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Course: Solid State II

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Anderson Localization

1 Introduction

Electrons in crystals are described by Bloch waves, which are periodic up to a phase. The foundation of this theory is the periodic nature of crystals. In this simplest non-interacting case, this theory implies that electrical resistance is zero for metals. Finite electrical conductivity is achieved when we make the plausible assumption that there are small imperfections in the lattice and that the electrons interact with the ions and imperfections. The electrical conductivity at low temperature in this weak-disorder limit is then given by

$$\sigma(T) = \sigma_0 - A\sigma_0^2 T^n, \quad (1)$$

where σ_0 and A positive are constants and n is a positive integer usually greater than or equal to two[1].

Unfortunately, from the experimental studies it turns out that in Eq. (1) A can either be positive or negative and n is typically $\frac{1}{2}$ for three dimensional systems. Also, as the disorder is increased, the electrons get localized and some materials (for example, granular Al) undergo metal-insulator transition[2]. Conventional description of electrons in the crystal by Bloch waves does not explain these behavior. Thus, we have to discard the weak-disorder limit and take into account the disorder from the outset.

2 Experimental motivation

The motivation for study of localization came from experiments investigating the effects of doping in Si. In 1955, Feher et al. measured electron spin resonance of P and As doped in Si[4]. They found that the characteristic electron spin frequency of P and As persisted for a timescale on the order of seconds to minutes. However, a simple Fermi golden rule calculation gives the expected lifetime for spin diffusion due to interaction with electrons of other atoms to range between 0.1 to $10^{-6}s$. Since the Si was extremely pure, Anderson argued that the absence of spin diffusion was due to disorder arising from the random distribution of impurities[6].

3 Basic concepts of Anderson localization

3.1 Weak Disorder Limit

In perfect crystals, electrons are described by delocalized Bloch waves. Unfortunately, crystals free of impurity hardly exist in nature. Disorder in crystals range from small impurities in an otherwise pure crystal to the strong disorder limit of alloys. In the weak disordered limit, the electrons are still described by delocalized Bloch waves that scatter off the impurities. The low-temperature resistivity is then given by solving the Boltzmann transport equation. The expression for resistivity has the form[1]

$$\rho(T) = \rho_0 + AT^n. \quad (2)$$

Here ρ_0 is the residual resistivity due to impurities, A is a positive constant and n is a positive integer usually greater than or equal to two. The case when n equals to two occurs when electron-electron scattering dominates.

3.2 Consequences of Disorder

It turns out that in disordered materials, the Boltzmann description of electronic conductivity is wrong[1]. The constant A could be positive or negative and n is usually $\frac{1}{2}$ for three dimensional systems.

Furthermore, it is found that in one and two dimensional systems, any amount of disorder will cause the electrons to be localized. Meanwhile, in three dimensional systems, there is a continuous metal to insulator transition as the disorder is increased. So we cannot approach the problem of disorder by assuming that electrons are described by delocalized Bloch waves scattering off almost perfect crystal. We will have to take into account the disorder from the outset.

3.3 Strong Disorder Limit

It was believed that the effect of scattering by random impurities would cause the Bloch electrons to lose their phase over some mean free path, although the electrons would still be

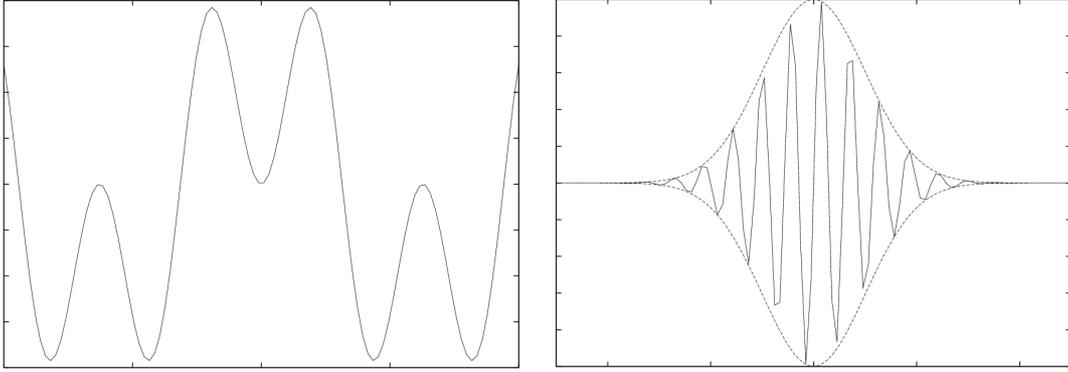


Figure 1: Typical delocalized (left) and localized (right) wave functions.

described by a delocalized wave function that extended throughout the sample. However, Anderson in 1958 showed that the electron wave function may be localized if the disorder is very strong[6]. In such cases, the envelope of the wave packet decays exponentially as shown in Fig. 1. Then the wave function can be described as

$$|\psi(r)| = \exp(-|r - r_0|/\xi) \quad (3)$$

where ξ is the localization length.

The existence of localized states can be explained as follows. In the limit of very strong disorder there is huge fluctuation in potential from one point to another. So the sample can be treated as a collection of potential wells of various depths. Since the electrons are bound inside the sample, the eigenstates in the first order of approximation are bound states or orbitals having exponentially decaying tails of varying lengths. The next order of approximation consists of admixture between different orbitals. However, the orbitals that are nearby in space have very different energy. Hence, the admixture is small because of big energy denominator. On the other hand, orbitals that are far apart have very small overlap integral. Thus, the higher orders of approximations do not produce linear combinations of infinitely many localized states. Intuitively, localization of electrons in presence of sufficiently random potential makes sense. In a periodic crystal, Bloch waves are the energetically lowest states. However, if there are potential wells due to impurities, electrons can lose kinetic energy by forming wave packets and being localized.

3.4 Computational example of localization in a one-dimensional chain

Analytically solving the Hamiltonian with random potential at various sites of a lattice is almost impossible. However, localization on a random lattice can be easily shown computationally. Here we follow the discussion of Šiber[7]. We consider the Hamiltonian

$$H = \sum_i E_i |i\rangle\langle i| + \sum_i T_i [|i+1\rangle\langle i| + |i\rangle\langle i+1|] \quad (4)$$

where $|i\rangle = |0, \dots, 1_i, \dots, 0_N\rangle$ denotes a particular site occupied by an excitation and T_i is the hopping matrix elements. In this basis, the Hamiltonian can be represented as a tridiagonal matrix:

$$H = \begin{pmatrix} E_1 & T_1 & 0 & 0 & \cdots & 0 & 0 \\ T_1 & E_2 & T_2 & 0 & \cdots & 0 & 0 \\ 0 & T_2 & E_3 & T_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & T_N & E_N \end{pmatrix} \quad (5)$$

To study the effect of random potential, Šiber chose E_i randomly in the interval $[e, 2e]$, $N = 900$ and $T_i = -0.1$. When Eq. 5 is solved, every eigenvectors turn out to be localized, as shown in Fig. 2.

4 Basic concepts of scaling theory

The localization of electrons in impurity doped sample can also be studied using scaling theory which was pioneered by Thouless[3]. This approach enables us to study the role of dimensionality in localization easily. The two fundamental assumptions of scaling theory are that the dimensionless conductance is a function of sample size only and scaling function is a function of conductance only. The dimensionless conductance is defined as

$$g(L) = \frac{G(L)}{e^2/\pi\hbar} \quad (6)$$

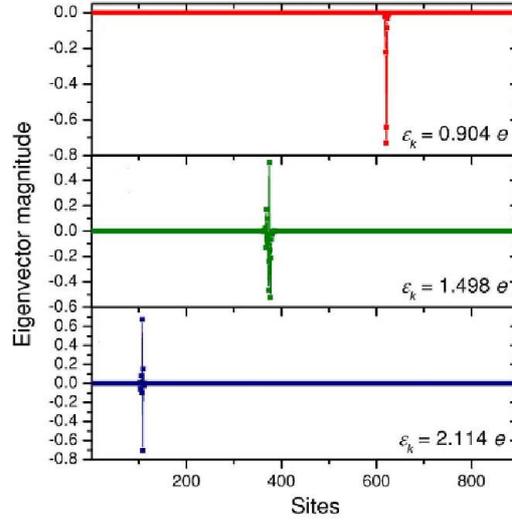


Figure 2: Localized eigenstates of a random potential in one-dimensional lattice for three different eigenvalues[7]

where G is the conductance in usual units and L is the sample size. The scaling function is defined as

$$\beta(g) = d(\ln g)/d \ln L. \quad (7)$$

In the strong disorder case, all the states are localized. Hence, we have

$$g(L) \approx e^{-\frac{L}{\xi}} \quad (8)$$

where ξ is the localization length. In the weak disorder limit, the conductance is proportional to the ratio of change in energy level spacing (ΔW) and energy of each eigenstate (ΔE) as the sample size is increased. The energy level spacing is given by the inverse of the number of particles in the system. So $\Delta W = (n_e L^d)^{-1}$. The shift in eigenstate is given by $\Delta E = \hbar/\tau$, where τ is the relaxation time[5]. If we take τ to be the time it takes for the electron to diffuse from the center to the edge of the sample, we have $\tau = (L/2)^2/D_0$, where D_0 is the diffusion constant. So we have for the conductance

$$g(L) = \frac{2\hbar}{e^2} \sigma L^{d-2} \quad (9)$$

where $\sigma = 2e^2 n_e D_0$.

5 Consequences of scaling theory

As described above, scaling function captures the essential physics in the scaling theory. If $\beta(g) > 0$ in the limit $L \rightarrow 0$, then $g(L)$ diverges implying extended states. On the other hand, if $\beta(g) < 0$ as $L \rightarrow 0$, then $g(L)$ monotonically tends to zero implying localized states. In the strong disorder limit, we get $\beta(g) = -\infty$. So all states are localized in strong disorder limit. In the weak disorder limit, we have $\beta(g) = (d - 2)$.

In one dimension we have $\beta(g) = -1$ in the weak disorder limit. Hence, any amount of disorder localizes the electrons.

In two dimensions, $\beta(g) = 0$ in the weak disorder limit. So in this case also any amount of disorder localizes the electrons.

In three dimensions, $\beta(g) = 1$ in the weak disorder limit. However, $\beta = -\infty$ in the strong disorder limit. Hence, a three dimensional sample undergoes a metal to insulator transition as disorder is increased.

6 Conclusions

Existence of disorder in a sample may cause electrons to be localized. According to Anderson, all electronic states are localized in the strong disorder limit. The effect of disorder can also be studied using scaling theory which postulates that conductance is a function of sample size only and that the scaling function captures all the essential aspects of disorder. According to the scaling theory, any amount of disorder will localize electrons in one and two dimensional samples. However, in three dimensions, there is a transition from metallic state to insulator as the disorder is increased.

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