Chapter 2

Theoretical Background

This chapter is devoted to a review of some theoretical background for approaching our problem: the physics of Anderson localization, Josephson tunneling effects, quantum vortex and its interaction.

2.1 Anderson Localization

Every levels of the electrons in a periodic potential in form an energy band: the electronic wave functions extend through out the system. When the periodicity is distorted the spatial extent of the wave functions is reduced in such a way that they are localized. This phenomenon is called *Anderson localization* (Anderson, 1958). Anderson considered a three-dimensional point lattice occupied by "atoms", each of which has just one single state E_n. If all E_n are equal, an energy band of width B results. For the discussion of the states in a disorders
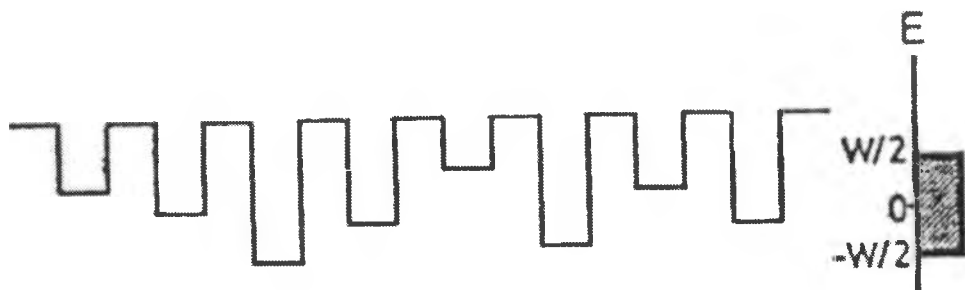
Figure 2.1: Anderson model: Potential wells of different depths at the lattice sites of a three-dimensional point lattice.

lattice, he maintains the positions of the atoms in the point lattice, but takes the E_n to be statistically distributed over a range of width W (Fig. 2.1).

The Hamiltonian can then be written as

$$H = \sum_n E_n c_n^\dagger c_n + \sum_{mn} V_{mn} c_m^\dagger c_n \qquad (2.1)$$

. where $c_n^\dagger$ is a creation operator, and c_n is an annihilation operator in the Wannier representation for site n. To simplify matters, in the second term only transitions between nearest neighbors are allowed and for them V_{mn} are asumed to take equal value V for all pairs mn. Starting from an initial state in which an electron is located at a given lattice point, one can inquire about the probability of finding the electron at this point again as $t \to \infty$. Diffusion of the electron in the lattice can, of course, occur since transitions are made possible by the second term in the Hamiltonian. If the initial position belongs to a localized state, the

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diffusion is restricted to a finite volume. The probability of return for $t \to \infty$ is then nonzero. If, however, the electron can diffuse to infinity, the probability of return is zero. Anderson was able to show that the magnitude of the ratio W/B decides between these two alternatives. In particular, for the state $E = 0$ (mean value of the E_n distribution in the disordered lattice, middle of the band in the ordered lattice) the probability of return is zero if W/B falls below a fixed value of the order of 5. The state is then delocalized (extended). For larger ratios W/B, i.e., when the width of the spread of energy levels significantly exceeds the band width B, the state $E = 0$ is localized.

This definition of localization does not allow us to distinguish in a real case between localized and extended states. It can, however, help us to understand the increasing localization of band states as the transition is made from an ordered to a disordered lattice.

We can follow this transition qualitatively, without having to go into the detailed calculations (Madelung, 1978). In solid, the periodicity of a lattice is the cause of the periodic potential, and the wave function which describes the system is the Bloch wave. The energy band is formed. To study the effect of defects on the lattice, it is instructive to consider a single defect in a periodic potential. We begin with the Schrödinger equation of an electron in a periodic lattice,

$$H_0 \Psi_n(\mathbf{k}, \mathbf{r}) \equiv \left[-\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \right] \Psi_n(\mathbf{k}, \mathbf{r}) = E_n(\mathbf{k}) \Psi_n(\mathbf{k}, \mathbf{r}) \qquad (2.2)$$

where $V(\mathbf{r})$ is the periodic lattice potential and $\Psi_n(\mathbf{k}, \mathbf{r})$ is the Bloch function.

The inclusion of defect modifies eq.(2.2) to

$$[H_0 + U(\mathbf{r})] \Psi = E\Psi. \qquad (2.3)$$

Here $U(\mathbf{r})$ is the additional potential introduced by the defect. For an impurity atom at a lattice position, for example, it is the potential of the impurity less than the potential of the lattice atom which has been substituted. $U(\mathbf{r})$ may, however, include the effect of a local lattice distortion caused by the impurity atom.

Since $U(\mathbf{r})$ can be either negative or positive, electrons can thus be bounded to the defect or repelled by it. We consequently anticipate that eq.(2.3) has solutions which are localized about the defect, and whose energy levels lie below or above the state of the energy band considered.

An analysis of eq.(2.3) for simple models indeed revealed this behavior (Madelung, 1978). We show one result in Fig. 2.2. The general feature is that the presence of the defect in an otherwise periodic potential leads to a split-off of one state from the original band. If $U(\mathbf{r})$ is positive, the uppermost state splits off; if $U(\mathbf{r})$ is negative the lowest splits off. In this case, there are only minor displacements of the states within the band. While the wave function in the band remains approximately a delocalized Bloch function, the one associated with the split-off state is localized. We shall not carry out the calculations which lead to Fig. 2.2.

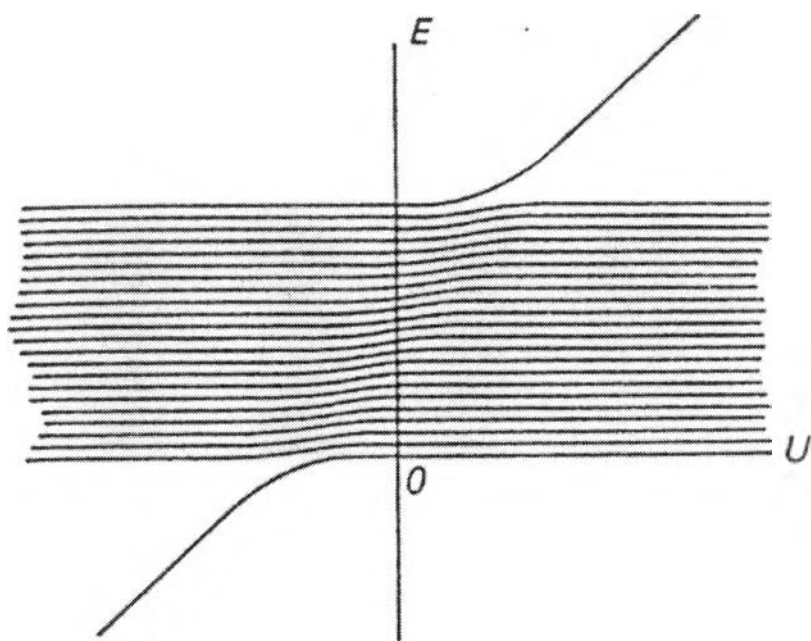From Fig. 2.2, we saw that a single imperfection leads to the split-off (and

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Figure 2.2: Energy band for a simple three-dimensional potential model (periodic potential with an isolated defect) as a function of the deviation U of the defect potential from the potential from the potential at an undisturbed lattice site. Depending on the sign of U, the state of highest or lowest energy splits out from the quasi-continuous band. The split-off state is spatially localized to the vicinity of the defect. The remaining delocalized band states are only displaced slightly in energy. This result justifies the retention of the band model and its extension with defect levels to describe crystals distorted by a small concentration of defects.

simultaneous localization) of a state from the band edge. With increasing number of imperfections, the number of localized states outside the band increases. The defect levels combine into a band (impurity band) which can overlap with the band of the delocalized states if the defect concentration is sufficiently high. We can imagine that the same phenomenon occurs with increasing disorder of a lattice. The states at the edges of an energy band become localized first, and simultaneously shift into the energy gap. These band this requires tails with localized occur states at its top and bottom edges. Fig. 2.3 shows the result of the calculation by Economou and Cohen (Economou, 1970). With growing disorder, the limits E_c and $E_{c'}$ approach one another from both sides and eventually meet at the middle of the band. When they meet, all band states are localized. This occurs just when the ratio W/B is fulfilled.

The electronic wave function in a random potential may be profoundly altered if the randomness is sufficiently strong. The traditional view had been that the scattering by the random potential causes the Block waves to lose phase coherence on the length scale of the mean free path l. Nevertheless, the wave function remains extended throughout the sample. Anderson pointed out that if the disorder is very strong, the wave function may become localized, in that the envelope of the wave function decays exponentially from some point in space, i.e.,

$$|\Psi(\mathbf{r})| \sim \exp(|\mathbf{r} - \mathbf{r}_0|/\xi) \tag{2.4}$$

and ξ is the localization length. This is illustrated in Fig. 2.4. This is expected if
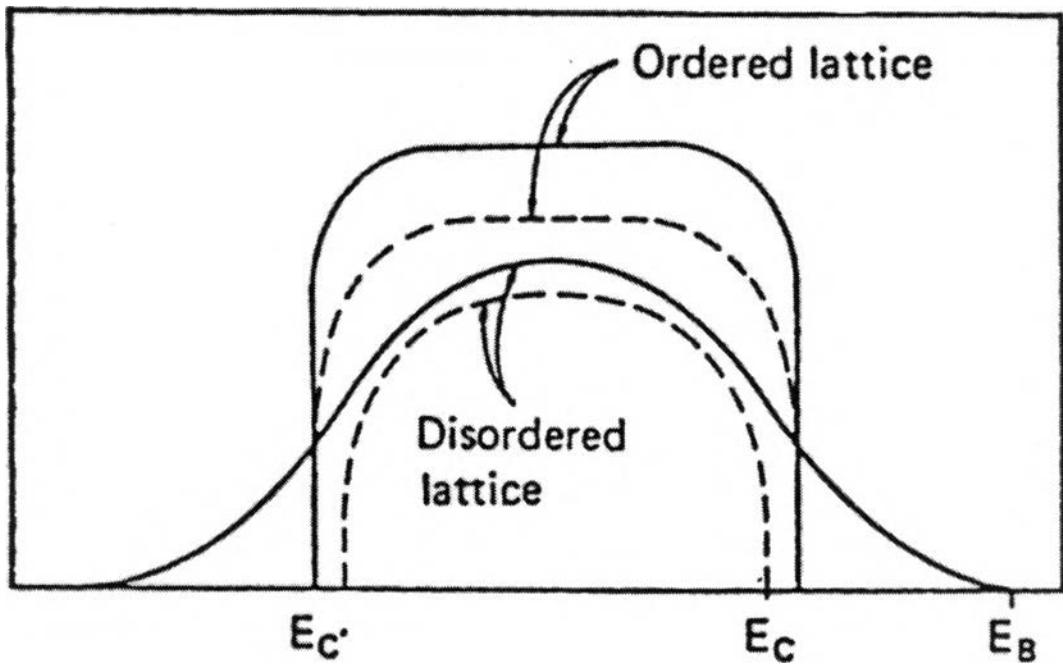
Figure 2.3: Density of states (solid curves) and distribution of the extended states (dashed curves) for an energy band of an ordered and a disordered lattice. E_B–band edge; E_c, $E_{c'}$–limits between localized and extended states.
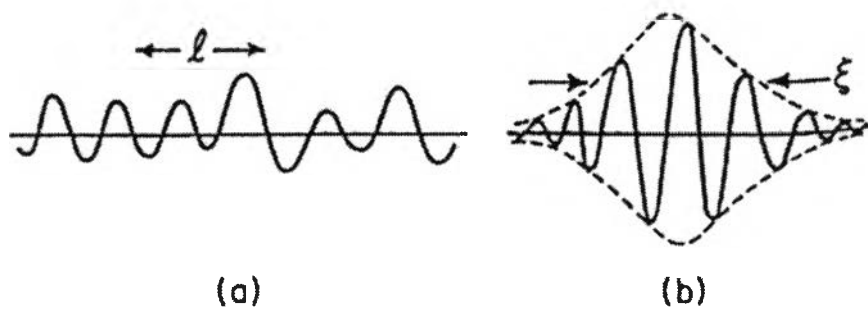
Figure 2.4: Typical wave function of (a) extended state with mean free path l; (b) localized state with localization length ξ.

the disorder is sufficiently strong or in energy regions where the density of states is sufficiently small. The energy regions with small densities of states are typically associated with the tails of quantum mechanically allowed energy bands. For weak disorder or energy regions with sufficient density of states, the wave functions will extend throughout the whole system with their phases and amplitudes varying randomly in space. Physically the disorder can be imagined to be commented with the presence of impurities (Kramer, 1993), vacancies and dislocations in an otherwise ideal crystal lattice. Another possibility is to distribute atoms or molecules at more or less random positions. Strong disorder can then be achieved by using a large concentration of impurities, for instance, independent of the strength of the individual impurities. A complete disordered assembly of atoms will be the one in which the atoms are sitting on sites that are chosen completely, independently and randomly.

The existence of the localized state is understood if we go to the limit

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of very strong disorder. Then a zeroth-order description of the eigenstate would be a bound state or a localized orbital bound by deep fluctuation in the random potential. We could then consider the admixture between different orbital as a perturbation. The main point is that such admixtures will not produce an extended state composed of linear combinations of infinitely many localized orbital. The reason is that the orbitals that are nearby in space, so that the wave functions overlap significantly, are in general very different in energy, so that the admixture is small because of the large energy denominator. On the other hand, states that are nearly degenerate are in general very far apart in space, so that the overlap is exponentially small. Thus, in the strongly disordered limit, the wave function will be exponentially localized.

Now that we understand the two limits of weak and strong disorder, the interesting question is what happens for intermediate disorder. Instead of varying the amount of disorder, we can also consider varying the energy of the eigenstates. We expect the states deep in the band tails to be localized, since these are states that are formed from localized orbital bound in deep potential fluctuations. The states in the center of the band have the best chance of remaining extended for a moderately disordered system. Thus, as a function of energy, the states must change their character from being localized to being extended. The critical energy at which this change occurs is called the mobility edge. Therefore, if the Fermi energy lies in a region of localized states, the conductivity at zero temperature would vanish, while the extended states give rise to a finite zero-temperature
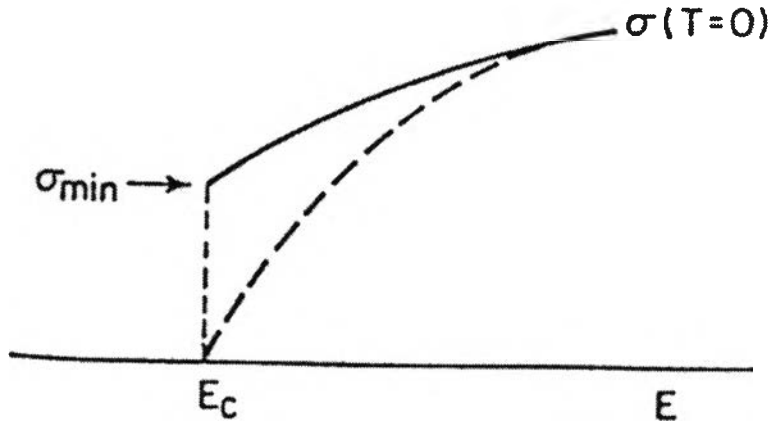
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Figure 2.5: Schematic illustration of the mobility edge E_c, which separate localized and extended states. The two possibilities of a continuous or discontinuous transition with σ_{min} are shown.

conductivity. The mobility edge marks the transition between a metal and an insulator. This is illustrated in Fig. 2.5.

Particles that occupy exponentially localized states are restricted to finite regions of space. They cannot contribute to transport at the absolute zero of temperature, $T = 0$ K, and therefore the coupling to other degrees of freedom, such as phonons and particle-particle interactions, has become negligible. On the other hand, particles in extended states can escape to infinity and contribute to transport. As a consequence, if there are only localized states near the Fermi energy the system will be an insulator, in the sense that, at $T = 0$ K, the DC conductivity (the zero frequency limit of the linear conductivity) vanishes. On the other hand, when the Fermi level lies in a region of extended states ($T = 0$

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K). The DC conductivity will be finite and the system will be metallic. The localization of the quantum mechanical wave functions as a consequence of the presence of disorder is one of the fundamental ingredients for the understanding of the existence of insulators and metals, and, in particular, the transition between the insulating and the metallic states of matter.

2.2 The Josephson Tunneling Effect

When two superconductors are separated by a thin layer of insulating material, electron pairs will tunnel through the insulator from one superconductor to the other. Josephson (Josephson, 1962) proposed that there should be a contribution to be current through an insulating barrier between two superconductors which would behave like direct tunneling of condensed pairs from one condensed gas of bound pairs at the Fermi surface to the other. The Hamiltonian for the problem of Josephson Effect is (Anderson, 1964)

$$H = H_1 + H_2 + \sum_{k,q} T_{kq} \left(C_{k\uparrow}^{\dagger} C_{q\uparrow} + C_{-q\downarrow}^{\dagger} C_{-k\downarrow} \right) + H.C. + \ldots \qquad (2.5)$$

where H_1 and H_2 are corresponding Hamiltonians of the two superconductors on both sides of the barrier; T_{kq} is the exponentially small tunneling matrix element from state k on one side to state q on the other. Eq.(2.5) is a standard form for many kinds of tunneling problems.

It is generally assumed, either because of the microcanonical assumption that the number of electrons is absolutely fixed, or because the system is in a

mixed state as a result of contact with an electron reservoir undergoing fluctuations, that the total phase of the sample as a whole is meaningless. It can be shown that the state of fixed number of Cooper pairs N is an average over all phase values. In fact, the total number N of Cooper pairs and the phase ϕ are conjugate variables obeying an uncertainty relation

$$\Delta N \Delta \phi \geq 2\pi. \tag{2.6}$$

It is, on the other hand, not necessarily meaningless to discuss the relative phases of two blocks of superconductor which are connected by an insulating barrier sufficiently thin for tunneling to occur. Clearly, again, the total phase of the assembly as a whole is not physical, but the relative phases can be meaningful when we observe that electrons can pass back and forth between the two through the barrier, leading to the possibility of coherence between states in which the total number of electrons is differently partitioned between the two sides: just as the phase coherence within the single block means that the number of electrons is not fixed locally and, for instance, there is coherence between the state with $N/2$ electrons in one half of the block and $N/2$ in the other, and that with $(N/2) + 2$ on one side and $(N/2) - 2$ on the other.

It thus may be meaningful to calculate the properties of the system assuming a given phase relationship. If we find that the energy is indeed a function of the relative phase, we must presume that the phase may adjust itself in such a way as to minimize the energy. If there are the possibility of quantum-mechanical

zero-point fluctuations or thermal fluctuations, as well as any external stresses, we can apply them to break up the coherence.

Now we simply write down the standard expression for the second-order energy perturbation using in eq.(2.5). We are also interested in the case in which the energy gaps on both sides differ in magnitude. In terms of the coherence factors u_k, v_k and v_q by which the Bogolyubov quasi-particles are defined,

$$\Delta E_2 = -2 \sum_{k,q} |T_{kq}|^2 \frac{|v_k u_q + v_k u_q|^2}{E_k + E_q} (1 - f_k - fq). \qquad (2.7)$$

Here we have allowed the energy gaps Δ_k and Δ_q to have arbitrary complex values, given by

$$2u_k v_k^* = \frac{\Delta_k}{E_k}, \qquad 2u_q v_q^* = \frac{\Delta_q}{E_q}$$

$$|u_k|^2 - |v_k|^2 = \frac{\epsilon_k}{E_k}, \qquad |u_q|^2 - |v_q|^2 = \frac{\epsilon_q}{E_q} \qquad (2.8)$$

$$E = \sqrt{\epsilon^2 + \Delta^2}$$

E and ϵ have the usual significance, and f_k and f_q are the Fermi distribution functions of E_k and E_q respectively. Here we have thrown away the terms with energy denominators $\pm(E_k - E_q)$ because they are not important except near T_c.

Let us rewrite eq.(2.7) using the relationships eq.(2.8)

$$\Delta E_2 = - \sum_{k,q} \frac{|T_{kq}|^2 (1 - f_k - f_q)}{E_k + E_q} \left(1 - \frac{\epsilon_k \epsilon_q}{E_k E_q} + Re \frac{\Delta_k \Delta_q^*}{E_k E_q} \right) \qquad (2.9)$$

This demonstrates explicitly the phase-dependent term. It will be interesting to calculate this term explicitly at the absolute zero. Let us assume Δ_k and Δ_q

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constant, namely equal to

$$\Delta_k = \Delta_1 \exp(i\phi_1), \qquad \Delta_q = \Delta_2 \exp(i\phi_2) \quad ; \qquad (2.10)$$

where Δ_1 and Δ_2 are real. Introducing the two densities of states of one spin in energy, N_1 and N_2, we obtain

$$
\begin{aligned}
\Delta E_2 &= -N_1 N_2 \Delta_1 \Delta_2 \langle |T_{kq}|^2 \rangle_{ave} \cos(\phi_1 - \phi_2) \\
&\times \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{d\epsilon_1 d\epsilon_2}{E_1 E_2 (E_1 + E_2)}.
\end{aligned} \qquad (2.11)
$$

It will lead to negligible error if we let the upper limits of the integrals to approach tend infinity. Then the integral is a complete elliptic integral:

$$
\begin{aligned}
\Delta E_2 &= -N_1 N_2 \langle |T_2| \rangle \cos(\phi_1 - \phi_2) \cdot \frac{4\pi \Delta_1 \Delta_2}{\Delta_1 + \Delta_2} K\left(\frac{|\Delta_1 - \Delta_2|}{|\Delta_1 + \Delta_2|} \right) \\
&\simeq -N_1 N_2 \langle |T_2| \rangle \cos(\phi_1 - \phi_2) \cdot 2\pi^2 \frac{\Delta_1 \Delta_2}{\Delta_1 + \Delta_2}.
\end{aligned} \qquad (2.12)
$$

From the energy expression E_2 we can easily deduce the Josephson current as follows. We first observe that eq.(2.11) is clearly not gauge invariant because it depends on the phase difference of the wave functions on the two sides. A gauge transformation which changes the phase can be performed, but only at cost of changing the vector potential $\mathbf{A}$. We can deduce, assuming-as by now is permissible-that the BCS theory gives gauge-invariant results, that had we calculated the energy in the presence of a vector potential $\mathbf{A}$ we should have obtained

$$\Delta E_2 = \Delta E_1 \cos\left(\phi_1 - \phi_2 - \frac{2e}{\hbar c} \int_1^2 \mathbf{A} \cdot d\mathbf{l}\right). \qquad (2.13)$$

Here we define ΔE as the result of the integration in eq.(2.11), i.e., the coefficient of $\cos(\phi_1 - \phi_2)$ in eq.(2.12) or the corresponding number at finite T. We use $2e$ in the $\mathbf{A}$ integration, of course, because Δ depends on the mean value of $\psi^*\psi^*$, and its phase therefore transforms with the doubled charge.

The current may be defined in term of the derivative of Hamiltonian with respect to the vector potential:

$$J = c\frac{\delta H}{\delta A}. \tag{2.14}$$

The dependence of the energy on the vector potential $\mathbf{A}$ implies immediately the existence of a certain density of supercurrent flow such that

$$\langle \mathbf{J} \rangle = c\frac{\delta \langle H \rangle}{\delta \mathbf{A}}. \tag{2.15}$$

In order to get mass flow per unit volume = current per unit area, we must note that ΔE in eq.(2.13) is a surface energy, and should be divided by w, the thickness of the barrier, to give volume energy. We then get

$$\langle J \rangle = \frac{2\Delta E e}{\hbar}\sin(\phi_1 - \phi_2 - \frac{2e}{\hbar c}|A|w) \tag{2.16}$$

Presuming that $\mathbf{A}$ is in the direction perpendicular to the surfaces. This then gives us the current (again at absolute zero):

$$J = J_1 \sin(\delta\phi) \tag{2.17}$$

where

$$J_1 = \frac{2e\Delta E}{\hbar} \cong \frac{4\pi^2 e}{\hbar} N_1 N_2 \langle T \rangle^2 \frac{\Delta_1 \Delta_2}{\Delta_1 + \Delta_2}. \tag{2.18}$$

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2.3   Quantum Vortex

In Type II superconductors it is observed that the magnetic flux is completely excluded only for the external field $B < B_{c1}$. Above the lower-critical field, B_{c1}, magnetic flux penetrates in the form of the flux tubes, discrete flux quanta, or vortices (Poole *et al.*, 1995). We have seen that an applied magnetic field B_{app} penetrates into a superconductor in the mixed-state, $B_{c1} < B_{app} < B_{c2}$. Penetration occurs in the form of tubes, called vortices (see Fig. 2.6), which serve to confine the flux. The strongest field is in the core which has a radius ξ. The core is surrounded by a region of larger radius λ within which magnetic flux and screening currents flowing around the core are present together, as shown in Fig. 2.6.

As the applied magnetic field increases, the density of vortices increases and they begin to overlap, making the vortex-vortex nearest-neighbor distance less than the penetration depth. The high-density case can be treated by assuming that the magnetic field at any point is a superposition of the fields from all of the overlapping vortices. At high density of vortices, the magnetic field between vortices B_{in} becomes very large and the variation of the field in the space between the cores becomes very small, as indicated in Fig. 2.7.

Since vortices is a flux lines through the superconductor, there are interaction potential between them. When two lines are separated by a distance r,
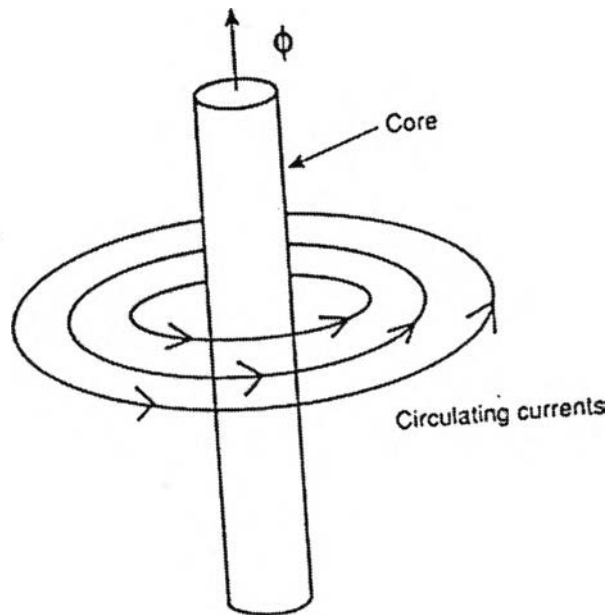
Figure 2.6: Sketch of shielding currents circulation around a vortex core. We can prove by using the Ginzberg-Landau theory that, the magnetic flux which penetrates into a superconductor in the mixed-state will be quantized in the unit of fluxoid Φ_0, where Φ_0 is the quantum of flux and equal to $\frac{h}{2e}$.

High concentration

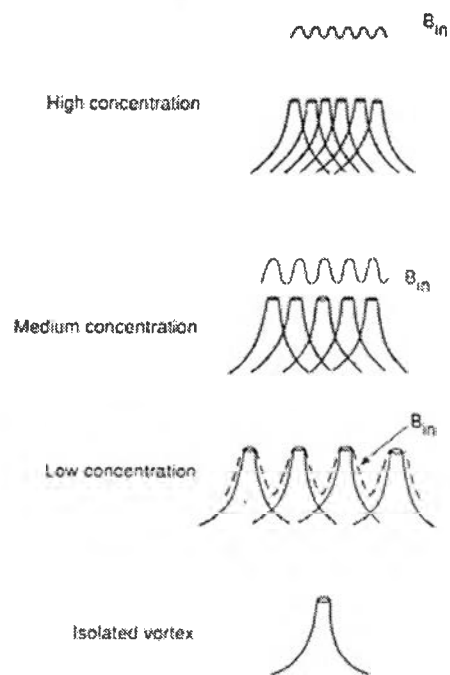Medium concentration

Low concentration

Isolated vortex

Figure 2.7: Sketch showing how the magnetic field B_{in} inside a superconductor increases as the concentration of vortices increases and their fields increasingly overlap.

there is a repulsive interaction potential $V(r) \propto K_0(r/\lambda)$, where $K_0(r/\lambda)$ is a Bessel function and λ is the London penetration depth. In general, the lattice spacing of the Josephson junction arrays fabricated in the laboratory is small in the order of micrometers. We therefore are interested in the limit of small r/λ in which case the Bessel function $K_0(r/\lambda) \simeq -\ln(r/\lambda)$. This motivates us to take $V(r) \propto \ln(r/\lambda)$ when we consider the problem of vortex transport in Chapter 5.