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Modified Fermi–Dirac Statistics of Fermionic Lattice Gas by the Back-Jump Correlations

T. Barszczak[1] **and R. Kutner**[1,2]

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The influence of the Bardeen–Herring back-jump correlations on the Fermi–Dirac statistics of the one-dimensional nonhomogeneous fermionic lattice gas is studied by the Monte Carlo simulation technique and semianalytically. The resulting distribution is obtained, exhibiting increased population of the lower levels in comparison to the Fermi–Dirac statistics.

KEY WORDS: Fermionic lattice gas; back-jump correlations; Fermi–Dirac statistics; Monte Carlo simulation; detailed balance conditions; two- and three-point occupancy joint probabilities; two- and three-point occupancy correlation functions; cluster expansions of joint probabilities.

1. INTRODUCTION

The present paper is concerned with the analysis of the distribution of correlated particles. The influence of the correlations on the distribution of structureless particles hopping in the one-dimensional nonhomogeneous fermionic lattice gas is studied here systematically by Monte Carlo simulation and semianalytically. By "fermionic lattice gas" we understand such a lattice gas in which double occupancy of the lattice sites is forbidden. This constraint plays a role analogous to Pauli's exclusion principle for usual fermions. In lattice gases defined in this way the undistinguishability of the particles, analogous to the quantum mechanical one, can easily be assured. The above-mentioned hopping process is interesting and complicated, since in the motion of the particles correlations with a fluctuating surroundings appear.

[1] Permanent address: Warsaw University, Department of Physics, PL-00-681 Warsaw, Hoża 69, Poland.

[2] Temporary address: Institut für Festkörperforschung, Forschungszentrum Jülich, Postfach 1913, D-5170 Jülich, Germany.

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Much work, numerical, phenomenological, and theoretical, has been devoted to the hopping of particles in concentrated fermionic lattice gases. In particular, effort has been made to analyze the basic mechanism for the correlations which accompanies a particle hopping in a concentrated fermionic lattice gas, i.e., Bardeen–Herring-type back-jump correlation effect.[1–10] Namely, when a particle exchanges with a vacancy, there is a strong tendency for the reverse exchange of this particle with the same vacancy, resulting just in a net backward correlation in a particle hopping.

Usually, this mechanism is studied in the context of diffusion, where it leads to, e.g., an essential reduction of the tracer diffusion coefficient. In the present paper we consider, however, this mechanism in a nondiffusion context.

We study a fermionic lattice gas in statistical equilibrium and consisting of undistinguishable particles hopping on a (vertical, one-dimensional, semi-infinite) "ladder." The rungs of the ladder are single-particle, hierarchical (for simplicity equally distributed) energy levels. The higher levels of the ladder have larger potential energies, since (for simplicity constant) external force has been applied vertically to the system. Hence, the observed population of the particles in the vertical direction is nonhomogeneous. Moreover, we assume that exchange between the different particles is impossible and any particle can jump only to the nearest-neighbor empty site. Apart from the double occupancy of the sites which we have excluded, there are no further mutual interactions between the particles.

To clarify the problem, let us classify all the current jumps of the particles in this model into two groups. In the first group we have jumps which occur against the external force, and in the second group those which occur in accordance with that force. Due to the back-jump correlation effect, the next (second) backward jumps of the particles from the first group lead to an increase of the population of the lower levels of the ladder. The analogous backward jumps for the particles from the second group lead to an increase of the population of the higher levels. Now the question arises as to the net result of both opposite tendencies.

It is decided here in the computer experiment (Section 2) and thanks to theoretical considerations (Section 3) that the sought net result is a distribution with a population of the lower levels higher than with the (standard) Fermi–Dirac statistics. Intuitively we could expect this result from the very beginning because the applied external force favors the downward (backward) jumps. The obtained result is systematically discussed, and Section 4 contains our concluding remarks.

2. NUMERICAL PROCEDURE AND RESULTS

Since the hopping process of the particles was carried out by the standard Monte Carlo simulation technique,[4–10] we will mention only some special features and characteristic steps of the present approach.

We usually work with short ladders of length $N = 20$–200 levels with blocking boundary conditions imposed at the bottom and at the top. (By blocking boundary conditions we mean that the jump of the particle being at the nearest-neighbor site to the wall cannot be performed in the direction of the wall.) To simulate the semi-infinite system, the length of the ladders was chosen so that the jumping particles could never reach the top of the ladder (during the computer experiment but after relaxation of the system to statistical equilibrium). The external (constant) force F was vertically applied against the h axis so that the (vertical) particle jump rate to an unoccupied site is defined, in the standard way, as

$$\Gamma_{\uparrow,\downarrow} = \begin{cases} \Gamma_0 \exp\left(-\dfrac{1}{2\alpha}\right) & \text{for jumps in accordance with the } h \text{ axis} \\ \Gamma_0 \exp\left(\dfrac{1}{2\alpha}\right) & \text{otherwise} \end{cases}$$

Here $\alpha = kT/\Delta\varepsilon$ will be called the "dimensionless temperature," where $\Delta\varepsilon = \varepsilon(h+1) - \varepsilon(h)$ is the energy difference between two consecutive energy levels $h+1$ and h, respectively (typically, in our simulations $\Delta\varepsilon = 0.02$ eV), and the energy level is $\varepsilon(h) = Fha$, with a the lattice constant (which has been assumed further as equal to unity); Γ_0 is an unbiased jump rate. The significant results discussed below were obtained for $\alpha \lesssim 1$, which means that we have to deal with a strongly degenerate fermionic lattice gas in this region. [The degeneration temperature T_0 is given here as $kT_0 \approx (\mathcal{N}_p - 1)\,\Delta\varepsilon$, where $\mathcal{N}_p$ is the fixed number of particles initially distributed on each ladder.]

We usually operate with a statistical ensemble consisting of $N = 80$ identical ladders to estimate experimentally the desired distribution $n(h)$, i.e., the average number of particles in a given state number h of energy $\varepsilon(h)$, when the system is in statistical equilibrium. The computer counts therefore the current total number of particles $\mathcal{N}(h)$ on a given level h (at the whole statistical ensemble) and then calculates the current occupancy as $\nu(h) = \mathcal{N}(h)/N$. For times shorter than $t_0 \approx 500$ Monte Carlo steps per particle (MCS/p) equilibrium was not yet established.

We average additionally the current occupancy number $\nu(h)$ over time beginning from t_0 up to $t \approx 5000$ MCS/p (then the relative statistical error is smaller than 0.1%). The resulting experimental distribution

$n(h) = \langle v(h) \rangle$ for correlated particles in a fermionic lattice gas is represented in Fig. 1 by the black circles. For comparison we also show, by open circles, the Fermi–Dirac statistics[11]

$$n_F(h) = \frac{1}{\exp[(h - h_F)/\alpha] + 1}$$

(where h_F is the Fermi level calculated numerically from the normalization condition) which only characterizes the uncorrelated fermions. This statistics is also reproduced (with a very good approximation) in an additional computer experiment where the horizontal jumps of the particles are permitted. (Then we treat our statistical ensemble of ladders as simply a two-dimensional lattice gas on a rectangular lattice.) We could expect such a result because now (generally speaking) the vacancies and the particles can easily depart and therefore the role of the back-jump correlation effect much decreases in this model. Moreover, in this case the Fermi level fluctuates from ladder to ladder, which strongly decreases the correlation effect.

In the vicinity of the Fermi level (cf. Fig. 1) a serious disagreement is seen between the experimental data (black circles) for the correlated

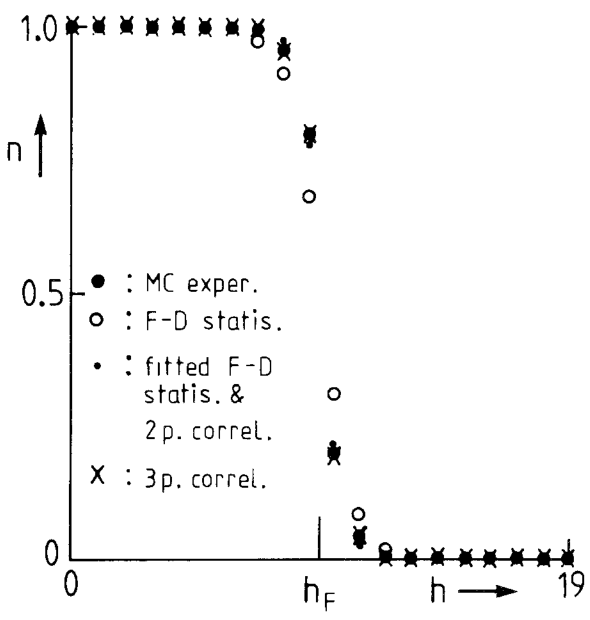

Fig. 1. Analysis of several statistics for the fermionic lattice gas as discussed in the text (here the absolute temperature $T = 150$ K).

particles and the Fermi–Dirac statistics (open circles), increasing when the temperature decreases and not exceeding here 15%. This is indeed the main experimental result of the present paper.

For example, to verify the stability of this result, we repeated our Monte Carlo simulation three times, using three different types of initial configurations of the particles, namely (i) homogeneous population of the sites (i.e., population of sites according to the Fermi–Dirac statistics at infinite temperature), (ii) distribution of the particles according to the Fermi–Dirac statistics at zero temperature, and (iii) at the real temperature. We can conclude that no changes in the final result were observed, although the system reaches the statistical equilibrium quickest in the third case.

The dots in Fig. 1 (very near the black circles) represent the fit of the (standard) Fermi–Dirac statistics to the experimental data, where the dimensionless temperature α was treated as a free fit parameter. (A very similar result, undistinguishable on the scale of the figure, was obtained when the Fermi level h_F was treated as an additional, second fit parameter.) However, a little deviation from the experimental data is still present. The result (which gives, as is seen, the Fermi–Dirac statistics at apparently lower temperature) is nevertheless qualitatively consistent with the experimental observation that the correlated particles of the fermionic lattice gas populate on the average the lower levels. The theoretical results, presented in Fig. 1 by crosses, are discussed in the next section, where "detailed balance conditions" involving three-point occupancy joint probabilities are exploited.

In Fig. 2 we show additionally the fitted effective dimensionless temperature α_{eff} as a function of α. The black circles were calculated for our one-dimensional model, while the open circles were obtained in an additional experiment where horizontal jumps of the particles were also permitted. (The crosslet in the same figure was obtained from the two-state model including only one active particle.) As is seen, a significantly decreasing temperature of the correlated particles is present for $\alpha \lesssim 1$. (We assumed a scaling factor $10^3 k/\Delta\varepsilon = 4.285\ \text{K}^{-1}$.)

3. FORMALISM

In this section we derive the difference recurrency equation for desired distribution. For simplicity we assume that all correlations can be described only by the two-point ones.

We therefore briefly consider the hierarchy of the detailed balance conditions which are fulfilled by our system at equilibrium. These conditions are the static version of the hierarchy of equations generated from the

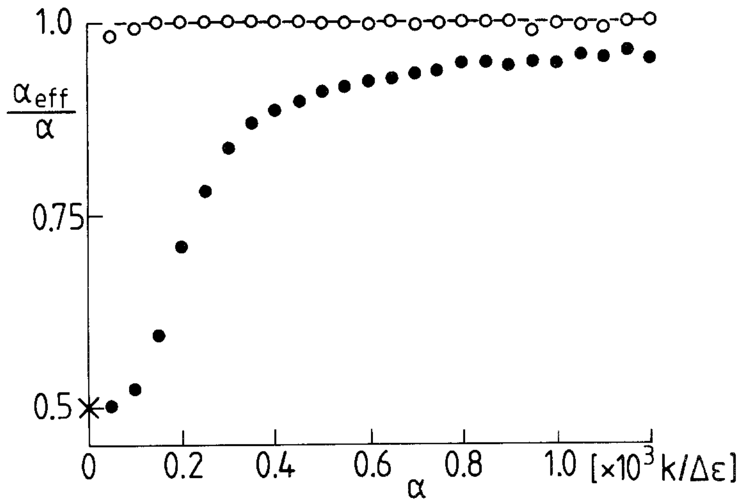

Fig. 2. The dimensionless, effective, relative temperature $\alpha_{\text{eff}}/\alpha$ as a function of the dimensionless temperature α for our one-dimensional system (black circles) and for the rectangular lattice (open circles; the crosslet is discussed in text).

Markovian master equation by appropriate summations. For example, one of the second-order detailed balance conditions for some static, two-point occupancy joint probabilities has the form

$$\Gamma_{\uparrow}(h)\, P_{10}(h) = \Gamma_{\downarrow}(h+1)\, P_{01}(h), \qquad h = 0, 1, 2,... \tag{1}$$

where, e.g., $P_{10}(h)$ is the static, two-point occupancy joint probability of finding a particle at level h and a vacancy at a higher, nearest-neighbor level $h+1$. In this notation $P_1(h)$ represents the desired distribution function. (In the whole formalism it is not necessary to assume that the levels should be equally distributed.) As is seen, (1) describes the balance between two local currents of probability [e.g., the left-hand side of (1) denotes the current probability of particles passing from site h up to the nearest-neighbor site]. If we would permit further decoupling of the two-point occupancy joint probabilities, e.g., by assuming that $P_{10}(h) = P_1(h)\, P_0(h+1)$, which is characteristic for the uncorrelated particles, we would easily find[12] the Fermi–Dirac statistics as a solution of (1).

Additionally, we have the third-order detailed balance conditions for some three-point occupancy joint probabilities. For example, one of these conditions takes the form

$$\Gamma_{\uparrow}(h)\, P_{101}(h) = \Gamma_{\downarrow}(h+1)\, P_{011}(h), \qquad h = 0, 1, 2,... \tag{2}$$

[where, e.g., $P_{101}(h)$ is the three-point occupancy joint probability of finding a vacancy at a level $h+1$ and the particles in the nearest-neighbor levels below and above].

To terminate the hierarchy we use the cluster expansion[13] (which is the one of the most effective factorization method) for describing the three-point occupancy joint probabilities in terms of the two-point occupancy correlation functions. For example,

$$P_{101}(h) \approx P_1(h)\, P_0(h+1)\, P_1(h+2) + P_1(h)\, F_{01}(h+1) + P_0(h+1)\, F'_{11}(h) + P_1(h+2)\, F_{10}(h) \tag{3}$$

where, e.g., $F_{01}(h+1)$ is the two-point occupancy correlation function defined as $F_{01}(h+1) = P_{01}(h+1) - P_0(h+1)\, P_1(h+2)$ [$F'_{11}(h)$ has an analogous definition, but for particles occupying levels h and $h+2$]. Our basic assumption here says that all three-point occupancy correlation functions vanish.

After straightforward but tedious calculations we derive (using the normalization and symmetry conditions fulfilled by the joint probabilities) a nonlinear second-order difference recurrency equation for the desired distribution function,

$$\begin{aligned}
&[-\gamma_{01} P_1(h) + P_1(h)\, P_1(h+1) + \gamma'_{01} P_1(h+1)] \\
&\quad \times [P_1(h+1) - \gamma_{01}][P_1(h+2) - \gamma_{12}] \\
&= [\gamma'_{12} P_1(h+2) + P_1(h+2)\, P_1(h+1) - \gamma_{12} P_1(h+1)] \\
&\quad \times [P_1(h) + \gamma'_{01}][P_1(h+1) + \gamma'_{12}]
\end{aligned} \tag{4}$$

where the abbreviated notation reads as follows:

$$\gamma'_{jj+1} = \gamma_{jj+1} - 1, \quad \gamma_{jj+1} = \frac{\Gamma_\uparrow(h+j)}{\Gamma_\downarrow(h+j+1)} \left[\frac{\Gamma_\uparrow(h+j)}{\Gamma_\downarrow(h+j+1)} - 1 \right]^{-1} \quad (j=0, 1)$$

We present this equation in the form which explicitly exhibits the required two kinds of symmetry conditions (the invariance under inversion of the external force and invariance under exchange of the roles of the particle and the vacancy).

The formalism obtained, e.g., under the assumption that the four-point correlations can be described by at the utmost the three-point ones, is only much more arithmetically complicated, while the idea of the derivation (in this case) of the nonlinear third-order difference recurrency equation is the same.

At present we have only numerical solutions of the derived recurrency equations, shown in Fig. 1 once more by dots for (4) (undistinguishable, on the scale of the figure, from the earlier discussed result of the fit of the Fermi–Dirac statistics to our experimental data) and by crosses for the mentioned more complicated approach. Note that because our equations are second- and third-order difference ones, they require, to determine the solutions, two and three additional (e.g., initial) conditions, respectively. To find numerical solutions it is easier to, e.g., in the more complicated case, treat the values $P_1(h=0)$, $P_1(h=1)$, and $P_1(h=2)$ as free parameters which can be obtained by the fit to the experimental data [as fit parameters we can also use any three consecutive values $P_1(h=j)$, $P_1(h=j+1)$, and $P_1(h=j+2)$, $j=0, 1,...$].

4. CONCLUDING REMARKS

As is seen from Fig. 1, the solution of the third-order recurrency equation (crosses) fits best the data of our computer experiment (we hope that this is so not only because it has the most free parameters). This result is quite consistent with the picture of the back-jump correlations where at least two consecutive jumps of a particle, and therefore at least three consecutive visited levels, are directly correlated, i.e., cannot solely be represented by the two-point occupancy correlation functions. In our formalism, however, the explicit form of the correlations was never used. Neither was it necessary to develop the more extended formalism to calculate higher-order occupancy correlation functions.

Roughly interpreting the results, we say that the correlated particles of the fermionic lattice gas behave as if they were colder. Alternatively, this can also be interpreted as an apparent increase of the energy differences between the levels (or possibly by both these phenomena occurring simultaneously). These observations are valid for the systems with metallic as well as with semiconductor structure.

Because the back-jump correlations accompany (with larger or smaller intensity) the hopping process even of noninteracting particles (except that double occupancy is forbidden), it would be interesting and important to have, e.g., the analytical solutions of our equations, and then analytically study the statistical, thermal physics of the fermionic lattice gas.

NOTE ADDED IN PROOF

Similar deviations from the distribution of the Fermi–Dirac type was also found for this model by the static calculations of R. Németh and

K. Kehr[14]. They directly counted by numerical means the number of possible configurations of the particles in the small system[15] and then calculated the partial and the total partition functions. Hence, by the usual way they numerically obtained the desired statistics for the fermionic lattice gas.

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