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Electron transport in one-dimensional disordered lattice

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We have studied the peculiarities of electron transport in one-dimensional disordered chain at the presence of correlations between on-site interaction and tunneling integrals. In the considered models, the disorder in host-lattice sites positions is caused by presence of defects, impurities, existence of electron-phonon interaction, etc. It is shown that for certain combination of parameters the localization of electron state inherited by a various of 1D disordered systems disappears, and electron transport becomes possible. The parameters of this transport are established.

Keywords: low-dimensional systems, disordered systems, electron transport.

1. Introduction

It is well known that in one-dimensional (1D) systems with random potential $U(r)$ and tunneling integrals $t(r)$ (where r is the coordinate) the localization of quantum states takes place [1, 2] for rather wide class of U and t. It means that all one-body wave functions are localized at some finite-size area (this size is called radius of localization R) and, hence, transport in such systems is impossible. For example, saying about electron transport, it means that transfer of energy, spin, information is impossible over 1D wires with disordered distribution of ions forming a host lattice. Note, if we consider finite size chain (with length N) and if $R \gtrsim N$ then the effects related to localization may not appear in measurements. As an example, we can cite waveguides, which with high accuracy represent one-dimensional systems with a non-ideal (disordered) surface.

The exact criteria for $U(r)$ and $t(r)$ guaranteeing the localization of quantum states are the following: Let $U(r)$ and $t(r)$ be random continuous functions with distribution densities f and g:

(i) space correlations should be absent: $\mathrm{Cov}[V(r),V(r')] = \mathrm{Cov}[t(r),t(r')] = \delta(r,r')$, $\mathrm{Cov}[V(r),t(r')] = 0$, where $\mathrm{Cov}[x,y] = \langle xy\rangle - \langle x\rangle\langle y\rangle$;

(ii) the distributions should be continuous; $f(x), g(x) > 0$ $\forall x \in (-\infty,\infty)$;

(iii) the distributions should be identical: $f(U(r)) = f(U(r'))$, $g(t(r)) = g(t(r'))$ (so-called homogeneous in mean).

Note that the proofs of corresponding theorems for (i)–(iii) are simple essentially in the case of discrete (lattice) models, where the positions of particles are bonded with host-lattice sites positions r_n, $n = 1, 2, \ldots$. That is why the main part of the investigations concerning one-body localization are carried out in the framework of discrete models.

Violation of any of these conditions makes transport possible, but of course does not guarantee its existence. In each case, it is necessary to solve the corresponding problem.

For example, in paper [2, 4, 5] in the framework of discrete Schrödinger equation was assumed the existence of correlations between U and t (i.e., requirement (i) is violated). As a result, for a certain combination of U and t, the localization is absent and electron transport takes place.

In [6–8], a 2-band model (discrete Dirac equation) with dimer correlations of potential U and discrete (Bernoulli) distribution of $f(U)$ (i.e., requirement (ii) is violated) was considered. As in the case above, for a certain combination of U parameters, the localization is absent and electron transport takes place.

The violation of condition (iii) means loss of mean homogeneity. This case is difficult to implement in practice and, hence, rarely studied.

2. Hamiltonian

In our study one-body 1D discrete Hamiltonian was chosen in the form

$$\hat{H} = -\sum_n \left(t_n \hat{c}_n^+ \hat{c}_{n+1} + t_n^* \hat{c}_{n+1}^+ \hat{c}_n \right) + \sum_n U_n \hat{c}_n^+ \hat{c}_n. \quad (1)$$

Here, index n enumerates host-lattice sites, $\hat{c}_n^+$ and $\hat{c}_n$ are the creation/annihilation operators of spin-less fermions on site n, t_n are the hopping constants and U_n is on-site potential.

The disorder in U_n and t_n is caused by the disorder in host-lattice site positions:

$$r_n = na_0 + x_n, \quad n = 0, 1, 2, \ldots . \quad (2)$$

Here, a_0 is the distance between the nearest host-lattice sites of ideal (unperturbed) lattice, and x_n are random variables, so that $-ca_0 \le x_n \le ca_0$ (in all our calculations $a_0 = 1$). The constant $0 \le c \le 1/2$ can be considered as a disorder parameter. Such choice of c allows us to avoid overlapping the host-lattice site positions r_n and facilitates the model.

Such disorder can be caused by presence of defects, impurities or phonon. As far as typical phonon frequencies ω_{ph} are much less than the frequencies of electron jumps ω_{el}, one can consider the deformations of lattice x_n as static random variables. If so, U_n describes electron-phonon on-site interaction and in the framework of Holstein model [9] it can be written as

$$U_n \sim \left(\hat{a}_n^+ + \hat{a}_n \right) = U_0 + G\left(x_{n+1} - x_{n-1} \right),$$

$$G, U_0 \in \mathbb{R}, \quad G, U_0 \ge 0, \quad (3)$$

where $\hat{a}_n^+$, $\hat{a}_n$ are the phonon creation/annihilation operators on site n (see, e.g., [2, 10, 11]) and U_0 and G are some constants.

The tunneling integrals were chosen in rather general form:

$$t_n = t(|r_{n+1} - r_n|) = Ae^{-b|r_{n+1} - r_n|},$$

where A and b are some constants. In the limit of weak disorder $c \ll 1$, one can expand t_n and in linear approximation we obtain

$$t_n = V - \Gamma(x_{n+1} - x_n),$$

where the constants $V, \Gamma \in \mathbb{C}$. Here and further, we will follow the notation from [2]. Hence, the tunneling integrals t_n can be written as

$$t_n = \sqrt{|V|^2 + |\Gamma|^2 (x_{n+1} - x_n)^2 - 2|V||\Gamma|(x_{n+1} - x_n)|\cos\theta} \times e^{i\phi_n}, \quad (4)$$

$$\tan\phi_n = \mathrm{Im}\, t_n / \mathrm{Re}\, t_n. \quad (5)$$

As it is shown in Appendix A, the complex phases ϕ_n do not affect on our results and can be omitted, and instead of (1) we will study the properties of real-valued Hamiltonian $\hat{\tilde{H}}$, which is tridiagonal with the following non-zero elements:

$$\hat{\tilde{H}}_{n,n} = U_n, \quad \hat{\tilde{H}}_{n,n-1} = -|t_{n-1}|, \quad \hat{\tilde{H}}_{n,n+1} = -|t_n|. \quad (6)$$

The proposed model with Hamiltonian (6) is similar to those, described in [2], but looks more realistic. We define the disorder in terms of random shifts of host-lattice sites with respect to "ideal" positions na_0 [see (2)]. The model described in [2] defines the disorder in terms of random distances between neighboring host-lattice sites $\Delta_{n,n+1}$. Besides the differences in distribution functions (distribution of $\Delta_{n,n+1}$ is the distribution of $x_{n+1} - x_n$), our model allows us to study consequently the transition from *weak* to *strong* disorder. Actually, an increase in Γ and G means an increase in the fluctuation of the host-lattice sites with respect to the "ideal" positions.

At the same time, in the model proposed in [2], $\Gamma = 0$ indeed corresponds to ordered chain, but any small, however nonzero values of Γ correspond to small mean distances between neighboring host sites. This, on own turn, corresponds to *strong* disorder. Moreover, as far as $\Delta_{n,n+1} \ge 0 \ \forall n$, this leads to either an increase or a decrease in all tunneling integrals t_n depending on the value of parameter $\phi - \theta$ (see, e.g., (2.1) of [2]). In our model, t_n can be larger or smaller than undisturbed value $t_n = |\Gamma|$ depending on sign of $(x_{n+1} - x_n)$ [see (4)].

In our model, the diagonal terms $U_n \sim \left(x_{n+1} - x_{n-1} \right)$ can be both positive and negative. This is physically reasonable: depending on compression or rarefication of host-lattice chain in the vicinity of nth site this term describes either energy gain or energy loss [9]. In the model proposed in [2], U_n are either all negative or all positive.

3. Results and discussion

We studied the solution of the time-dependent Schrödinger equation with Hamiltonian (6)

$$\hat{\tilde{H}} |\tilde{\Psi}(x_n, t)\rangle = i \frac{\partial |\tilde{\Psi}(x_n, t)\rangle}{\partial t} \quad (7)$$

with the following initial condition:

$$|\Psi'(x_n, t = 0)\rangle = \delta(x_n, x_0).$$

This condition corresponds to the localization of an electron at site with index $n = 0$ at time moment $t = 0$.

Motion of an electron means "spreading" of $|\tilde{\Psi}(x_n, t)\rangle$ as the function of time t. The most informative characteristics describing electron transport in terms of $|\tilde{\Psi}(x_n, t)\rangle$ is time dependence of variance $D(t)$ (see, e.g., [2, 8]):

$$D(t) = \langle x(t)^2 \rangle - \langle x(t) \rangle^2 = m^{(2)}(t) - \left(m^{(1)}(t) \right)^2. \quad (8)$$

Here, $m^{(1)}(t)$ and $m^{(2)}(t)$ are the corresponding moments:

$$m^{(k)}(t) = \langle \tilde{\Psi} | (\hat{x})^k | \tilde{\Psi} \rangle. \quad (9)$$

Note that, as it is shown in Appendix A, the moments do not depend on complex phases of off-diagonal matrix elements of the Hamiltonian.

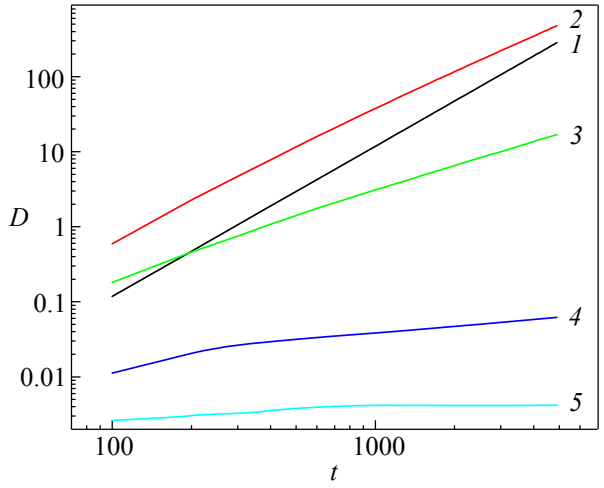

Fig. 1. (Color online) Time dependencies of the variance $D(t)$ (8) $|V|=1$, $G=|\Gamma|$ and the number of host-lattice sites $N=10000$. Curve *1* (black line) corresponds to the ordered chain ($G=0$), exponent $\alpha=2$ [see (10)]; the case of ballistic transport. Curve *2* (red line) corresponds to $G=0.25$ and $\theta=90°$, $\alpha=1.6$; the case of superdiffusive transport. Curve *3* (green line) corresponds to $G=0.2$ and $\theta=0°$, $\alpha=1$; the case of diffusive transport. Curve *4* (blue line) corresponds to $G=0.5$ and $\theta=0°$, $\alpha=0.35$; the case of subdiffusive transport. Curve *5* (cyan line) corresponds to $G=0.75$ and $\theta=0°$, $\alpha=0.01$; the case of absence of transport.

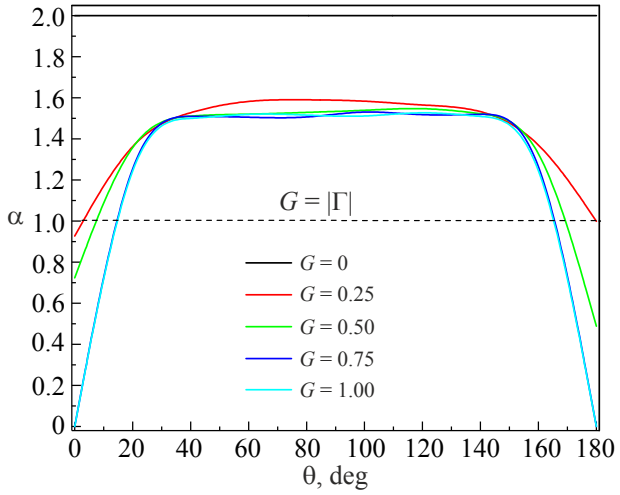

Fig. 2. (Color online) The dependencies of exponent α [see (10)] on parameter θ for different values of $G=\Gamma$. In all these calculations, $V=1$, and the number of host-lattice sites $N=20000$.

Approximation of $D(t)$ by power low dependence

$$D(t)\sim t^{\alpha},\quad t\gg 1 \tag{10}$$

allows us to establish the existence (or absence) of transport and, if transport exists, the character of the transport. For example, $\alpha=0$ corresponds to absence of transport, $0<\alpha<1$ is so-called subdiffusive transport, $\alpha=1$ is diffusive motion, $1<\alpha<2$ is superdiffusive transport, and $\alpha=2$ corresponds to ballistic (free to move) transport.

We studied the solution of (7) numerically using 8th order Runge–Kutta method. To avoid an influence of finite-size effects, we checked the probability of finding an electron on the last (Nth) site of our 1D disordered chain. In all our calculations $|\tilde{\Psi}(x_N,t)|^2<\varepsilon=10^{-10}$ for all t in the considered time range $0\le t\le N/2$.

To check the obtained result, we performed additional calculations of (8) using spectral data of operator $\hat{\tilde{H}}$ [see (6)]: the eignevalues $\{\lambda_k\}_{k=1}^{N}$ and eigenvectors $\{\psi_k(x_n)\}_{k,n=1}^{N}$. These values were obtained numerically too. Such approach is applicable for rather "small" systems with length $N\approx 1000$–3000 because calculation time of spectral data increases as N^3. In terms of spectral data, the wavefunction of (7) can be written as

$$|\tilde{\Psi}(x_n,t)\rangle=\sum_{k=1}^{N}\psi_k(x_n)\psi_k(x_0)\mathrm{e}^{i\lambda_k t}. \tag{11}$$

The vectors $\psi_k(x_n)$ are real-valued and complex conjunction in (11) is omitted. The results obtained using (7) and (11) are in full agreement.

Typical dependencies $D(t)$ for $N=10000$ and certain combinations of the parameters G, Γ, and θ are presented in double-log scale in Fig. 1. In all these calculations $V=1$. One can see that all possible transport regimes can be realized in the framework of proposed model: from localization of states up to ballistic transport.

Approximation of $D(t)$ by the expression (10) at $t\gg 1$ allows us to obtain the dependencies of exponent α on tunneling (V, Γ, θ) and hopping (G) parameters. These dependencies are shown in Fig. 2. One can see that in rather wide range of $0<G=|\Gamma|\le 1$ and $20°\lesssim\theta\lesssim 160°$ superdiffusive transport regime is realized. For $0<\theta\lesssim 20°$ and $160°\lesssim\theta<180°$ transport regime depends on $G,|\Gamma|$: if $0<G=|\Gamma|<0.22$ the transport is superdiffusive; if $G=|\Gamma|>0.22$ the transport is subdiffusive. If $\theta=0°$ or $\theta=180°$ and $G=|\Gamma|>0.5$ electron transport is absent.

It should be noted that the proposed model was formulated within the framework of the linear expansion of on-site potential U_n (3) and tunneling integrals t_n (4) with respect to random lattice deformations x_n (2), i.e., in the limits of $G\sim|\Gamma|\ll|V|$. Nevertheless, we extended the area of G and $|\Gamma|$ up to $G,|\Gamma|\le 1$. In this case, of course, the Hamiltonian (6) can be considered as model only.

As was shown in [2], the case of $G=|\Gamma|$ is of special interest due disappearing the scattering. Hence, this case is the most prospective for electron transport. An influence of G and Γ on $D(t)$ is presented in Fig. 3.

An absence of transport at $\theta=0°,180°$ and $G=|\Gamma|>0.5$ (see Fig. 4) is of special interest. To understand the reason of such a peculiarity, we performed additional investigations using Lyapunov exponent [3, 8].

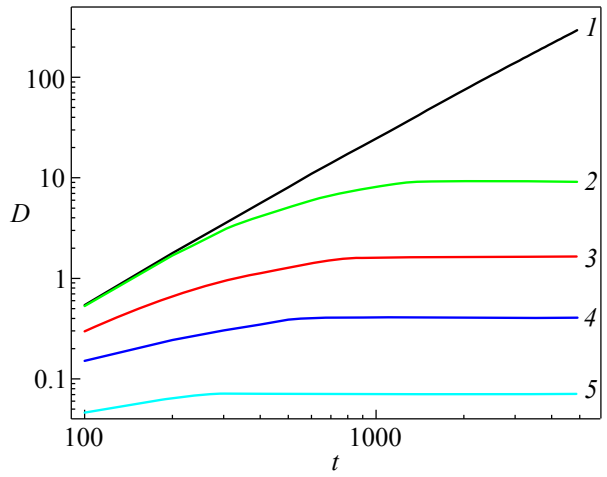

Fig. 3. (Color online) Time dependencies of the variance $D(t)$ (8) in double-log scale. In all these calculations, $|V|=1$, $\theta=90°$ and the number of host-lattice sites $N=10000$. Curve *1* (black line) corresponds to $G=|\Gamma|=0.5$, exponent $\alpha=1.5$ [see (10)]. Curve *2* (red line) corresponds to $G=0.5$ and $|\Gamma|=0$, $\alpha=0$. Curve *3* (green line) corresponds to $G=0$ and $|\Gamma|=0.5$, $\alpha=0$. Curve *4* (blue line) corresponds to $G=0.5$ and $|\Gamma|=1$, $\alpha=0$; Curve *5* (cyan line) corresponds to $G=1$ and $|\Gamma|=0.5$, $\alpha=0$.

Applying Fürstenberg theorem [12, 13], one can write Lyapunov exponent γ as the following:

$$\gamma(\lambda)=\lim_{n\to\infty}\frac{1}{n}\ln\left(\left\|\prod_{k=n}^{1}\hat{T}_k(\lambda)\right\|\right). \qquad (12)$$

Here, the transfer matrices $\hat{T}_k$ have the form [3, 12, 8]

$$\hat{T}_k(\lambda)=\begin{pmatrix}\dfrac{U_k-\lambda}{|t_k|} & -\dfrac{|t_{k-1}|}{|t_k|}\\ 1 & 0\end{pmatrix}. \qquad (13)$$

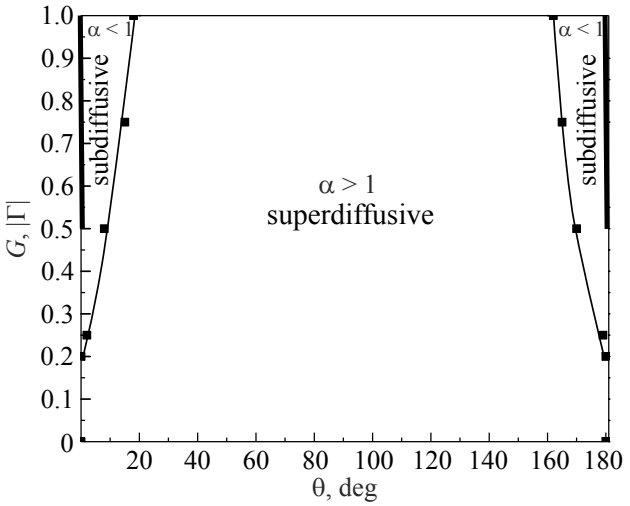

Fig. 4. "Phase diagram" based on the analysis of the dependence of exponent α (10) on the parameters $G=|\Gamma|$ and θ. Wide vertical solid lines at and $\theta=180°$ correspond to localization area ($\alpha=0$).

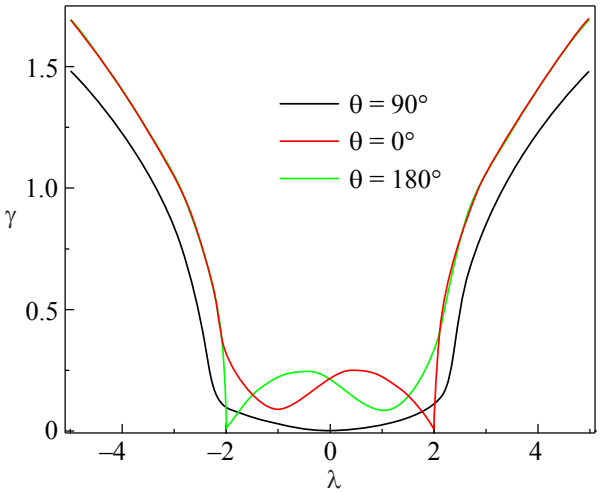

Fig. 5. (Color online) The dependencies of the Lyapunov exponent γ on energy λ. $|V|=1$, $G=|\Gamma|=0.5$ and the number of host-lattice sites $N=10000$. Black line corresponds to $\theta=90°$. Red line corresponds to $\theta=0°$ and green line corresponds to $\theta=180°$.

As far as typical values of Lyapunov exponent $\gamma\sim R^{-1}\sim D^{-1/2}(t\to\infty)$, where R is the localization radius, the zeros of γ indicate on possible delocalization of the states (more exactly, the condition $\gamma=0$ is necessary, but not sufficient for delocalization of the states, see, e.g., [3, 8]).

The results of our calculations are presented in Fig. 5. We see that at $\theta=90°$ the behavior of Lyapunov exponent γ in the neighborhood of root $\gamma(0)=0$ is $\gamma(\lambda)\sim\lambda^{\beta}$, where $\beta>1$. At the same time at $\theta=0°$ and $\theta=180°$ the behavior Lyapunov exponent γ in the neighborhood of roots $\gamma(\pm2)=0$ is $\gamma(\lambda)\sim\left(\pm(2-\lambda)\right)^{\beta}$, where $\beta<1$. It was shown in [3, 8] that such root-like singularities may not lead to delocalization of states.

4. Conclusions

We have studied electron transport properties in 1D disordered chain in the framework of one-body Schrödinger equation. In the presented model the disorder is caused by an influence of defects, impurities or phonons on the positions of ions, forming host-lattice chain. We have shown, that such disorder affects both on the values of on-site potential U and on tunneling integrals t. Just due to the correlations between random U and t electron transport becomes possible. We have studied and influence of model parameters on this transport. The areas of localization, superdiffusion and subdiffusion transport have been established. It has been shown that for certain combinations of model parameters ($|V|=1$, $G=|\Gamma|>0.5$ and for $\theta=0°,180°$) electron transport is impossible, despite the fact that Lyapunov exponent vanishes in the considered energy region.

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Appendix A

Tridiagonal Hermitian matrix $\hat{H}$ (1) can be reduced to symmetric (real-valued) form $\tilde{\hat{H}}$ using unitary transformation

$$\tilde{\hat{H}} = \hat{U}^{-1}\hat{H}\hat{U}, \tag{A1}$$

where unitary matrix $\hat{U}$ is diagonal:

$$U_{11} = 1, \quad U_{nn} = \mathrm{e}^{-i\sum_{k=1}^{n-1}\alpha_k}, \quad n = 2, 3, \ldots.$$

Here, α_k are the complex phases of off-diagonal elements (4), (5).

Let $|\Psi(x_n,t)\rangle$ be the solution of time-dependent Schrödinger equation with Hamiltonian $\hat{H}$ (1) and $|\tilde{\Psi}(x_n,t)\rangle$ be the corresponding solution of Schrödinger equation with Hamiltonian $\tilde{\hat{H}}$ (6), (14).

We will show that the unitary transformation do not affect on the moments $m^{(k)}(t)$ (9), i.e.,

$$m^{(k)}(t) = \langle\Psi|(\hat{x})^k|\Psi\rangle = \langle\tilde{\Psi}|(\hat{x})^k|\tilde{\Psi}\rangle,$$

$$\left((\hat{x})^k\right)_{\alpha,\beta} = \alpha^k\delta_{\alpha,\beta},$$

and, hence, do not affect on $D(t)$ (8).

According to the definition,

$$m^{(k)}(t) = \sum_n (x_n)^k |\Psi(x_n,t)|^2.$$

The relationship between $|\Psi\rangle$ and $|\tilde{\Psi}\rangle$ is

$$\Psi_j = \sum_{\alpha=1}^{N} U_{j,\alpha}\tilde{\Psi}_\alpha.$$

Hence,

$$m^{(k)} = \sum_{j=1}^{N}(x^k)_{j,j}\Psi_j\Psi_j^*$$

$$= \sum_{j=1}^{N}\sum_{\alpha=1}^{N}\sum_{\beta=1}^{N}(x^k)_{j,j}U_{j,\alpha}U_{j,\beta}^*\tilde{\Psi}_\alpha(\tilde{\Psi}_\beta)^*.$$

As far as $\hat{U}$ is unitary, $U_{j,\beta}^* = U_{\beta,j}^{-1}$. Thus,

$$m^{(k)} = \sum_{j=1}^{N}\sum_{\alpha=1}^{N}\sum_{\beta=1}^{N}(x^k)_{j,j}U_{j,\alpha}U_{\beta,j}^{-1}\Psi'_\alpha(\Psi'_\beta)^*$$

$$= \sum_{j=1}^{N}\sum_{\alpha=1}^{N}\sum_{\beta=1}^{N}U_{\beta,j}^{-1}(x^k)_{j,j}U_{j,\alpha}\Psi'_\alpha(\Psi'_\beta)^*$$

$$= \sum_{j=1}^{N}\sum_{\alpha=1}^{N}\sum_{\beta=1}^{N}(\tilde{x}^k)_{\beta,\alpha}\Psi'_\alpha(\Psi'_\beta)^*,$$

where

$$\left(\hat{\tilde{x}}^k\right)_{\beta,\alpha} = \sum_{j=1}^{N}U_{\beta,j}^{-1}(x^k)_{j,j}U_{j,\alpha}$$

are the matrix elements of operator $\hat{x}^k$ in new basis. As far as $\hat{x}^k$ and $\hat{U}$ are diagonal:

$$\left(\hat{\tilde{x}}^k\right)_{\beta,\alpha} = \sum_{j=1}^{N}U_{\beta,j}^{-1}(x^k)_{j,j}U_{j,\alpha}$$

$$= \sum_{j=1}^{N}U_{\beta,j}^{-1}\delta_{\beta,j}(x^k)_{j,j}U_{j,\alpha}\delta_{\alpha,j} = \left(x^k\right)_{\beta,\alpha}.$$

Finally, we have

$$m^{(k)} = \langle\Psi|(\hat{x})^k|\Psi\rangle = \sum_{\alpha=1}^{N}\sum_{\beta=1}^{N}(\tilde{x}^k)_{\alpha,\beta}\tilde{\Psi}_\alpha(\tilde{\Psi}_\beta)^*$$

$$= \langle\tilde{\Psi}|\hat{x}^k|\tilde{\Psi}\rangle.$$

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Транспорт електронів в одновимірній невпорядкованій ґратці

V. Slavin, Y. Savin, M. Klimov, M. Kiyashko

Досліджено особливості транспорту електронів в одновимірному невпорядкованому ланцюжку за наявності кореляцій між амплітудами взаємодії електронів з вузлами ґратки та амплітудами тунелювання. У розглянутій моделі невпорядкованість позицій вузлів ґратки зумовлена наявністю дефектів, домішок, електрон-фононною взаємодією тощо. Показано, що за певної комбінації параметрів локалізація електронних станів зникає і стає можливим транспорт електронів. Параметри цього транспорту встановлено.

Ключові слова: низьковимірні системи, невпорядковані системи, електронний транспорт.