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HOPPING OF ELECTRON LOCALIZATION POSITIONS IN 1D RANDOM SYSTEM

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We consider an electron in a 1D random adiabatically changing potential. We demonstrate that the positions of the maxima of an electron eigenstate probability density do not move even when the change of the potential is significant. We show that at the same time the main maximum hops by a distance of the order of the size of the system. We present arguments that such hopping of electron localization position happens also in two and three dimensions.

It is well established that there are two main different types of electron transport, which depend on the extended or localized nature of the eigenstates of electrons. Since Anderson[1] demonstrated localization of a quantum particle in a random potential, this phenomenon was extensively studied analytically, numerically and experimentally[2–5]. Studies included the zero-temperature properties, effect of electron–electron and spin-orbit interactions and finite temperature. Under consideration were also the resonance tunneling, wave function phase randomization, nature and stability of ensemble averages; fluctuations[6,7]; nonlinearities[8]. In all these studies randomness was related to atoms and ions with only small thermal fluctuations around their quenched positions. An experimental observation of a positron moving in a dense low temperature helium gas[9] presented an extension of the localization problem[10,11].

Light quickly moving particle sees heavy slowly (adiabatically) moving atoms as frozen. In the case, when the energy of this light particle is below the mobility edge, it is localized by a random potential. Still, slow motion of atoms may lead to the diffusion of the localization positions and hence of the light particle itself. The dynamics of motion of localization positions of a light particle might be interesting theoretically. The results of this investigation might be important for charge transfer in dense gases and liquids.

In this paper we consider an electron in a set of randomly located potential barriers. We show that in a 1D case adiabatic motion of these potential barriers leads to hopping of the localization position of an electron. We treat the electron localization position dynamics numerically. We show that this position is not moving during time interval $t \sim \tau$, where τ is the characteristic time, when potential barriers shift on average by the distance of the order of the distance a between them. Then the electron localization position hops by the distance $l_h \sim L$, where L is the size of the system. We suggest that such hopping of electron localization position happens also in two and three dimensions.

Let us first consider an electron moving in a 1D random set of infinite barriers. In this case electrons are confined in potential wells between the barriers. When the barriers move the width of the wells is changing. It results in a considerable change of the electron eigenenergies as the eigenenergy difference equals to $\Delta E \sim \hbar^2/2ml^2$, where m is the electron mass, and l is the width of the well. The motion of barriers results in their collisions and reflections. Due to these collisions positions of the barriers are fluctuating in a vicinity of a stationary position with an amplitude which is of the order of the distance between them. The same fluctuations arise for the positions of the wells and thus for the confined electrons.

Now let us suppose that the 1D barriers are high but finite. The same reasoning related to the localization positions of individual well eigenstates remains valid also in this case. The only difference is that the decay of each eigenstate probability density is related to the superposition of all barriers outside the eigenstate well, *i.e.* to the "barrier average"[12]. It is almost unchanged by the diffusion of the potential barriers. The new factor, imposed by finite barriers, is the possibility of the nearest neighbor interaction with adjacent wells. In virtue of the Sturm-Liouville theorem, 1D levels never cross (thus, they may be labelled and followed when a 1D potential adiabatically changes). The corresponding eigenenergy change is therefore $\propto 1/N$ (N is the number of sites) and very small. However, when the eigenenergy increase switches to decrease, the eigenstae changes the well[13] (and typically moves a macroscopic distance $\sim$ the size of the system).

Finally, let us assume low 1D potential barriers. Their superposition yields self-consistent deep wells, and thus very high total effective barriers[12]. This reduces the problem to the previous case. The same reasoning is applicable to any dimensionality. We verify these results

with numerical simulations for a $1D$ case.

We perform the numerical simulations for a potential $V(x)$, which is a sum of N identical δ-function potential barriers with an amplitude $V_0 > 0$. These δ-function potential barriers are located at a random set of points x_n with an averaged distance a between them, *i.e.*

$$V(x) = V_0 \sum_{n=1}^{N} \delta(x - x_n). \tag{1}$$

We find, following[14,15], the transmittance T as a function of the electron energy E. The maxima of the transmittance correspond to the electron eigenenergies[12,14]. We calculate the electron wave function $\Psi(x)$ at the eigenenergies and find the eigenstate probability density distribution $\rho(x) = \left|\Psi(x)\right|^2$. The main maximum of $\rho(x)$ determine the electron localization position (with the accuracy of the electron localization length ξ). We simulate the adiabatic motion of the δ-function potential barriers simultaneously shifting their positions by the distance $d \ll a$. We choose the shift direction (to the right or to the left) randomly for each of the δ-function potential barriers. We keep these directions to be the same until a collision of two certain δ-function potential barriers occurs after a sequence of shifts. We consider a model where colliding δ-function potential barriers are elastically reflected from each other. Therefore, we change the shift direction for both colliding δ-function potential barriers to opposite ones after a collision occurs. We calculate the transmittance $T(E)$ for the resulting potential $V(x)$ and trace the values of the eigenenergies and electron localization position.

The accuracy of electron localization position can not exceed the localization length ξ [12]. The eigenstate probability density distribution $\rho(x)$ course grained on the scale $a \ll |x - x_0| < \xi$, is given by the equation

$$\rho(x) = \rho_0 \exp\left(-\frac{|x - x_0|}{\xi}\right), \tag{2}$$

where x_0 is electron localization position, and ρ_0 is a normalization constant. Thus, to calculate the value of ξ we use the relation:

$$\frac{1}{x - x_0} \int_{x_0}^{x} \ln\left[\rho(x)\right] dx = Const - \frac{1}{2} \frac{|x - x_0|}{\xi}. \tag{3}$$

which is valid for $|x - x_0| \gg \xi$.

The specific numerical simulations were done for $N = 100$, $d = a/30$, $a = 1$ and the amplitude

$$V_0 = \frac{\hbar^2}{2ma}. \tag{4}$$

The initial positions of the δ-function potential barriers were located in the interval $0 < x < 100\,a$.

We choose the electron wave function $\Psi(x)$ in the interval $x_{n-1} < x < x_n$ in the form

$$\Psi(x) = A \exp\left[\frac{G_n}{2}\right] \cos\left[k(x - x_{n-1}) - \frac{\varphi_n}{2}\right]. \tag{5}$$

where $k = \sqrt{2mE}/\hbar$ is the wave vector and A is the overall amplitude. The two independent solutions for the wave function $\Psi(x)$ are obtained by taking the initial phase values to be equal to $\varphi_1 = 0$ and $\varphi_1 = \pi$. The initial value for the exponent G_n is $G_1 = 0$. A straightforward calculation leads then to the following formulae for the exponent G_n and the phase φ_n:

$$\exp\left(G_{n+1} - G_n\right) = 1 + 4\alpha \frac{\alpha + \tan\left(\frac{\varphi_n}{2} - k\Delta_n\right)}{1 + \tan^2\left(\frac{\varphi_n}{2} - k\Delta_n\right)}, \tag{6}$$

$$\tan\left(\frac{\varphi_{n+1}}{2}\right) = 2\alpha + \tan\left(\frac{\varphi_n}{2} - k\Delta_n\right), \tag{7}$$

$$\Delta_n = x_n - x_{n-1}, \tag{8}$$

$$\alpha = \frac{1}{2ka}. \tag{9}$$

and the transmittance $T(E)$ is given then by the expression[14,15]:

$$T = \frac{4}{\left[\exp(G) + \exp(G') + 2\right]}, \tag{10}$$

where G and G' are the values of G_{N+1} for $\varphi_1 = 0$ and $\varphi_1 = \pi$.

Typical results of the numerical simulations are presented in Fig. 1, 2. For the data shown in Fig. 1, 2 the initial eigenenergy corresponds to the initial wave vector $k = k_0 = 1.83256/a$. Using Eq. (3) we calculate the value of the localization length ξ. We find it to be equal to $\xi \approx 5 \pm 1$. The characteristic dynamics of the main maximum of the probability density distribution $\rho(x) = \left|\Psi(x)\right|^2$ is presented in Fig. 1 for a sequence of 16 shifts of the δ-function potential barriers. It is seen from Fig. 1, that within the accuracy of $\xi \approx 5$ the electron localization position eather do not move, or hops by the distance of the order of L. The characteristic dynamics of the probability density distribution $\rho(x)$ is presented in Fig. 2 on a large scale for the same sequence of 16 shifts. We show in Fig. 2 the normalized ratio $\rho(x)/\rho_{\max}$ as a function of x in the interval $20 < x < 30$, where $\rho_{\max}$ is the maximum value of $\rho(x)$ in the same interval. Fig. 2 covers only the distance $\pm\xi$ from its center, *i.e.*, just within the accuracy of the very definition of a local-

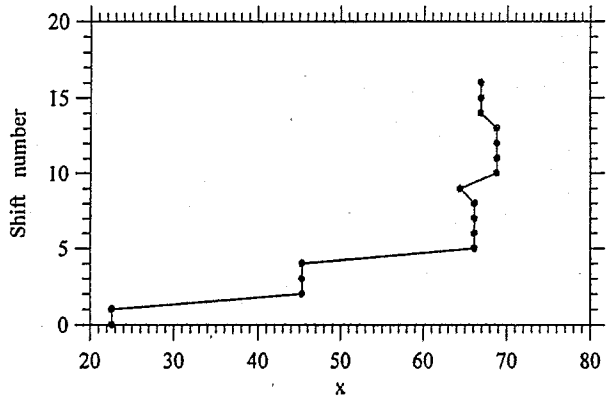

Fig. 1. Position of the main maximum of $\rho(x)$ (x-axis) calculated for a sequence of 16 shifts (y-axis).

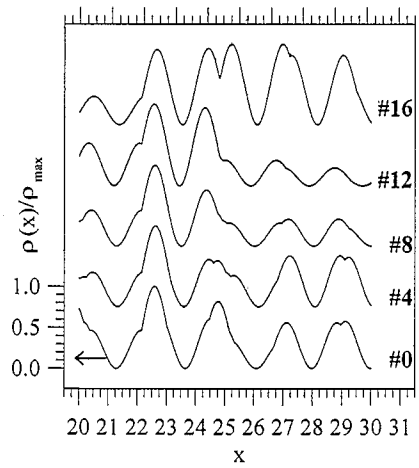

Fig. 2. Normalized probability density distribution $\rho(x)/\rho_{\max}$ for the shifts #0, #4, #8, #12, #16 from the sequence of 16 shifts, which are arbitrary lifted with respect to each other.

ization position (hence little different heights of the $\rho(x)$ maxima). Multiple nods are related to $\sim$ 10 strongly interacting potential wells. Nevertheless, it is seen from Fig. 2, that within the accuracy of a small fraction of the average distance between the potential barriers a the maxima of $\rho(x)$ are localized at the same positions while the potential $V(x)$ is changing significantly. The relative heights of these maxima are changing with the shifts of the δ-function potential barriers, which is the reason for the hopping of the main maximum of $\rho(x)$ *i.e.*, of the electron localization position.

As long as the electron localization position does not change (*i.e.*, on the time scale $t \sim \tau$), adiabatic transport on this time scale does not feel atomic motion and thus does not distinguish between gas, liquid and disordered solid with quenched atoms, which were extensively studied[2–5]. Since localization positions are randomly situated in a system[12], an electron randomly hops in a system, and one should find how the time to diffuse from one end of the system to another scales with L. Slow atomic motion results also in the change in motion of eigenenergies. It enhances or suppresses the Mott hopping, and allows for the possibility of resonance tunneling when eigenenergies in different wells coincide. Since the eigenenergy width in localization is extremely small[12], the equality of the eigenenergies with the accuracy of their width happens for a very short time only, even though atoms move slowly. The temperature, below which the resonance tunneling becomes possible, may allow for the experimental measurement of the resonance tunneling time.

We consider in this paper the case of elastic scattering of atoms which is true if the temperature of the system is relatively low. Similar reasoning as above is applicable to the case of nonelastic scattering of atoms leading to the same results.

To summarize we show that for a $1D$ random adiabatically changing potential the positions of the maxima of electron eigenstate probability density distribution do not move even when the change of the potential is significant. We show that at the same time the main maximum hops by a distance of the order of the size of the system. We suggest that such hopping of electron localization position happens also in two and three dimensions.

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