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Dynamics of two interacting electrons in a one-dimensional crystal with impurities

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Abstract

We investigated the role that the electron–electron interaction plays on the propagating properties of wave packets in a one-dimensional crystal with impurities. We considered two interacting particles with opposite spins in a band, where we treated their interaction along the Hubbard model. We have obtained the density of states of the crystal for different values of the interaction term, as well as solved the dynamical Schrödinger equation by varying the initial conditions. We have introduced a method through which we were able to follow the time evolution of the wave packets for both spins showed in three-dimensional plots, and have evaluated, for each particle, the corresponding mean-square displacement and the centroids as function of time. These measurements allow us to determine the influence of the interaction on dynamical properties. We discussed the combined effect that the extension of the initial wave packets and the interaction strength have on propagating properties. Under certain conditions we obtained an oscillatory movement of the overlapping packets associated with both spins that takes place in a small region of the lattice.

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1. Introduction

According to the scaling theory of localization developed by Abrahams et al. [1] in low-dimensional systems (one and two dimensions), any degree of disorder will prevent the appearance of a metallic phase. Moreover, former experiments done with two-dimensional electron systems fabricated on semiconductor surfaces showed a logarithmic increase of resistivity while lowering the temperature [2–5]. This behavior lends support to the scaling theory of localization, since this happens in case of a weak electron–electron interaction. These results were in agreement with theoretical predictions [6] that *weak* electron–electron interaction increases localization. The above experiments were done with samples of high density of electrons, i.e., systems for which the associated Wigner radius $r_s \ll 1$, which is the ratio of the Coulomb energy to Fermi energy.

However, such a scaling theory does not take into account the electron–electron interaction which was lately believed to be responsible for a metal–insulator transition, observed in several experiments performed at zero magnetic field described below. In the metallic phase, one observes a strong temperature dependence (a steep $d\varrho/dT > 0$) caused by the delocalizing effects produced by the interaction between the particles.

As the density is reduced such that $r_s \gg 1$, the interaction becomes dominant, for that regime. Finkelstein [7] and Castellani et al. [8] predicted that for sufficiently strong interactions, a 2D system should present a conducting phase as the temperature is lowered. Since recently the fabrication of 2D samples of high quality with very small amount of randomness was possible, measurements were done at very low particle densities. In this way the strongly

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interacting regime ($r_s \gg 1$) has become experimentally accessible. For instance for $r_s > 10$ experiments done on low-disordered 2D silicon samples demonstrated that with increasing electron density one can cross from the insulating regime, where the resistance *diverges* with decreasing temperature, to a regime where the resistance *decreases* strongly with decreasing temperature, clearly showing metallic behavior [9–12].

In addition to that, in an extensive numerical analysis of the two-dimensional Anderson model with dimerized disorder, we have reported the existence of several dynamical regimes [13,14].

As far as we are concerned there is no a theoretical explanation that describes adequately the metal–insulator transition in 2D systems, as well as the dramatic increase of the spin susceptibility in its vicinity. Comprehensive studies of the state of the art of this intriguing problem are presented by Abrahams et al. [15] and Kravchenko and Sarachik [16].

In 1D systems with random disorder of any intensity, all states are exponentially localized as shown in the pioneering work by Anderson [17] in dealing with diagonal disorder, i.e., a model where the on-site energies are randomly distributed. On the other hand, when some correlation is included in the model, and without considering interaction between particles, this picture is substantially modified, giving the appearance of extended states and, consequently, carriers are able to propagate through the system. Several structures with correlated disorder show vanishing of localization, when one considers nearest-neighbors hopping. Among them one can quote the random-dimer model that can explain the high conductivity of polymers [18–21]. Another example that shows correlated disorder, responsible for particle diffusion in 1D, is provided by the structures where the on-site energies follow the Fibonacci and Thue–Morse sequences [22–26]. One should also mention the Harper model of a quasicrystal which presents a mobility edge when the strength of the potential equals the half-bandwidth. Starting with a well-localized particle in the lattice, as long as the Harper potential is less than half-bandwidth, we encounter ballistic propagation [27–30]. The purpose of this work is to analyze the role the electron–electron interaction plays on propagation in some 1D nonperiodic structures. First, we present in Section 2 the model assumed for the interaction between two particles in a band, namely the Hubbard Hamiltonian. The two electrons are assumed to be in the singlet state in order to detect the effect of the Hubbard term, since it acts on opposite spins. We show the density of states for different strengths of the interaction. The dynamics tools introduced in order to characterize the dynamical behavior are presented in Section 3, namely, the time evolution of the mean square displacement (MSD) and the centroids associated with each of the particles, as well as the construction of 3D graphs of the wave packets evolution. In Section 4 we discuss the interplay between the strength of the interaction U with the initial wave packet extension. In Section 5 we present the results concerning a 1D crystal with impurities. In Section 6 we present the conclusion to which we arrived in this work.

2. The Hubbard Hamiltonian for two electrons interacting in a band

With the aim to study the influence of the Coulomb interaction between carriers in a 1D lattice, we treat the electron–electron interaction along the Hubbard model [31] in a crystalline system with impurities. As the experiments show, the electron–electron interaction should modify the behavior of the carriers as obtained in a one particle non-interacting scheme. In our work, we introduce two interacting particles in an otherwise empty band. The study of such a problem has deserved a number of interesting works due to the relevant question of what is the role of the interaction between electrons on propagating properties in low-dimensional disordered systems [32–38]. We assume that by solving the present problem one can get a better understanding of the role the interaction plays in real systems.

We consider a 1D lattice of N sites with lattice parameter d, for which the Hubbard Hamiltonian is

$$H = \sum_{r,s} c^{+}_{r,s} c_{r,s} \varepsilon_r + V \sum_{r,s} (c^{+}_{r+1,s} c_{r,s} + \text{c.c.}) + U \sum_{r} \hat{n}_{r\uparrow} \hat{n}_{r\downarrow}, \tag{1}$$

where ε_r is the on-site energy, $c^{+}_{r,s}(c_{r,s})$ is the Fermi creation (destruction) operator for an electron of spin s at site r, V is the hopping term and $\hat{n}_{r\uparrow}(\hat{n}_{r\downarrow})$ is the number operator for spin up (spin down) at site r. As it was stated above, in order to analyze the role the U term plays on the dynamics, we treat the case of electrons with opposite spins, the singlet.

2.1. Energy spectrum for a crystal

To obtain the energy spectrum for the singlet in an impurity-free 1D lattice, we solve the stationary Schrödinger equation in the Wannier representation where we expand the eigenfunction in terms of the kets $|ns, ms'\rangle$ that represent the state with one electron of spin s at site n and the other with spin s' at site m:

$$\Phi_E = \sum_{ns,\, ms'} g(ns, ms'; E) |ns, ms'\rangle. \tag{2}$$

In the Wannier representation we obtain the following set of equations corresponding to energy E:

$$V(g_{n+1,m} + g_{n,m+1} + g_{n-1,m} + g_{n,m-1}) + (\gamma_n + \gamma_m + U\delta_{n,m}) g_{n,m} = E g_{n,m}. \tag{3}$$

In this equation the first index refers to a particle with spin *up* and the second for spin *down*. The Wannier amplitudes $g_{n\uparrow,\, m\downarrow}$ do not depend on time. For simplicity we omit the label E in the Wannier amplitudes.