violation is found for all non-zero field cases of DDS or lattice gas system.

To have a better understanding of collective behavior of the system dynamics, we turn to simulations. We demonstrate how one can alternatively understand the driven diffusive lattice gas system by means of numerical Monte Carlo simulations. The system is in contact with a heat reservoir, which keeps the temperature T constant. During one Monte Carlo step, which is our time unit, each particle on average could move to an empty neighbor site. The dynamics is governed by the Metropolis algorithm. A jump is realized with a probability of 1 if the new location is energetically favorable; otherwise, it is demonstrated by the probability Min(1,exp[$-\beta(\Delta H - \vec{E}.\vec{L})$]). We then present an extensive numerical study that supports the theoretical predictions. We performed the simulations according to the update rule and then compared the simulation results with those analytical results obtained from the previous section.

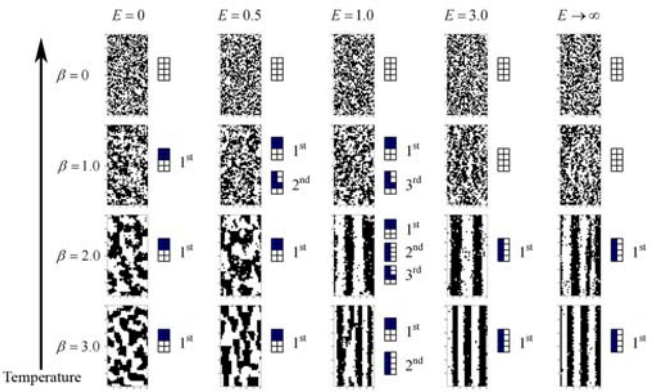

Fig. 13 Typical configurations of a 30×60 system along the inverse temperature (β) and the external field (E). The right-side of each typical configuration presents the representative configuration of any groups of the 2×4 system on the same conditions. In some case, the 2×4 system has more than one obviously dominant configuration. It is necessary to indicate the level of observable configuration, i.e. the 1st represents the highest probability of finding those configurations then 2nd and 3rd most likely configurations. An empty lattice means that there are no dominant configurations.

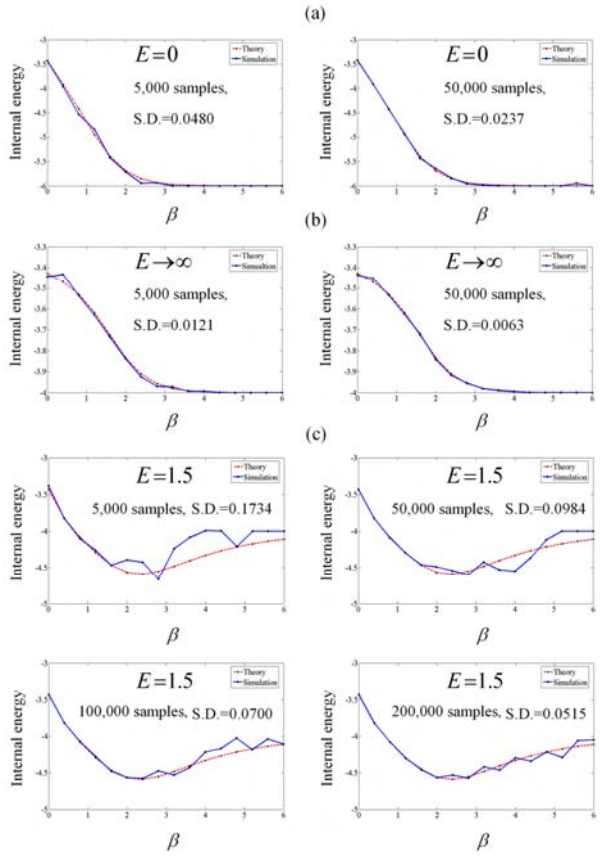

Fig. 14 The internal energy versus β for E = 0, E = 1.5, and E = ∞. The standard deviations (S.D.) of the data from exact solution and simulation are shown on the figures.

Fig. 14 shows typical configurations of a 30x60 system for various β and E. The right-side of each typical configuration presents the representatives of the most likely configuration of the 2x4 systems on the same conditions. It is seen that the system tends towards the ordered phase with decreasing temperature. Hence, we can approximate the critical point temperature to be between 0.5 and 1. Overall, it was found that the results on large systems agree surprisingly well with those on small systems.

Fig.14 presents a comparison between simulation and analytical results of the internal energy vs. β for E = 0 (see Fig.17a), E = ∞ (see Fig. 17b) and E = 1.5 (see Fig. 17c). In each case of the external field, we compare the simulation results of those from the ensemble average over 5000 and 50,000 samples (for case of E = 1.5, 5000 50,000 100,000 and 200,000 samples) to see the deviation of the predicted results from the theoretical values. It was found that the simulation results are in good agreement with analytical results especially for the large ensemble average. The internal energy is inversely proportional to β or is directly proportional to the temperature as expected. The measured standard deviation consistently decreases with the sample size.

An example of a bigger sized system which is closely related to our systems has been studied by Katz, Lebowitz and Spohn [24]. They investigated the phase transitions in stationary non-equilibrium states of a lattice gas system via Monte-Carlo simulation. Their systems contained two species, particles and holes, of states. The particle-vacancy exchanges follow the Kawasaki dynamics [20] with periodic boundary condition and the number of particles is conserved. They found that for a non-equilibrium steady state, the systems went into the ordered state, namely strips configurations, that consistent with our prediction. It should also be pointed out that, with a finite temperature, the correlation will play a greater role in contrast with the infinite temperature situation. This is mainly due to how each moving particle interacts with its environment. As seen that even though the considered small model is simple, allowing the analytical solution to be obtained, it provides a basis for the description of a variety of larger systems.

IV. Concluding Remarks

The study of non-equilibrium systems has attracted increasing interest in recent years, mainly due to the lack of theoretical frameworks, unlike their equilibrium counterparts. In this work, we used DLG model to investigate non-equilibrium phenomena and their stochastic properties. The stochastic physical properties at non-equilibrium steady state were particularly focused upon. Our aim was to find out about the possible patterns and dynamics in stationary states. The study used the master equation and solved for the probability distribution function as well as violation of detailed balance in term of the fluctuation-dissipation theorem using the small system via analytical method and simulating the large system by Monte Carlo simulations to validate the analytic results

Our overall results show that the probability distributions are controlled by such interactions via parameters including particle interaction, field strength, temperature and excluded volume. As analytically seen the interactions, which influences over others, also determine its state on the system. We support our analytic results by means of computer simulations of a two-dimensional lattice with nearest-neighbor interactions. We simulated the dependence of the configuration changes, energy, and energy fluctuation on various conditions of temperatures and fields. All simulation results are well consistent with analytical ones.

Finally, we would like highlight that the studied interacting lattice gas, driven into non-equilibrium steady states by an external field, exhibits remarkable properties such as its non-Hamiltonian nature, the violation of the fluctuation-dissipation

theorem, the occurrence of anisotropic critical behavior. Because of the model's simplicity and yet enough realisticity, its stochastic mathematics and its predictions of physical properties make it a valuable part of statistical mechanics research.

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