Universal scheme to generate metal–insulator transition in disordered systems

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Abstract
We propose a scheme to generate metal–insulator transition in the random binary layer (RBL) model, which is constructed by randomly assigning two types of layers along the longitudinal direction. Based on a tight-binding Hamiltonian, the localization length is calculated for a variety of RBLs with different cross section geometries by using the transfer-matrix method. Both analytical and numerical results show that a band of extended states could appear in the quasi-one-dimensional RBLs and the systems behave as metals by properly tuning the model parameters, due to the existence of a completely ordered subband, leading to a metal–insulator transition in parameter space. Furthermore, the extended states are irrespective of the diagonal and off-diagonal disorder strengths. Our results can be generalized to two- and three-dimensional disordered systems with arbitrary layer structures, and may be realized in Bose–Einstein condensates.

1. Introduction
One of the most important issues in condensed-matter physics is Anderson localization [1], which predicts that the electronic wavefunctions may become localized in imperfect crystals and leads to a disorder-induced metal–insulator transition (MIT), owing to the quantum interference between multiple scatterings of an electron with random impurities and defects [2–4]. Another seminal work along this direction is the scaling theory of localization [5], which indicates that all electronic states are exponentially localized in low-dimensional noninteracting systems even for infinitesimal disorder and become localized in three-dimensional (3D) systems with sufficiently large disorder strength. In fact, Anderson localization is a universal wave phenomenon and has been observed experimentally in a wide variety of systems, including light [6–9], microwaves [10], acoustic waves [11, 12], and matter waves [13–17].

The simplest one-dimensional (1D) example exhibiting Anderson localization is the random binary alloy, where the two constituents A and B are randomly distributed in the lattice (see figure 1(a)) and all eigenmodes are localized within a small region (see the solid line in figure 1(c)). However, Anderson localization breaks down in the random binary alloy when correlations are introduced in the disorder distribution. A discrete number of extended states have been reported in the random-dimer model [18–20] and its generalized versions [21, 22], where one or both sites always appear in n-mer. A band of extended states will emerge in the binary alloy when the site energies are long-range correlated [23]. In addition, other theoretical models have been suggested to produce conducting states in low-dimensional disordered systems [24–33], and some of them...
Schematic views of (a) random binary alloy and of (b) RBL model. The former is composed of two different sites (atoms) A and B with constant nearest-neighbor hopping integral $t$, while the latter is constituted by assigning two types of layers $L_A$ and $L_B$ at random, where $L_A$ ($L_B$) contains only A (B) sites. The coupling parameters within $L_A$ and $L_B$ layers are $\lambda_A$ and $\lambda_B$, respectively. (c) Typical wavefunctions of a random binary chain $L=200$ (see equation (1)). All of the wavefunctions are bounded in a small region and both systems behave as insulators. However, a band of extended states will emerge in the RBLs by introducing a relation between $\varepsilon_A, \lambda_A$, and $\varepsilon_B, \lambda_B$ (see text).

have been corroborated in GaAs–AlGaAs superlattices [34] and Bose–Einstein condensate (BEC) [14]. Nevertheless, we notice that all electronic states become localized in these correlated disordered systems when the disorder degree is extremely large. Recently, a band of extended states has been found in a peculiar two-dimensional (2D) disordered system [35].

In this paper, we explore the electronic and localization properties of a quasi-1D random binary layer (RBL) model, which can be constructed by coupling identical random binary chains along the transverse direction or equivalently by stochastically assigning two types of layers $L_A$ and $L_B$ along the longitudinal direction in the lattice, as illustrated in figure 1(b). One expects that since a single random binary chain behaves as an insulator, all electronic states should be localized in the RBL model (see the dashed line in figure 1(c)). However, contrary to this physical intuition and the scaling theory of localization that all electronic states are localized in low-dimensional disordered systems, we show that a continuous band of extended states could emerge in the quasi-1D RBLs and the disordered systems behave as metals in the thermodynamic limit by introducing a simple relation for the model parameters within a single layer, giving rise to an MIT in parameter space. This is due to the presence of a perfectly ordered subband. Besides, the mobility edges can be determined analytically and the extended states are independent of the strengths of the diagonal and off-diagonal disorders. Our results still hold in 2D and 3D disordered systems with arbitrary layer structures, and may be implemented in the BECs more easily. We point out that the mechanism to generate extended states in the RBLs is different and simpler as compared with the previous works [18–26, 29–33], where the electronic delocalization is driven by introducing long- or short-range correlations among the on-site energies while keeping the hopping integrals as constant.

2. Model

The Hamiltonian of the RBL model can be written in the tight-binding form:

$$H = \sum_{i,j} \epsilon_{ij} c_{ij}^\dagger c_{ij} + \sum_{(i,m,j)} \lambda_{ij} c_{ij}^\dagger c_{mj} + t \sum_{(i,y,n)} \epsilon_{ij} c_{in}^\dagger,$$

where $c_{ij}^\dagger$ ($c_{ij}$) is the creation (annihilation) operator of an electron at site $(i, j)$, with subscripts $i \in [1, S]$ labeling a chain and $j \in [1, L]$ denoting a layer. $S$ is the number of chains and can also describe the cross section geometry, and $L$ is the length. The site energy $\epsilon_{ij}$ for the $L_A$ ($L_B$) layer is taken as $\epsilon_A$ ($\epsilon_B$), the interchain hopping integral $\lambda_{ij}$ is set to $\lambda_A$ ($\lambda_B$) within the $L_A$ ($L_B$) layer, and $t$ is the intrachain hopping integral. The dot represents the nearest-neighbor sites. In what follows, the most disordered case is considered with probability $\frac{1}{2}$ for each layer, $\epsilon_A = 0$ is chosen as the energy reference point, and all energy parameters are in units of $t$. Consequently, the diagonal disorder degree is $W = \epsilon_B$.

It is convenient to study the localization properties of the RBLs by using the transfer-matrix method [36–38], i.e., the Lyapunov exponents $\gamma_i$ can be obtained from the QR decomposition together with the Gram–Schmidt reorthonormalization. The localization length $\xi$ is then defined as the reciprocal of the smallest positive $\gamma_i$. The conductance can be calculated from the Landauer–Büttiker formula [39]: $G = \frac{2e^2}{h}T \text{Tr}[\Gamma_L G^1 \Gamma_R G^2]$. The Green’s function $G^j = (G^j)^\dagger = (E I - \Sigma_L \Sigma_R)^{-1}$ and $\Gamma_L/R = i(\Sigma_L/R - \Sigma_L^*/R)$, with $E$ the Fermi energy and $\Sigma_L/R$ the retarded self-energy due to the coupling to the left/right lead. Here, the left and right leads consist of $A$ atoms only. Our results are averaged over an ensemble of disorder configurations to reach convergence.

In the site representation, the Schrödinger equation $H(\Psi) = E(\Psi)$ can be expressed as

$$(EI - H_j)\Psi_j = t(\Psi_{j-1} + \Psi_{j+1}).$$

Here, $I$ is the $S \times S$ identity matrix, $H_j$ is the sub-Hamiltonian matrix of the $j$th layer, and $\Psi_j = (\psi_{1j}, \psi_{2j}, \ldots, \psi_{Sj})^T$ with $\psi_{ij}$ the amplitude of the wavefunction at site $(i, j)$ and $T$ the transpose. It is clear that there are two different Hermitian matrices $H_j$, namely $H_A$ and $H_B$. Both $H_A$ and $H_B$ can be diagonalized by a single unitary matrix $U$ through $P_j = U^\dagger H_j U$, and the diagonal elements of $P_j$ are the eigenvalues of $H_j$. Thus, equation (2) can be transformed into

$$(EI - P_j)\Phi_j = t(\Phi_{j-1} + \Phi_{j+1}),$$

with $\Phi_j = U^\dagger \Psi_j = (\phi_{1j}, \phi_{2j}, \ldots, \phi_{Sj})^T$. Then the RBL model is decoupled into the following Schrödinger equations:

$$(E - \nu_{kj})\phi_{kj} = t(\phi_{k,j-1} + \phi_{k,j+1}).$$

Figure 1. Schematic views of (a) random binary alloy and of (b) RBL model. The former is composed of two different sites (atoms) A and B with constant nearest-neighbor hopping integral $t$, while the latter is constituted by assigning two types of layers $L_A$ and $L_B$ at random, where $L_A$ ($L_B$) contains only A (B) sites. The coupling parameters within $L_A$ and $L_B$ layers are $\lambda_A$ and $\lambda_B$, respectively. (c) Typical wavefunctions of a random binary chain $L=200$ (see equation (1)). All of the wavefunctions are bounded in a small region and both systems behave as insulators. However, a band of extended states will emerge in the RBLs by introducing a relation between $\varepsilon_A, \lambda_A$, and $\varepsilon_B, \lambda_B$ (see text).
where $v_{kj}$ is the $k$th eigenvalue of $H_j$. When the cross section is a line, the eigenvalue $v_{kj}$ is

$$v_{kj} = \epsilon_j + 2\lambda_j \cos \frac{k\pi}{S+1}. \quad (5)$$

When the cross section is a rectangle with $S = S_y \times S_z$, the $v_{kj}$ with integer index $k = (k_y - 1)S_y + k_z$ is

$$v_{kj} = \epsilon_j + 2\lambda_j \left( \cos \frac{k_y \pi}{S_y + 1} + \cos \frac{k_z \pi}{S_z + 1} \right). \quad (6)$$

Here, $\epsilon_j = 0$ and $\lambda_j = \lambda_A$ when $H_j = H_A$, $\epsilon_j = \epsilon_B$ and $\lambda_j = \lambda_B$ when $H_j = H_B$, $k \in [1, S_y]$, $k_y \in [1, S_y]$, and $k_z \in [1, S_z]$. It clearly appears that the RBLs can be decoupled into $S$ chains, each of which is a random binary chain with site energies $v_{kA}$ and $v_{kB}$ determined by equation (5) or (6); and $\lambda_j$ only contributes to the site energies, and hence the electronic and localization properties of the RBLs could be strongly changed by varying $\lambda_j$ only. One notices that when $v_{kA} = v_{kB}$, the $k$th decoupled chain is a perfectly ordered one with constant site energy $v_{kA}$ and nearest-neighbor hopping integral $t$, and the electronic states are Bloch-like states in the energy interval $[v_{kA} - 2t, v_{kA} + 2t]$, with the mobility edges being at $E = v_{kA} \pm 2t$. This result will be verified numerically for several RBLs with different cross sections (see below).

### 3. Results and discussions

We first consider the simplest case of $S = 2$, namely the two-leg ladder model [33], which has been used to simulate the charge transport through double-stranded DNA. In this respect, the site energies of two decoupled chains are $v_{1A} = \lambda_A$, $v_{1B} = \epsilon_B + \lambda_B$ and $v_{2A} = -\lambda_A$, $v_{2B} = \epsilon_B - \lambda_B$, respectively. Accordingly, the energy spectrum of the disordered two-leg ladder, composed of the energy bands of individual decoupled chains, can be written as

$$[v_{1A} - 2t, v_{1A} + 2t] \cup [v_{1B} - 2t, v_{1B} + 2t]$$

$$[v_{2A} - 2t, v_{2A} + 2t] \cup [v_{2B} - 2t, v_{2B} + 2t]. \quad (7)$$

Figures 2(a) and (b) display, respectively, the density of states (DOS) and the localization length $\xi$ with $\epsilon_B = 0.5$, $\lambda_A = -2.5$, $\lambda_B = -3$ (solid lines), $\epsilon_B = 0.5$, $\lambda_A = \lambda_B = 2.5$ (dashed lines), and $\epsilon_B = 0$, $\lambda_A = -2.5$, $\lambda_B = -3$ (dotted lines). The inset displays the two-terminal conductance. The DOS is calculated by diagonalizing the Hamiltonian for a single disorder configuration and is almost the same when other disorder configurations are employed, since the system size is very large. In the gray energy region, $\xi$ is averaged in a small energy window of width 0.1 around $E$ to avoid numerical fluctuations.

Figure 2. (a) DOS and (b) localization length for disordered two-leg ladders with $\epsilon_B = 0.5$, $\lambda_A = -2.5$, $\lambda_B = -3$ (solid lines), $\epsilon_B = 0.5$, $\lambda_A = \lambda_B = 2.5$ (dashed lines), and $\epsilon_B = 0$, $\lambda_A = -2.5$, $\lambda_B = -3$ (dotted lines). The inset displays the two-terminal conductance. The DOS is calculated by diagonalizing the Hamiltonian for a single disorder configuration and is almost the same when other disorder configurations are employed, since the system size is very large. In the gray energy region, $\xi$ is averaged in a small energy window of width 0.1 around $E$ to avoid numerical fluctuations.

As a comparison, figure 2 shows DOS and $\xi$ by changing only one parameter of the two-leg ladder, namely, replacing $\lambda_B$ with $-2.5$ (dashed lines) and $\epsilon_B$ with 0 (dotted lines), respectively. In contrast, all states become localized for both two-leg ladders with $G = 0$ (see inset) and constant localization length at fixed energies (from figure 3(b) we obtain $\beta = -1$), due to the Anderson localization effects, although they possess either the diagonal disorder (dashed lines) or the off-diagonal disorder (dotted lines) and are more ordered than the former case.

4 When the long-range intrachain hopping is considered, our results still hold and the RBLs may present better conducting behavior, due to the emergence of additional propagating channels for electrons. When the interchain hopping integrals $\lambda_A$ and $\lambda_B$ randomly fluctuate within an energy interval, it can be deduced from equation (5) or (6) that the completely ordered decoupled chain will become disordered and all states are localized. However, when the width of this energy interval is small, the localization length remains very large. Here, we emphasize that a band of extended states could appear in the disordered systems in the presence of off-diagonal disorder only, see point (iv) in the last paragraph of this section.
Figures 4(a)–(d) show various situations and are shifted toward lower energies by increasing $W$. The states are extended in the thermodynamic limit if $\xi \propto L^\alpha$ and for (a) $\epsilon_B = 0.5$, $\lambda_A = -2.5$, $\lambda_B = -3$ and for (b) $\epsilon_B = 0.5$, $\lambda_A = \lambda_B = -2.5$. The dependence of $\xi$ on $L$ can be fitted exactly by a simple function $\xi \propto L^\alpha$, as shown by the solid, dashed, and dotted lines. $\xi$ versus $W$ for (c) $\lambda_A = -2.5$, $\lambda_B = -2.5 - W$ and for (d) $\lambda_A = \lambda_B = -2.5$. The inset presents the enlarged view of $\xi$ versus $W$ in the region of $W < W_c$ with $W_c = E + 2r - \lambda_B$, and the corresponding fitting curves $\xi \propto W^\alpha$. The parameter $\alpha$ in the vertical scale of (b) and (d) is employed to separate the lines. $\alpha = 2, 1, 0.5$ for $E = -2.5, -1.7, -0.9$, respectively.

Figures 3(c) and (d) plot $\xi$ versus $W$ for the two-leg ladders with $\lambda_A = -2.5$, $\lambda_B = -2.5 - W$ and $\lambda_A = \lambda_B = -2.5$, respectively. Contrary to the previous works that all states become localized in the disordered systems when the disorder degree is very large [18–33], we can see from figure 3(c) that $\xi$ is independent of $W$ for the former ladder and all states are always extended in the gray energy region (figure 2(b)), because $\psi_{1A} = \psi_{1B} = -2.5$ and the left subband denotes a completely ordered chain and does not move with $W$. Meanwhile, for the latter ladder, a crossover $W_c$, dividing strong and weak dependence of $\xi$ on $W$, exists in all the curves (figure 3(d)), similar to that observed in the experiments [8, 13, 17]. $\xi$ is strongly declined by increasing $W$ up to $W_c = E + 2r - \lambda_B$, due to the gradually enhanced scatterings from the potential barriers at B sites. The behavior of $\xi$ versus $W$ can be fitted by a power law relation for $W < W_c$ (see inset), $\xi \propto W^\alpha$ for $W > W_c$ (see equation (7)). In this situation, the state at $E$ is formed by A sites only and the electron is usually confined inside a single A site, leading to the localization length $\xi \approx 1$. We then consider the RBLs of various cross sections.

Figures 4(a)–(d) show $\xi$ versus $E$ for several values of $\epsilon_B$, $\lambda_B$, $L$ by fixing $S = 5$ and $\lambda_A = 5$. The $\epsilon_B$ and $\lambda_B$ are chosen so that $\psi_{1A} = \psi_{1B}$ is satisfied for specific $k$ and a perfectly ordered chain always appears. A band of extended states as well as the mobility edges can be observed in all the situations and are shifted toward lower energies by increasing $W_c$; and the wavefunction in the metallic regime will spread over the entire system (see the dashed line of the inset). In this regard, the RBLs may be used as switching devices and their electronic structure could be controlled by changing $\epsilon_B$ and $\lambda_B$ while keeping other parameters fixed. However, the localized state can survive in the metallic regime (see the solid line of the inset), due to the superposition of extended and localized subbands, as can be inferred from equation (5). Similar results can be obtained for the RBLs of square cross sections, even when $\lambda_A = 0$ (figures 4(e)–(f)). Therefore, we conclude that a band of extended states will appear in the RBLs with any value of $S$ except for $S = 1$ and $S = 2$, the systems behave as metals by implementing a relation between $\epsilon_B$, $\lambda_A$ and $\epsilon_B$, $\lambda_B$, leading to an MIT in parameter space. These are irrespective of the diagonal and off-diagonal disorder strengths.

Finally, we discuss the generalization of our results and the possible relevance to realistic systems. (i) In contrast to the random-dimer model in which the extended states vanish when it contains more than two different sites [18–22], our results can still hold when the site energies are randomly selected from a certain probability distribution. For example, we consider $\epsilon_j$ uniformly distributed within $[-\frac{W}{2}, \frac{W}{2}]$. By properly choosing the interchain hopping integral that

\begin{align*}
\text{Figure 3.} & \quad \text{Scaling behaviors of the normalized localization length at several energies for the corresponding two-leg ladders in figure 2.} \\
& \quad \text{The states are extended in the thermodynamic limit if } \xi \propto L^\alpha \text{ or increased by increasing } W, \text{ and are localized otherwise.} \\
& \quad \text{The states are extended in the thermodynamic limit if } \xi \propto L^\alpha \text{ and for (a) } \epsilon_B = 0.5, \lambda_A = -2.5, \lambda_B = -3 \text{ and for (b) } \epsilon_B = 0.5, \lambda_A = \lambda_B = -2.5. \text{ The dependence of } \xi \text{ on } L \text{ can be fitted exactly by a simple function } \xi \propto L^\alpha, \text{ as shown by the solid, dashed, and dotted lines.} \\
& \quad \text{The states are extended in the thermodynamic limit if } \xi \propto L^\alpha \text{ and for (a) } \epsilon_B = 0.5, \lambda_A = -2.5, \lambda_B = -3 \text{ and for (b) } \epsilon_B = 0.5, \lambda_A = \lambda_B = -2.5. \text{ The dependence of } \xi \text{ on } L \text{ can be fitted exactly by a simple function } \xi \propto L^\alpha, \text{ as shown by the solid, dashed, and dotted lines.} \\
& \quad \text{The states are extended in the thermodynamic limit if } \xi \propto L^\alpha \text{ and for (a) } \epsilon_B = 0.5, \lambda_A = -2.5, \lambda_B = -3 \text{ and for (b) } \epsilon_B = 0.5, \lambda_A = \lambda_B = -2.5. \text{ The dependence of } \xi \text{ on } L \text{ can be fitted exactly by a simple function } \xi \propto L^\alpha, \text{ as shown by the solid, dashed, and dotted lines.} \\
& \quad \text{The states are extended in the thermodynamic limit if } \xi \propto L^\alpha \text{ and for (a) } \epsilon_B = 0.5, \lambda_A = -2.5, \lambda_B = -3 \text{ and for (b) } \epsilon_B = 0.5, \lambda_A = \lambda_B = -2.5. \text{ The dependence of } \xi \text{ on } L \text{ can be fitted exactly by a simple function } \xi \propto L^\alpha, \text{ as shown by the solid, dashed, and dotted lines.} \\
& \quad \text{The states are extended in the thermodynamic limit if } \xi \propto L^\alpha \text{ and for (a) } \epsilon_B = 0.5, \lambda_A = -2.5, \lambda_B = -3 \text{ and for (b) } \epsilon_B = 0.5, \lambda_A = \lambda_B = -2.5. \text{ The dependence of } \xi \text{ on } L \text{ can be fitted exactly by a simple function } \xi \propto L^\alpha, \text{ as shown by the solid, dashed, and dotted lines.} \\
& \quad \text{The states are extended in the thermodynamic limit if } \xi \propto L^\alpha \text{ and for (a) } \epsilon_B = 0.5, \lambda_A = -2.5, \lambda_B = -3 \text{ and for (b) } \epsilon_B = 0.5, \lambda_A = \lambda_B = -2.5. \text{ The dependence of } \xi \text{ on } L \text{ can be fitted exactly by a simple function } \xi \propto L^\alpha, \text{ as shown by the solid, dashed, and dotted lines.}
\end{align*}
$v_{ij} = E_c$ always holds for specific $k$ (equation (5)) or $k_y, k_z$ (equation (6)) with $E_c$ a constant, a band of extended states will emerge in the energy region $[E_c - 2t, E_c + 2t]$. (ii) Our results remain valid for other 2D and 3D disordered systems when $v_{ij} = E_c$ is satisfied. For an $S \times L$ disordered system, the number of the condition $v_{ij} = E_c$ is $\frac{2S-1+(1-1)^5}{2}$, except for the case $\cos \frac{k_x}{k} = 0$ which leads to an ordered system. Similarly for an $S \times S \times L$ disordered system, the number is $\frac{2S^2-1+(1-1)^5}{4}$. (iii) These results also hold for the disordered systems with various layer structures, such as rectangle and hexagon, as long as the $v_{ij}$ for fixed $k$ (or $k_x, k_y$) are constant or follow a periodic distribution by increasing $j$. (iv) Another interesting phenomenon is that a band of extended states could appear in the presence of off-diagonal disorder only, no matter how large the disorder strength is. For example, we consider $\epsilon_j = 0$ and $\lambda_j$ being any random number. In this situation, the electronic states are extended within the energy interval $[-2t, 2t]$ for the 2D systems with odd number of chains and for the 3D systems with square layer structure. This is due to the fact that the off-diagonal disorder will not contribute to the site energies of one decoupled chain when the cosine function is zero (see equation (5) or (6)). (v) Besides the double-stranded DNA, we believe our results to be relevant for the BECs, which offer an ideal platform for studying Anderson localization [13–17]; and the model parameters can be precisely controlled [40].

4. Conclusions

In summary, we suggest a scheme to produce metallic states in a series of disordered systems. Our results indicate that a band of extended states could emerge in the thermodynamic limit and the disordered systems behave as metals by properly adjusting the model parameters, generating a metal–insulator transition in parameter space. The results are independent of the diagonal and off-diagonal disorder strengths, and still hold in two- and three-dimensional disordered systems.

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