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Full-band extended states with random phases in one-dimensional disordered system with specific impurities

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Abstract. We investigate transport properties of electrons in a one-dimensional (1D) disordered system consisting of a host chain attached with specific impurities. Every impurity, labelled by j and possessing site energy ϵ_j, is side-coupled to two adjacent sites of the host chain with hopping integral t_{1j} and changes the original nearest-neighbor (NN) hopping to t_{2j}. We show that if $t_{2j} = -\epsilon_j/2$ and $t_{1j} = \sqrt{t_0^2 - (\epsilon_j/2)^2}$ for all impurities, with t_0 being the NN hopping of the host chain, the states in the whole band are extended, even though ϵ_j's and positions of impurities are random. The phases of these states, however, are spatially random, corresponding to finite free path and infinite localization length in such a 1D system.

PACS. 72.15.Rn Localization effects (Anderson or weak localization) – 72.80.Ng Disordered solids – 73.20.Jc Delocalization processes

Since the pioneering work of Anderson on the nature of states in disordered systems [1], the metal-insulator transition originated from the Anderson localization has drawn extensive attention [2,3]. It has been predicted from the one-parameter scaling theory that all the states are localized in one-dimensional (1D) and 2D disordered systems [4]. In 1D, however, several exceptional disordered models emerge in which some extended states at specific energies exist. One example is the random-dimer model which has one extended state at the resonance energy [5]. This idea has been extended to continuous Kronig-Penny model with randomly placed identical multibarrier structures in which several reflectionless resonances were found [6]. It was shown by Maciá et al. that in Kronig-Penny models with short-range correlated disorder there exist infinitely many resonances that give rise to a band of extended states [7]. Extended states can exist in a range of energy in models with long-range correlated disorder [8,9]. Recently it is shown that some states exhibit extended characteristics in 1D Anderson model with long-range hoppings [10]. A specific type of impurities in 1D system, each of which is side-coupled to two nearest-neighbor sites of the host chain, is proposed and investigated in reference [11]. In this paper we prove that for this type of disorder the states in the *whole band* are fully extended, but the phases of wavefunctions are random in the space due to the scattering of impurities, if the hopping integrals and site energy of every impurity satisfies given conditions. In this sense the localization length is infinite, independent of the energy. The combination of the full transmission and the random phases leads to a classical-like ballistic behavior of the particle diffusion. On the other hand, this provides a possible method for controlling the phase of a wavefunction by designing the energy and coupling strength of impurities in a 1D conductor.

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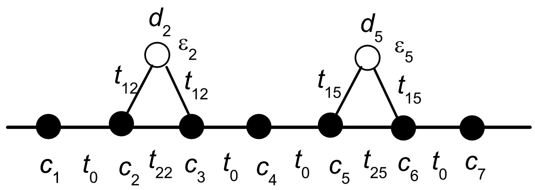

Fig. 1. Impurities, denoted by d_j, doubly side-coupled to a host chain for which the sites are labelled as c_i.

The system consists of a 1D host chain and attached impurities with random site energies and positions, as shown in Figure 1. An impurity, at position j and having site energy ϵ_j, is side-coupled to two adjacent sites of the host chain, j and $j+1$, with hopping integral t_{1j} and changes the original nearest-neighbor (NN) hopping between them to t_{2j}. The Hamiltonian of the model can be expressed as

$$H = \sum_{i \notin \mathcal{S}} t_0 \left(c_i^\dagger c_{i+1} + \text{h.c.} \right) + \sum_{j \in \mathcal{S}} \Big[\epsilon_j d_j^\dagger d_j + t_{1j} \left(c_j^\dagger d_j + c_{j+1}^\dagger d_j + \text{h.c.} \right) + t_{2j} \left(c_j^\dagger c_{j+1} + \text{h.c.} \right) \Big], \quad (1)$$

where $c_i^\dagger$ and $d_j^\dagger$ are the creation operators for electron on the ith site of the host chain and on the impurity at position j, respectively, t_0 is the NN hopping integral in

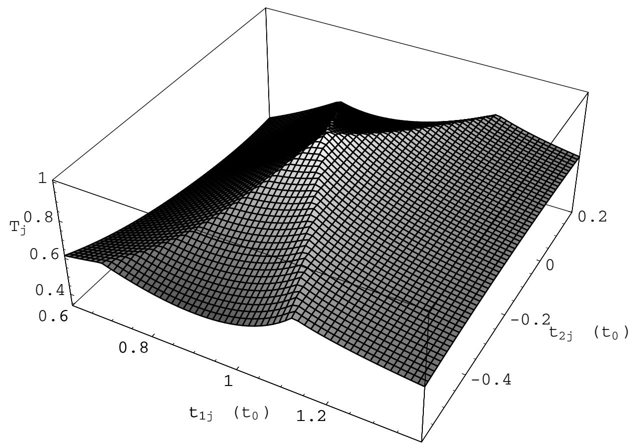

Fig. 2. Mean value of transmission coefficient averaged over the whole band (T_j) as a function of t_{1j} and t_{2j} for $\epsilon_j = 0.4t_0$.

the host chain, and $\mathcal{S}$ is the set of all impurity positions. Here, the position of an impurity j is defined as that of the left one of two adjacent sites in the host chain to which the impurity is side-coupled.

If we consider the transmission of an electron through one impurity labelled as j in set $\mathcal{S}$, a plane wave incident from the left part of the host chain will be partially transmitted to the right part with transmission amplitude τ_j. From the Schrödinger equation $H\psi = E\psi$, with ψ being the wavefunction and E the energy of electron, τ_j is energy dependent and can be easily calculated as

$$\tau_j(k) = \frac{2\mathrm{i}t_0 \sin k[t_{1j}^2 - t_{2j}(\epsilon_j - 2t_0\cos k)]}{(t_{2j} + t_0 e^{-\mathrm{i}k})\left[(e^{-\mathrm{i}k}t_0 - t_{2j})(\epsilon_j - 2t_0\cos k) + 2t_{1j}^2\right]}, \quad (2)$$

where k is the wave vector of the incident electron determined by $E = 2t_0 \cos k$. Thus, for given values of ϵ_j, t_{1j} and t_{2j}, there may exist finite number of resonance energies for which the transmission coefficient $|\tau_j(k)|^2$ is one. However, if the impurity level is in the host band ($|\epsilon_j| \le 2t_0$), and t_{1j} and t_{2j} satisfy

$$t_{1j} = \sqrt{t_0^2 - (\epsilon_j/2)^2},\ t_{2j} = -\epsilon_j/2, \quad (3)$$

one has

$$\tau_j(k) = \frac{e^{2\,\mathrm{i}\,k}\left(2\,t_0 - e^{-\mathrm{i}\,k}\,\epsilon_j\right)}{2\,t_0 - e^{\mathrm{i}\,k}\,\epsilon_j}, \quad (4)$$

and the corresponding transmission coefficient $|\tau_j|^2 = 1$, independent of the energy of electrons and ϵ_j. This means that under conditions (3) impurity j is transparent for electrons in the whole band. In order to show how the whole-band transmission coefficient is changed if the values of t_{1j} and t_{2j} are shifted from conditions (3), in Figure 2 we show the mean value of the transmission coefficient averaged over the whole band, defined as $T_j = \frac{1}{2\pi}\int_0^{2\pi} dk|\tau_j(k)|^2$, as a function of t_{1j} and t_{2j}. Due to the averaging over the whole band, T_j is not related to the transmission of an electron with a given energy, but is a measure of how strict the condition (3) is for the whole-band full transmission. The top of the hill in Figure 2 ($T_j = 1$) is at values of t_{1j} and t_{2j} satisfying condition (3), corresponding to the full transmission in the whole band. The slope near the top of the hill is rather small, implying relatively large tolerance of condition (3) for the full transmission.

Then we consider a chain containing a set of impurities, random in positions and site energies (ϵ_j's) located within the host band, but with all the corresponding hoppings t_{1j} and t_{2j} satisfying condition (3). If an electron, with any energy in the band, is incident from the left, it will completely be transmitted to the right, in spite of the randomness in the impurity positions and site energies. By this way we define a new type of 1D random systems in which the states of the whole band are extended.

Although the transparency is complete for the whole band, the phases of electron wavefunctions are spatially random due to the randomness of impurity positions and site energies. By passing through the jth impurity the electron wave function acquires a phase determined with

$$\phi_j = 2k + 2\arcsin\frac{\epsilon_j \sin k}{\sqrt{4t_0^2 - 4t_0\epsilon_j\cos k + \epsilon_j^2}}. \quad (5)$$

If ϵ_j's are uniformly distributed in range of $[-W/2, W/2]$, the phase shift acquired in passing through an impurity is also random, ranging from

$$\phi_{01} = 2k - \arcsin\frac{W\sin k}{\sqrt{4t_0^2 + 2t_0 W\cos k + W^2/4}}$$

to

$$\phi_{02} = 2k + \arcsin\frac{W\sin k}{\sqrt{4t_0^2 - 2t_0 W\cos k + W^2/4}},$$

and satisfies a probability depending on wave vector k. This probability can be written as

$$P(\phi_j) = \begin{cases} \frac{t_0[A\sin(\phi_j - k) - \sin(\frac{\phi_j}{2} - k)\sin\frac{\phi_j}{2}\sin(\phi_j - 2k)]}{A^2 W}, \\ \text{for } \phi_j \text{ in between } \phi_{01} \text{ and } \phi_{02}, \\ 0, \text{ otherwise.} \end{cases} \quad (6)$$

with

$$A = \sin^2\left(\frac{\phi_j}{2} - k\right) - \sin^2 k.$$

From this we can calculate the average phase shift through one impurity, $\langle\phi_j\rangle$, as a function of wave vector k for different disorder strength W,

$$\bar{\phi_j} = 2k + \frac{\sin k(\eta_- - \eta_+)}{W} + \frac{t_0 \sin 2k}{W}\ln\frac{\eta_- - 2t_0\cos k + W/2}{\eta_+ - 2t_0\cos k - W/2}, \quad (7)$$

with

$$\eta_\pm = \sqrt{\left(\frac{W}{2} \pm 2t_0\cos k\right)^2 + 4t_0^2\sin^2 k}.$$

The mean free path of electrons is determined by $\bar{l} = 2\pi/[(\langle\phi_j\rangle - 2k)n]$ depending on k, with n being the density of impurities. For most k states the mean free path is finite except specific values of k at which $\langle\phi_j\rangle - 2k = 0$.

The characteristics of electron motion in such systems can be illustrated by the diffusion of a wave packet. We suppose that at $t = 0$ a δ-function wave packet is located at site $i = 0$ in a system where $\mathcal{S}$ is the set of all odd numbers. The evolution of the wave packet can be numerically solved from the time-dependent Schrödinger equation. The second moment of the corresponding spatial probability distribution can be written as

$$\sigma^2(t) = \sum_i (i - i_0)^2 |\psi_i(t)|^2, \tag{8}$$

where $\psi_i(t)$ is the wave function at site i and time t. The long-time asymptotic limit of $\sigma^2(t)$ can be fitted with a power law [12,13],

$$\sigma^2 \sim At^{\alpha}, \tag{9}$$

where A is a prefactor and α is the exponent. The value of exponent α characterizes the behavior of electron motion: $\alpha < 1$ corresponds to the localization, $\alpha = 1$ is for the ordinary diffusion, $\alpha > 1$ is related to the super-diffusion, and $\alpha = 2$ stands for the ballistic motion. From Figure 3, the motion of electrons is ballistic with $\alpha \sim 2$, as can be expected from the complete transparency for the whole band. By increasing the disorder strength W and keeping the average impurity site energy unchanged, A is slightly degreased, as can be seen from the comparison between the solid and dotted lines in Figure 3. This suggests the weak effect of this type of disorder on the motion of electrons. On the other hand, by varying the average impurity site energy, a large change of A is caused, as shown by the dashed line. This is due to the variation of the band width from the change of the average value of ϵ_j.

In practice, one of such impurities can be produced by attaching an atom or an atom cluster to a host chain such as conducting polymer or carbon nanotube. Condition (3) for the full transmission of the whole band requires some method of tuning the distance of the impurity from the host chain and the spacing between two host sites to which the impurity is attached. This can be realized with careful choosing of the impurity energy level and the attaching method. In a mesoscopic system such an impurity can be used for adjusting the phase of a wave function and keeping its module unchanged. This may be useful for the manipulation of quantum states in future nano-scale devices.

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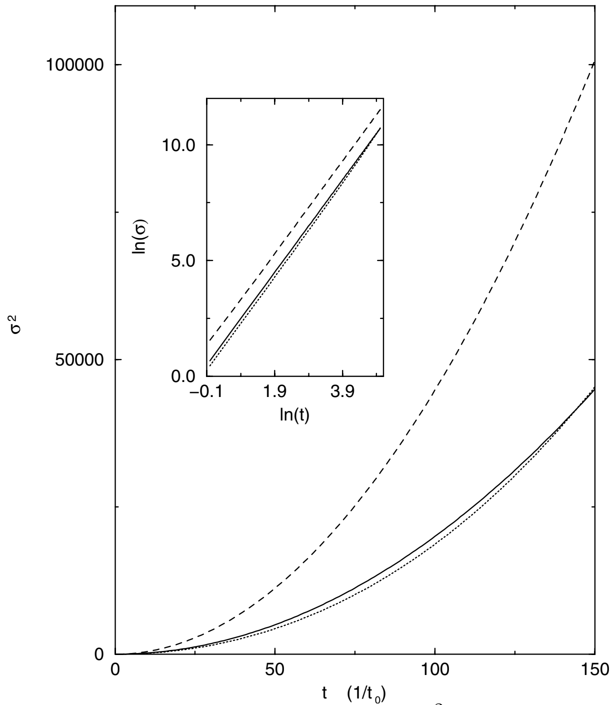

Fig. 3. Evolution of the second moment σ^2 for a wave packet. The inset is the log-log plot. Solid line: $\epsilon_j = 0$ for all impurities, corresponding to $W = 0$. It can be fitted with parameters $A = 2.0$ and $\alpha = 2.0$. Dotted line: ϵ_j's are uniformly distributed in $[-1.5t_0, 1.5t_0]$, and the obtained fitting parameters are $A = 1.606$ and $\alpha = 2.021$. Dashed line: $\epsilon_j = -t_0$ for all impurities, it is fitted with $A = 4.874$ and $\alpha = 2.009$.

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