BCS Theory, Energy Gap

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A theoretical explanation of superconductivity was sought early on. Albert Einstein, for example, had suggested that superconductivity is caused by molecular chains (similar to Ampère's molecular currents). In a manuscript of March 1922 entitled "*Theoretical Remarks on the Superconductivity of Metals*" (*Theoretische Bemerkungen zur Supraleitung der Metalle*; published in September 1922), Einstein had discussed the superconducting state as follows:

> It therefore seems inevitable that the superconducting currents are carried by closed molecular chains (conduction chains), whose electrons constantly undergo cyclic permutations. Kamerlingh Onnes therefore compares the closed currents in superconductors with Ampère's molecular currents. … It may be regarded as improbable that different kinds of atoms can form conducting chains with each other. So perhaps the transition from one superconducting metal to another is never superconducting.

However, Kamerlingh Onnes was already interested in the contact between two different superconductors. At the end of the mentioned manuscript, Albert Einstein writes in a short P.S.: "*The last hinted assumptions … are partly disproved by an important experiment, which Kamerlingh Onnes carried out in the last months. He showed that at the contact point of two different superconductors (lead and tin), no measurable ohmic resistance appears.*"

The question of the behavior of a contact between two superconductors was taken up again in 1932, when Walther Meissner showed in experiments together with Ragnar Holm that the mechanical contact between two superconductors is also superconducting, which is incompatible with molecular chains. We will come back to the contact between two superconductors in Chapter 7 when discussing the Josephson effect.

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Phenomenological theories such as the London theory and the Ginzburg–Landau theory meant important stations in theoretical understanding. However, a microscopic explanation of the mechanism was still missing. The list of those who had tried this is long. Besides Albert Einstein, we mention the names of Felix Bloch, Niels Bohr, Léon Brillouin, Jakov I. Frenkel, Werner Heisenberg, Ralph Kronig, Lew Dawidowitsch Landau and Wolfgang Pauli.

In 1957, John Bardeen, Leon Cooper and Robert Schrieffer achieved a decisive progress. Their "BCS theory" was quickly accepted. The reason why it took so long to find a convincing theoretical explanation of superconductivity is that the energy difference of the electrons between their normal and superconducting states is extremely small and much smaller than the Fermi energy. However, the calculation of the various individual contributions to the energy of the electrons in the crystal is much less accurate than the energy gain achieved during the transition to the superconducting state.

The BCS theory is based on the idea that at low temperatures, there is an attractive force between two electrons, so that two electrons combine to form pairs in a certain way. The binding energy thus obtained leads to a reduction in energy. Leon Cooper had already theoretically deduced such pair formation and energy lowering in 1956. Therefore, the pairs of electrons are called "Cooper pairs." The attraction during the formation of the Cooper pairs is caused by distortions of the crystal lattice in the vicinity of the individual electrons. Phonons therefore play a role here.

Herbert Fröhlich and independently John Bardeen had developed an important basic idea for this in 1950. They had realized that an electron distorts the crystal lattice in its environment. Due to the electron–phonon interaction, an electron moving through the crystal lattice is surrounded by a cloud of virtual phonons, which are continuously emitted and reabsorbed. The formation of Cooper pairs is due to the exchange of virtual phonons between the two electrons. This process is shown schematically in Fig. 6.1. An electron with the wave vector $\mathbf{k}$ emits a virtual phonon $\mathbf{q}$, which is absorbed by an electron $\mathbf{k}'$. The virtual phonon scatters $\mathbf{k}$ to $\mathbf{k} - \mathbf{q}$ and $\mathbf{k}'$ to $\mathbf{k}' + \mathbf{q}$. Since the process is virtual, energy conservation does not have to be maintained. The exchange of phonons between the electrons leads to an attraction when one of the electrons is surrounded by a positive shielding charge through the lattice, which overcompensates the negative elementary charge. The other electron is then attracted by the net positive charge.

Experimental observations of the so-called isotope effect had already indicated the important role of the crystal lattice in superconductivity in the early 1950s. The term isotope effect is used when the result depends on the mass of the atomic nuclei at constant electric charge of the nuclei, i.e., on the number of neutrons in

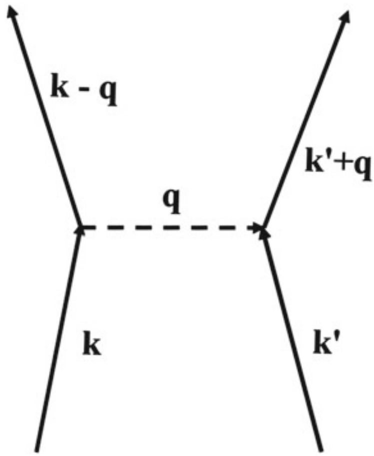

Fig. 6.1 Exchange of a virtual phonon **q** between the electrons with the wave vectors **k** or **k′**

the atomic nucleus. In various specially produced isotopically pure superconducting metals (lead, mercury, and tin), it was found that the critical temperature T_C is inversely proportional to the square root of the mass M of the lattice atoms:

$$T_c \sim 1/M^{\alpha} \tag{6.1}$$

The exponent was $\alpha = 0.5$. The crystal lattice therefore had to play a role in superconductivity.

The Cooper pairs always consist of two electrons with oppositely directed intrinsic angular momentum, so that the total spin of the individual Cooper pair disappears. In this case, the Pauli principle is invalid and all Cooper pairs can occupy the same quantum state. This quantum state is described by a macroscopic quantum mechanical wave function. However, the formation of Cooper pairs and the macroscopic quantum state is restricted to a certain small energy range in the vicinity of the Fermi surface (and thus to a small part of the conduction band).

At the heart of the BCS theory is the idea of an energy gap in the energy spectrum of electrons at the Fermi energy. Above the critical temperature T_C, the energy gap disappears, and below T_C, it grows in a certain way as the temperature decreases, reaching its maximum at 0 K. First indications of a gap in the energy spectrum of the electrons had already been obtained by optical absorption experiments on superconducting thin films. In 1960, Ivar Giaever provided impressive proof of the energy gap through his famous tunnel experiment (Fig. 6.2). At that time, he had been particularly fascinated by the quantum mechanical tunneling

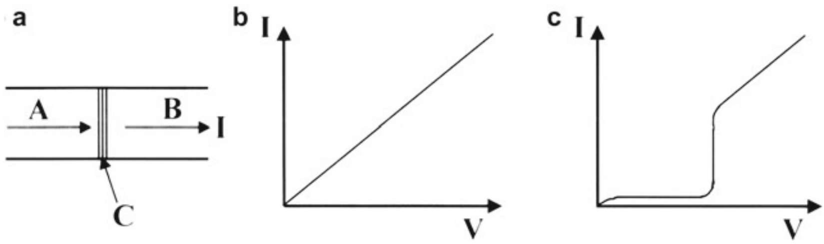

Fig. 6.2 Experimental proof of the energy gap in a superconductor by the tunnel experiment of Giaever. **a** A superconducting electrode A and a normal electrode B are separated from each other by a thin, electrically insulating barrier C, so that the flow of electric current through the barrier is only possible by the quantum mechanical tunnel effect. **b** Electric current I as a function of voltage V, when both electrode metals are in the normal state. **c** Electrical current I as a function of the voltage V, if one metal electrode is superconducting. Only when the potential difference between the two electrodes has reached the value of the energy gap can the electric current flow begin

process for quite some time. After hearing about the new BCS theory and its prediction of a gap in the energy spectrum of electrons, he succeeded in demonstrating the energy gap directly by means of the electric current flow between a superconducting and a normal electrode: If the two electrodes are separated from each other by a thin electrically insulating barrier, the electric current flow can only come about through the quantum mechanical tunnel effect. In such a "tunnel contact," the wave function of the particles extends to the other side of the barrier. However, the tunnel current cannot yet flow if no permitted energy states are available on the other side in the superconductor. The electric current only begins to flow when the potential difference between the two sides of the contact has reached the value of the energy gap. If both electrodes are superconducting, it is similar. In this way, Giaever succeeded in determining the energy gap with a simple measurement of electrical voltage and electrical current. Such tunnel experiments on superconductors have subsequently become very important.

The formation of Cooper pairs in superconductivity is also expressed in the size of the magnetic flux quantum discussed above. Since the Cooper pairs consist of two elementary charges, it follows that the magnetic flux quantum $\varphi_o = h/2e$ is only half as large as in the case where only a single elementary charge is involved.