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# Thermodynamics of an extended Hubbard model chain. I: Atomic limit for the half-filled band*

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For an infinite linear chain we consider the atomic limit of an extended Hubbard model which takes into account the nearest-neighbor interatomic electron-electron repulsion. The specific heat, static magnetic susceptibility, and density-density correlation function are studied exactly at any temperature for the half-filled-band case. We discuss also the quarter-filled band in the limit of infinite intra-atomic Coulomb repulsion.

## I. INTRODUCTION

This is the first of a series of papers presenting a study of an extended one-dimensional Hubbard model.[1] Our modified Hubbard Hamiltonian is

$$H=-t\sum_{i,\sigma}(c^\dagger_{i,\sigma}c_{i+1,\sigma}+\mathrm{H.c})+U\sum_i n_{i,\uparrow}n_{i,\downarrow}+V\sum_i n_i n_{i+1}\,, \tag{1}$$

$$n_{i\uparrow}=c^\dagger_{i\uparrow}c_{i\uparrow}\,,\quad n_i=n_{i\uparrow}+n_{i\downarrow}\ .$$

The first two terms constitute the standard Hubbard Hamiltonian; $t$ is the electron-transfer integral connecting states localized on nearest-neighbor molecules; $c^\dagger_{i,\sigma}$ and $c_{i,\sigma}$, respectively, create and destroy an electron spin on the $i$th site; $U$ is the intramolecular Coulomb repulsion. The third term, which represents the intermolecular electron repulsion, may be considered as a first step towards taking into account the long-range character of the electron-electron interaction.

The simplest version of the Hubbard model has been extensively studied[2] and applied to various physical systems. For example, Epstein *et al.*[3] have discussed the metal-insulator transition of N-methyl phenazinium (NMP) tetracyanoquinodimethan (TCNQ) on the basis of the strongly correlated Hubbard model ($t \ll U$). Also a considerable number of the theoretical studies of this model have been undertaken and many properties of it are now well known.[4]

More generally, unidimensional electron systems are the object of an increasing interest, especially in connection with the behavior of substances containing TCNQ. These substances offer an example of one dimensional, or quasi-one-dimensional electronic systems[5] crystallizing in form of linear chains of molecular anions separated by atomic or molecular cations. The chains are separated by comparatively large distances which allow us, in first approximation, to consider them independently. Theoretically, such quasi-one-dimensional systems should possess fascinating properties. They may be metals, dielectrics, antiferromagnets, or superconductors,[6,13] depending on the number of particles and the character of the interaction between them. But the problem of what are the possible states of a linear electron system is far from being fully clear at present. For some special models like the Hubbard model or a gas of $\delta$-function interactions, exact solutions can be found.[7-12] So far, however, much understanding of one-dimensional electronic systems has been gained through approximate theories.[4,13]

As already remarked, the Hubbard model has been rather successfully applied to TCNQ systems.[14] But in view of the crudeness of a two-parameter model to describe a system of organic molecules, various extensions have been proposed. Chaikin *et al.*[15] have suggested that, in the presence of strongly electronically polarizable molecules, excitonic polarons may form which could modify the $U$, $t$ parameters as determined experimentally. Subsequently, a unification of the half-filled-band Hubbard Hamiltonian with Holstein's molecular-crystal model[16] has been discussed by one of the authors[17] and is presently under investigation in our group.

Apart from electron-phonon effects we feel that the two-parameter Hubbard Hamiltonian may fail to describe correctly such systems as the TCNQ salts by explicitly neglecting the finite range of the Coulomb forces. Epstein *et al.*[3] regarded $U$ as an effective interaction representing the Coulomb energy difference in making a charge-transfer excitation, i.e., the difference between the repulsion of two electrons on the same site and the reuplsion of the two electrons on separated sites. This point of view, however, may not always be appropriate. In fact, if we consider, for example, a half-filled chain in the $t=0$ limit, we notice that the ground state configuration consists of one electron per site if $V<\frac{1}{2}U$ but it consists of alternating pairs if $V>\frac{1}{2}U$ (see Fig. 1).

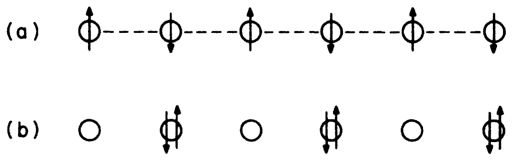

FIG. 1. Possible ground-state configurations are: (a) the ground-state energy per site $E(a) = V$ and in (b) the ground state energy per site $E(b) = \frac{1}{2}U$. Configuration (b) prevails if $V > \frac{1}{2}U$.

Thus if $V > \frac{1}{2}U$ we cannot take into account the effect of intermolecular repulsion by simply renormalizing $U$. This will be shown more clearly below.

Actually this effect was first pointed out by Bari[18] who investigated the role of electron-lattice interactions in a very narrow half-filled band. His Hamiltonian, which incorporates electron-electron and electron-lattice interactions, can be decoupled via a canonical transformation and, in one dimension, reduces to Eq. (1) with $t = 0$. Bari approached the problem within a modified Hartree-Fock approximation and showed that for a three-dimensional system, the Mott insulator can undergo a phase transition to a quite different insulating state as the temperature is lowered. This state is characterized by a charge density wave in which alternate atomic sites are doubly occupied. Bari proved also that, in one dimension, while there cannot be such phase transition, we have alternating pairs in the ground state, if $V$ exceeds $\frac{1}{2}U$, as we have previously remarked.

There is another physical situation that our model, Hamiltonian (1), may help to clarify. Consider a typical TCNQ salt. The separation distances between chains largely exceed the interplanar distance between TCNQ molecules within a given chain. We have seen that this allows us to describe the electronic structure as a one-dimensional one with the only transfer occurring along the TCNQ chain axis and zero transfer otherwise. However, it has been pointed out[3] that in a crystal-like NMP-TCNQ the energy involved in making the charge-transfer excitation should be significantly reduced as a result of the presence of the highly polarizable NMP cations in the nearby NMP chains. This reduction[19] is the result of induced electric dipoles on the NMP molecules in response to the electric fields resulting from the local charge fluctuations in the TCNQ chains.

We see, therefore, that even in the absence of any transfer, the TCNQ chains may be coupled via the oscillating electric dipoles on the NMP cations. In general, the induced polarization can be divided into two components: lattice polarization described by phonons[20] and electron polarization described by excitons.[21] As a first step towards the description of this interchain coupling, we may thus consider the following model (Fig. 2):

$$H = \sum_{j=1}^{N_B} \left[ U n_{2j,\uparrow} n_{2j,\downarrow} + h\omega \alpha_{2j+1}^{\dagger} \alpha_{2j+1} - A n_{2j} (x_{2j-1} - x_{2j+1}) \right] . \tag{2}$$

The first term is the intramolecular Coulomb repulsion acting when two electrons reside on the $2j$th TCNQ molecule. ($N_B$ is the number of sites counted perpendicularly to a given chain; $n_{2j,\uparrow}$ is the number operator for electrons of spin up residing at the $2j$th site.) The second term describes a harmonic oscillator of frequency $\omega$ with $\alpha_{2j+1}^{\dagger}$ and $\alpha_{2j+1}$, respectively, creating and destroying a boson at the $(2j+1)$th site. The last term represents the coupling between the oscillating dipoles on NMP and the charge fluctuation on TCNQ, with coupling constant $A$. The displacement of the $j$th oscillator equilibrium position is given by

$$x_j = [\hbar / 2M_0\omega]^{1/2} (\alpha_j^{\dagger} + \alpha_j) ,$$

where $M_0$ is the mass of the oscillator.

Since we work in the representation where $n_{2j,\sigma}$ is diagonal, we may perform a linear transformation to remove coupling. Let

$$\alpha_j^{\dagger} = \beta_j^{\dagger} + \epsilon_j , \tag{3}$$

where $\epsilon_j$ is a $c$ number.

Substituting (3) into (2) and choosing

$$\epsilon_{2j+1} = (A/\hbar\omega)(\hbar/2M_0\omega)^{1/2} (n_{2j+2} - n_{2j}) , \tag{4}$$

we obtain immediately

$$H = (U - 4E_b) \sum_{j=1}^{N_B} n_{2j,\uparrow} n_{2j,\downarrow} + 2E_b \sum_{j=1}^{N_B} n_{2j} n_{2j+2} + \hbar\omega \sum_{j=0}^{N_B} \beta_{2j+1}^{\dagger} \beta_{2j+1} - 2E_b \sum_{j=1}^{N_B} n_{2j} , \tag{5}$$

where $E_b = A^2/2M_0\omega^2$ is a sort of "binding energy."

Except for the irrelevant last two terms, Eq. (5) is of the same form of Hamiltonian (1) with $t = 0$, i.e., the polarizability of the cation introduces an effective interchain repulsion. This pro-

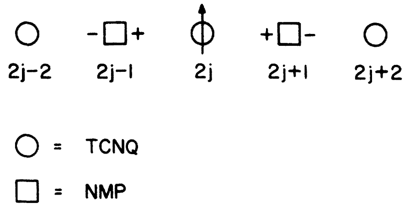

FIG. 2. Schematic interchain coupling. An electron on the $2j$th TCNQ distorts the oscillators on the neighboring NMP molecules giving rise to an effective interaction between TCNQ chains.

vides us with another reason for studying the properties of the model described by the extended Hubbard Hamiltonian, i.e., Eq. (1).

The specific purpose of the present work is to analyze the model for $t=0$ and electron density $\rho = N/N_A = 1$ ($N$ is the number of electrons and $N_A$ is the number of sites). As we have seen, this model, while not realistic, shows some features of physical problems and, at the same time, is susceptible to exact analysis. In this work we discuss also the $\rho = \frac{1}{2}$ case with infinite intramolecular repulsion. In subsequent papers we will consider (a) the quarter-filled-band case ($\rho = \frac{1}{2}$) for arbitrary $U$, and (b) the effects of transfer.

## II. TRANSFER MATRIX

We start with the Hamiltonian

$$H = \sum_{i=1}^{N_A} \left[ U n_{i\uparrow} n_{i\downarrow} + V n_i n_{i+1} - \mu n_i - h(n_{i\uparrow} - n_{i\downarrow}) \right] , \tag{6}$$

where $\mu$ is the chemical potential (to be set by fixing the number of particles) and $h = \mu_B B$; $\mu_B$ being the Bohr magneton and $B$ a magnetic field in which our system is supposed to be placed.

All the terms of the Hamiltonian commute with each other and are diagonal in the $n_{i\sigma}$ representation. It is therefore convenient to use the transfer-matrix method[22] to find the grand partition function $Z$ and the density-density correlation functions of the system. The typical element of the transfer matrix for the Hamiltonian (6) is given by

$$\begin{aligned} P_{i,i+1} = \exp\{ -\beta[ & \tfrac{1}{2} U n_{i\downarrow} n_{i\uparrow} + \tfrac{1}{2} U n_{i+1\uparrow} n_{1+1\downarrow} \\ & + V n_i n_{i+1} - \tfrac{1}{2} \mu n_i - \tfrac{1}{2} \mu n_{i+1} \\ & - \tfrac{1}{2} h(n_{i\uparrow} - n_{i\downarrow}) - \tfrac{1}{2} h(n_{i+1\uparrow} - n_{i+1\downarrow})]\} , \end{aligned} \tag{7}$$

where $\beta = 1/KT$; $K$ is the Boltzmann constant, and $T$ is the temperature.

Thus our problem is reduced to diagonalize the symmetric matrix $P$

$$P = \begin{pmatrix} 1 & m x_0 & m^{-1} x_0 & w_0 x_0^2 \\ m x_0 & m^2 x_0^2 y & x_0^2 y & m w_0 x_0^3 y^2 \\ m^{-1} x_0 & x_0^2 y & m^{-2} x_0^2 y & m^{-1} w_0 x_0^3 y^2 \\ w_0 x_0^2 & m w_0 x_0^3 y^2 & m^{-1} w_0 x_0^3 y^2 & w_0^2 x_0^4 y^4 \end{pmatrix} , \tag{8}$$

where $x_0 = e^{\beta\mu/2}$; $w_0 = e^{-\beta U/2}$, $y = e^{-\beta V}$, and $m = e^{\beta h/2}$.

It is straightforward to see that three eigenvalues of $P$ are the roots $\lambda_l$ ($l = 1, 2, 3$) of the cubic equation (9) while the fourth eigenvalue vanishes ($\lambda_4 = 0$).

$$\begin{aligned} & \lambda^3 - \lambda^2 (1 + Mxy + y^4 x^2 w) \\ & \quad - \lambda x (1-y)[M + Mwx^2 y^4 + wx(1+y^2)(1+y)] \\ & \quad - Mwx^3 y(-1 + 2y - 2y^3 + y^4) = 0 . \end{aligned} \tag{9}$$

In Eq. (9), $x = x_0^2$, $w = w_0^2$; and $M = m^2 + m^{-2} = 2\cosh\beta h$. This equation, in the $h = 0$ limit, coincides with Eq. (C5) of Ref. 19. Bari did not proceed further in the analysis of the model but used this eigenvalue equation to prove that there is no phase transition in one dimension.

So far we have not specified the number of particles in the chain. This must be done in the usual way by solving the equation

$$N = - \left. \frac{\partial \Omega}{\partial \mu} \right|_{\beta} , \tag{10}$$

where $\Omega$ is the thermodynamic potential, $\Omega = -KT \ln Z$. When $N_A$ is large ($N_A \to \infty$) the grand partition function is given by[22] $Z = \lambda_M^{N_A}$ where $\lambda_M$ is the maximum eigenvalue (assumed to be nondegenerate). Therefore Eq. (10) may be rewritten

$$\frac{\partial \lambda_M}{\partial x} = \rho \frac{\lambda_M}{x} . \tag{11}$$

In principle, we should first find $\lambda_M$ from Eq. (9) and then use Eq. (11) to find $x$, from which all the eigenvalues would be known as function of the temperature and the parameters $U$ and $V$. This can always be done numerically but in particular cases algebraic solutions are possible. The rest of this paper is devoted to the analyses of two of these cases.

## III. QUARTER-FILLED BAND ($N/N_A = \frac{1}{2}$) : $U = \infty$

The quarter-filled-band case is not easily handled algebraically and its study will be the subject of a subsequent paper. However, some insight into the nature of the problem can be gained immediately by looking at the $U = \infty$ limit.

For infinite intramolecular repulsion there are no doubly occupied sites and the transfer matrix $P$ reduces to ($h = 0$)

$$P = \begin{pmatrix} 1 & x_0 & x_0 \\ x_0 & x_0^2 y & x_0^2 y \\ x_0 & x_0^2 y & x_0^2 y \end{pmatrix} , \tag{12}$$

with eigenvalues

$$\lambda_3 = 0, \quad \lambda_{1,2} = \tfrac{1}{2}\{1 + 2xy \pm [(1-2xy)^2 + 8x]^{1/2}\} . \tag{13}$$

Using Eq. (11) with $\lambda_M = \lambda_1$ and $\rho = \frac{1}{2}$ we have directly $x = 1/2y$ and $\lambda_{1\,2} = 1 \pm e^{\beta V/2}$, from which the thermodynamics follows trivially.

Aside from the usual thermodynamic quantities, one is more interested in the correlations between electrons at different lattice sites. Such correlations are observable experimentally in $x$-ray diffraction effects.

We define the correlation function between sites $i$ and $i+k$ in the usual way:

$$G_{ik} = \langle n_i n_{i+k}\rangle - \langle n_i\rangle^2 \ , \qquad (14)$$

where $\langle\cdots\rangle$ stands for thermal average. As shown in the appendix, this correlation function can be conveniently written

$$G_{ik} = G_k = \frac{1}{\lambda_m^k} \sum_{m\neq M} \lambda_m^k \langle M|\tilde{n}|m\rangle^2 \ , \qquad (15)$$

where $\tilde{n}$ is the matrix defined by (A4); $|m\rangle$ and $|M\rangle$ are the eigenstates of $P$ corresponding to the eigenvalues $\lambda_m$ and $\lambda_M$, respectively; and the summation includes all the eigenvalues $\lambda_m$ except the largest one, i.e. $\lambda_M$.

From Eq. (15) we have immediately

$$G_k = \tfrac{1}{4}[-\tanh(6V/4)]^k, \qquad (16)$$

which is essentially the correlation function for the spin-one-half Ising chain. Indeed, the entire model is, in this case, equivalent to an Ising chain in which one of the states is double degenerate.

## IV. HALF-FILLED BAND

This case can be solved exactly for arbitrary $U$. In fact for $\rho = 1$ we find

$$x = 1/y^2\sqrt{w} \ . \qquad (17)$$

This equation is obtained in the following way.[18] We differentiate Eq. (9) with respect to $x$, then we substitute Eq. (11) into it and thus obtain another cubic equation. This can be solved simultaneously with Eq. (9) only if (17) is satisfied. In general, however, this procedure does not lead to a simple result if $\rho \neq 1$.

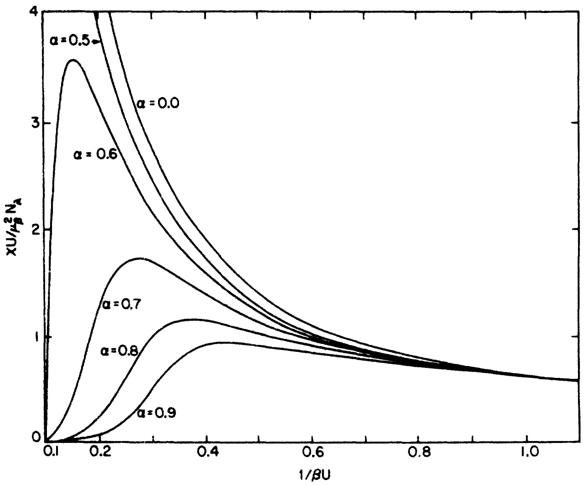

FIG. 3. Temperature dependence of the static magnetic susceptibility for various values of $\alpha = V/U$. The curves for $0 < \alpha < 0.5$ fall in the region between the $\alpha = 0$ and 0.5 curves.

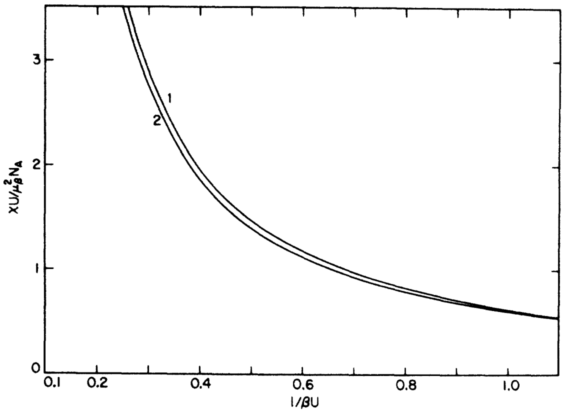

FIG. 4. Temperature dependence of the static magnetic susceptibility for (a) $\alpha = 0.2$ and for (b) $\alpha = 0$ with renormalized Coulomb repulsion $U \to 0.8U$.

From (17) we obtain the chemical potential

$$\mu = \tfrac{1}{2}U + 2V \qquad (18)$$

and by substituting in Eq. (9) the eigenvalues

$$\begin{aligned} &\lambda_4 = 0, \quad \lambda_3 = 1 - e^{2\beta V}, \\ &\lambda_{1,2} = \tfrac{1}{2}[p \pm (p^2 - q)^{1/2}] \ , \\ &p = 1 + e^{2\beta V} + 2e^{\beta(V+U/2)}\cosh\beta h \ , \\ &q = 8e^{\beta(V+U/2)}(1 - e^{\beta V})^2\cosh\beta h \ . \end{aligned} \qquad (19)$$

From the grand partition function $Z = \lambda_M^{N_A} = \lambda_1^{N_A}$ we find the static magnetic susceptibility

$$\begin{aligned} \chi &= -\mu_B^2 \lim_{h\to 0} \frac{\partial^2\Omega}{\partial h^2} \\ &= 2\mu_B^2 N_A \beta e^{\beta(V+U/2)} \frac{\lambda_M - (1 - e^{\beta V})^2}{\lambda_M(2\lambda_M - p)} \end{aligned} \qquad (20)$$

which is shown in Fig. 3 as a function of the temperature for various values of $\alpha = V/U$. Note that for $\alpha > \frac{1}{2}$ the susceptibility vanishes exponentially at $T = 0$, corresponding to a configuration of paired electrons in the ground state [see Fig. 1(b)].

We believe that this behavior persists in the presence of a small transfer, $t$. Thus for $\alpha > \frac{1}{2}$ a simple renormalization of $U$ (and neglect of $V$) would lead to an incorrect description of the system. On the other hand, if $\alpha$ is small we may actually neglect $V$ and renormalize $U$ without any qualitative change in the behavior of $\chi$, as shown in Fig. 4.

From the grand partition function it is also straightforward to evaluate the specific heat

$$\begin{aligned} \frac{C_V}{N_A K} &= \beta^2 \frac{d^2}{d\beta^2} \ln\lambda_M \\ &= \frac{\beta^2}{\lambda_M^2(2\lambda_M - p)^3}\{\gamma_1\lambda_M(2\lambda_M - p)^2 - \gamma_2[2\lambda_M - (2\lambda_M - p)\gamma_3]\} \ , \end{aligned}$$

$$\gamma_1 = 4\lambda_M V^2 e^{2\beta V} + \tfrac{1}{2}e^{\beta(V+U/2)}[(1+2V)^2(\lambda_M - 1) - 2(1+4V)^2 e^{\beta V} + (1+6V)^2 e^{2\beta V}] \ ,$$

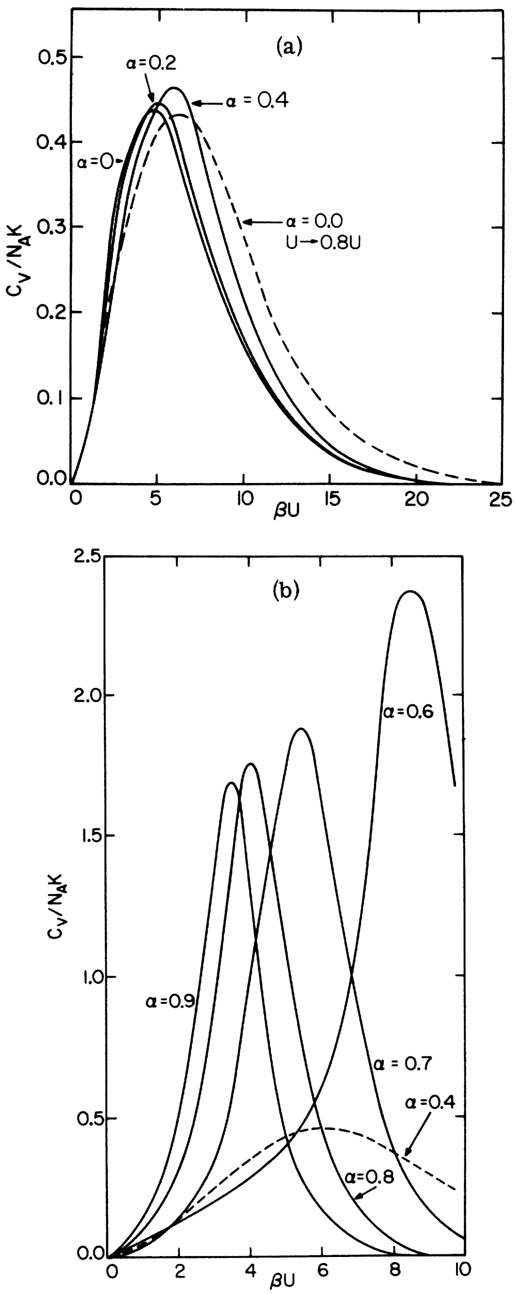

FIG. 5. Inverse temperature dependence of the specific heat for (a) $\alpha < \frac{1}{2}$ and (b) $\alpha > \frac{1}{2}$. The dashed curve in (b) is shown for comparison. Note the "jump" in specific heat at $\alpha \sim \frac{1}{2}$. In (a) the dashed curve shows the specific heat for $\alpha = 0$ and renormalized $U \rightarrow 0.8U$. This should be compared with the $\alpha = 0.2$ curve. The agreement is worse than for the corresponding susceptibility curves.

$$\gamma_2 = \lambda_M[2Ve^{2\beta V} + (2V+1)e^{\beta(V+U/2)}]$$
$$- 2(1 - e^{\beta V} e^{\beta(V+U/2)}[(\tfrac{1}{2} + V) - e^{\beta V}(\tfrac{1}{2} + 3V)] ,$$
$$\gamma_3 = 2\lambda_M[2Ve^{2\beta V} + (2V+1)e^{\beta(V+U/2)}] - 1 . \qquad (21)$$

Figures 5(a) and 5(b) show the inverse temperature dependence of the specific heat at typical values of $\alpha$. Comparing these figures, note how the features of the specific heat versus temperature change with the relative magnitude of $U$ and $V$. Again we distinguish two regions: for $\alpha < \frac{1}{2}$ the specific heat has a peak at lower temperatures for higher values of $\alpha$. The reverse is true for $\alpha > \frac{1}{2}$. This can be easily understood by means of an elementary argument. By looking at Fig. 1 we may infer that the energy to excite an electron above the ground state should be of the order of $U$ for $\alpha = 0$, $\frac{1}{2}U$ for $\alpha = \frac{1}{2}$, and $2U$ for $\alpha = 1$. The minimum should occur for $\alpha = \frac{1}{2}$. As we decrease $\alpha$ below $\frac{1}{2}$ the thermal energy required for an excitation increases and thus the peak in the specific heat shifts towards higher temperature. The same happens as we increase $\alpha$ above $\frac{1}{2}$. Another interesting feature of the specific heat is the sudden increase at $\alpha = \frac{1}{2}$, which can also be easily understood by the previous elementary argument.

From the calculation of the static magnetic susceptibility and the specific heat, we have drawn a rather well-defined picture of the thermal behavior of our system. In order to obtain more detailed information, we have evaluated the temperature dependence of the density-density correlation function, as defined by Eq. (14).

We again use expression (15) to calculate $G_k$, except that the matrix $\tilde{n}$ is this time given by (A3). It is straightforward to find the eigenvectors of $P$ and we finally obtain

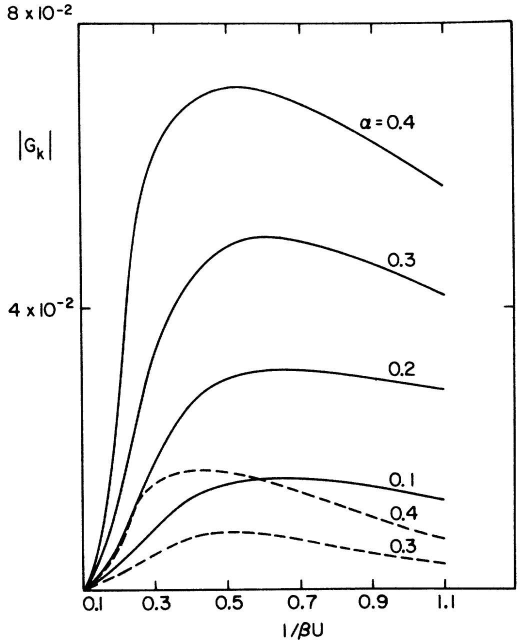

FIG. 6. Temperature dependence of the correlation function for $k = 2$ (dashed) and 1 (solid).

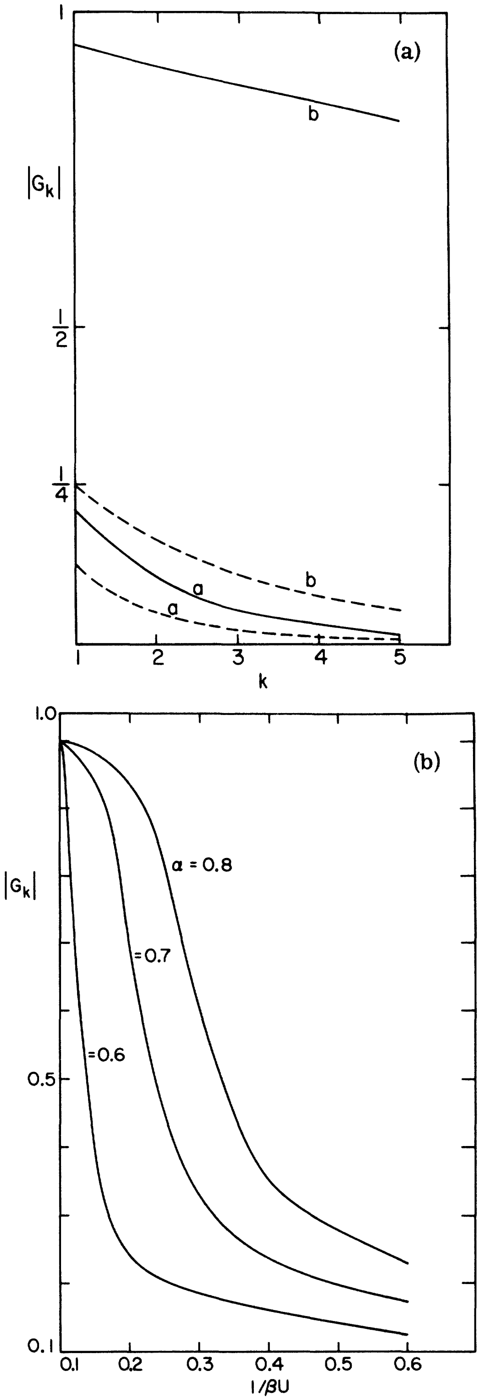

FIG. 7. (a) Correlation function for $\alpha = 0.6$ (dashed) and $\alpha = 0.8$ (solid) at temperatures (a) $KT/U = 0.6$ and (b) $KT/U = 0.2$. (b) $|G_k|$ as a function of temperature at $k = 1$.

$$\begin{aligned} G_k &= \left(\frac{1-e^{2\beta V}}{\lambda_M}\right)^k \sin^2\delta \,, \\ \delta &= \tan^{-1}\frac{\lambda_M - 2e^{\beta(V+U/2)}}{2e^{\beta(V+U/4)}} \;. \end{aligned} \tag{22}$$

Again we note a sharp distinction between the $\alpha > \frac{1}{2}$ and $\alpha < \frac{1}{2}$ case. At $T = 0$, in the former case, $G_k = (-1)^k$ while, in the latter case $G_k$ vanishes. In both cases $G_k$ obviously vanishes as $T \to \infty$. Thus for $\alpha < \frac{1}{2}$ the correlation function has a maximum. This is shown in Fig. 6 for $k = 1$ and 2.

Instead for $\alpha > \frac{1}{2}$ we observe an exponential decay of $G_k$ with $k$ (Fig. 7). The range of the correlation increases with $\alpha$ and its temperature dependence is shown in Fig. 8. Note the change of scale between Figs. 8(a) and 8(b) which indicates the strong dependence of the correlation on $\alpha$.

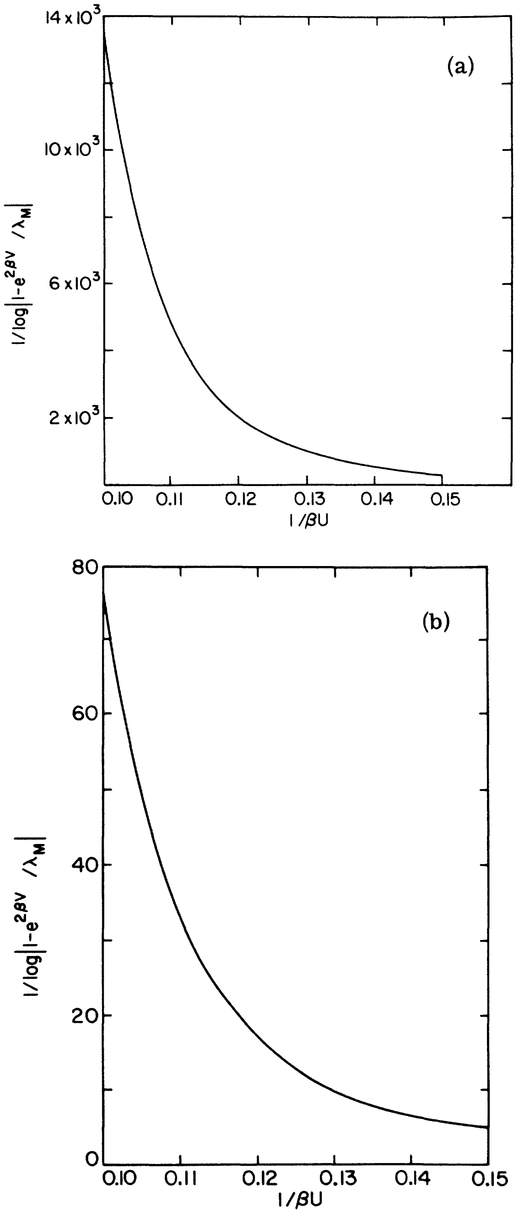

FIG. 8. Temperature dependence of the range of the density-density correlation function for (a) $\alpha = 0.8$ and (b) $\alpha = 0.6$.

## V. CONCLUSION

It is believed that a thorough understanding of exactly solvable models might shed light on some of the unresolved questions concerning a one-dimensional electron system. This paper has investigated the basic thermodynamic properties of the Hubbard model with nearest-neighbor interactions in the atomic limit. The principal result is found in Eq. (19) which gives the grand partition function of the system. From it we have evaluated the magnetic susceptibility [Eq. (20)], the specific heat [Eq. (21)], and the density-density correlation function [Eq. (22)].

The basic motivation for this study was provided by the need to justify the neglect of any sort of intermolecular electron-electron repulsion in dealing with unidimensional systems such as TCNQ salts. The point of view of taking into account $V$ simply by renormalizing $U$ does not lead to the correct description of the system if $V$ exceeds $\frac{1}{2}U$ (at least in the atomic limit). This was first pointed out by Bari[18] and actually Epstein *et al.*[3] cautioned that the simple renormalization of $U$ would fail for large enough $V$. Another interesting aspect of the present study is provided by the existence of a regime $(\alpha > \frac{1}{2})$ in which the electrons form correlated pairs. Similarly correlated pairs form in an *attractive* Hubbard model.[25] Whether the formation of such pairs can lead to superconductivity in a one-dimensional system is not known but appears to be a fascinating problem.

Finally we remark that our efforts have been directed toward laying the groundwork for further study of this model.

## ACKNOWLEDGMENTS

We would like to thank Professor P. Chaikin and Professor D. Scalapino for several useful discussions.

## APPENDIX

In this appendix, Eq. (15) will be derived. First we find an expression for the average electric density $\langle n_i \rangle$. By definition

$$\langle n_i \rangle = (1/Z)\,\mathrm{Tr}(e^{-\beta H} n_i)\ . \tag{A1}$$

This equation can be rewritten using the transfer matrix $P$ as

$$\langle n_i \rangle = (1/Z)\,\mathrm{Tr}(P^{i-1}\tilde{P}P^{N_A - i})\ , \tag{A2}$$

where $\tilde{P} = P\tilde{n}$. The matrix $\tilde{n}$ is defined by

$$\tilde{n} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix} \tag{A3}$$

in the vector space of (8) and by

$$\tilde{n} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{A4}$$

in the vector space of (12).

Now we introduce the unitary matrix $S$ which diagonalizes $P$, i.e., $S^\dagger P S = D$ where $D$ has matrix elements $D_{ij} = \lambda_i \delta_{ij}$. Thus, we may rewrite (A2) as

$$\langle n_i \rangle = \frac{1}{Z}\,\mathrm{Tr}(D^N S^\dagger \tilde{n} S) = \frac{1}{Z}\sum_i \lambda_i^{N_A}\Big(\sum_m S_{mi}^2 \tilde{n}_m\Big)\ , \tag{A5}$$

where $\tilde{n}_m$ is the $m$th row matrix element of $\tilde{n}$ and $S_{mi}$ is the $(m, i)$ matrix element of $S$. Finally, assuming the nondegeneracy of the largest eigenvalue, i.e., $\lambda_M$ we obtain $(N_A \rightarrow \infty)$

$$\langle n_i \rangle \simeq \frac{1}{Z}\lambda_M^{N_A}\sum_m S_{mM}^2 \tilde{n}_m = \sum_m S_{mM}^2 \tilde{n}_M\ . \tag{A6}$$

By following the same procedure which led us from (A1) to (A5) we find a convenient expression for $\langle n_i n_{i+k} \rangle = (1/Z)\,\mathrm{Tr}(e^{-\beta H} n_i n_{i+k})$, namely,

$$\begin{aligned} \langle n_i n_{i+k} \rangle &= \frac{1}{Z}\,\mathrm{Tr}(D^{N_A - k} S^\dagger \tilde{n} S D^k S^\dagger \tilde{n} S) \\ &= \frac{1}{Z}\sum_{i,m,p,q} \lambda_i^{N_A - k}\lambda_m^k S_{qi} S_{pi} S_{qm} S_{pm} \tilde{n}_q \tilde{n}_p \end{aligned} \tag{A7}$$

which, in the limit of large $N_A$ $(N_A \rightarrow \infty)$, gives

$$\langle n_i n_{i+k} \rangle \simeq \frac{1}{\lambda_M^k}\sum_m \lambda_m^k\Big(\sum_p S_{pM} S_{pm} \tilde{n}_p\Big)^2\ . \tag{A8}$$

Finally from (A6) and (A8) we obtain

$$\langle n_i n_{i+k} \rangle - \langle n_i \rangle^2 = \frac{1}{\lambda_M^k}\sum_{m \neq M} \lambda_m^k\Big(\sum_p S_{pM} S_{pm} \tilde{n}_p\Big)^2 \tag{A9}$$

which is Eq. (15).

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