# DEFINING METALLICITY AND MOTT LOCALIZATION IN CORRELATED NANOSCOPIC SYSTEMS\*

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Exact ground state properties are presented by combining the exact diagonalization in the Fock space (including the *long-range* Coulomb interaction) with an *ab initio* optimization of the single-particle (Wannier) functions. The quasiparticle mass is almost divergent at the localization threshold, where the particle distribution of the Fermi-Dirac type gets smeared out. The analysis is performed using 1*s*-like Gaussian-type orbitals.

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### 1. Introduction

In spite of the development of the physics of one dimensional systems such as nanotubes, quantum rings and wires, and organic metals, the understanding of these correlated fermionic systems is still lacking. This is because in their description the role of the long-range Coulomb interaction is crucial, as the charge screening becomes less effective. The exact solutions of the parametrized models with inclusion of intersite interactions [1] prove the existence of the metal-insulator transition for the half-filled-band case, in contradistinction to the corresponding Hubbard-model solution [2], for which the system is insulating even for an arbitrarily small Coulomb repulsion. A separate question concerns the appearance of the Tomonaga-Luttinger liquid behavior [3] in the metallic state, for which some evidence has been gathered [4]. In brief, the delocalization of the states in d = 1provides a crucial case for the analysis of the localization as a quantum phase transition in a rigorous manner. Here we address the question of the metallicity appearance in a correlated nanoscopic atomic chain or ring.

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#### 2. Model Hamiltonian and the optimized ground state energy

We focus here on the so-called  $Extended\ Hubbard\ Model$  with Hamiltonian of the form

$$H = \epsilon_a^{\text{eff}} \sum_i n_i + t \sum_{i\sigma} \left( a_{i\sigma}^{\dagger} a_{i+1} + \text{h.c.} \right) + U \sum_i n_{i\uparrow} n_{i\downarrow} + \frac{1}{2} \sum_{ij}' K_{ij} \delta n_i \delta n_j, \quad (1)$$

where  $\delta n_i \equiv n_i - 1$ ,  $\epsilon_a^{\text{eff}} = \epsilon_a + N^{-1} \sum_{i < j} (2/R_{ij} + K_{ij})$  (Ry) is the effective atomic level defined including the mean-field part of the Coulomb interaction, t is the nearest-neighbor hopping integral, and U,  $K_{ij}$  are the intraand inter-site Coulomb repulsion amplitudes, respectively.

The Hamiltonian (1) is diagonalized in the Fock space with the help of Lanczos technique. As the microscopic parameters  $\epsilon_a^{\text{eff}}$ , t, U, and  $K_{ij}$  are calculated numerically in the Gaussian STO-3G basis, the inverse orbital size  $\alpha$  of the 1s-like state is subsequently optimized to obtain the ground state energy  $E_G$ . This procedure follows the idea of recently developed method combining first- and second-quantization schemes [5,6]. We have already shown [6] that such a combined exact diagonalization — *ab initio* study of the one dimensional system leads to the precise values of the localization threshold, the electron-lattice couplings, and the dimerization magnitude. However, the convergence of the results obtained with the Slater-type orbitals is not sufficient to perform the finite-size scaling with the lattice size  $N \to \infty$ . This is because, when calculating the microscopic parameters in the single-particle (Wannier) basis, one ignores the three- and the four-site interaction terms, that represents an uncontrolled approximation.

In contrast, for the Gaussian-type orbitals, we can treat the three- and four-site terms exactly. Their effects on the convergence of the results for the ground-state energy  $E_G$  and the optimal inverse orbital size  $\alpha_{\min}$  are shown in Fig. 1 for  $N = 6 \div 10$  atoms. These results were used to extrapolate the value of the variational parameter  $\alpha_{\min}$  to larger N to speed up the computations. Fig. 1 illustrates also the Hubbard localization criterion. Namely, for the interatomic distance  $a \approx 3a_0$  ( $a_0$  is the Bohr radius) the energy of the metallic state crosses over to that representing the Mott insulating state. The critical value of a is very close to obtained for the 1s Slater-type orbitals [6].

#### 3. The quantum critical behavior

The the electron momentum distribution  $n_{k\sigma} \equiv \langle a_{k\sigma}^{\dagger} a_{k\sigma} \rangle$  is shown in Fig. 2 for  $N = 6 \div 14$  atoms. The continuous lines represent the formula

$$n_{k\sigma} = \frac{1}{2} + \operatorname{sgn}(k - k_F)[\alpha |k - k_F|^2 + \beta |k - k_F| - \gamma], \qquad (2)$$



Fig. 1. The ground state energy per atom for the linear chain of  $N = 6 \div 10$  with periodic boundary conditions. The Gaussian-type orbitals (STO-3G basis) have been used. The energies of the *purely* metallic (M) and insulating (INS) states are shown for comparison [7]. The *inset* provides the optimal inverse orbital size  $\alpha_{\min}$ .

with fitted parameters  $\alpha$ ,  $\beta$ , and  $\gamma$ . We obtain the critical distance in the range  $a_{\rm crit} = 3.56 \div 4.18 a_0$  (cf. Table I), at which the interpolated Fermiridge discontinuity  $\Delta n_F = 2 \gamma$  disappears, signaling the electron localization. No Luttinger-liquid effects were observed in the system with one-electron per atom. A clear metallic behavior is evidenced by the presence of the Fermi ridge, since the energy-level spread produces remarkably smaller variations of  $n_{k\sigma}$  than  $\Delta n_{\rm F}$  for  $a < a_{\rm crit}$ .

TABLE I

The fitted parameters of the critical exponent formula for the quasiparticle mass  $m^*/m_{\rm B} \equiv (\Delta n_{\rm F})^{-1} = A|a - a_{\rm crit}|^{-\gamma}$ .

N	A	$a_{ m crit}$	$\gamma$	N	A	$a_{ m crit}$	$\gamma$
8	$3.5 \pm 2.6$	4.18(1)	1.39(14)	12	$7.0 \pm 1.1$	4.030(5)	1.29(10)
10	$6.5\pm2.3$	3.900(3)	1.32(7)	14	$7.4 \pm 0.4$	3.56(2)	1.58(7)

With the help of the interpolation formula (2) we can determine the quasiparticle mass enhancement  $m^*/m_{\rm B}$  by equating it with  $(\Delta n_{\rm F})^{-1}$ . The resulting parameters of fitted critical formula  $m^*/m_{\rm B} = A|a - a_{\rm crit}|^{-\gamma}$  are gathered in Table I. The values of critical exponent are in agreement with those obtained for Slater-type orbitals [6]. It would be very important to test experimentally this result, as it represents the critical behavior of the Fermi discontinuity  $\Delta n_{\rm F} \sim |a - a_{\rm crit}|^{\gamma}$  at the localization border reached from the metallic side.



Fig. 2. Momentum distribution  $n_{k\sigma}$  for electrons on a linear ring of  $N = 6 \div 14$  atoms; the interatomic distance *a* is specified in units of Bohr radius  $a_0$ . The continuous line represents the parabolic interpolation (2).

In summary, we have determined the microscopic criterion for the *cross-over* transition from the nanoscopic metal to the localized spin system in one dimension. The new method of optimizing the single-particle wave functions in the correlated state proves thus executable in an exact treatment of nanoscopic systems for both Slater- and Gaussian-type basis sets. A quantum critical behavior at the metal-insulator boundary is suggested.

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