Journal of Statistical Physics, Vol. 65, Nos. 3/4, 1991

Distribution for Fermionic Discrete Lattice Gas within the Canonical Ensemble

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

Received May 22, 1991

The distinct deviations from the Fermi–Dirac statistics ascertained recently at low temperatures for a one-dimensional, spinless fermionic discrete lattice gas with conserved number of noninteracting particles hopping on the non-degenerated, well-separated single-particle energy levels are studied in numerical and theoretical terms. The generalized distribution is derived in the form $n(h) = \{Y_h \exp[(\varepsilon_h - \mu)\beta] + 1\}^{-1}$ valid even in the thermodynamic limit, when the discreteness of the energy levels is kept. This distribution demonstrates good agreement with the data obtained numerically both by the canonical partition function technique and by Monte Carlo simulation.

KEY WORDS: Fermionic lattice gas; canonical and grand canonical ensembles; complete, incomplete, and specific canonical partition functions; Fermi–Dirac statistics; Monte Carlo simulation.

1. INTRODUCTION

Recently we ascertained,[1] mainly by the Monte Carlo simulation, that the one-dimensional, spinless fermionic discrete lattice gas with conserved number of particles does not obey the conventional Fermi–Dirac statistics as one would expect.[2] This surprising result is systematically studied in the present paper by numerical and theoretical means, leading to a closed formula for the sought generalized distribution for this lattice gas within the canonical ensemble, valid even in the thermodynamic limit when the discreteness of the lattice is kept.

We consider a system in statistical equilibrium and consisting of N_p undistinguishable, spinless particles hopping on a ladder constructed of N

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

[2] Temporary address: Tokyo Institute of Technology, Department of Applied Physics, O-okayama 2-12-1, Meguro-ku, Tokyo 152, Japan.

0022-4715/91/1100-0813$06.50/0

equally distributed nondegenerate, well-separated, single-particle energy levels. The higher levels have of course larger potential energies, which can be realized e.g., by the application to the lattice gas of a biased field (acting against the vertical axis). The length of the ladder was chosen so that the jumping particles never reach (in practice) the top of the ladder and, analogously, the holes do not reach its bottom (nevertheless, blocking boundary conditions were imposed for the system). We assume that any particle can hop only up (with jump rate $\Gamma_\uparrow$) and down (with jump rate $\Gamma_\downarrow$) to the nearest-neighbor empty site, and exchange between different particles is forbidden. Apart from double occupancy of the sites, which we have excluded (this is an analog of Pauli's exclusion principle), there are no other mutual interactions between particles. Such a model can represent some general statistical physics aspects of real fermionic systems; it also should be possible to verify the above mentioned result directly in real experiments.[3] So we do not study the ideal quantum Fermi gas, but a discrete lattice gas with a site exclusion principle imposed on the system.

We consider mainly the most important, low-temperature region, i.e., the one for which the dimensionless temperature $\tau \lesssim 1$ {here we define $\tau = [\ln(\Gamma_\downarrow/\Gamma_\uparrow)]^{-1} = (\beta\, \Delta\varepsilon)^{-1}$, where $\beta = 1/k_B T$ and $\Delta\varepsilon$ is the discreteness i.e., the energy difference between two consecutive energy levels}, since earlier[1] we found, in principle, by Monte Carlo simulation, that deviations from the Fermi–Dirac statistics are then enhanced, especially in the vicinity of the Fermi level.

In Section 2 we develop an algorithm for numerical calculation of the canonical partition functions and hence evaluate in the standard way[4] the sought distribution (and its deviation from the Fermi–Dirac statistics). Section 3 (together with the Appendix) is devoted to the theoretical derivation of the sought distribution. Section 4 presents our current numerical and theoretical results and their comparison with the data of Monte Carlo simulation (obtained earlier[1]), as well as a discussion and concluding remarks.

2. THE ALGORITHM

It is commonly known that the equilibrium statistics of noninteracting fermions can be exactly expressed within the canonical ensemble by the following (general) relation[4] which is suitable as the starting point of the present considerations:

$$n(h) = \frac{1}{\exp(\beta\varepsilon_h)\, Z_h(N-1, N_p)/Z_h(N-1, N_p-1) + 1}, \qquad h = 0,..., N-1 \tag{1}$$

where, e.g., the conventional, "incomplete," canonical partition function $Z_h(N-1, N_p)$ is defined (for $N_p \leqslant N-1$) in standard terms as

$$Z_h(N-1, N_p) = \sum_{n_0,\ldots,n_{N-1}}^{(h)} \exp[-(n_0\varepsilon_0 + \cdots + n_{N-1}\varepsilon_{N-1})\beta] \qquad (1a)$$

This sum is extended over all levels except the fixed number h one, excluded from the system. The conventional "complete," canonical partition function is of course defined analogously while the sum is extended over all levels in the system. The occupation numbers n_j are $n_j = 1$ or 0 for each level j when it is occupied by a particle or not, and satisfies here the conservation condition

$$\sum_{j=0}^{N-1}{}^{(h)} n_j = N_p$$

The aim of the considerations in the present section is to find the algorithm for numerical calculation of the ratio of the incomplete partition functions used in (1). The algorithm for this calculation[3] is based on the recurrence relations fulfilled by the canonical partition functions. By using the standard definition of the canonical partition function and by performing explicitly the summation over two possible values of the occupation number n_{N-k-2} we get

$$\begin{aligned} Z'_h(N-k-1, N_p-m) &= Z'_h(N-k-2, N_p-m) \\ &\quad + Z'_h(N-k-2, N_p-m-1)\exp(-\beta\varepsilon_{N-k-2}) \qquad (2) \\ k &= 0,\ldots, N-4; \qquad m = 0, 1,\ldots, N_p-2 \end{aligned}$$

where, e.g., $Z'_h(N-k-1, N_p-m)$ is the "specific," canonical partition function having k topmost consecutive levels and m particles excluded from the summation in definition (1a) of the incomplete, canonical partition function (note that $N_p - m \leqslant N-k-2$). We consider here an auxiliary, incomplete system in which the energy level previously denoted as ε_h is excluded and therefore not taken into account by the k-index numeration. Additionally, we can write the following necessary boundary relations:

$$Z'_h(K, 1) = \sum_{j=0}^{K-1} \exp(-\beta\varepsilon_j), \qquad Z'_h(K, K) = \prod_{j=0}^{K-1} \exp(-\beta\varepsilon_j)$$
$$K = 1,\ldots, N$$

[3] The computer programs used in refs. 1 and 2, and in this paper are available on a DSDD disc 5.25″ or/and 3.5″ for microcomputers compatible with an IBM PC.

which complete the algorithm. This is a recurrence procedure which begins at $k = N - 4$ and $m = N_p - 2$ and runs down to the final values of $k = m = 0$. It is at these values of indexes that the procedure is terminated, giving the sought partition functions: $Z_h(N-1, N_p) = Z'_h(N-1, N_p)$ and $Z_h(N-1, N_p-1) = Z'_h(N-1, N_p-1)$. (We see that this algorithm provides more partition functions than we currently need.) The proposed algorithm is not as effective as, e.g., the one developed in ref. 5, but simple enough and appropriate for the present study.

3. THEORETICAL CONSIDERATIONS

In the present section we simplify primary expression (1) by relating the incomplete, canonical partition function $Z_h(N-1, N_p-1)$ to the $Z_h(N-1, N_p)$ one, to find the closed analytical formula for the sought distribution $n(h)$.

The following quite general Taylor expansion (both for the complete and incomplete, canonical partition function) can be written (if $\Delta N_p \ll N_p$):

$$\ln Z_{(h)}(I, N_p - \Delta N_p) \approx \ln Z_{(h)}(I, N_p) - \Delta N_p \, \alpha_{(h)} + (\Delta N_p)^2 \, \gamma_{(h)}/2 \qquad (3)$$

where $\alpha_{(h)}(I, N_p) = [\ln Z_{(h)}(I, N_p)]'$ and $\gamma_{(h)} = [\alpha_{(h)}]'$ (here the prime denotes the partial derivative over the second argument, and $N_p \leqslant I$). By a combining expansion (3) (for $\Delta N_p = 1$) with expression (1) we obtain the formula

$$n(h) = \{ Y_h \exp[(\varepsilon_h - \mu)\, \beta] + 1 \}^{-1} \qquad (4)$$

where the correction term $Y_h = \exp(\beta\mu + \alpha_h - \gamma_h/2)$ [here $\alpha_h = \alpha_h(N-1, N_p)$ and $\gamma_h = \gamma_h(N-1, N_p)$]; $\mu = -\alpha/\beta (> 0)$ is the chemical potential or Fermi level (discussed later).

When deriving the conventional Fermi–Dirac statistics, only the first two terms in expansion (3) are taken into account[4]; all other terms are neglected. It is easy to prove that in such a case the α coefficient is h-independent. Hence, the correction term $Y_h = 1$ independently of the number of the level.

Our case is more complicated, since we take into account the first three terms in expansion (3); such an approach is particularly important at low temperatures for finite discreteness. The principal aim of this study is eventually to find the analytical closed expression for the correction term Y_h. This is performed in the Appendix, since several tedious mathematical steps are required.

By a similar procedure one can easily calculate the joint probability $n(h, k)$ of finding a particle at level h and another particle at a different

level k, in order to discuss the static correlation effect. We can prove that this joint probability (in the general case) cannot be factorized, i.e., $n(h, k) \neq n(h)\, n(k)$, which means that the particles are correlated. However, the particles would be uncorrelated if all higher terms, except the first two, were neglected in an expansion like (3) (which is equivalent e.g. to the transition from the discrete to the continuous distribution of the energy levels, as we point out in the next section). These conclusions are consistent with our earlier observations,[1] where we tried to interpret the correlations in dynamic terms, as caused e.g., by the back-jump effect. Very recently it was proved[6] that the dynamics of this nonhomogeneous correlated fermionic discrete lattice gas can be described in terms of the XXZ-Heisenberg model.

In Section 4 the sought distribution $n(h)$ given by (4) and the correction term Y_h given by the formula (A3) are compared with our numerical data.

4. RESULTS AND DISCUSSION

As already mentioned, in the model developed here we assumed that the hopping particles never reach (during the long-time computer experiment) the top of the ladder, and likewise the holes never reach its bottom, which in practice eliminates the influence of the boundary condition (uninteresting for the present considerations). From the above it follows that to a good approximation we have the Fermi level $\mu = (N_p - 1/2)\, \Delta\varepsilon$; hence we have $\gamma = -\beta\, \Delta\varepsilon - \tau^{-1}$. Eventually these values of μ and γ are used in our calculations. In the half-filled case $N_p/N = 1/2$ this result is exact because of the particle–hole symmetry condition. In general, in a finite system the formula for the Fermi level is satisfied only at a sufficiently low temperature and/or sufficiently large discreteness. Here we study the important region $\tau \lesssim 1$ where the obtained distribution differs essentially from the conventional Fermi–Dirac statistics, and the latter one distinctly differs from the Boltzmann distribution. It is seen that the limit $\gamma \Rightarrow 0$ occurs when the transition from discrete to the continuous energy spectrum takes place and/or the temperature tends to infinity, i.e., when relative discreteness $\Delta\varepsilon/kT \Rightarrow 0$ and/or the energy $(N_p - 1)\, \Delta\varepsilon \Rightarrow \varepsilon > 0$.

In Fig. 1 our results for the distribution of the fermionic lattice gas are compared with the conventional Fermi–Dirac statistics at $\tau = 0.646$ (which is equivalent to, e.g., 150 K when $\Delta\varepsilon = 0.02$ eV). We present four types of results, obtained by: (i) Monte Carlo (MC) simulation discussed earlier[1] (having error bars distinctly smaller than the dimension of the circles), (ii) direct numerical calculations with the use of canonical partition functions (PF) according to the algorithm described in Section 2, (iii) predictions of

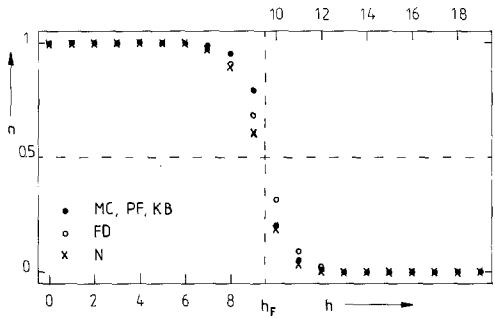

Fig. 1. Analysis of several statistics for the one-dimensional fermionic lattice gas at $\tau = 0.646$. The black circles present results of (i) Monte Carlo (MC) simulation, (ii) direct calculation by the canonical partition functions (PF), and (iii) our theoretical predictions (KB), which, on the scale of the figure, are indistinguishable. The open circles represent the conventional Fermi–Dirac (FD) statistics, and the crosses show predictions of the Németh (N) theory.

our theoretical approach (KB) discussed in Section 3 and in the Appendix, (iv) conventional Fermi–Dirac (FD) statistics, and (v) predictions of the Németh (N) theory.[3] As is seen, the first three types of results are indistinguishable on the scale of the figure. The agreement demonstrated here is better than that reached recently by Németh. Moreover, the first two results are indistinguishable even in a more suitable scale; we can conclude that these results are equivalent, though the first one is burdened with some small statistical error. It follows that the dynamic and static calculations provide the same equilibrium static distribution. In a more subtle scale one can observe, for $\tau \gg 1$, a slight difference between the first two types of results (numerical) and the third one (theoretical), which is due to the approximation used in formula (3).

The results presented in Fig. 1 confirm the earlier observations[1,3] that the equilibrium distribution for the fermionic discrete lattice gas derived within the canonical ensemble differs from the Fermi–Dirac statistics, especially for low temperatures in the vicinity of the Fermi level. The discrepancy does not vanish even if one increases the size of the system keeping the single-particle energy spectrum discrete, because this discrepancy eventually follows from the discreteness of the level spacing of the (energetic) ladder.

However, within the grand canonical ensemble, when the number of particles on an individual ladder fluctuates, the above-mentioned discrepancy disappears[1,3] thanks to the fluctuation of the Fermi level. This means that the canonical and grand canonical treatments given here quite different results for the occupation numbers,[3] even in the thermodynamic limit, as opposed to the ideal quantum Fermi gas.

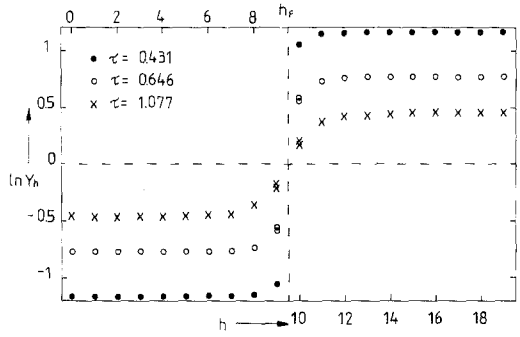

Fig. 2. The correction term Y_h vs. energy $\varepsilon_h - \mu$ for three different values of dimensionless temperature τ.

In Fig. 2 we present the correction term Y_h vs. energy $\varepsilon_h - \mu$ on a semilogarithmic scale, for three characteristic values of dimensionless temperature τ (note that $\tau = 0.431$ is equivalent to 100 K and $\tau = 1.077$ to 250 K when $\Delta\varepsilon = 0.02$ eV). In the figure the results obtained by the partition function technique and those found theoretically are compared. On the scale of the figure, however, we cannot distinguish between these two types of results (therefore they are labeled by the same markers), although for temperatures $\tau \gtrsim 0.5$, at points nearest to the Fermi level, the absolute values of the theoretical predictions are slightly smaller than the numerical data. The Y_h term for the conventional Fermi–Dirac statistics is represented by the horizontal dashed line.

Finally, for possible comparison of our results with real experiments, we should at least: (i) extend our considerations for non-equally-distributed levels in the energy spectrum, (ii) consider particles with spin, which leads to the extension of the formula (4) for the case of a twofold spin-degeneracy, and (iii) permit jumps of particles also to the next-nearest and further neighbors.

APPENDIX. DERIVATION AND SOLUTION OF EQUATION FOR Y_h

Here we derive and solve the fourth-order algebraic equation for the correction term Y_h, by using known relations[4] between the canonical partition functions (complete and incomplete) analogous to (2). The relations for three consecutive values of the number of particles in the system can be written in the following brief way:

$$Z(N, N_p + \eta) = Z_h(N-1, N_p + \eta) + Z_h(N-1, N_p - 1 + \eta)\exp(-\beta\varepsilon_h) \quad \text{(A1)}$$

where $\eta = -1, 0, 1$ (and $N_p + 1 \leqslant N - 1$) are assumed consecutively. By expanding both sides of the above relation [as was done in (3)] and by dividing the first relation with $\eta = -1$ by the second one with $\eta = 0$, and then that with $\eta = 1$ also by the relation with $\eta = 0$, we obtain two independent equations for the $\exp(\alpha_h)$ and $\exp(\gamma_h/2)$ unknown variables. After simple arithmetic operations we finally obtain the sought equation for the combined variable Y_h [$= \exp(\beta\mu + \alpha_h - \gamma_h/2)$] in the form

$$(Y_h)^4 + b \cdot (Y_h)^3 + d \cdot Y_h + e = 0 \tag{A2}$$

where

$$b = \exp[-(\varepsilon_h - \mu)\beta] - \exp(-\gamma/2)$$
$$d = \exp[-(\varepsilon_h - \mu)\beta - \gamma/2]\{\exp[-(\varepsilon_h - \mu)\beta] - \exp(\gamma/2)\}$$
$$e = -\exp[-2(\varepsilon_h - \mu)\beta]$$

As is seen, if $\gamma = 0$, then $Y_h = 1$ is a constant solution of (A2), as expected, and then distribution $n(h)$ is exactly given by the Fermi–Dirac statistics. In Section 4 we briefly discuss the physical conditions which make possible the important transition $\gamma \Rightarrow 0$. If we put (formally) $\varepsilon_h = \mu$, then $Y_{h=\mu/\Delta\varepsilon} = 1$ would be the solution of Eq. (A2) for any arbitrary γ (as expected). Moreover, from Eq. (A2) it is easy to find two characteristic asymptotic solutions. On the one hand, by assuming that $\varepsilon_h - \mu \gg -\gamma/2$ (note that γ is negative), we simply obtain $Y_h \approx \exp(-\gamma/2)$. On the other hand, for $\varepsilon_h - \mu \ll \gamma/2$, we have $Y_h \approx \exp(\gamma/2)$. Moreover, when $T \Rightarrow 0$ (at fixed $\Delta\varepsilon$) then from (A2) follows that also $Y_h \approx \exp(-\gamma/2)$ for $\varepsilon_h - \mu > 0$, and $Y_h \approx \exp(\gamma/2)$ for $\varepsilon_h - \mu < 0$. Nevertheless, precisely at $T = 0$ both statistics are identical and equal to the (discrete) step function.

The exact solution of (A2), which is consistent with the above-mentioned special cases, is derived in the standard way and has the form

$$Y_h = (-(b + A) + \{(b + A)^2 - 16[y + (by - d)/A]\}^{1/2})/4 \tag{A3}$$

where $A = \pm(8y + b^2)^{1/2}$. For $\gamma = 0$ the plus sign must be assumed, at any arbitrary value of energy ε_h. For $\gamma \neq 0$ the plus sign is also correct, but only for $\varepsilon_h \leqslant \mu$, while for $\varepsilon_h > \mu$ we must assume the minus sign. The value y is a real solution of the following third-order algebraic equation:

$$8y^3 + (2bd - 8e)\, y - (eb^2 + d^2) = 0 \tag{A4}$$

The solution y is

$$y = u_- - u_+$$

where $u_{\pm} = [(q^2 + p^3)^{1/2} \pm q]^{1/3}$, with $q = -(eb^2 + d^2)/16$ and $p = (bd - 4e)/12$. The real solution y can be represented in such a form because q and p are real and, what is most important, $p > 0$ except for the cases when $\varepsilon_h = \mu$ or/and $\gamma = 0$; but then $q = 0$ and we have $y = 0$, for any arbitrary p. Note that the values A, b, d, e, q, p, $u_{\pm}$, and y are (in general) h-dependent, although this index was omitted to simplify the notation.

The extension of the present approach for the h-dependent level spacing is straightforward (which means that it was no necessary to assume in the whole consideration that energy $\varepsilon_h = h\,\Delta\varepsilon$, $h = 0,..., N-1$, where $\Delta\varepsilon$ is h-independent).

We conclude that the closed analytical and not too complicated formula (A3) has been obtained for the correction term Y_h.

NOTE ADDED IN PROOF

After completing this paper we found refs. 7–10 where authors studied metallic fine particles and/or granular superconductors suggesting existence of the phenomena related to that discussed here.

ACKNOWLEDGMENTS

We thank R. Németh, D. Stauffer, K. Kitahana, K. Kehr, I. Sosnowska, and J. Spałek for helpful discussions. This work was partially supported by project RPBR RRI.14 of the Polish Ministry of National Education, and partially by the International Cooperation Program of the Ministry of Education of Japan.

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Communicated by D. Stauffer