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Wave Functions in Disordered Systems

Michael J. Stephen[1]

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Particular solutions of the stationary Schrödinger equation for a d-dimensional disordered tight binding model are found. The particular solution is defined by boundary conditions on one face of the system. The determination of the rate of growth of the mean square wave function leads to an exactly soluble eigenvalue problem in $d-1$ dimensions. For $d \geqslant 2$ there are three types of particular wave functions in which the mean square amplitude (a) grows exponentially (b) decays exponentially (c) does not grow or decay but oscillates.

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The properties of the electronic states of disordered quantum systems are of considerable interest. Most of the known exact results are for one-dimensional ($d = 1$) systems, and in this case it has been established under quite general conditions that all eigenstates are localized. A review of this work has been given by Ishii.[1] Most of the discussions of this problem consider particular solutions of the stationary Schrödinger equation, i.e., solutions for given energy with boundary conditions prescribed on one edge of the system, and show that the solution grows exponentially with probability unity. It is then argued (Borland[2]) that eigenstates for a long but finite system occur at those energies where an exponentially growing wave function on the left can be matched to an exponentially growing function from the right. It is thus of considerable interest to investigate the properties of particular solutions of the Schrödinger equation for disordered systems in higher dimensions. In this paper we show that the problem of particular solutions can be exactly solved in any dimension for tight binding models with diagonal disorder. The determination of the rate of growth of the mean square wave function in d dimensions leads to an

[1] Physics Department, Rutgers University, Piscataway, New Jersey 08854. Supported in part by the National Science Foundation under grant No. DMR 78-10276.

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eigenvalue problem. This eigenvalue problem is equivalent to determining the eigenvalues of a single impurity in an otherwise periodic system in $d-1$ dimensions. We show that in disordered systems with $d \geqslant 2$ there are three kinds of particular wave functions, those where the mean square amplitude (a) grows exponentially, (b) decays exponentially, and (c) does not grow or decay but oscillates.

We begin by considering the tight binding Anderson model[3] in two dimensions with Schrödinger equation

$$Ea_{i,j} = \epsilon_{i,j} a_{i,j} + a_{i+1,j} + a_{i-1,j} + a_{i,j+1} + a_{i,j-1} \tag{1}$$

where E is the energy, $a_{i,j}$ is the wave function amplitude on the site in row i column j of a two-dimensional square lattice, and ϵ_{ij} is the energy of this site. The units of energy have been chosen so that the nearest neighbor transfer energy is unity. The ϵ_{ij} are mutually independent, random variables with a common distribution. The zero of energy is chosen so that $\langle \epsilon_{ij} \rangle = 0$ and the second moment is

$$\langle \epsilon_{ij}^2 \rangle = \sigma \tag{2}$$

The lattice is semi-infinite in the row direction to the right and each column has N sites and periodic boundary conditions are imposed in this direction. The amplitudes of the wave function in the first two columns on the left (say 0 and 1) are given. We denote these by $\mathbf{a}_0 \equiv a_{10} \cdots a_{N0}$ and $\mathbf{a}_1 = a_{11} \cdots a_{N1}$. Alternatively we could consider a lattice infinite in the row direction with the left half ordered and the right half disordered. A wave function of energy E on the left in the ordered region is given and we ask how this wave function grows in the disordered region.

We define a $2N$ column vector of the amplitudes in columns $i-1$ and i by

$$\begin{Bmatrix} \mathbf{a}_i \\ \mathbf{a}_{i-1} \end{Bmatrix} = \{ a_{1,i}, a_{1,i-1}, \ldots, a_{N,i}, a_{N,i-1} \} \tag{3}$$

We can then find a $2N \times 2N$ transfer matrix $T^{(i)}$ for column i which relates the amplitudes in columns i and $i+1$ to those in $i-1$ and i:

$$\begin{Bmatrix} \mathbf{a}_{i+1} \\ \mathbf{a}_i \end{Bmatrix} = T^{(i)} \begin{Bmatrix} \mathbf{a}_i \\ \mathbf{a}_{i-1} \end{Bmatrix} \tag{4}$$

The transfer matrix is conveniently written as an $N \times N$ matrix in which each element is a 2×2 matrix. The elements of this latter matrix are denoted by $T_{jk}^{(i)}$ $(j, k = 1 \ldots N)$ and are

$$\begin{aligned} T_{jj}^{(i)} &= W_j^{(i)} = \begin{pmatrix} E - \epsilon_{ij}, & -1 \\ 1, & 0 \end{pmatrix} \\ T_{j,j\pm 1}^{(i)} &= Q = -\tfrac{1}{2}(1 + \sigma_z) \end{aligned} \tag{5}$$

where σ_z is the Pauli matrix $(\sigma_z^2 = 1)$.

From (4) the mean square amplitudes in columns L and $L+1$ of the disordered region are

$$\langle |\mathbf{a}_{L+1}|^2 + |\mathbf{a}_L|^2 \rangle = (\mathbf{a}_1^*, \mathbf{a}_0^*) M_L \begin{Bmatrix} \mathbf{a}_1 \\ \mathbf{a}_0 \end{Bmatrix} \tag{6}$$

where

$$M_L = \langle \tilde{T}^{(1)} \cdots \tilde{T}^{(L)} T^{(L)} \cdots T^{(1)} \rangle \tag{7}$$

and $\tilde{T}$ is the transpose of T. We are thus led to consider the eigenvalues of the matrix equation

$$\lambda M_L = \langle \tilde{T} M_L T \rangle \tag{8}$$

The eigenvalues λ determine the rate of growth of the mean square amplitudes (6) because $\langle |\mathbf{a}_L|^2 \rangle \sim \lambda^L$. To solve this equation we must decide on the form of the $2N \times 2N$ matrix M_L. We write it as an $N \times N$ matrix with each element a 2×2 matrix, and from the symmetry of the problem this block matrix must be cyclic. It is thus determined by its first row, which we denote by $m_1 \cdots m_N$, where each m_j is a 2×2 matrix. The recursion relations for the m_j from (8) and (5) are [omitting the column index i in (5)]

$$\begin{aligned} \lambda m_j = \langle \tilde{W}_1 m_j W_j + \tilde{W}_1 (m_{j-1} + m_{j+1}) Q \\ + Q(m_{j-1} + m_{j+1}) W_j + Q(m_{j-2} + 2m_j + m_{j+2}) Q \rangle \end{aligned} \tag{9}$$

We are thus led to consider a one-dimensional problem, the elements of which are 2×2 matrices. There is a single impurity (at site 1), which results from the average of the first term on the right of (9) for $j = 1$, in an otherwise periodic system.

We first solve (9) for the special case $E = 0$, i.e., the center of the band. The matrices m_j are real and symmetric and a convenient representation in terms of Pauli matrices σ_x and σ_z is

$$m_j = \tfrac{1}{2} U_j (1 + \sigma_z) + \tfrac{1}{2} V_j (1 - \sigma_z) + W_j \sigma_x \tag{10}$$

Substituting (10) in (9) and carrying out the average, the coefficients in (10) satisfy

$$\begin{aligned} \lambda U_j &= (2 + \sigma \delta_{j,1}) U_j + V_j + U_{j-2} + U_{j+2} - 2(W_{j-1} + W_{j+1}) \\ \lambda V_j &= U_j \\ \lambda W_j &= U_{j-1} + U_{j+1} - W_j \end{aligned} \tag{11}$$

In the absence of disorder ($\sigma = 0$) these equations are solved by setting

$$(U_j, V_j, W_j) = (U, V, W) e^{ikj} \tag{12}$$

with $k = 2\pi l / N$ ($l = 1 \cdots N$). The eigenvalues are

$$\lambda = 1, e^{\pm 2ik} \tag{13}$$

and are distributed on the unit circle in the complex plane. These solutions correspond to propagating waves in the original two-dimensional lattice with wave vector $\pi - k$ (for $E = 0$) along the rows. We get three eigenvalues because the eigenvalues of T in the perfect lattice are $e^{\pm ik}$ and the eigenvalues of the matrix equation (8) are the three different products of these two eigenvalues.

In the presence of the single impurity the problem may be completely solved (see Maradudin *et al.*[4]). The eigenvalues of (11) are determined by the dispersion relation

$$1 = \frac{\sigma}{N} \sum_k \frac{\lambda(\lambda + 1)}{(\lambda - 1)(\lambda - e^{2ik})(\lambda - e^{-2ik})} \tag{14}$$

The sum on k in (14) gives (for N even)

$$1 = \frac{\sigma\lambda}{(\lambda - 1)^2} \frac{\lambda^{N/2} + 1}{\lambda^{N/2} - 1} \tag{15}$$

There is one eigenvalue with $|\lambda| > 1$ given by (in the $N \to \infty$ limit)

$$\lambda_0 = 1 + \frac{\sigma}{2} + \left(\sigma + \frac{\sigma^2}{4}\right)^{1/2} \tag{16}$$

The remaining eigenvalues are of the form $\lambda_k = e^{2ik}(1 - \sigma\delta_k/N)$ where δ_k has a positive real part. These eigenvalues lie inside the unit circle but as the width of the strip $N \to \infty$ $|\lambda_k| \to 1$. In general the wave function will contain a part which grows exponentially due to the large eigenvalue (16) and given by

$$\langle |\mathbf{a}_{L+1}|^2 + |\mathbf{a}_L|^2 \rangle \sim \exp(L \log \lambda_0) \tag{17}$$

This is similar to results in $d = 1$.[2] The important difference between $d = 1$ and $d = 2$ is that for $d = 1$ there is one growing and one decaying exponential solution while for $d = 2$ there is one growing (for $E = 0$) and $O(N)$ solutions in which the wave function does not grow or decay. It can be shown that it is possible to choose the initial boundary conditions so that the particular wave function is of this latter type, i.e., is not exponentially growing or decaying. There thus exist extended particular wave functions in $d = 2$.

The dispersion relation (14) is easily generalized to the case $E \neq 0$ in $d = 2$ and higher dimensions. In d dimensions we consider a semi-infinite

[2] In the $d = 1$ case the large eigenvalue is given by

$$\lambda = \frac{\sigma}{2} + \left(1 + \frac{\sigma^2}{4}\right)^{1/2} \qquad \text{for } E = 0$$

hypercubic lattice with a cross section with side containing N atoms. Periodic boundary conditions are imposed in the $d-1$ transverse directions and we introduce wave vector $k_\alpha = 2\pi l_\alpha / N$, $\alpha = 1 \cdots d-1$ and $l_\alpha = 1 \cdots N$. For fixed energy E we define

$$\cos\theta(k) = E/2 - (\cos k_1 + \cdots + \cos k_{d-1}) \tag{18}$$

Physically θ is the propagation constant along the semi-infinite direction. For E within the band of the ordered crystal θ assumes real values when the modulus of the right-hand side is < 1 and is complex when this modulus > 1. The solutions of (18) where θ is complex correspond to exponentially growing or decaying surface states. For E outside the band it is always complex. The solution of the problem in d dimensions follows the same method as for $d = 2$ and the dispersion relation for the eigenvalues of (8) is

$$1 = \frac{\sigma}{N^{d-1}} \sum_{(k_\alpha)} \frac{\lambda(\lambda+1)}{(\lambda-1)(\lambda - e^{2i\theta(k)})(\lambda - e^{-2i\theta(k)})} \tag{19}$$

From (17) and (18) it can be shown that for E within the band the distribution of eigenvalues for $N \to \infty$ is of the form shown in Fig. 1. The eigenvalues with $|\lambda| = 1$ lie around the unit circle and those with $\lambda > 1$ and $\lambda < 1$ along the real axis. For E outside the band only eigenvalues with $\lambda > 1$ and $\lambda < 1$ exist. We thus find for all $d \geqslant 2$ that for E within the band there exist particular wave functions whose mean square amplitudes either grow exponentially, decay exponentially, or oscillate around the initial

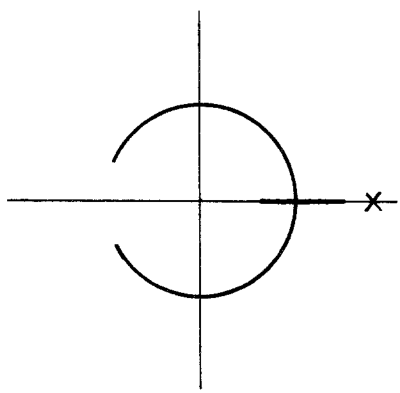

Fig. 1. Distribution of eigenvalues of the dispersion relation for E within the band (denoted by heavy lines and cross). Propagating solutions lie on the unit circle, exponentially growing and decaying surface states lie on the positive real axis, and the exponentially growing solution due to disorder is denoted by a cross.

values.[3] These wave functions are not directly related to the eigenfunctions of the system. However, it is reasonable to argue, as in the $d = 1$ case, that eigenstates for a large finite system occur at those energies where states from the left match those from the right. The exponentially growing particular wave functions are then associated with localized eigenstates and the extended particular wave functions with extended eigenstates. Of course this argument is not rigorous nor does it indicate for which energies we expect localized or extended eigenstates. The above results on the particular wave functions do suggest the existence of both kind of states in disordered systems with $d \geqslant 2$.

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REFERENCES

1. K. Ishii, *Prog. Theor. Phys.* (*Suppl.*) **53**:77 (1973).
2. R. E. Borland, *Proc. R. Soc. London Ser. A* **274**:529 (1963).
3. P. W. Anderson, *Phys. Rev.* **109**:1492 (1958).
4. A. A. Maradudin, E. W. Montroll, and G. H. Weiss, *Solid State Physics*, Suppl. 3, F. Seitz and D. Turnbull, eds. (Academic Press, New York, 1963).

[3] In the special case $d = 2$, $E = 0$ the exponentially decaying solutions are absent.