ELECTRONIC PROPERTIES
OF SOLID

Simple Method for Exact Calculation of Thermodynamic Properties of the 1D Hubbard Model with Infinite Repulsion

K. A. Sidorov[a,b], S. G. Ovchinnikov[a,b,*], and N. V. Tikhonov[b]

[a]*Kirensky Institute of Physics, Siberian Branch, Russian Academy of Sciences, Krasnoyarsk, 660036 Russia*
[b]*Siberian Federal University, Krasnoyarsk, 660041 Russia*
*e-mail: sgo@iph.krasn.ru
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Abstract—It is shown that the canonical partition function in the 1D Hubbard model with $U = \infty$ in the nearest neighbor approximation is determined by the product of canonical partition functions of spinons and holons. In this approximation, the concentration and temperature dependences of the free and internal energies, as well as of the chemical potential, entropy, and heat capacity, are calculated for electron concentrations of $0 \leq n_e < 1$.

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1. INTRODUCTION

The Hubbard model is one of a few basic models in condensed state physics. Its exact solution using the Bethe ansatz [1] is one of the fundamental results in the physics of strongly correlated systems. The spectrum of both charge and spin elementary excitations was analyzed at $T = 0$ in [2]. In the limit $U \longrightarrow \infty$, the exact wavefunction is simplified upon elimination of local two-particle states and can be written in the form of the product of the spin and charge functions [3].

The thermodynamics of the 1D model was investigated by various methods (based on the Bethe ansatz with the string hypothesis [4, 5] and using the quantum transfer matrix [6]). All these methods are rather complicated; therefore, it would be interesting to obtain exact results using a simpler method. In this study, we will use the splitting of spin and charge degrees of freedom [3], which leads to factorization of the partition function in the form of the product of the partition functions of spinons and holons. For $U \longrightarrow \infty$, the exchange interaction between the nearest neighbors is $J = 2t^2/U \longrightarrow 0$; therefore, we have a chain of noninteracting spins with partition function $Z^{(s)} = 2^{N_e}$, where N_e is the total number of electrons in the chain. The partition function $Z^{(h)}$ for holons can easily be estimated owing to exact diagonalization of the Hamiltonian of interatomic jumps for spinless fermions. As a result, simple relations were derived between the thermodynamic parameters of electrons and spinless fermions (holons).

Eliminating the states of twos from the complete basis of local states $|0\rangle$, $|\sigma\rangle = a_\sigma^\dagger|\sigma\rangle$, and $|2\rangle = a_\uparrow^\dagger a_\downarrow^\dagger|0\rangle$, we in fact project the Hubbard model onto

the t–J model, which can be written for $U \longrightarrow \infty$ in the form

$$H = \sum_{f,\sigma} \varepsilon X_f^{\sigma\sigma} - \sum_{f,m,\sigma} t_{fm} X_f^{\sigma 0} X_m^{0\sigma}. \quad (1)$$

Here, $X_f^{pq} = |p\rangle\langle q|$ represents the Hubbard operator constructed on the truncated local basis for site f containing three states $|0\rangle$, $|\uparrow\rangle$, and $|\downarrow\rangle$. In this case, the electron–hole symmetry is broken and we therefore cannot consider the half-filled band with electron concentration $n_e = N_e/N = 1$ (N is the total number of sites). Our solutions are valid for concentrations of $0 \leq n_e < 1$. In this study, we take into account only the jumps t_{fm} between the nearest neighbors.

The article has the following structure. In Section 2, we analyze multielectron wavefunctions and write the exact expression for the partition function in the nearest neighbor approximation. In Section 3, the exact solution is obtained in the atomic limit ($t = 0$). The concentration and temperature dependences of the thermodynamic parameters of electrons, which are obtained from the exact solution for finite values of hopping parameter t, are considered in Section 4. Finally, in Section 5, we compare our results with the available data. The appendix contains proof of factorization of the partition function in the form of the product of the partition functions for holons and spinons.

2. ANALYSIS OF MULTIELECTRON STATES

For spinless fermions, the basis of local states at site f consists of only two vectors $|0\rangle_f$ and $|1\rangle_f = a_f^\dagger|0\rangle_f$. The

holon creation operator at site f is X_f^{10}. The condition for the completeness of the basis assumes the form

$$X_f^{00} + X_f^{11} = 1. \qquad (2)$$

The Hamiltonians for holons have the form

$$H = \sum_f \varepsilon X_f^{11} - \sum_{f,m} t_{fm} X_f^{10} X_m^{01}, \qquad (3)$$

and holons satisfy the conventional commutation relation typical of free fermions:

$$[X_f^{10}, X_m^{01}] = X_f^{10} X_m^{01} + X_m^{01} X_f^{10}$$
$$= \delta_{fm}(X_f^{11} + X_f^{00}) = \delta_{fm}. \qquad (4)$$

It should be noted that the electron creation and annihilation operators obey a more complex commutation relation:

$$[X_f^{\sigma 0}, X_m^{0\sigma}] = X_f^{\sigma 0} X_m^{0\sigma} + X_m^{0\sigma} X_f^{\sigma 0}$$
$$= \delta_{fm}(X_f^{00} + X_m^{\sigma\sigma}) = \delta_{fm}(1 - X_f^{\bar{\sigma}\bar{\sigma}}). \qquad (5)$$

For operators (1) and (3), a very convenient basis of the functions exists in which the matrices of these operators can be written. Namely, for such a basis it is convenient to take wavefunctions of the form

$$|\psi\rangle = |\psi\rangle_1 |\psi\rangle_2 \ldots |\psi\rangle_N = \prod_{i=1}^{N} |\psi\rangle_i, \qquad (6)$$

where

$$|\psi\rangle_i = \begin{cases} |0\rangle_i, & \text{if site } i \text{ is not occupied by an electron,} \\ |1\rangle_i, & \text{if site } i \text{ is occupied by an electron,} \end{cases} \qquad (7)$$

$$|\psi\rangle_i = \begin{cases} |0\rangle_i, & \text{if site } i \text{ is not occupied by an electron,} \\ |\uparrow\rangle_i, & \text{if site } i \text{ is occupied by an electron with spin } 1/2, \\ |\downarrow\rangle_i, & \text{if site } i \text{ is occupied by an electron with spin } -1/2, \end{cases} \qquad (8)$$

for a nonzero spin.

Dimensionality g of the Hilbert space of wavefunctions of the electron system is related to dimensionality $g^{(h)}$ of the Hilbert space of the spinless (holon) system by the obvious relation

$$g = 2^{N_e} g^{(h)}, \qquad (9)$$

where

$$g^{(h)} = \frac{N!}{N_e!(N - N_e)!}. \qquad (10)$$

The basis is defined by relations (6)–(8) to within the numbering of the basis vectors, which, however, does not affect the physical results being derived. Having defined the basis, we can consider the matrices of operators (1) and (3) in these bases. It will be rigorously proved in the Appendix proceeding from such analysis and general considerations that the canonical partition function in the limit $U \longrightarrow \infty$ can be factorized into the product of partition functions for holons and spinons:

$$Z = Z^{(h)} Z^{(s)}, \qquad (11)$$

where

$$Z^{(h)} = \mathrm{Sp}\left(\exp\left(-\frac{H^{(h)}}{k_B T}\right)\right), \qquad (12)$$

and $Z^{(s)}$ is defined as

$$Z^{(s)} = 2^{N_e}. \qquad (13)$$

Relations (11)–(13) are very important because these formulas determine the relation between the canonical partition functions for the spinless and non-

zero-spin cases and they make it possible to calculate the thermodynamic parameters of a system with nonzero spin if these parameters for the spinless system are known. Namely, introducing the notation

$$x = 1 - n_e \qquad (14)$$

for the hole concentration and using the well-known identities of statistical physics and thermodynamics, we immediately obtain the following relations:

$$f = f^{(h)} - k_B T(1-x)\ln 2 \qquad (15)$$

for the free energy,

$$s = s^{(h)} + k_B(1-x)\ln 2 \qquad (16)$$

for the entropy,

$$u = u^{(h)} \qquad (17)$$

for the internal energy,

$$c = c^{(h)} \qquad (18)$$

for the heat capacity at constant volume and number of particles, and

$$\mu = \mu^{(h)} - k_B T \ln 2 \qquad (19)$$

for the chemical potential. It should be noted that each formula in (15)–(19) has the following general form:

$$a = a^{(h)} + a^{(s)}, \qquad (20)$$

where $a^{(h)}$ is the contribution to quantity a from factor $Z^{(h)}$ in equality (11) (holon contribution) and $a^{(s)}$ is the contribution from factor $Z^{(s)}$ in the same equality (spinon contribution).

3. ATOMIC LIMIT

In atomic limit $t = 0$, Hamiltonians (1) and (3) assume the form

$$H^{(h)} = \sum_f \varepsilon X_f^{11} \qquad (21)$$

for holons and

$$H = \sum_{f, \sigma} \varepsilon X_f^{\sigma\sigma} \qquad (22)$$

for electrons.

The canonical partition functions for the systems described by Hamiltonians (21) and (22) are given, respectively, by

$$Z^{(h)} = \frac{N!}{N_e!(N - N_e)!} \exp\left(-\frac{N_e \varepsilon}{k_B T}\right), \qquad (23)$$

$$Z = \frac{2^{N_e} N!}{N_e!(N - N_e)!} \exp\left(-\frac{N_e \varepsilon}{k_B T}\right). \qquad (24)$$

It can be seen from these relations that the validity of equalities (11) and (13) is obvious in this case. Expanding the factorials in formulas (23) and (24) by Stirling's formula $n! \approx (n/e)^n$, we obtain the following expressions for the partition functions:

$$Z^{(h)} = \frac{N^N}{N_e^{N_e}(N - N_e)^{N - N_e}} \exp\left(-\frac{N_e \varepsilon}{k_B T}\right), \qquad (25)$$

$$Z = \frac{2^{N_e} N^N}{N_e^{N_e}(N - N_e)^{N - N_e}} \exp\left(-\frac{N_e \varepsilon}{k_B T}\right). \qquad (26)$$

Using these expressions for partition functions with notation (14) for the hole concentration, we can calculate all thermodynamic parameters of the system progressively. For the free energy per atom, we obtain, in accordance with the identity $F = -k_B T \ln Z$,

$$f^{(h)} = \varepsilon(1 - x) + k_B T(x \ln x + (1 - x) \ln(1 - x)), \quad (27)$$

$$f = \varepsilon(1 - x) + k_B T$$
$$\times (x \ln x + (1 - x) \ln(1 - x) - (1 - x) \ln 2). \qquad (28)$$

These expressions can be used to directly calculate the specific entropy and internal energy for holons and electrons:

$$s^{(h)} = -k_B(x \ln x + (1 - x) \ln(1 - x)), \qquad (29)$$

$$s = -k_B((1 - x) \ln 2 - (x \ln x + (1 - x) \ln(1 - x))), \quad (30)$$

$$u^{(h)} = u = \varepsilon(1 - x). \qquad (31)$$

Note that relations (29) and (30) are in complete agreement with the Boltzmann formula, according to which

$$s = -k_B \overline{\ln w} = -k_B \sum_k w_k \ln w_k. $$

Then, heat capacity $c = (\partial u / \partial T)_{V, N_e}$ in the atomic limit is zero:

$$c^{(h)} = c = 0. \qquad (32)$$

This result has a simple interpretation: the form of Hamiltonians (21) and (22) implies that all their eigenvalues are identical and equal to $N_e \varepsilon$ so that the internal energy remains unchanged upon a variation of temperature. Finally, the chemical potential

$$\mu = \frac{\partial F}{\partial N_e} = \frac{\partial F}{\partial x} \frac{\partial x}{\partial N_e} = -\frac{1}{N} \frac{\partial F}{\partial x}$$

can be written in the form

$$\mu^{(h)} = \varepsilon - k_B T \ln \frac{x}{1 - x}, \qquad (33)$$

$$\mu = \varepsilon - k_B T \ln \frac{2x}{1 - x}. \qquad (34)$$

It is important that relations (27)–(34) derived above are in complete conformity with relations (15)–(19).

4. EXACT CALCULATION OF THERMODYNAMIC PROPERTIES FOR FINITE VALUES OF THE HOPPING PARAMETER

Commutation relation (4) for holons, which is typical for free fermions, makes it possible to easily diagonalize Hamiltonian (3) using simple Fourier transformation. As a result, we obtain the exact expression for the spectral function:

$$\langle X_k^{10} X_k^{01} \rangle = \left\{ \exp\left(\frac{t(k) - \mu^{(ns)}}{k_B T} \right) + 1 \right\}^{-1} \qquad (35)$$
$$= f_{FD}(t(k)),$$

which coincides with the expression for the Fermi–Dirac free electron distribution function. In expression (35), $t(k)$ is the conventional band spectrum, which has the following form in the 1D case in the nearest neighbor approximation:

$$t(k) = -2t \cos(ka). \qquad (36)$$

To calculate the thermodynamic parameters of the system, we must primarily solve the equation for the chemical potential,

$$\sum_k \left\{ \exp\left(\frac{t(k) - \mu^{(h)}}{k_B T} \right) + 1 \right\}^{-1}$$
$$= \frac{N}{\pi} \int_0^\pi dy \left\{ \exp\left(\frac{-2t \cos y - \mu^{(h)}}{k_B T} \right) + 1 \right\}^{-1} = N_e, \qquad (37)$$
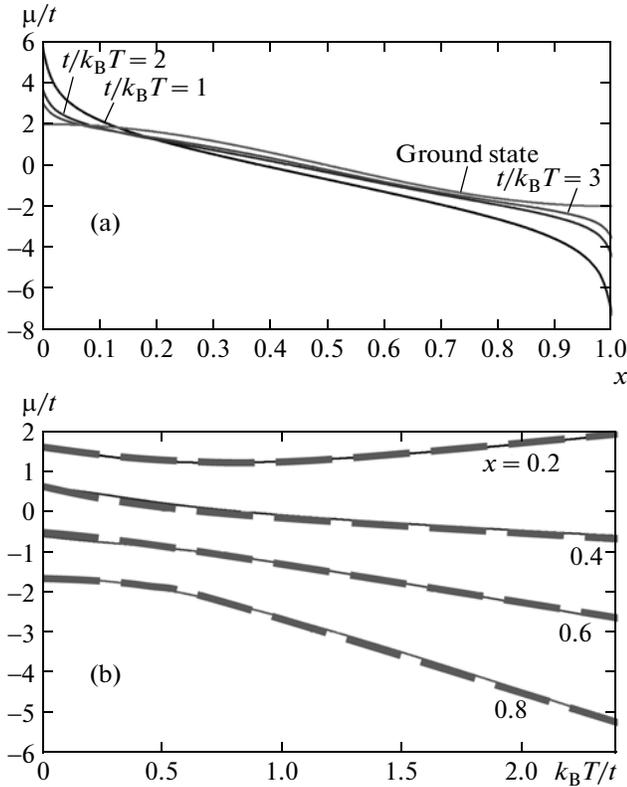
Fig. 1. (a) Concentration and (b) temperature dependences of the electron chemical potential. Bold dashed curves in (b) are the results from [8].
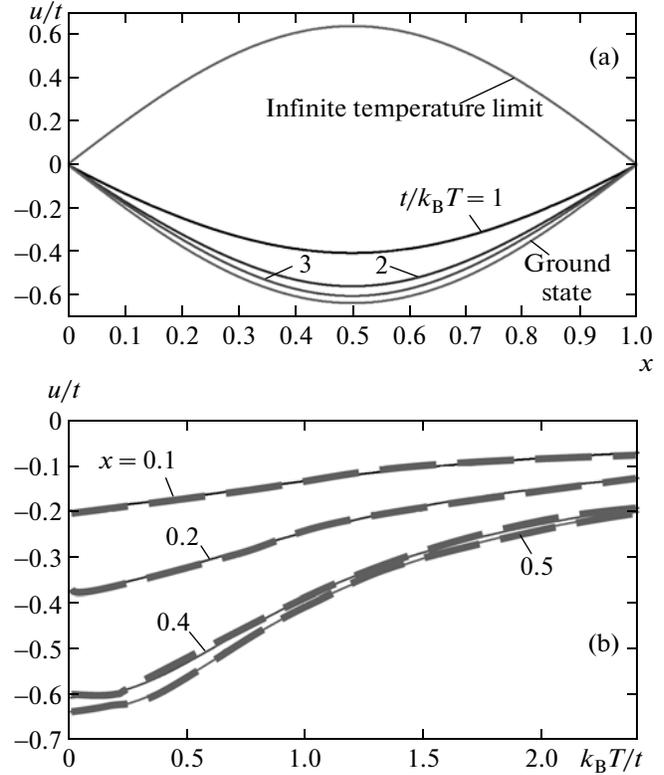

Fig. 2. (a) Concentration and (b) temperature dependences of the electron internal energy. Bold dashed curves in (b) are the results from [8].

where summation is carried out over all vectors **k** from the first Brillouin zone. At the second stage, we calculate the internal energy of the holon system:

$$u^{(h)} = \frac{1}{N}\sum_k t(k) f_{FD}(t(k))$$

$$= -\frac{2t}{\pi}\int_0^\pi \cos y \, dy \left\{ \exp\left(\frac{-2t\cos y - \mu^{(h)}}{k_B T}\right) + 1 \right\}^{-1}. \tag{38}$$

This expression is used to successively calculate the heat capacity for a constant volume and number of electrons, entropy, and free energy:

$$c^{(h)} = \left(\frac{\partial u^{(h)}}{\partial T}\right)_{V, N_e}, \tag{39}$$

$$s^{(h)} = \int_0^T \frac{c^{(h)}}{T} dT, \tag{40}$$

$$f^{(h)} = u^{(h)} - Ts^{(h)}. \tag{41}$$

As a result, we obtain the well-known dependences describing the behavior of an ideal Fermi gas [7]. It should be noted that the total number of states per atom in the holon band is unity; therefore, in the nearest neighbor approximation, the concentration

dependence for the chemical potential is antisymmetric, while for other thermodynamic characteristics of holons, it is symmetric with respect to a concentration of $x = 1/2$.

Let us now calculate the thermodynamic parameters of a system with nonzero spin. As mentioned above, such thermodynamic parameters can be calculated using relation (11). It is with this relation that we have derived formulas (15)–(19). The results of our numerical calculation for the chemical potential are shown in Fig. 1. By virtue of relation (19), the energy and the Fermi wavenumber of the electron system do not differ from their values for the holon system. In the latter system, these values are calculated from the familiar elementary considerations. As a result, we obtain the radius of the 1D Fermi sphere,

$$k_F^{(h)} = \frac{N_e}{N}\frac{\pi}{a} = (1-x)\frac{\pi}{a} \tag{42}$$

and the Fermi energy,

$$\varepsilon_F^{(h)} = -2t\cos(\pi(1-x)) = 2t\cos(\pi x). \tag{43}$$

Thus, at $T = 0$, the dependence of the chemical potential on the hole concentration has the form of a conventional cosine. However, as soon as the temperature becomes nonzero, the chemical potential for $x = 0$ and $x = 1$ turns to $+\infty$ and $-\infty$, respectively. This is visually
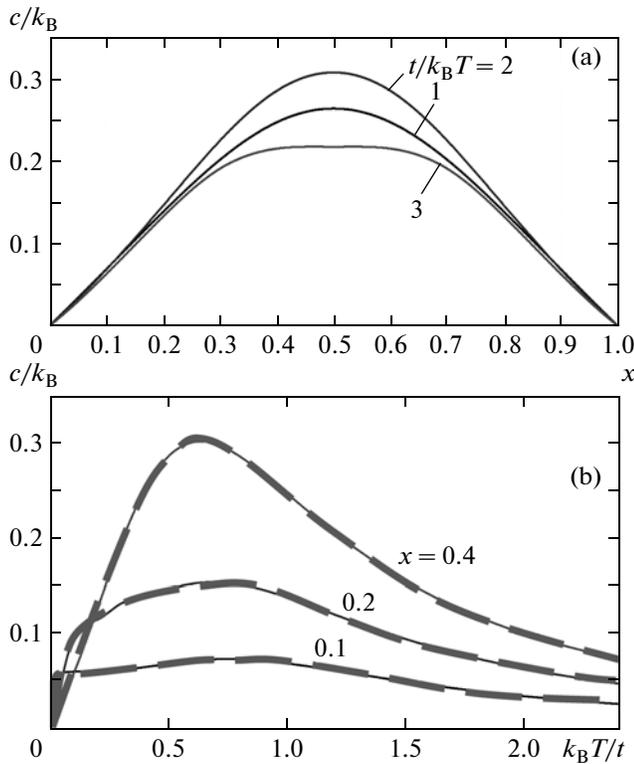
Fig. 3. (a) Concentration and (b) temperature dependences of the electron heat capacity taking into account equality (18). Bold dashed curves in (b) are the results from [8].
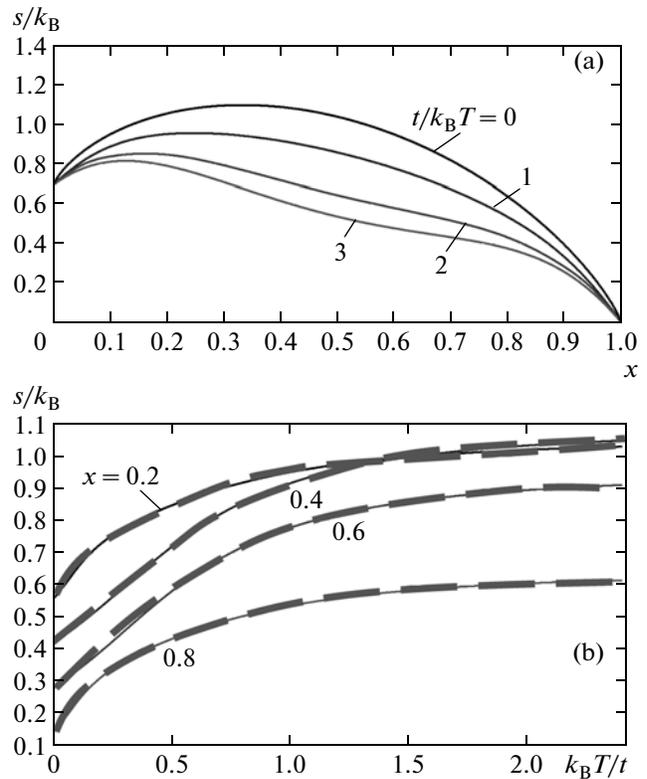

Fig. 4. (a) Concentration and (b) temperature dependences of the electron entropy.

demonstrated the best using Eq. (37), which was considered above for holons. For $x = 0$, we have $N_e = N$. However, the sum consisting of N terms can be equal to N iff each term separately is equal to unity. This condition can be satisfied either by setting $\mu^{(h)} \geq 2t$ and $T = 0$ (in accordance with relation (43), we see that $\mu^{(h)} = 2t$ in this case), or setting $\mu^{(h)} = +\infty$ and $T \neq 0$. In accordance with relation (19), if the system has a non-zero spin, the curve describing the function

$$\frac{\mu}{t} = \frac{\mu}{t}\left(x, \frac{t}{T} = \text{const}\right)$$

is simply shifted downwards along the ordinate axis. The case when $x = 1$ can be analyzed similarly.

In accordance with relations (17) and (18), the internal energy and the heat capacity of electrons coincide with the corresponding quantities for holons. Let us briefly consider the results (Figs. 2 and 3). All dependences $u(x, T/t = \text{const})$ lie between the curve describing the ground state,

$$u^{(h)}(T = 0) = \frac{1}{N} \sum_{k=-k_F}^{k_F} \varepsilon(k)$$

$$= -\frac{t}{\pi} \int_{-(1-x)\pi}^{(1-x)\pi} \cos y\, dy = -\frac{2t}{\pi}\sin(\pi x), \quad (44)$$

and the curve corresponding to an infinitely high temperature,

$$u^{(h)}(T = \infty) = 2\frac{1}{\pi} \sum_{k=\pi x/a}^{\pi/a} \varepsilon(k)$$

$$= -\frac{2t}{\pi} \int_{\pi x}^{\pi} \cos y\, dy = \frac{2t}{\pi}\sin(\pi x). \quad (45)$$

Thus, upon an increase in temperature, the curve smoothly shifts from its position (44) at $T = 0$ to the limiting position (45) as $T \longrightarrow \infty$.

Naturally, analogous behavior is also observed for the temperature dependences of internal energy $u(k_B T/t, x = \text{const})$: the curves originate at points $(0, -(2t/\pi)\sin(\pi x))$ and tend to horizontal asymptote (45) for $T \longrightarrow \infty$.

Curves $c(x, T/t = \text{const})$ describing the concentration dependence of the heat capacity for a constant volume and number of electrons increase with temperature from their initial position $c = 0$ at $T = 0$, attain a certain critical (uppermost) curve, and then collapse, tending to zero for $T \longrightarrow \infty$. The same physical peculiarity is also observed when analyzing the temperature dependence of the heat capacity.

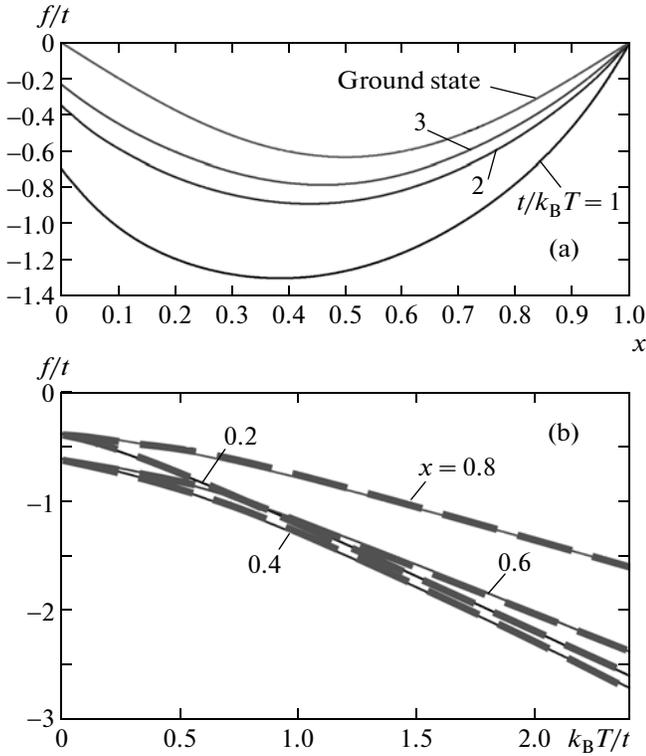In accordance with formula (16), the entropy increases by $k_B(1 - x)\ln 2$ as compared to the contribu-

Fig. 5. (a) Concentration and (b) temperature dependences of the electron free energy.
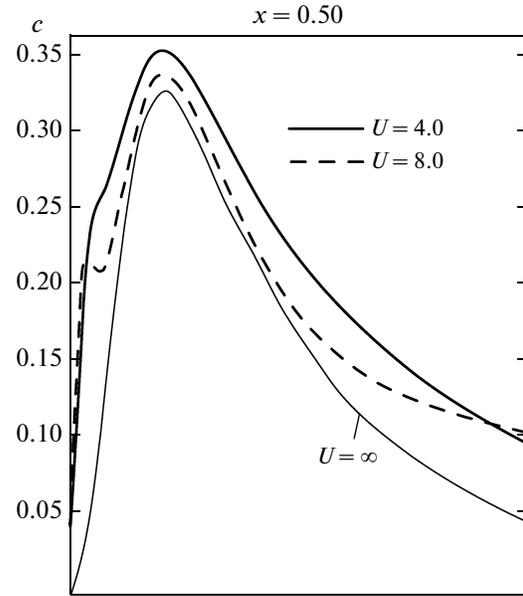

Fig. 6. Comparison of the temperature dependences of heat capacity from [6] calculated for $U/t = 4$ and 8 with the curve calculated in this study for infinitely strong repulsion.

tion of holons. The concentration dependences resulting from such an increment are shown in Fig. 4a. For $x = 0$, we observe the well-known result $s(x = 0) = k_B \ln 2$; i.e., the entropy is determined by localized spins $\sigma = 1/2$. Further, upon an increase in ratio $t/k_B T$, the $s(x)$ curve "passes" from its initial position described by equality (30) to the straight line described by the equation $s = k_B(1 - x)\ln 2$. The $s(k_B T/t)$ curves "emerge" from point $(0, k_B(1 - x)\ln 2)$ and tend to their asymptote described by equality (30) for $k_B T/t \longrightarrow \infty$ (Fig. 4b).

Finally, let us consider the behavior of the free energy. Upon an increase in the $t/k_B T$ ratio, the $f(x)$ curve (Fig. 5a) tends from minus infinity to the "critical" curve $f(x, T = 0) = u(x, T = 0) = -(2t/\pi)\sin(\pi x)$, which, in accordance with relation (15), is described by the same equation for spinless systems and for systems with a nonzero spin. The $f(k_B T/t)$ curves emerge from point $(0, -(2t/\pi)\sin(\pi x))$ and asymptotically approach the straight lines described by the equation

$$f = \frac{2t}{\pi}\sin(\pi x)$$
$$-k_B T((1 - x)\ln 2 - x\ln x - (1 - x)\ln(1 - x)) \qquad (46)$$

as $k_B T/t \longrightarrow \infty$ (Fig. 5b).

5. COMPARISON WITH RESULTS OF OTHER STUDIES

The temperature dependences of thermodynamic quantities were calculated in [8] for the 1D Hubbard model for $U = \infty$ without employing the idea about the spin–charge splitting. It can be seen from the temperature dependences depicted in Figs. 1b, 2b, 3b, 4b, and 5b that our results completely coincide with the data from [8]. However, the concentration dependences were not reported in the literature. For finite values of U, the temperature dependences of heat capacity reported in [5, 6] have two peaks at small values of x. The narrow low-temperature peak is associated with spin excitations and is attained at $T \sim J/k_B \sim t^2/k_B U$; this peak is not observed in the limit $U \longrightarrow \infty$. The broader high-temperature peak is due to charge excitations. It exhibits a weak dependence on U and is attained at $T_{max} \approx 0.6 t/k_B$ for $U = 4t$ and $U = 8t$ at $x = 0.5$. In view of the weak dependence of this peak on the value of U, it can be compared with our results for $U \longrightarrow \infty$ (lower curve in Fig. 6). It can be seen that the value of T_{max} as well as the value of heat capacity $c/k_B \approx 0.3$ at the point of maximum are very close to those reported in [6]. As noted in [5], an increase in the hole concentration smears the two (holon and spinon) peaks in the temperature dependence of the heat capacity because the interrelation between the charge and spin excitations is restored in the metallic system.

APPENDIX

Let us prove formula (11), which is of fundamental importance for the entire paper. We introduce the following notation for operators:

$$H_0^{(h)} = \sum_f \varepsilon X_f^{11}, \qquad (47)$$

$$H_t^{(h)} = \sum_{g,m} t_{gm} X_g^{10} X_m^{01}, \qquad (48)$$

$$H_0 = \sum_{f,\sigma} \varepsilon X_f^{\sigma\sigma}, \qquad (49)$$

$$H_t = \sum_{g,m,\sigma} t_{gm} X_g^{\sigma 0} X_m^{0\sigma}. \qquad (50)$$

We can verify by direct calculations that

$$[H_0^{(h)}, H_t^{(h)}] = [H_0, H_t] = 0. \qquad (51)$$

The equality of these commutators to zero entails the following matrix equalities:

$$\exp\left(-\frac{H_0^{(h)} + H_t^{(h)}}{k_B T}\right)$$
$$= \exp\left(-\frac{H_0^{(h)}}{k_B T}\right) \exp\left(-\frac{H_t^{(h)}}{k_B T}\right), \qquad (52)$$

$$\exp\left(-\frac{H_0 + H_t}{k_B T}\right) = \exp\left(-\frac{H_0}{k_B T}\right) \exp\left(-\frac{H_t}{k_B T}\right). \qquad (53)$$

Then, considering that matrices $\exp(-H_0^{(h)}/k_B T)$ and $\exp(-H_0/k_B T)$ are diagonal matrices containing $\exp(-N_e \varepsilon/k_B T)$ on both diagonals, we obtain the following expressions for the canonical partition functions for the spinless and nonzero spin cases, respectively:

$$Z^{(h)} = \exp\left(-\frac{N_e \varepsilon}{k_B T}\right) \mathrm{Tr}\left(\exp\left(-\frac{H_t^{(h)}}{k_B T}\right)\right), \qquad (54)$$

$$Z = \exp\left(-\frac{N_e \varepsilon}{k_B T}\right) \mathrm{Tr}\left(\exp\left(-\frac{H_t}{k_B T}\right)\right). \qquad (55)$$

Let us now consider the action of operator $H_t^{(h)}$ on a state of type (6), in which $|\psi\rangle_i$ are defined by equalities (7). We have

$$H_t^{(h)} \begin{vmatrix} 1 & 1 & \dots & 1 \\ f_1 & f_2 & & f_{N_e} \end{vmatrix} \Bigg\rangle$$

$$= \sum_{m \in \{f_1, f_2, \dots, f_{N_e}\}} \sum_{g \in h\backslash\{f_1, f_2, \dots, f_{N_e}\}} (-1)^{\Delta N_{gm} + 1}$$

$$\times t_{gm} \begin{vmatrix} 1 & 1 & \dots & 0 & \dots & 1 & \dots & 1 \\ f_1 & f_2 & & m & & g & & f_{N_e} \end{vmatrix} \Bigg\rangle,$$

where the left-hand side contains the vector symbolizing the state in which holons are at sites $f_1, f_2, \dots, f_{N_e}$ and holes are at the remaining sites; braces $\{f_1, f_2, \dots, f_{N_e}\}$ indicate a set consisting of sites $f_1, f_2, \dots, f_{N_e}$; h is the set of all sites of the system; symbol "\" indicates the difference of sets; and ΔN_{gm} is the number of holons located strictly between sites g and m. Clearly, all vectors appearing on the left-hand side of the last equality are different. The coefficients of these vectors are also different. Forming the scalar product of this equality and a bra vector from

$$\frac{N!}{N_e!(N - N_e)!}$$

possible vectors, we obtain the matrix element either equal to zero or to $(-1)^{\Delta N_{ij} + 1} t_{ij}$, where $i \in \{f_1, f_2, \dots, f_{N_e}\}$ and $j \in h\backslash\{f_1, f_2, \dots, f_{N_e}\}$. It should be noted by the way that we have proved an important statement. For its formulation, we will refer to a pair of vectors on which the given matrix element is constructed as the pair generating this element. Then the above arguments lead to the conclusion that a matrix element differs from zero iff the vectors of the pair generating this matrix element can be transformed into each other by a jump of only one electron from one position to the other. Analogously, for a system with a nonzero spin, the matrix element differs from zero iff one of the vectors of the pair generating this matrix element can be transformed into the other by a jump of a single electron from one position to the other (which preserves its spin). This statement can be proved by analyzing the action of operator H_t on a state of type (6), there $|\psi\rangle_i$ are now defined by equality (8).

We can now easily determine the algorithm for obtaining the matrix of operator H_t from the matrix of operator $H_t^{(h)}$. Obviously, each matrix element is transformed into a $2^{N_e} \times 2^{N_e}$ block. It is clear now that if this matrix element is zero, it is transformed into the zero block. This statement holds if only due to the fact

that any matrix element of the block under investigation is generated by a pair of vectors such that a transition from one vector to the other by a jump of a single electron from one position to the other is ruled out (because the matrix element being transformed is zero). If, however, the matrix element is equal to the hopping parameter between the nearest neighbors with the minus sign, the diagonal elements of the block are equal to this element. Indeed, for a pair generating a diagonal element, there exists a transition from one vector of the pair to the other by a jump of only one electron, whose spin is preserved. The directions of the remaining spins for the vectors in the pair generating a diagonal element coincide (because we are considering precisely the diagonal element). Conversely, for off-diagonal elements, the directions of the spins of at least one pair of electrons located in two vectors generating the matrix element under consideration and located in the same position are necessarily different (due to the fact that the element itself is off-diagonal). Thus, the matrix of operator H_t can be obtained from the matrix of operator $H_t^{(h)}$ by transforming each matrix element into a $2^{N_e} \times 2^{N_e}$ block with the numbers on the diagonal equal to the element being transformed, while all off-diagonal elements are zeros.

In accordance with the rule of multiplication of block matrices, we can readily conclude (taking into account the definition of the matrix exponential as a matrix series) that matrix exponential $\exp(-H_t/k_B T)$ can be formed from exponential $\exp(-H_t^{(h)}/k_B T)$ by transforming each matrix element into a $2^{N_e} \times 2^{N_e}$ block with the numbers on the diagonal equal to the matrix element being transformed and with zero off-diagonal elements. This immediately leads to relation (11).

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