Physics Letters A 380 (2016) 1450–1454

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Metal–insulator transition in an one-dimensional half-filled interacting mesoscopic ring with spinless fermions: Exact results

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ARTICLE INFO

Article history:
Received 17 November 2015
Received in revised form 8 February 2016
Accepted 16 February 2016
Available online 20 February 2016
Communicated by R. Wu

Keywords:
Metal–insulator transition
Coulomb interaction
Spinless fermions
Persistent current
Drude weight
Exact results

ABSTRACT

We calculate persistent current of one-dimensional rings of fermions neglecting the spin degrees of freedom considering only nearest-neighbor Coulomb interactions with different electron fillings in both ordered and disordered cases. We treat the interaction exactly and find eigenenergies by exact diagonalization of many-body Hamiltonian and compute persistent current by numerical derivative method. We also determine Drude weight to estimate the conducting nature of the system. From our numerical results, we obtain a metal–insulator transition in half-filled case with increasing correlation strength U but away from half-filling no such transition is observed even for large U.

1. Introduction

The metal–insulator (MI) transition is one of the most significant phenomena in condensed matter physics [1–5]. The usual band structure predictions are not capable of exploring many experimental evidences. For example, according to the band structure analysis, Iron (II) Oxide (FeO), Nickel Oxide (NiO) and Cobalt Oxide (CoO) are shown to be metallic but experimentally they exhibit insulating phase. Similarly, the absence of magnetism in several high-temperature superconductors verified in experiments contradict theoretical results which suggest finite magnetism. Likewise a strong mismatch has also been observed between theoretical predictions and experimental observation in the determination of band-gap for many semi-conductors [4]. Considering Hubbard correlation, when calculating the electronic band structures, it has flourished all the experimental results quite strongly. If the Hubbard correlation is much greater than the bandwidth of a material, the MI transition becomes extremely relevant, and, compounds containing rare earth ions with localized $4f$ electrons or partially filled d-band elements show this type of transition. On the other hand, if bandwidth is higher than the Hubbard correlation, then the electron–electron interaction can be excluded and the experimental evidences for those systems can be explained by conventional band structure predictions [4]. It is not only true for the macroscopic bulk systems but Hubbard correlation has an effective impact on low-dimensional transport phenomena [6,7].

Persistent current in an isolated 1D small conducting ring threaded by a magnetic flux is a well established phenomenon in mesoscopic regime. There exist many controversial issues involving current amplitude, sign and its periodicity between theoretical and experimental results [6–21], and in the last few decades people have attempted a lot to remove these discrepancies by improving their models [6,7,19–21]. But still, it is an open challenge to remove the disparity exactly. People have also explored the role of interactions on persistent current and to some extent the enhancement of current has been observed in presence of interaction [7]. In the early 90s Bouzerar et al. have performed the calculation of persistent current in 1D ring considering spinless electrons. Utilizing a Wigner–Jordon transformation on the tight-binding (TB) Hamiltonian they have found the ground state energy from Lanczos algorithm and determined the current using conventional method. It has been shown that the ring exhibits a MI transition at the half-filled band case due to correlation, and, away from half-filling the interaction has no such strong influence [6]. Studying persistent current in finite two-dimensional (2D) arrays of semiconducting quantum dots in presence of magnetic field perpendicular to the 2D plane the phenomenon of MI transition in the half-filled band case has also been reported in a nice work [22] by Das Sarma and his co-worker. However, the persistent current in 2D quantum dot arrays has important differences compared to established persistent current in one-dimensional ring structure subjected to

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http://dx.doi.org/10.1016/j.physleta.2016.02.022
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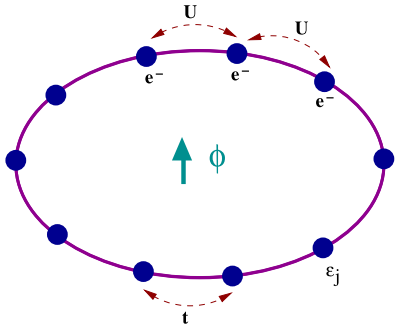

Fig. 1. (Color online.) 1D ring with interacting spinless electrons threaded by an AB flux ϕ where the filled blue circles represent the atomic sites.

Aharonov–Bohm (AB) flux ϕ. In that work (Ref. [22]) several qualitative features of persistent current as functions of both on-site and extended electron–electron interactions have been put forward where the current has been computed by determining ground state energy through Lanczos diagonalization technique. Here it is important to note that the understanding of the MI transition in 1D system of spinless fermions in other context has already been established several years ago where response functions have been calculated [23] in a solvable model. These response functions, on the other hand, cannot be computed by Bethe ansatz though this ansatz allows us to get rigorous statements on many-body system of interacting 1D spinless fermions [24–26].

The aim of this paper is to treat the interacting Hamiltonian *exactly* and find ground state energy from exact diagonalization of many-body TB Hamiltonian. Evaluating ground state energy we compute persistent current using conventional method both for ordered and disordered cases. Our model comprises a 1D finite ring of spinless fermions with nearest-neighbor (NN) Coulomb correlation. From our analysis we find that in the limit of half-filling current amplitude decreases sharply with correlation strength U and drops to almost zero (insulating phase) for moderate U, while a metallic phase is always observed in the non-half-filled cases irrespective of U. To substantiate the role of U more precisely on conducting properties, in the present work, we also discuss the variation of Drude weight [27] for different electron fillings, and, from these results sharp transition between two conducting phases is noticed. Finally, we discuss scaling behavior of persistent current with ring size.

The rest of the work is arranged as follows. Section 2 describes the model and theoretical approach and Sec. 3 presents the numerical results. Finally, we summarize our findings in Sec. 4.

2. Model and formalism

The model is shown in Fig. 1 where we consider an AB ring of spinless fermions with nearest-neighbor Coulomb interaction. Under nearest-neighbor hopping approximation the TB Hamiltonian of such a N-site ring reads,

$$\mathbf{H} = \sum_j \epsilon_j n_j - t \sum_j \left[e^{i\theta} c_j^\dagger c_{j+1} + e^{-i\theta} c_{j+1}^\dagger c_j \right] + U \sum_{j=1} n_j n_{j+1} \quad (1)$$

where $c_j^\dagger$ and c_j are the usual creation and annihilation operators, respectively, ϵ_j describes the site energy, t is the NN hopping integral and U measures the NN Coulomb interaction. The phase factor θ $(= 2\pi\phi/N\phi_0)$ arises due to AB flux ϕ, where $\phi_0 = ch/e$. For ordered ring, all site energies are identical and therefore we set them to zero without loss of generality. While, for disordered rings we choose site energies randomly from a 'Box' distribution function of width W within the range $-W/2$ and $W/2$.

To find ground state energy of the system first we construct the many-body Hamiltonian matrix considering the interaction exactly where the matrix elements are obtained following the prescription: $\mathbf{H}_{mn} = \langle\psi_m|\mathbf{H}|\psi_n\rangle$. Here $|\psi_m\rangle$ and $|\psi_n\rangle$ are the basis vectors associated with total number of spinless fermions N_e in the ring. For example, for a two-electron system we define them as $|\psi_m\rangle = c_p^\dagger c_q^\dagger|0\rangle$ and $|\psi_n\rangle = c_k^\dagger c_l^\dagger|0\rangle$ where $|0\rangle$ is the null state. Likewise we define basis vectors for higher-electron systems and construct appropriate matrices. Once the matrix is constructed, we compute ground state energy by exact diagonalization method.

The persistent current in such a system at absolute zero temperature ($T = 0$ K) can be determined from the relation [17], $I(\phi) = -\partial E_0(\phi)/\partial\phi$, where $E_0(\phi)$ is the ground state energy.

Finally, we calculate Drude weight D from the expression [27],

$$D = \frac{N}{4\pi^2}\left[\frac{\partial^2 E_0(\phi)}{\partial\phi^2}\right]_{\phi\to 0}. \quad (2)$$

Finite value of D corresponds to the metallic phase while it drops to zero for the insulating one, as originally put forward by Kohn.

3. Results and discussions

Below we present our results. In our numerical calculations we choose $c = e = h = 1$ and measure the energy in unit of t which is fixed at 1 eV. Since we are dealing with exact many-body Hamiltonian, dimension of the matrix increases sharply with electron filling, and therefore, we restrict ourselves to the rings with few electrons due to computation limitations. But, the point is that with these results we can easily analyze the characteristic features of current as well as conducting properties for larger rings with higher N_e as all the basic features will remain invariant with our numerical results presented here.

Fig. 2 displays the current–flux characteristics of some typical ordered half-filled mesoscopic rings for three distinct values of correlation strength U where (a), (b), (c) and (d) correspond to $N = 4$, 6, 8 and 10, respectively. In the absence of Coulomb correlation, current exhibits sharp transitions at $\phi = 0$ (for even N_e) or ± 0.5 (for odd N_e) associated with the energy level crossing, while it becomes continuous as long as interaction is included. Most interestingly we see that for a specific U current decreases sharply as we increase ring size, and, for large U it practically drops to zero (blue line). This is solely due to the repulsive Coulomb interaction U. In the limit of half-filling all sites are occupied by single

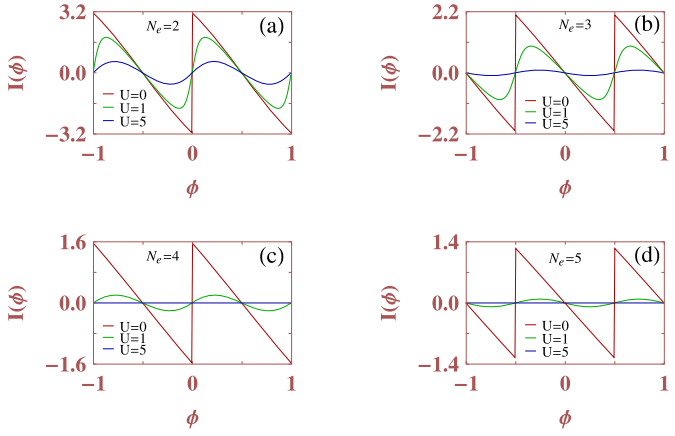

Fig. 2. (Color online.) $I(\phi)$ vs. ϕ characteristics for three distinct values of U in the ordered ($W = 0$) half-filled ($N_e = N/2$) rings where (a), (b), (c) and (d) correspond to $N = 4$, 6, 8 and 10, respectively.