Tight-binding electrons on open chains: Density distribution and correlations

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The ground state of the tight-binding electrons on finite open chains is studied for arbitrary band filling. Analytic expressions for the distribution of electron density and the density-density correlation functions within the system are found and discussed as a function of chain size. Particular attention is paid to the study of boundary effects.

I. INTRODUCTION

In this work we study in detail the $T=0$ K ground state of the electronic Hamiltonian in the form

$$H=\sum_{\substack{\langle i,j\rangle \\ \sigma}}(c_{i\sigma}^{\dagger}c_{j\sigma}+c_{j\sigma}^{\dagger}c_{i\sigma}) , \tag{1}$$

where $c_{i\sigma}^{\dagger}$ ($c_{i\sigma}$) creates (destroys) an electron on a site i of a regular lattice with z projection of its spin equal to σ, $\langle i,j\rangle$ denotes a pair of nearest neighbors, and $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$. $c_{i\sigma}$ is the number operator at site i.

The density of electrons in the state $|\psi\rangle$ is described by the band-filling factor $r=\sum_{\sigma}r_{\sigma}$:

$$\begin{aligned} r&=\left[\sum_{\sigma}\left\langle\psi\left|\sum_{i}n_{i\sigma}\right|\psi\right\rangle\right]\Big/N \\ &\equiv\left[\sum_{\sigma}N_{e\sigma}\right]\Big/N , \end{aligned} \tag{2}$$

where N denotes the number of lattice sites in the system. Here we limit ourselves to the nonmagnetic case $N_{e\sigma}=N_{e\,-\sigma}$. The Hamiltonian (1) serves as a "free" term in considering electronic systems with $H'=H+V$, where V is the electron-electron interaction.

For the case of periodic boundary conditions (1) is exhaustively treated in most of the textbooks.[1,2] The case of open boundary conditions (OBC) has been less studied. The purpose of this work is to derive and study the properties of the ground state of (1) of finite chains of length N with OBC, i.e., the Hamiltonian

$$H=\sum_{\substack{i=1 \\ \sigma}}^{N-1}(c_{i\sigma}^{\dagger}c_{i+1\,\sigma}+c_{i+1\,\sigma}^{\dagger}c_{i\sigma}) . \tag{3}$$

The Hamiltonian (3) appears in the study of renormalization for fermion systems[3-5] and in the calculations for quantum spin chains.[6] It serves also as a starting point for the analysis of properties of electronic aggregates.[7]

In the following we will determine the ground-state wave function of Eq. (3) for arbitrary r and N and study the distribution of density and the density-density correlation functions. Special attention will be devoted to the influence of the boundary effects.

II. CALCULATIONS AND RESULTS

The Hamiltonian (4) is diagonalized by introducing new Fermion operators $d_{l\sigma}^{\dagger}$ defined as[5]

$$c_{i\sigma}^{\dagger}=\left[\frac{2}{N+1}\right]^{1/2}\sum_{l=1}^{N}\sin(q_l i)d_{l\sigma}^{\dagger} . \tag{4}$$

The transformation (4) corresponds to "standing" normal modes of the finite system and the OBC read now

$$\begin{aligned} &c_{N+1\,\sigma}^{\dagger}\,|\,0\rangle=0 , \\ &c_{0\,\sigma}^{\dagger}\,|\,0\rangle=0 , \end{aligned} \tag{5}$$

giving the quantization condition

$$q_l=\frac{\pi}{N+1}l , \quad 1\le l\le N . \tag{6}$$

With (4) and (5) we obtain the transformed Hamiltonian

$$H=2\sum_{\substack{l=1 \\ \sigma}}^{N}(\cos q_l)d_{l\sigma}^{\dagger}d_{l\sigma} . \tag{7}$$

The ground-state wave function $|\psi_0\rangle$ of Eq. (7) corresponds to the consecutive filling of allowed wave vectors q_l and is equal to

$$|\psi_0\rangle=\prod_{\sigma}\prod_{l=N-N_{e\sigma}+1}^{N}d_{l\sigma}^{\dagger}\,|\,0\rangle , \tag{8}$$

with $\langle\psi_0\,|\,\psi_0\rangle=1$, where $N_{e\sigma}=\langle\psi_0\,|\sum_{i=1}^{N}n_{i\sigma}\,|\,\psi_0\rangle$. The ground-state energy $E_0^{(N)}=\langle\psi_0\,|\,H\,|\,\psi_0\rangle$ is obtained from

$$\begin{aligned} E_0^{(N)}&=2\sum_{\sigma}\sum_{l=1}^{N_{e\sigma}}\cos\left[\pi\frac{N-N_{e\sigma}+l}{N+1}\right] \\ &=-2\sum_{\sigma}\frac{\cos\dfrac{\pi(N_{e\sigma}+1)}{2(N+1)}\sin\dfrac{\pi N_{e\sigma}}{2(N+1)}}{\sin\dfrac{\pi}{2(N+1)}} , \end{aligned} \tag{9}$$

and it gives the ground-state energy per site $e_0^{(N)}=E_0^{(N)}/N$

$$e_0^{(N)} = -2\sum_\sigma r_\sigma \frac{\cos\frac{\pi(N_{e\sigma}+1)}{2(N+1)}\sin\frac{\pi N_{e\sigma}}{2(N+1)}}{N_{e\sigma}\sin\frac{\pi}{2(N+1)}} . \quad (10)$$

To obtain the expectation value of the density we calculate the matrix elements $\rho_{i\sigma} = \langle \psi_0 \mid n_{i\sigma} \mid \psi_0 \rangle$ and obtain

$$\rho_{i\sigma} = \frac{N_{e\sigma}}{N+1}\left[1 - \frac{\cos\frac{\pi i(N_{e\sigma}+1)}{N+1}\sin\frac{\pi i N_{e\sigma}}{N+1}}{N_{e\sigma}\sin\frac{\pi i}{N+1}}\right] . \quad (11)$$

To obtain the density-density correlation function in $\mid \psi_0 \rangle$ we calculate $g_{ij\sigma} = \langle \psi_0 \mid n_{i\sigma} n_{j\sigma} \mid \psi_0 \rangle$ and obtain

$$g_{ij\sigma} = \delta_{ij}\rho_{i\sigma} + \rho_{i\sigma}\rho_{j\sigma} - \left[\frac{N_{e\sigma}}{N+1}\right]^2 \left[\frac{\cos\frac{(N_{e\sigma}+1)(i-j)\pi}{2(N+1)}\sin\frac{N_{e\sigma}(i-j)\pi}{2(N+1)}}{N_{e\sigma}\sin\frac{(i-j)\pi}{2(N+1)}} - \frac{\cos\frac{(N_{e\sigma}+1)(i+j)\pi}{2(N+1)}\sin\frac{N_{e\sigma}(i+j)\pi}{2(N+1)}}{N_{e\sigma}\sin\frac{(i+j)\pi}{2(N+1)}}\right]^2 . \quad (12)$$

Since in Eq. (3) the translation invariance is lost, we observe that $\rho_{i\sigma}$ explicitly depends on i, and $g_{ij\sigma}$ does not depend on $(i-j)$ only.

The general expressions of Eqs. (10), (11), and (12) simplify in the limit $N \to \infty$:

$$e_0^{(\infty)} = -2\sum_\sigma \frac{\sin r_\sigma \pi}{\pi} , \quad (13)$$

$$\rho_{i\sigma}^{(\infty)} = r_\sigma \left[1 - \frac{\sin 2r_\sigma \pi i}{2r_\sigma \pi i}\right] , \quad (14)$$

$$g_{ij\sigma}^{(\infty)} = \delta_{ij}\rho_{i\sigma}^{(\infty)} + \rho_{i\sigma}^{(\infty)}\rho_{j\sigma}^{(\infty)} - r_\sigma^2 \left[\frac{\sin\pi r_\sigma (i-j)}{\pi r_\sigma (i-j)} - \frac{\cos\pi r_\sigma (i+j)}{\pi r_\sigma (i+j)}\right]^2 . \quad (15)$$

These equations applied to the half-filled-band case ($r_\sigma = r_{-\sigma} = \frac{1}{2}$) give

$$e_0^{(\infty)} = -\frac{4}{\pi} , \quad (16)$$

$$\rho_{i\sigma}^{(\infty)} = \text{const} = \tfrac{1}{2} , \quad (17)$$

$$g_{ij\sigma}^{(\infty)} = \tfrac{1}{2}\delta_{ij} + \tfrac{1}{4} - \frac{1}{\pi^2}\left[\frac{\sin\frac{\pi}{2}(i-j)}{(i-j)} - \frac{\cos\frac{\pi}{2}(i+j)}{(i+j)}\right]^2 . \quad (18)$$

III. DISCUSSION

It is instructive to visualize Eqs. (10), (11), and (12) for a general value of band filling. To this end we have plotted in Fig. 1 the ground-state energy per site as a function of $1/N$. We have traced for simplicity the continuous lines. Except for $r = 1$, where a small curvature is present, a linear extrapolation gives the asymptotic values with great accuracy. A development of Eq. (10) in terms of $1/N$ shows this explicitly. As expected, the minimum is attained for the half-filled band, giving us the well-known result $e_0^{(\infty)} = -4/\pi$.

In Fig. 2 we have plotted the local density $\rho_{i\sigma}$ as a function of coordinate i ($1 \le i \le 32$) for $\frac{1}{4}$-filled band and for different chain lengths $N = 20$, 32, 72, and 200. One notices rather large density oscillations, with amplitude increasing from the center of the chain towards its ends. Exactly at the chain ends an abrupt reduction of electronic density is observed. The amplitude of the density oscillations inside the chain decreases strongly as a function of N and converges towards 0 as N goes to infinity. In contrast the reduction of these oscillations as a function of N is very weak at and near the ends.

According to Eq. (14) for $r_\sigma < 1$ $\rho_{i\sigma}(r_\sigma) = 1 - \rho_{i\sigma}(1 - r_\sigma)$. Consequently, for $r > 1$ we have a significant increase of electronic density at the ends.

In Fig. 3 we have plotted the electronic density symmetrically with respect to the center of chains with $N = 20$, 32, 72, and 200 sites for a $\frac{1}{4}$-filled band. The decrease in amplitude of the oscillations near the center of the chain is clearly visible. In Fig. 4 we have presented

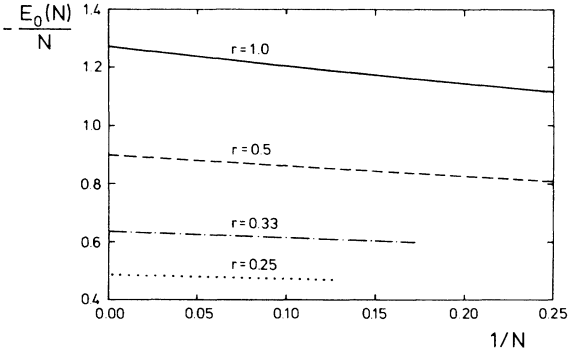

FIG. 1. Ground-state energy per site $e_0^{(N)}$, as a function of $1/N$ for different band fillings r.

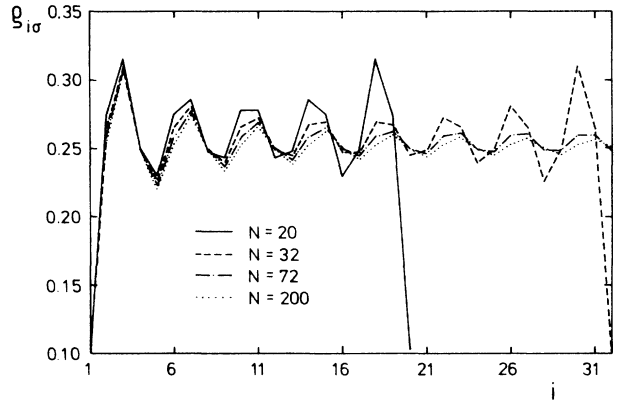

FIG. 2. Local electronic density $\rho_{i\sigma}$ calculated from Eq. (11) for a $\frac{1}{4}$-filled band as a function of coordinate i ($i=1,2,\ldots,32$; $i=1$ at the beginning of the chain) for different chain lengths $N=20$, 32, 72, and 200.

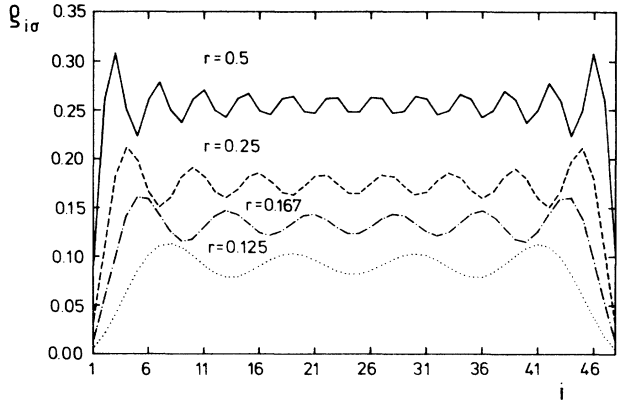

FIG. 4. Local electronic density $\rho_{i\sigma}$ for different band fillings r calculated from Eq. (11) as a function of coordinate i ($i=1,2,\ldots,48$; $i=1$ at the beginning of the chain) for a chain of $N=48$ sites.

the electronic density for a whole chain with $N=48$ for different band fillings. The period of the oscillations depends on the band filling and on the average density. The period is $\pi/k_F=1/r_\sigma$, which can be seen from Eq. (14) too. The last follows from the relation between the Fermi vector k_F and the density in one dimension, $k_F=(\pi/2)r$. In fact we are dealing here with Friedel-type density oscillations which are induced by the finite size of the chain and its boundaries. The relative decrease of density at the boundary, i.e., the ratio $\rho_\sigma(i=1)/\rho_\sigma(i=24)$ is a decreasing function of band filling.

The density-density correlation function $g_{ij\sigma}$ for $i=1$, $j=1,2,\ldots,32$ for a $\frac{1}{4}$-filled band for $N=20$, 32, 72, and 200 is presented in Fig. 5. A characteristic feature is a drastic decrease of $g_{ij\sigma}$ at a first neighbor ("correlation hole," see Ref. 8), followed by very weak oscillations of the same period as for the density $\rho_{i\sigma}$. The amplitude of these oscillations again decreases when moving towards the center of the chain. However this effect is only visible for large N. For $N\leq 50$ the boundary effects dominate and no such decrease can be seen. Similar results are obtained for $r>1$ and $i>1$. The Hamiltonian (3) can be diagonalized in any dimension but exact calculations of appropriate expectation values are no longer evident.

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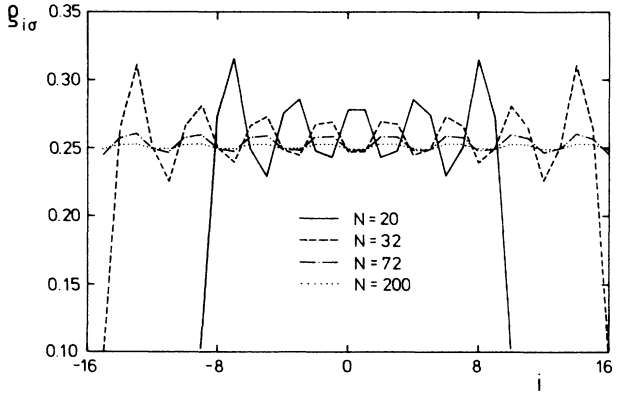

FIG. 3. Local electronic density $\rho_{i\sigma}$ for a $\frac{1}{4}$-filled band calculated from Eq. (11) as a function of coordinate i ($-16\leq i\leq 16$; $i=0$ at the center of the chain) for different chain lengths $N=20$, 32, 72, and 200.

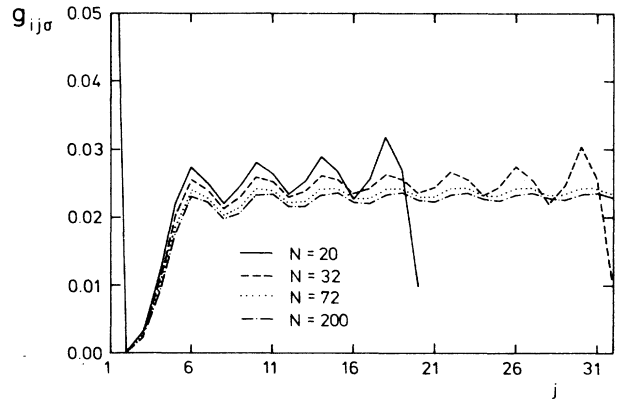

FIG. 5. Density-density correlation function $g_{ij\sigma}$ for a $\frac{1}{4}$-filled band, calculated from Eq. (12) as a function of coordinate j ($j=1,2,\ldots,32$; $i=1$ at the beginning of the chain) for different chain lengths $N=20$, 32, 72, and 200. Note that the value of $g_{12\sigma}$ is of the order of 10^{-4} and is not zero.

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