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State vector evolution localized over the edges of a square tight-binding lattice

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We study the time evolution of a state vector in a square tight-binding lattice, focusing on its evolution localized over the system surfaces. In this tight-binding lattice, the energy of atomic orbital centred at surface site is different from that at the interior (bulky) site by an energy shift U. It is shown that for the state vector initially localized on a surface, there exists an exponential law ($y = ae^{x/b} + y_0$) determined by the absolute value of the energy shift, $|U|$, which describes the transition of the state evolving on the square tight-binding lattice, from delocalized over the whole lattice to localized over the surfaces.

Keywords: Anderson localization, surface states, state vector evolution
PACC: 7200, 7290

1. Introduction

Edge states or surface states, which are localized at a boundary of a system, have significant effects on physical phenomena, such as the zero bias conductance peak structure in anisotropic superconductivity,[1,2] single-layer graphite,[3] and the boundary local moment on an edge of hexagonally bonded honeycomb sheets consisting of B, N, and C atoms.[4] Especially, in a graphene, it is now widely understood that there exist important edge states, which are related to the chiral symmetry of the system and the Dirac cone spectrum. In metal–semiconductor interfaces, an interface state, known as the metal induced gap state, plays an important role in understanding Fermi level pinning.[5] In disordered one-dimensional solids (disordered chain) with short-range interaction, the Anderson localization is well known to occur, i.e. the energy spectrum is pure point and eigenstates are exponentially localized. It was found that the localization of eigenstates has a profound influence on the propagation of an initially localized state: not only slowing but also effectively blocking this propagation through the chain.[6−8] Similarly, in disordered two-dimensional or three-dimensional solids that are due to impurities, interfaces, boundaries and atoms non-uniformly distributed in the materials, there could be localized eigenstates, in particular surface states, consequently influencing the propagation of an initially localized state.[9]

Self-consistent calculations of metal surfaces indicated different ionization energies for surface sites and bulky sites.[10] This is expected realistically in metallic particles with clean surfaces and in those with chemisorbed atoms. Recently, Gascón and Pastawski[11] therefore used a simple tight binding model with shifts in ionization energy of surface atoms with respect to bulky atoms to explore the effects of surface states, which contribute to an over-broadening of the NMR absorption spectra, determined by the Knight shift distribution of magnetic nuclei. In realistic materials, including nanostructure materials such as nanoparticles, nanoislands[12] and nanowires with a coating, such as Ag nanowires with Ni coating,[13] Au coated ZnO nanowires,[14] the energies of atomic orbital centred at surface site are different from those of bulky atoms: not only smaller but also sometimes larger than those of bulky atoms.

Grain refinement can strengthen the metals but often simultaneously lead to a pronounced reduction in conductivity. This is due to the introduction of more grain boundaries, which are barriers to intra-grain dislocation motion, thereby making the material harder to deform, and also increase the scattering of conducting electrons, thus increasing the electrical resistivity of the metal.[15] In nano-materials, there are a large numbers of grain boundaries, and the electrical resistivity of nano-material is determined by its

composition (nanoparticles) and grain boundaries. In order to understand the electrical resistivity of nanomaterial, we use the tight-binding model provided in Ref.[11] to investigate the time dependence of a state vector influenced by surface or edge (acts as grain boundary) in which the surface site has an additional energy shift U with respect to bulky site.

2. Model

For simplicity, we here consider a two-dimensional lattice, whereon N ($N = L \times L$) sites are arranged on a two-dimensional square lattice. We believe that qualitatively similar results would be displayed by the three-dimensional square lattice. Similar to the Hamiltonian in Ref.[11], the model Hamiltonian here is expressed as

$$H = \sum_{i=1}^{N} E_i c_i^+ c_i + \sum_{j>i}^{N} \sum_{i=1}^{N} (V_{ji} c_j^+ c_i + V_{ij} c_i^+ c_j), \quad (1)$$

where E_i is the energy of atomic orbital centred at site i of the lattice. $V_{ij} = V$ that is the kinetic energy involved in hopping between the nearest neighbouring sites i and j. We define surface site as the site that is centred at the surface (on the edge) of the lattice and has additional energy shift U. The remaining sites are bulky (or interior) sites with $E_i = E$, even though they may belong to the faces of the lattice with unshifted site energies, thereby different ratios of surface to bulk are allowed to be regarded as N constants. It is pointed out that periodic boundary conditions are not imposed on this model.

We restrict our attention to a single particle (or an excitation) propagating through the square lattice. The dynamics can be described in a position-occupation basis of which the states are denoted by $\{|i\rangle, i = 1, ..., N\}$ such that $|i\rangle = |00...1_i...0\rangle$, where i refers to a particular site occupied by an excitation, N denotes the total number of sites. Correspondingly, $c_i^+ |0\rangle = |i\rangle$, $c_i |i\rangle = |0\rangle$, and $c_i |j\rangle = 0$, $(i \neq j)$, where $|0\rangle$ denotes the vacuum state.

In such a position-occupation basis, the matrix representation of Eq.(1) is easy to construct and diagonalize numerically, accordingly we can study the time evolution of any state vector by using the evolution operator $U(t) = \mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar}$, but unfortunately, the exact diagonalization is restricted to a small system size. It is also very CPU time-consuming even if the matrix representation is exactly diagonalized into a system of 961 sites. Contrary to the exact diagonalization, the second order differencing scheme,[16−18] which consists of a given initial state $|\psi(0)\rangle$, is expressed as

$$|\psi(t + \Delta t)\rangle = |\psi(t - \Delta t)\rangle - 2\mathrm{i}\Delta t H |\psi(t)\rangle, \quad (2)$$

which allows one to investigate the dynamics on very large systems with about one million sites. To obtain a good accuracy for our results, the evolution time t ($t = m\Delta t$, m=0,1,2,...) is chosen to be not too long, however.

Using the exact diagonalization method for Hamiltonian, we explore the dynamics of a small size system with site number $N = L \times L$, $L \sim 10$, 20, and use the second order differencing scheme to investigate larger systems in a reasonable evolution time.

3. Simulation and discussion

In the course of our simulation, the energy of atomic orbital centred at bulky site i is set to be $E_i = E = e$, the hopping matrices between the nearest neighbouring sites i and j are fixed as $V_{ji} = V = -0.1e$, while the energy of atomic orbital centred at surface site has an additional energy shift U with respect to bulky site, that is, $E_i = E - U$, where U is chosen from the interval [–0.9e, 0.9e], attempting to include realistic materials and fictitious materials. Note that e denotes the energy scale wherewith to scale time as $\hbar/e$.

We now study the dynamics of a small size system by using the exact diagonalization method. By diagonalizing numerically the matrix of Eq.(1), one can obtain all values of eigenvalue ε_k and eigenvector $|\xi_k\rangle$ of the Hamiltonian H. Introducing energy shift to surface sites means 'disordering' the lattice. As mentioned in Section 1, this would induce the occurrence of surface states, whose projections in interior sites are very small or even naught. Figure 1 shows two such states as examples.

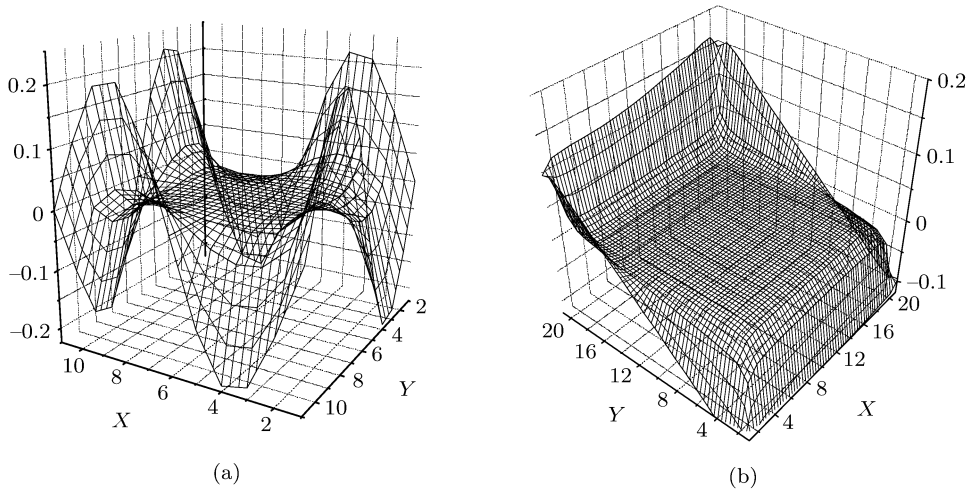


Fig.1. Two examples for surface states whose eigenvalue ε=0.322 in the lattice of L=11, U=0.5 (a), and ε=0.280 in the lattice of L=21, U=0.5 (b).

With the knowing of eigenvalues ε_k and eigenvectors $|\xi_k\rangle$ of the Hamiltonian H, the developed state $|\psi(t)\rangle$, originating from an arbitrary initial state $|\psi(t=0)\rangle$ ($|\psi(t=0)\rangle = \sum_{i=1}^{N} b_i |i\rangle$, where $\sum_{i=1}^{N} {b_i}^2 = 1$), is thus obtained as[6]

$$\begin{aligned}|\psi(t)\rangle &= \sum\nolimits_k \langle\xi_k|\psi(t=0)\rangle \exp(-\mathrm{i}\varepsilon_k t/\hbar)\,|\xi_k\rangle \\ &= \sum\nolimits_{i=1}^{N} \sum\nolimits_k b_i \langle\xi_k|i\rangle \exp(-\mathrm{i}\varepsilon_k t/\hbar)\,|\xi_k\rangle\,.\end{aligned} \tag{3}$$

In the case where the initial state, $|\psi(t=0)\rangle$, is selected to be localized on a edge, say, on the left edge of the square lattice, that is, $|\psi(t=0)\rangle = \frac{1}{\sqrt{L}} \sum_{i_l=1}^{L} |i_l\rangle$, thereby a particle is imagined as being initially localized on the left edge), the $|\psi(t)\rangle$ becomes $|\psi(t)\rangle = \frac{1}{\sqrt{L}} \sum_k \sum_{i_l}^{L} \langle\xi_k|i_l\rangle \exp(-\mathrm{i}\varepsilon_k t/\hbar)\,|\xi_k\rangle$, consequently we obtain the probability $P_{m,l}(t)$, with which at time t the particle initially localized on the left edge is found at site m, as

$$P_{m,l}(t) = \left| \sum_k \sum_{i_l}^{L} \frac{1}{\sqrt{L}} \langle\xi_k|i_l\rangle \langle m|\xi_k\rangle \exp(-\mathrm{i}\varepsilon_k t/\hbar) \right|^2 . \tag{4}$$

Consider the dynamics of a particle initially localized on the left edge of a small square lattice with 441 (N=21×21) sites. From Fig.2, the probability P_{in} with which the particle is found to be at interior site is shown as a function of time t. Figure 2(a) is for the cases of U= 0, 0.2, 0.5. In these cases only the outmost layer does consist of the surface of the lattice. For the system of U=0, i.e. no difference was introduced between the energies of atomic orbital E_i of all bulky and surface sites, the value of P_{in} fluctuates mightily with time t around a largest value,

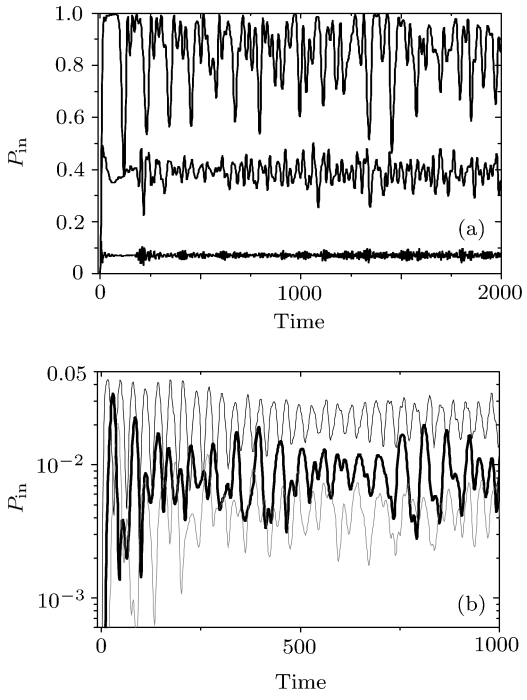


Fig.2. Curves for probability P_{in} versus time t in some systems characterized by the thickness of surface (or coating) and the energy shift U. The size of each system is N=21×21. (a) From top to bottom, U= 0, 0.2, 0.5, respectively. The thickness of surface for each system is one. (b) The grey, the dark grey and the light grey lines are for the case of U=0.5 with the thicknesses being 2, 4, and 6, respectively.

relative to the other cases. It implies that the particle propagates over the whole lattice. For the systems of U=0.2 and 05, the values of $P_{\rm in}$ are smaller than that in the system of U=0, from which it may be concluded that in the systems with a large energy shift in surface sites, the particle propagates mainly or even exclusively over the surface layer, rarely penetrating into the interior layer of the system. In order to involve the material with a coating or the nanoparticle 'coated' by grain boundary in our study, the outmost layer together with some layers near to the outmost is referred to as the coating, and the layer is called 'surface layer' correspondingly. Figure 2(b) illustrates that the thicker the coating is, the smaller the probability $P_{\rm in}$ will be. This means that the degree of the particle propagating over the coating increases with the increase of the coating thickness.

The system we study is of finite size, and the dynamics of the particle initially localized on the left edge therefore describes its propagation and reflection in the system. Figure 2 shows the dynamics in a shorter period of time, say, $0 \le t \le 2.0 \times 10^3$. To obtain the probability distribution of the particle in the system, we investigate the averaged probability with which the particle is found to be at site i. Note here that the probability is averaged over the evolution time. From expression (4), we obtain

$$P_{m,l} = \lim_{T\to\infty} \frac{\int_0^T P_{m,l}\,(t)\,\mathrm{d}t}{T} = \sum_k \sum_{i_l=1}^{L} \left[\frac{1}{\sqrt{L}} \langle \xi_k | i_l \rangle \langle m | \xi_k \rangle\right]^2, \qquad (5)$$

where $P_{m,l}$ denotes the averaged probability with which a particle initially localized on the left edge is found to be at site m. According to expression (5), we have the averaged probability distributions in the systems with U and the thicknesses being 0.0, 1; 0.2, 1; 0.5, 1; 0.2, 2; 0.5, 4; and 0.5, 6, respectively (see Fig.3). From Fig.3 it follows that the degree of localization of the particle over the surface or coating increases with energy shift U and coating thickness increasing.

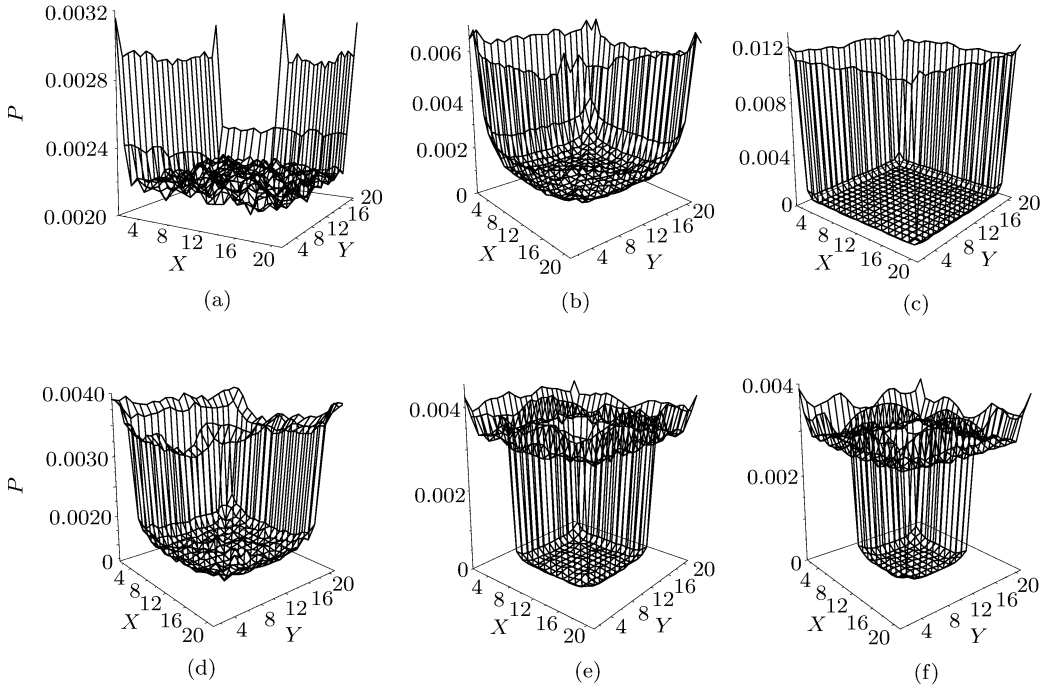


Fig.3. The averaged probability distributions in some systems distinguished by the energy shift U and the thickness of the surface, where panels (a), (b), and (c) are for the systems each with a thickness of 1 and U=0.0, 0.2, 0.5, respectively; panel (d) is for the system with a thickness of 2 and U= 0.2; panels (e) and (f) are for the systems of U=0.5 with the thicknesses being 4 and 6, respectively.

In the systems of $U \neq 0$, there are some eigenvectors which are localized over the surface layer (i.e. their components on interior sites are very small or even naught), and whose localization at the surface site is nonvanishing (see Fig.1). The variation of U would change the number and the configurations of such eigenvectors. From expression (5), we know that the propagation of particle localized mainly over the surface layer is related to the fact that the projections of the initially localized state have a significant magnitude only for several such localized eigenvectors, while the magnitudes of the projections on the other eigenvectors including delocalized eigenvectors almost vanish.

The systems mentioned above only roughly reflect their edge effect or surface effect by a difference in energy between the atomic orbital centred at surface site to that at the interior sites. Before going further, we first set up such a coordinate system in the square lattice that i_x=1, 2, ..., L, from left to right; and j_y= 1, 2, ..., L, from bottom to top. Furthermore, a distance from the geometry centre of the square lattice is arranged to each site (i_x, j_y), so that $R_{i_x,\ j_y} = \sqrt{(i_x - c_x)^2 + (j_y - c_y)^2}$, where c_x and c_y are coordinates of the geometry centre. At any time t, the probability distribution over $R_{i_x,\ j_y}$ is easy to obtain and so is the mean position R of the particle relative to the centre (c_x, c_y). To expose the edge effect as completely as possible, we take an average of R over the whole evolution time and study how the averaged R depends on the characteristic quantity U. In the following, the averaged R is denoted by $< R >$, and for convenience, $< R >$ is normalized as $< R > /R_{\max}$, where $R_{\max} = \sqrt{(1 - c_x)^2 + (1 - c_y)^2}$. In a strongly disordered macroscopic system, the wavefunctions decay exponentially away from the specific site at which the carrier is present. This means that there is no long-range wavelike behaviour in the carrier character. The standard indicator that depicts the degree of localization over the edge of system is the localization length from the edge. For a nanoscopic system, however, the localization length from the edge does not work well, since it may be larger than the size of nanoscopic system. We find that for a nanoscopic system, $< R > /R_{\max}$ is a good indicator to characterize the degree of the evolution of state localized on the edge of system.

Using expression (5), we acquire a function $< R > /R_{\max}$ that depends on U, for two system sizes, i.e. N=11×11 and N=21×21, separately (see Fig.4). $< R > /R_{\max}$ reflects the following behaviours of averaged probability distribution: (1) the smaller the value of $< R > /R_{\max}$ is, the more deeply the particle will penetrate into the interior layer, i.e. the smaller the value of $< R > /R_{\max}$ is, the higher the degree of delocalization of the propagation will be; (2) the larger the value of $< R > /R_{\max}$ is, the smaller the probability with which the particle is found in interior layer will be, i.e. the larger the value of $< R > /R_{\max}$ is, the higher the degree of localization over surface layer of the propagation will be. That may be confirmed by comparing Fig.4 with Fig.3. From Fig.4 we find that the function $< R > /R_{\max}$ is even with respect to U, that is, $< R > /R_{\max}$ depends on the absolute value of energy shift, $|U|$. With the increase of absolute value $|U|$, the value of $< R > /R_{\max}$ increases according to an exponential law (beginning with some value of $|U|$), i.e. $y = ae^{x/b} + y_0$, where y and x denote $< R > /R_{\max}$ and $|U|$ respectively. For the system with N=11×11, the parameters a, b and y_0 are –0.48914±0.00921, –0.14661± 0.00203 and 0.81099± 0.00045, respectively; while for the system with N=21×21, a=–0.4539±0.01038, b=–0.15316± 0.004 and y_0=0.811± 0.00127 respectively. So we say that there exists an exponential law that describes the transition of the particle propagating on the square tight-binding lattice, from delocalized over the whole lattice to localized over the surface of lattice. We point out that there exist exponential laws similar to the above in systems with the thicknesses of surface being larger than one.

To consider the system larger than the mentioned above in size, we will use the second order differencing scheme as depicted in Eq.(2). In Refs.[16, 17], Eq.(2) was applied to explore the time evolution of a wavepacket in the tilings, and it was numerically integrated in time steps of 0.05 till t=10^4. Similarly, we here take the time step Δt=0.01 and integrate Eq.(2) till $t = T = 10^4$ (i.e. $0 < t \leq T = 10^6 \Delta t$). In this case, Eq.(5) becomes $P_{m,l} = \left[\int_0^T P_{m,l}\,(t)\,\mathrm{d}t\right] \Big/ T$, where T=10^4, as a result, we obtain the important quantity $< R > /R_{\max}$ for each system.

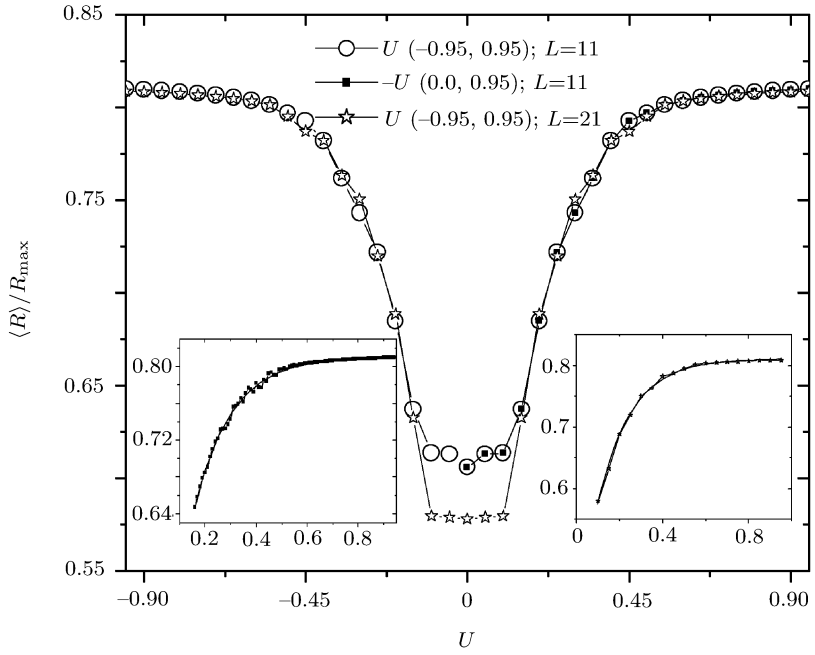


Fig.4. Curves for $< R > /R_{\max}$ versus U in two systems with size L=11 and 21, separately, where the thickness of surface is one for each system and the two insets, where the left inset is for the system of L=11 and the right one for the system of L=21, show the exponential law of $< R > /R_{\max}$ with respect to U.

From Fig.5, which comes from the second method, $< R > /R_{\max}$ is shown as a function of U in the interval of [0.0, 0.9] and system size L, where $N = L \times L$. The exponential law also holds for systems with different system sizes in the evolution time $0 \leq t \leq T$.

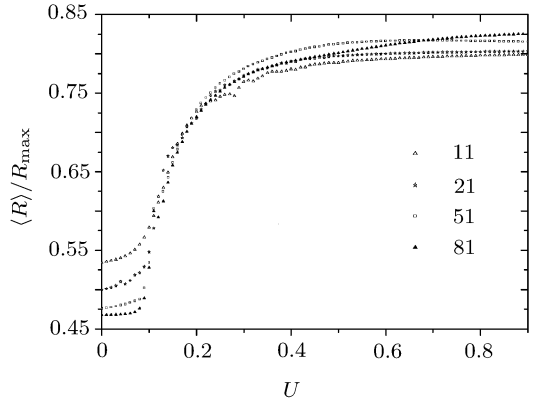


Fig.5. Curves for $< R > /R_{\max}$ versus U in some systems with size L =11, 21, 51, and 81, separately, with the thickness of surface being one for each system.

The values of parameters a, b and y_0 in the exponential law, $y = ae^{x/b} + y_0$, are shown in Table 1 for different values of system size L. One can find that even for the same system, there exists a difference between the functions of $< R > /R_{\max}$ with respect to U, obtained by using the first method and the second method, separately. This difference results from the fact that the evolution time that we adopted is finite in the second method, that is, $< R > /R_{\max}$ in the second method was averaged over finite time T, not over infinite time as used in the first method. Fortunately, however, as an approximate method for the Schrödinger equation, the second order differencing scheme, for our case, is qualitatively efficient, and consequently it exhibits the law of $< R > /R_{\max}$ with U like that in the first method.

Table 1. The parameters in $y = ae^{x/b} + y_0$, where y is substituted for $< R > /R_{\max}$ and x for U..

size L	a	b	y_0
11	–0.56658	–0.10221	0.79582
	±0.01388	±0.00197	±0.00066
21	–0.7196	–0.08887	0.79995
	±0.02647	±0.00223	±0.00093
51	–0.78733	–0.09161	0.81498
	±0.01862	±0.0018	±0.0011
81	–0.82268	–0.080792	0.80272
	±0.03072	±0.00252	±0.0016

Our model is also used to simulate a single particle (i.e. a carrier) or particles (carriers), among which there is no interaction, propagating from left to right through the lattice. For the lattice with the energy of

atomic orbital centred at surface site being different from those of bulky atoms, the carrier initially localized on the left edge is scattered by bulky atoms, that is, all bulky atoms act as a barrier. The exponential law ($y = ae^{x/b} + y_0$), which is determined by the absolute value of the energy shift, $|U|$, and describes the transition of the state evolving on the square tight-binding lattice, from delocalized over the whole lattice to localized over the surfaces, is helpful for understanding the electrical resistivity of nano-material. The larger the value of $|U|$ is, the higher the degree of localization over surface layer of the propagation will be, i.e. the smaller the transmission coefficient for carrier propagating from left to right through the interior of system or the larger the scattering cross section of bulky sites will be. In macroscopic conductors, the resistance that is found to exist at their contact is related to the bulky conductivity and to the dimensions of the conductor as well. In short, this relationship is expressed as $R = L/(\sigma A)$, where σ is the conductivity and L and A are the length and the cross-sectional area of the conductor, respectively. For a two-dimensional conductor, such as a thin sheet of metal, the conductivity is the conductance per square, and the cross-sectional area is just the width W. For the bulky nanomaterial that is comprised of nanoparticles, the carriers initially localized on grain boundaries propagate over the grain boundaries, rarely penetrating into the interior of nanoparticles. It means that the cross-sectional area of bulky nanomaterial is smaller than that of its conventional counterpart, and this is why the resistance of bulky nanomaterial is often larger than that of its conventional counterpart. From the mentioned above, one can conclude that reducing the difference between the energy of atomic orbital centred at surface site or at grain boundary and that at the interior (bulky) site may be an effective way to reduce the resistance of bulky nanomaterial.

4. Conclusion

In this paper we have studied the time evolution of a state vector initially localized on a surface of a square tight-binding lattice in which the energy of atomic orbital centred at surface site is different by an energy shift U from that of the interior (bulky) site. It is found that for the state vector initially localized on a surface, there exists an exponential law ($y = ae^{x/b} + y_0$) determined by the absolute value of the energy shift, $|U|$, which describes the transition of the state evolving on the square tight-binding lattice, from delocalized over the whole lattice to localized over the surfaces. We point out that there is no qualitative difference between the results obtained in the case of the state vector initially localized only at on only a surface site and those obtained in the case of the state vector initially localized on an edge of system. The model is two-dimensional, but qualitatively similar results would be displayed by a three-dimensional square lattice. Note that our model reflects the fact that in some realistic materials, there is the difference between the energy of atomic orbital centred at surface site and that centred at the bulky site.[10,19] So our results may be helpful for essentially understanding some properties of realistic materials such as the electrical conductivity, in particular, the electrical conductivity of nanostructure materials.

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