ON METAL–INSULATOR TRANSITION FOR A ONE-DIMENSIONAL CORRELATED NANOSCOPIC CHAIN*

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We have applied our novel numerical scheme combining Lanczos diagonalization in the Fock space with an *ab initio* renormalization of the single-particle (Wannier) functions, to study the ground state properties of the *Extended Hubbard Model*. Through the *finite-size scaling* we determine the discontinuity of the momentum distribution Fermi surface. Our results imply *Fermi-liquid behavior* for lattice parameter $a \lesssim 3a_0$ (a_0 is the Bohr radius) and zero-temperature transition to the localized spin system for larger a. Possible further applications of the method are listed at the end.

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One of the central issues in the physics of strongly correlated electron systems (which relevance is crucial in the modeling of *high-*T_c superconductors [1]), is the question whether the electron behavior in such system is or is not Fermi-liquid-like. This problem also appears in recently studied one-dimensional systems (1D), which range from organic metals [2] to quantum rings and wires [3], and to nanotubes [4]. In their canonical description, provided by the Hubbard-model-methodology [5], the non-Fermi-liquid behavior is predicted (away from half-filling) by the renormalization group mapping onto the Tomonaga–Luttinger model [6]. Numerical evidence for this behavior has also been gathered [7]. However, as the exact solutions of the modified Hubbard model with inclusion of intersite interactions [8] prove the existence of the metal-insulator transition (MIT) even for the half-filled-band case, the role of the *long-range* interactions has to be crucial in the theoretical understanding of the correlated 1D systems. The existence of such MIT has also been discussed [9] within the density-matrix renormalization group (DMRG) method when the second-neighbor hopping is included.

In this paper we complement our previous study [10] of the electron localization in 1D, 1s-band system with both the long-range (Coulomb) interactions and the nearest-neighbor hopping [11]. Finite-size scaling is applied for

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the first time to determine whether the system shows Fermi- or non-Fermi-liquid-like behavior at the localization threshold. But first, let us briefly summarize the basic features of the homogeneous conductors, following [7].

In a Fermi liquid quasiparticles are well defined, which implies: *(i)* a nonzero quasiparticle pole strength Z in a single particle propagator

$$G(\boldsymbol{k},\omega) = \frac{Z}{\omega - (\epsilon_{\boldsymbol{k}} - \epsilon_{\mathrm{F}}) + i\delta \mathrm{sgn}(k - k_{\mathrm{F}})} + G_{\mathrm{incoh}}(\boldsymbol{k},\omega) \tag{1}$$

(with standard notation), and *(ii)* a finite discontinuity $\Delta n_{\boldsymbol{k}}$ of the momentum distribution $n_{\boldsymbol{k}} = \left\langle a^{\dagger}_{\boldsymbol{k}} a_{\boldsymbol{k}} \right\rangle$ at the Fermi ridge ($k = k_{\mathrm{F}}$). Moreover, in a Fermi-liquid the discontinuity $\Delta n_{\boldsymbol{k}}$ is equal to the inverse quasiparticle mass renormalization Z.

In a system of finite size N, however, $\Delta n_{\boldsymbol{k}}(N)$ is always nonzero due to the finite distance between neighboring states in the first Brillouin zone. Nevertheless, its asymptotic behavior for $N \to \infty$ can belong to one of three categories: (a) $\Delta n_{\boldsymbol{k}}(N) \to A^{-N}$ *(insulator)*, (b) $\Delta n_{\boldsymbol{k}}(N) \to N^{-\theta}$ *(marginal conductor)*, (c) $\Delta n_{\boldsymbol{k}}(N) \to$ const *(normal conductor)*. Although it is, in principle, straightforward to justify whether a correlated electron liquid is a Fermi liquid, provided finite-size scaling can be performed on $\Delta n_{\boldsymbol{k}}(N)$, one should carefully check the condition *(i)*, concerning the quasiparticle pole strength Z in Eq. (1). This part of an analysis can also be done with the help of Lanczos diagonalization technique [12], and will be presented elsewhere [13].

For the Fermi-liquid regime (c), one can expand $\Delta n_{\boldsymbol{k}}(N)$ in powers of $1/N$, to obtain the following extrapolation formula for large lattice size N:

$$\Delta n_{\boldsymbol{k}}(N) = \Delta n_{\boldsymbol{k}} + a(1/N) + b(1/N)^2 + \ldots . \tag{2}$$

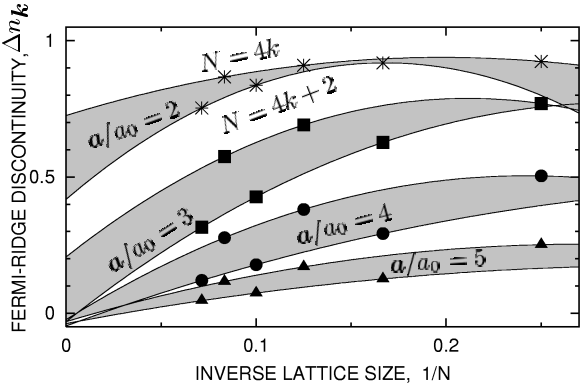

Fig. 1. The finite-size scaling of the Fermi-ridge discontinuity $\Delta n_{\boldsymbol{k}}(N)$. The extrapolation with $1/N \to 0$ is performed separately for $N = 4k$ and $N = 4k + 2$. The lattice parameter a is expressed in the units of Bohr radius a_0.

A sample of numerical results for $N = 4 \div 14$ with corresponding extrapolation parabolas of the form (2) are shown in Fig. 1. All the results were obtained for *Extended Hubbard model* [11], within a combined exact diagonalization-*ab initio* approach [10]. The extrapolated values of $\Delta n_{\boldsymbol{k}}$ for $1/N \to 0$, are presented in Fig. 2 as a function of the lattice parameter a. The source data for $N = 4 \div 14$, used for finite-size scaling, are provided with the inset. Both curves for $N = 4k$ and $N = 4k+2$ shows clear transition-like behavior for $a_{\rm crit} \approx 3a_0$ in contradistinction to the corresponding numerical results for *pure* Hubbard model [7]. The values of $a_{\rm crit}$ are in agreement with the Hubbard localization criterion [10].

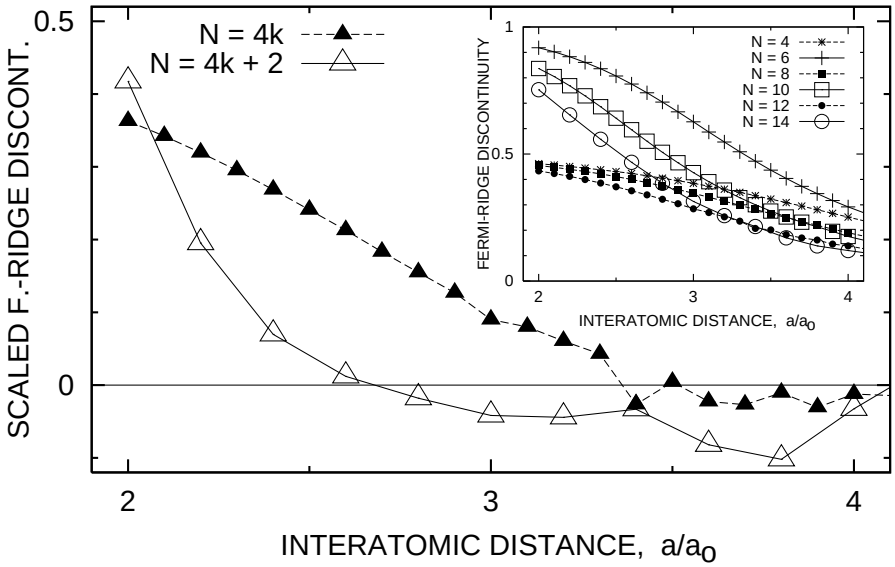

Fig. 2. Fermi-ridge discontinuity $\Delta n_{\boldsymbol{k}}$ obtained through the finite-size scaling with $1/N \to 0$, and the original data *(inset)* for $N = 4 \div 14$.

In summary, we presented a first numerical evidence for the possible metal–insulator transition in one-dimensional, 1*s*-band system with *long range* Coulomb interactions using the finite-size scaling. The results, obtained via the combined exact diagonalization — *ab initio* approach [10] are in agreement with an exact solution of the modified Hubbard model by Strack and Vollhardt [8]. Among the future applications of our method are the following problems:

(i) A direct treatment of the realistic 1D systems with the single-band extended Hubbard model. This most straightforward application concerns only a limited class of materials. However, as the Hilbert space of various organic conductors can be effectively reduced by choosing only the highest occupied-(HOMO) or the lowest unoccupied molecular orbital (LUMO) per structural unit, this direction seems realizable [14].

(ii) The combination of the approximate methods of solving parametrized Hamiltonians with an *ab initio* readjustment of the Wannier functions. This approach, *i.e.* for the case of Gutzwiller method (possibly combined with a few Lanczos steps) will allow us to consider 3-dimensional systems of a larger size. The study of the correlated electrons in such materials as the metallic hydrogen, or truly 1D systems (*e.g.* carbon nanotubes), looks possible.

(iii) The use of the Gaussian-type orbitals (GTO) provides us with an insight into a system containing heavier atoms or ions (such as CuO planar cluster in a *high-*T_c superconductor). However, the computational complexity of the method increases with the fourth power of the number of Gaussians per site, so this particular application seems to be limited to small clusters, even with modification *(ii)*.

It would also be very interesting to test experimentally presented results on a "toy" nanoscopic systems, such as linear chains of single-electron quantum dots (with steered gate potential), or K/Na atoms wrapped with C_{60} fullerenes.

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