A simple approach to Anderson localization in one-dimensional disordered lattices

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We present a simple approach to Anderson localization in one-dimensional disordered lattices. We introduce the tight-binding model in which one orbital and a single random energy are assigned to each lattice site, and the hopping integrals are constant and restricted to nearest-neighbor sites. The localization of eigenstates is explained by two-parameter scaling arguments. We compare the size scaling of the level spacing in the bare energy spectrum of the quasi-particle (in the ideal lattice) with the size scaling of the renormalized disorder seen by the quasi-particle. The former decreases faster than the latter with increasing system size, giving rise to mixing and to the localization of the bare quasi-particle wave functions in the thermodynamic limit. We also provide a self-consistent calculation of the localization length and show how this length can be obtained from optical absorption spectra for Frenkel excitons. © *2004 American Association of Physics Teachers.*
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I. INTRODUCTION

Low temperature quantum phenomena in crystalline solids, such as charge and energy transport, optical absorption and thermal properties, can be understood in terms of quasi-particles. According to Bloch's theorem, a quasi-particle wave function in a periodic lattice is the product of a periodic function, which reflects the full translational symmetry of the lattice, and a plane wave.[1] Consequently, the quasi-particle probability amplitudes are extended over the entire lattice, that is, the states are delocalized in space.

Noncrystalline matter, such as amorphous metals and semiconductors or molecular aggregates, is characterized by random arrangements of atoms or molecules.[2] Because the crystal potential is nonperiodic, Bloch's theorem is no longer valid. Therefore, quasi-particle states are not expected to be Bloch functions. The simplest model that describes the nature of one-particle states in disordered matter was introduced by Anderson.[3] In this seminal paper, Anderson established that the quasi-particle states in three dimensions became localized for sufficiently large disorder. Localization means that the quasi-particle probability amplitude is nonvanishing only in a finite region of the solid. In 1977, Anderson, Mott, and van Vleck were awarded the Nobel prize ''for their fundamental theoretical investigations of the electronic structure of magnetic and disordered systems.''[4] Despite its forty-year history, Anderson localization still excites much interest among researchers.

We note that Anderson localization in low-dimensional disordered solids has its own peculiarities. In this context, Mott and Twose made the statement that in one dimension all the states of random systems become exponentially localized for any amount of disorder.[5] Abrahams *et al.*[6] confirmed this statement by introducing a single-parameter scaling theory of localization and extended the Mott–Twose conclusion to two-dimensional systems as well. (See Refs. 7–9 for a comprehensive review.) The single-parameter scaling theory works remarkably well in random media with time-reversal symmetry, uncorrelated disorder, and finite-range hopping.

In this paper we consider the tight-binding model in which one orbital and a single random energy are assigned to each site of a one-dimensional lattice, while the intersite coupling does not fluctuate. The localization of the wave function is explained by the different size scaling of two parameters, namely the level spacing of the bare quasi-particle energy spectrum (in the ideal lattice) and the renormalized disorder seen by the quasi-particles. For this reason, quasi-particle states in this model are always localized in the thermodynamic limit. We also provide a self-consistent rule for estimating the localization length and discuss the effects of disorder on the optical response of the quasi-particles known as Frenkel excitons.[10–12]

II. TIGHT-BINDING MODEL

We first consider an electron moving in a potential $V(\mathbf{r})$ and assume that $V(\mathbf{r})$ is the superposition of atomic potentials $v_k(\mathbf{r})$. Although we will mostly discuss one-dimensional systems, we introduce the tight-binding framework for arbitrary dimension d. We are interested in the stationary Schrödinger equation for the wave function $\Psi(\mathbf{r})$

$$\left[-\frac{1}{2m}\nabla^2+\sum_k v_k(\mathbf{r}-\mathbf{r}_k)\right]\Psi(\mathbf{r})=E\Psi(\mathbf{r}), \tag{1}$$

where $\mathbf{r}_k$ is the position of the kth atom and the sum runs over all atoms in the solid. The Planck constant $\hbar$ is set to unity throughout the paper. We assume that each atom supports only one bound state, although more complicated situations can be handled in a similar fashion.

We seek a solution of Eq. (1) in the form

$$\Psi(\mathbf{r})=\sum_j \psi_j\chi_j(\mathbf{r}-\mathbf{r}_j), \tag{2}$$

where $\chi_j(\mathbf{r}-\mathbf{r}_j)$ and ψ_j are the jth atomic orbital and its amplitude, respectively. The atomic orbitals $\chi_j(\mathbf{r}-\mathbf{r}_j)$ can be found by solving the corresponding Schrödinger equation for a single atom

$$\left[-\frac{1}{2m}\nabla^2+v_j(\mathbf{r}-\mathbf{r}_j)\right]\chi_j(\mathbf{r}-\mathbf{r}_j)=\varepsilon_j\chi_j(\mathbf{r}-\mathbf{r}_j), \tag{3}$$

where ε_j is the electron energy in the jth atom when the other atoms are far apart. If we substitute Eq. (2) into Eq. (1) and use Eq. (3), we obtain

$$\sum_j \left[\varepsilon_j - E + \sum_{k\neq j} v_k(\mathbf{r}-\mathbf{r}_k)\right]\psi_j\chi_j(\mathbf{r}-\mathbf{r}_j)=0. \tag{4}$$

We proceed in the standard fashion to obtain the electron amplitude ψ_j at any site. We multiply Eq. (4) by $\chi_l^*(\mathbf{r}-\mathbf{r}_l)$ from the left and perform the integration over the volume of the solid. By doing so, we are led to the following algebraic equation for the amplitudes:

$$\sum_j \left[(\varepsilon_j - E)\widetilde{A}_{l,j} + \sum_{k\neq j}\widetilde{B}_{l,k,j}\right]\psi_j=0, \tag{5a}$$

where

$$\widetilde{A}_{l,j}=\int d\mathbf{r}\chi_l^*(\mathbf{r}-\mathbf{r}_l)\chi_j(\mathbf{r}-\mathbf{r}_j), \tag{5b}$$

$$\widetilde{B}_{l,k,j}=\int d\mathbf{r}\chi_l^*(\mathbf{r}-\mathbf{r}_l)v_k(\mathbf{r}-\mathbf{r}_k)\chi_j(\mathbf{r}-\mathbf{r}_j) \quad (k\neq j). \tag{5c}$$

Equation (5) is valid for any superposition of arbitrary atomic potentials v_j. The coefficients $\widetilde{A}_{l,j}$ and $\widetilde{B}_{l,k,j}$ depend only on the particular choice for the atomic potentials v_j. Their values for the one-dimensional Kronig–Penney model with δ-function potentials are found in Ref. 13.

To find the electron wave function (2), we must solve Eq. (5a). Clearly, this is hardly possible when the number of atoms is very large. We will consider a suitable approximation to reduce the number of coefficients involved in the calculation. We suppose that the electrons are tightly bound, so that the overlap between the orbitals of neighboring atoms is negligible. Whenever this condition holds, we can replace $\widetilde{A}_{l,j}$ by δ_{lj}. For the three-center integrals in Eq. (5c), we assume that the only nonvanishing coefficients are $\widetilde{B}_{l,l,l+z}$, where z indicates nearest-neighbor sites, that is, only nearest-neighbor interactions are significant. Further simplification is achieved by assuming that $\widetilde{B}_{l,l,l+z}$ do not fluctuate and have the value $\widetilde{B}_{l,l,l+z}=-J$ ($J>0$ without lose of generality). This assumption implies that we restrict our consideration to a regular but realistic lattice because the on-site energies ε_j may fluctuate. This model is usually referred to as the tight-binding model with diagonal disorder. The Schrödinger equation for the amplitudes is now

$$\varepsilon_l\psi_l - J\sum_z \psi_{l+z}=E\psi_l, \tag{6}$$

where the sum runs over nearest-neighbor sites. Equation (6) was used by Anderson in his work on the localization–delocalization transition in three-dimensional systems.[3]

III. NONDISORDERED LATTICE

The tight-binding equation (6) can be easily solved in the limit of nonfluctuating on-site energies: $\varepsilon_l=\overline{\varepsilon}=$constant, that is, for an ideal lattice. As an example, let us consider a simple cubic lattice in a d-dimensional space with N atoms along each spatial direction. Thus, the lattice consists of $\mathcal{N}=N^d$ identical atoms. We assume periodic boundary conditions and use the Bloch theorem, which allows us to write the solution of Eq. (6) in the form

$$\psi_l^0(\mathbf{K})=\frac{1}{\sqrt{\mathcal{N}}}\exp(i\mathbf{K}\cdot\mathbf{R}_l), \tag{7}$$

where $\mathbf{K}=(2\pi/Na)(k_1,k_2,\ldots,k_d)$ is the d-dimensional crystal momentum of the electron state, $\mathbf{R}_l=(l_1a,l_2a,\ldots,l_da)$ denotes the d spatial coordinates, a is the lattice spacing, and l_j, k_j are integers $(0\leqslant l_j,k_j\leqslant N-1)$. Note that the probability $|\psi_l^0(\mathbf{K})|^2$ of finding the electron at one particular atom of the solid is constant and equals $1/\mathcal{N}$, that is, the electron is extended uniformly over the lattice. If we substitute Eq. (7) into Eq. (6), we obtain the dispersion relation for a d-dimensional cubic lattice

$$E_{\mathbf{K}}^0=\overline{\varepsilon}-2J\sum_{j=1}^{d}\cos(K_j). \tag{8}$$

The superscript 0 refers to the absence of disorder and $K_j=2\pi k_j/N$. The energy width of the spectrum in the simple d-dimensional lattice is then given by $W=4Jd$.

IV. DISORDERED LATTICE: PERTURBATIVE LIMIT

In a disordered lattice, the on-site energies ε_l are different for different sites. In the following, we will consider only one-dimensional systems. Then the equation of motion (6) can be rewritten as

$$D_l\psi_l+\overline{\varepsilon}\psi_l-J\psi_{l+1}-J\psi_{l-1}=E\psi_l, \tag{9}$$

where $D_l\equiv\varepsilon_l-\overline{\varepsilon}$ is the deviation of the site energy from its mean $\overline{\varepsilon}$. We will assume that D_l is uncorrelated for different sites and distributed according to a Gaussian distribution

$$\mathcal{P}(D_l)=(2\pi\sigma^2)^{-1/2}\exp(-D_l^2/2\sigma^2), \tag{10}$$

where $\langle D_l\rangle=0$ and the standard deviation $\sigma=\langle D_lD_l\rangle^{1/2}$. The angular brackets $\langle\ldots\rangle$ denote an average over the distribution $\mathcal{P}$.

We now rewrite Eq. (9) in the K-representation. To do so, we multiply Eq. (9) by the Bloch wave in Eq. (7) and sum over the site numbers. We obtain

$$(E-E_K^0)\psi(K)=\sum_{K'}V_{KK'}\psi(K'), \tag{11}$$

where E_K^0 is given by Eq. (8) with $d=1$, and the other variables are

$$\psi(K)=\frac{1}{\sqrt{N}}\sum_l\psi_l e^{iKla}, \tag{12a}$$

$$V_{KK'}=\frac{1}{N}\sum_{l=0}^{N-1}D_le^{i(K-K')la}. \tag{12b}$$

The diagonal matrix elements, V_{KK}, simply give an energy shift of the corresponding Kth state

$$\Delta E_K=V_{KK}=\frac{1}{N}\sum_{l=0}^{N-1}D_l, \tag{13}$$

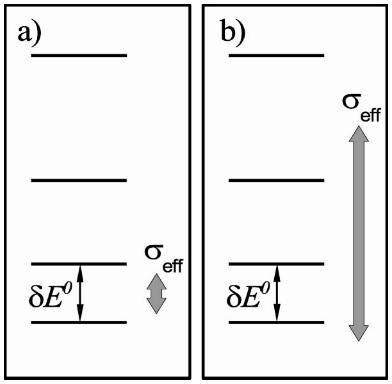

Fig. 1. Schematic diagram of (a) perturbative and (b) nonperturbative disorder. The solid lines are the lowest energy levels in the ideal lattice, and δE^0 is the level spacing. The thick arrows indicate the value of the effective disorder, $\sigma_{\rm eff} = \sigma/\sqrt{N}$.

and turn out to be independent of the state, but dependent on the particular realization of the random variables $\{D_l\}$. The shift has zero mean because $\langle D_l \rangle = 0$. The variance is nonzero and is given by

$$B_{KK} \equiv \langle (\Delta E_K)^2 \rangle = \frac{1}{N^2} \sum_{l,l'=0}^{N-1} \langle D_l D_{l'} \rangle$$
$$= \frac{1}{N^2} \sum_{l=0}^{N-1} \langle D_l^2 \rangle = \frac{\sigma^2}{N}. \tag{14}$$

We have used the fact that $\langle D_l D_{l'} \rangle = 0$ for $l \neq l'$. For an ensemble of lattices, the disorder-induced energy shift results in inhomogeneous broadening of the quasi-particle levels.

The off-diagonal matrix elements elements, $V_{KK'}$, describe mixing (or scattering) of the quasi-particle states; they are the quantities that are responsible for localization. Again we obtain $\langle V_{KK'} \rangle = 0$ because $\langle D_l \rangle = 0$, while the variance is

$$B_{KK'} = \langle |V_{KK'}|^2 \rangle = \frac{\sigma^2}{N}, \tag{15}$$

which is equal to the variance of the energy shift given in Eq. (14). Thus, $\sqrt{B_{KK'}} = \sigma/\sqrt{N}$ represents the typical fluctuation of the coupling $V_{KK'}$ between different K states. For a given lattice size, the disorder is perturbative provided that $V_{KK'}$ is small compared to the level spacing δE^0 in the ideal lattice [see Fig. 1(a)]:

$$\delta E^0 \gg \frac{\sigma}{\sqrt{N}} = \sigma_{\rm eff}. \tag{16}$$

In this case, the mixing of Bloch states is weak and the perturbed states are expected to remain extended over the whole lattice. The electron (or any other quasi-particle) sees an effective (averaged) disorder whose magnitude is $1/\sqrt{N}$ smaller than the bare magnitude of the disorder, σ. This effect is known as *exchange narrowing*. Note that it is the exchange-narrowed value of disorder that we must compare with the level spacing in the ideal system to determine whether the disorder is perturbative or not.

From these arguments we cannot conclude whether the states will remain extended or will be localized in the thermodynamic limit $N \to \infty$. According to the standard scaling theory, they should be localized.[6] The reasoning relies on the fact that δE^0 and $\sigma_{\rm eff}$ scale with the system size N in a different way. Let us consider the bottom of the unperturbed spectrum, $K \ll 1$, where the dispersion relation (8) is parabolic, $E_K^0 = \overline{\varepsilon} - 2J + JK^2$, and the level spacing is a minimum. Then for δE^0 we obtain

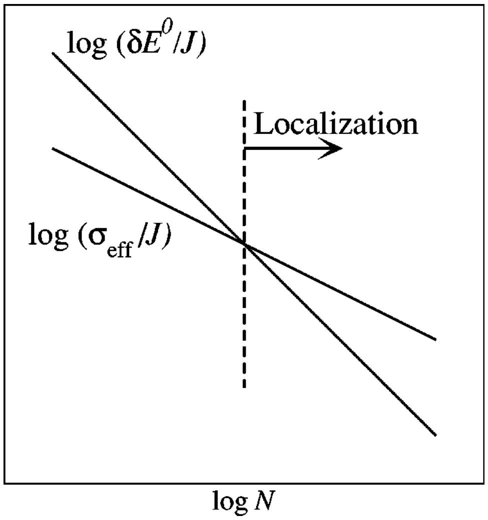

Fig. 2. Schematic of the scaling of the level spacing in the ideal lattice, δE^0, and the effective magnitude of disorder, $\sigma_{\rm eff}$, for small enough σ.

$$\delta E^0 \simeq \frac{4\pi^2 J}{N^2}. \tag{17}$$

We see that δE^0 decreases faster than $\sigma_{\rm eff}$ with increasing N. In other words, if the disorder is perturbative for a given N, it will be nonperturbative for a larger N and the inequality (16) would be reversed (see Fig. 2). Consequently, for a large enough system, the Bloch states are always strongly mixed and localization occurs as expected. Therefore, the condition,

$$\delta E^0 = \sigma_{\rm eff}, \tag{18}$$

indicates the onset of localization for a given lattice size, in the sense that the localization length becomes smaller than the lattice length.

V. DISORDERED LATTICE: NONPERTURBATIVE LIMIT

For moderately high disorder and large systems, the states are spatially localized. Despite the underlying randomness, some regularities are observed in the energy spectrum, specifically at the band edges. We briefly recall the local (hidden) energy structure of localized one-dimensional quasi-particles, which was shown to exist in the vicinity of the band edge.[14–16] The idea is that the low-energy eigenfunctions for a fixed realization of the disorder are localized at nonoverlapping segments (see Fig. 3) of typical size N^* (localization length). Some of these localized states can be grouped into local groups of two (or sometimes more) states that are localized at the same N^* segment (see the states joined by ellipses in Fig. 3). In each segment, the lowest levels are arranged according to Eq. (8), but with N replaced by the segment length, N^*. Note that the wave functions associated with each segment resemble a particle in a box, that is, they have an almost perfect reflection symmetry and the number of nodes increases with energy.

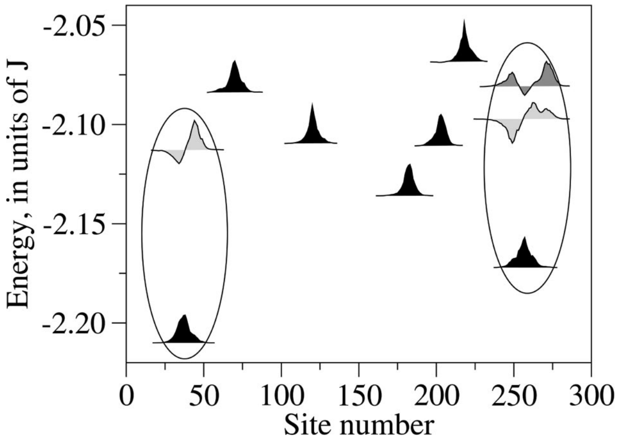

Fig. 3. States in the vicinity of the bottom of the band. The states are obtained by diagonalizing of Eq. (9) for a disordered linear chain of 300 sites. The magnitude of the disorder is $\sigma=0.2J$. The energy of each state is in units of J. The wave function amplitude is in arbitrary units. It is clearly seen that some lower states can be grouped into local groups (the groups are joined by ellipses). The states within each group are localized at the same segment of typical size N^*.

To estimate N^* we follow Ref. 14. We should use the fact that the lowest levels within a localization segment resemble the levels of an ideal lattice of size N^*. In such a case, the localization length is exactly the system length (that is, the segment length), and we can then use the onset condition (18) with N replaced by N^*. We obtain

$$N^*=\left(\frac{4\pi^2 J}{\sigma}\right)^{2/3}=11.59\left(\frac{J}{\sigma}\right)^{2/3}. \tag{19}$$

The numerical factor depends slightly on the boundary conditions, and it is found that $N^*=(3\pi^2 J/\sigma)^{2/3}\simeq 9.57(J/\sigma)^{2/3}$ for an open chain. In spite of the simplicity of the underlying reasoning, Eq. (19) for estimating N^* yields surprisingly good results. An extensive numerical analysis[17] has showed that $N^*=8.71(J/\sigma)^{0.67}$. In addition, the concept of N^* works well for correlated disorder.[16]

VI. OPTICAL ABSORPTION BY FRENKEL EXCITONS

It is well established that the lowest optical excitation in linear molecular aggregates (more specifically, J-aggregates[18,19]) are Frenkel excitons (see, for instance, Ref. 20). These quasi-particles arise due to the resonant dipole–dipole interaction of molecules[10] and drive the energy transport and optical properties in molecular aggregates. In the nearest-neighbor approximation, the wave functions of Frenkel excitons obey Eq. (9), in which $\varepsilon_l=\overline{\varepsilon}+D_l$ now should be considered as the energy of transition in the lth molecule. Thus, the previous results regarding localization also can be applied to Frenkel excitons in J-aggregates.

The major contribution to the linear optical response in J-aggregates $(J>0)$ is determined by the states in the vicinity of the bottom of the exciton band. For aggregates small compared to the emission wavelength, where the dipole approximation for the light-matter interaction becomes valid, the absorption band (J-band) is found to be

$$I(E)=\frac{1}{N}\left\langle\sum_{\nu=0}^{N-1} F_\nu^2\,\delta(E-E_\nu)\right\rangle, \tag{20a}$$

where F_ν^2 is the dimensionless oscillator strength of the νth state,

$$F_\nu^2\equiv\left(\sum_l \psi_l(\nu)\right)^2, \tag{20b}$$

and the oscillator strength of an isolated molecule is set to unity. From Eq. (20b) it follows that only exciton wave functions at the bottom of the band contribute to the absorption because only they have noticeable oscillator strengths.

For an ideal circular J-aggregate, where the exciton wave functions are Bloch functions (7), $F_K=N\delta_{K0}$, that is, the state with $K=0$ carries the entire oscillator strength and is the only one that is coupled to light. Consequently, the absorption spectrum contains only one peak located exactly at the bottom of the exciton band, $E^0_{K=0}=\overline{\varepsilon}-2J$. In particular, this fact explains the experimentally observed redshift of the J-band with respect to the absorption spectra of isolated molecules.

If we introduce a small Gaussian disorder which is perturbative in the sense of Eq. (16), the peak is broadened. However, exciton wave function keeps the Gaussian form and is again centered at the bottom of the band, $E^0_{K=0}=\overline{\varepsilon}-2J$. Its standard deviation, equal to $\sqrt{B_{00}}=\sigma/\sqrt{N}$, is a factor of $1/\sqrt{N}$ smaller than that for decoupled molecules, resembling the exchange narrowing effect in the exciton absorption spectra.[21]

In the nonperturbative limit, the exciton wave functions that contribute to the J-band are mostly those that have no nodes within the localization segments (see Fig. 3). They are extended over segments of length N^* given by Eq. (19). Therefore, absorption spectra provide a unique way to measure N^*.[22] The standard deviation of the J-band (denoted by σ^*) can be estimated by replacing N by N^* in the corresponding expression for the perturbative limit, $\sigma/\sqrt{N}$. We obtain

$$\sigma^*=\frac{\sigma}{\sqrt{N^*}}=\frac{1}{(4\pi^2)^{1/3}}J\left(\frac{\sigma}{J}\right)^{4/3}=0.29J\left(\frac{\sigma}{J}\right)^{4/3}. \tag{21}$$

As we have mentioned, the J-band is shifted to the red by an amount $2J$ relative to the monomer absorption spectrum. In this way, we can estimate the hopping integral J with enough precision. Furthermore, the J-band often appears as an isolated peak, so that its width also can be easily measured. We also assume that the magnitude of σ can be extracted from the monomer absorption spectrum. In this way, all the parameters are known for calculating N^* using Eq. (21). We only need to replace the numerical factor 0.29 in Eq. (21) by 0.42, as suggested by numerical simulations.[23]

VII. CONCLUSIONS

We have discussed Anderson localization in one-dimensional disordered lattices in the vicinity of the band edges. We treated these systems within the tight-binding model, in which the hopping integrals do not fluctuate and are restricted to nearest-neighbor sites, while on-site energies are uncorrelated (for different sites) random numbers. We made use of the fact that the size scaling of the bare level spacing (in the ideal lattice) differs from that for the renormalized disorder (seen by the quasi-particles). The former ($\sim N^{-2}$) becomes small compared to the latter ($\sim N^{-1/2}$) for $N \rightarrow \infty$. Therefore, the bare wave functions will be strongly mixed by the disorder, giving rise to localization of the quasi-particle states in the thermodynamic limit. Similar reasoning also applies for the center of the band where the bare level spacing scales as N^{-1}. Nevertheless, the spacing decreases with N faster than the renormalized magnitude of disorder. Consequently, all the states in the tight binding model are localized for sufficiently large enough N, no matter how small the degree of disorder.

We formulated a simple self-consistent relation for estimating the localization length and discussed a relevant experimental procedure to measure it in linear molecular aggregates (J-aggregates), where localized quasi-particles are represented by Frenkel excitons. Due to the strong coupling of Frenkel excitons to light, their localization length can be measured by analyzing the linear optical response.

We stress that the validity of the scaling arguments presented in the paper is not restricted to one-dimensional systems. Indeed, it is well established that the standard three-dimensional Anderson model shows a localization–delocalization transition at the band center. In this model, the bare level spacing at the band center decreases as N^{-1}, while the magnitude of the effective disorder decreases faster, $\sim N^{-3/2}$, and is thus unable to localize the states at the band center for moderate disorder. Strong disorder (large compared to the bandwidth) localizes the states. This reasoning gives us insight into why the three-dimensional Anderson model shows a localization–delocalization transition. Thus, scaling arguments provide a basis for understanding of several localization problems. The underlying ideas are based on standard perturbation theory, and knowledge of advanced quantum mechanics or field theory is not required. Thus, we believe that our approach is suitable for introductory courses in solid state and condensed matter physics.

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