Chapter 2
Superconducting Gap Structure and Magnetic Penetration Depth

Abstract The BCS theory proposed by J. Bardeen, L. N. Cooper, and J. R. Schrieffer in 1957 is the first microscopic theory of superconductivity. In this theory, Fermi surface becomes gapped to avoid the instability caused even by an infinitely small interaction if it is attractive, which drives the system into the superconducting condensate state at low temperatures. The wave function that describes the electron pair, which serves as the order parameter, is related to the superconducting energy gap. Therefore, identifying the detailed superconducting gap structure is a major step toward clarifying the interactions that produce the pairing. Since the magnetic penetration depth is directly connected to the superfluid density, the measurement of the penetration depth is a powerful method to elucidate the superconducting gap structure, particularly the presence or absence of nodes. In this chapter, we will give a brief account of superconductivity and magnetic penetration depth.

Keywords Superconducting pairing symmetry · Superconducting gap structure · Low-energy quasiparticle excitations · Magnetic penetration depth

2.1 Superconducting Pairing Symmetry

In the BCS theory [1], the electron-phonon interaction leads to an effective attraction between electrons near the Fermi surface with opposite momenta and opposite spins, which eventually causes superconductivity. Below a critical temperature (T_c), the electron pairs (the so-called Cooper pairs) condense into a coherent macroscopic quantum state, which is separated from the excited state by an energy gap 2Δ. This means that the amount of energy of at least 2Δ is required in order to break up one Cooper pair. Thus, the energy spectrum of quasiparticles E_k in a singlet superconducting state can be given by $E_k = \sqrt{\xi_k^2 + \Delta_k^2}$, where ξ_k represents the energy of an electron relative to the chemical potential with momentum k. Since the interaction of electrons with phonons is isotropic in the k-space, the Cooper pairs

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are formed in a state with zero orbital angular momentum (s-wave pairing), which leads to a fully gapped superconducting state. On the other hand, unconventional superconductivity is mostly characterized by the anisotropic superconducting gap function with zeros (nodes) along certain directions in the momentum space. Thus, the superconducting gap structure is closely related to the paring interaction responsible for the superconductivity. Therefore detailed knowledge of the gap structure will give a strong guide to establishing the pairing mechanism of superconductivity.

The superconducting gap function $\Delta^{\ell}_{s_1,s_2}(k)$, which is proportional to the amplitude of the wave function of a Cooper pair $\Psi^{\ell}_{s_1,s_2}(k) = \langle \psi_{k,s_1}\psi_{-k,s_2}\rangle$, serves as an order parameter of the system [2]: it is non-zero only in the superconducting state. Here, k is the quasiparticle momentum, l is the orbital angular momentum, s_i is the electron spin, and ψ is the electron annihilation operator. In the simplest case where the spin-orbit coupling is negligible, the total angular momentum L and total spin $S = s_1 + s_2$ are good quantum numbers, and $\Psi^{\ell}_{s_1,s_2}(k)$ can be expressed in the form of a product of the orbital and spin parts,

$$\Psi^{\ell}_{s_1,s_2}(k) = g_{\ell}(k)\chi_s(s_1, s_2), \tag{2.1}$$

where $g_{\ell}(k)$ is the orbital wave function and $\chi_s(s_1, s_2)$ is the spin wave function. According to the Pauli's exclusion principle, the total wave function should change its sign under the exchange of two particles;

$$g_{\ell}(-k)\chi_s(s_2, s_1) = -g_{\ell}(k)\chi_s(s_1, s_2). \tag{2.2}$$

The orbital part $g_{\ell}(k)$ can be expanded in terms of spherical harmonics $Y_{\ell m}(\hat{k})$, which are the eigenfunctions of the angular momentum operator with the momentum ℓ and its z-projections m,

$$g_{\ell}(k) = \sum_{m=-\ell}^{\ell} a_{\ell m}(k) Y_{\ell m}(\hat{k}), \tag{2.3}$$

where $\hat{k} = k/k_{\mathrm{F}}$ represents the direction of the momentum. $g_{\ell}(k)$ is even for even values of ℓ and odd for odd values of ℓ, $g_{\ell}(k) = (-1)^{\ell} g_{\ell}(-k)$, and superconductors with $\ell = 0, 1, 2, \ldots$ are labeled as $s, p, d, \ldots$ -wave, respectively. Hence, the spin component of a paired state with even (odd) orbital angular momentum ℓ should be antisymmetric (symmetric) under the exchange of particles.

The spin wave function of the Cooper pair $\chi_s(s_1, s_2)$ is a product of the one-particle spin wave functions,

$$\alpha_{\lambda} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |\uparrow\rangle \text{ and } \beta_{\lambda} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |\downarrow\rangle, \tag{2.4}$$

which are eigenstates of the operators s^2 and s_z:

$$s_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad s_z\alpha_\lambda = \frac{\hbar}{2}\alpha_\lambda, \quad s_z\beta_\lambda = -\frac{\hbar}{2}\beta_\lambda. \tag{2.5}$$

In the singlet state, $S = 0$, the spin part of the wave function is antisymmetric with respect to the particle exchange. Therefore, the eigenfunction corresponding to the spin singlet state can be given by

$$\alpha_{1\lambda}\beta_{2\lambda} - \beta_{1\lambda}\alpha_{2\lambda} = \ |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = i\sigma_y, \tag{2.6}$$

where σ_i $(i = x, y, z)$ is the Pauli matrix,

$$\sigma_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{2.7}$$

As a result, the total wave function of the Cooper pair with $S = 0$ is given by

$$\Psi^{\ell}_{singlet}(k) = g_\ell(k) i\sigma_y, \tag{2.8}$$

where ℓ is even.

For spin triplet pairing ($S = 1$), the spin wave functions corresponding to the three different spin projections on the quantization axis, which are symmetric under the exchange of particles, are given by

$$S_z = \begin{cases} 1, & \alpha_{1\lambda}\alpha_{2\mu} = |\uparrow\uparrow\rangle = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \\ 0, & \alpha_{1\lambda}\beta_{2\mu} + \beta_{1\lambda}\alpha_{2\mu} = |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ -1, & \beta_{1\lambda}\beta_{2\mu} = |\downarrow\downarrow\rangle = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}. \end{cases} \tag{2.9}$$

Consequently, the total wave function can be written as

$$\Psi^{\ell}_{triplet} = g_1(k)\,|\uparrow\uparrow\rangle + g_2(k)(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) + g_3(k)\,|\downarrow\downarrow\rangle = \begin{pmatrix} g_1(k) & g_2(k) \\ g_2(k) & g_3(k) \end{pmatrix}, \tag{2.10}$$

where $g_\alpha(k)$ is defined as the amplitudes of states with $S_z = 1, 0$, and -1, respectively,

$$g_\alpha(k) = \sum_{m=-l}^{l} a^{\alpha}_{lm} Y^m_l(\hat{k}) \qquad \alpha = 1, 2, 3. \tag{2.11}$$

This equation can be rewritten as the following form by using the basis of the symmetric matrices $i\sigma\sigma_y = (i\sigma_x\sigma_y, i\sigma_y\sigma_y, i\sigma_z\sigma_y)$,

$$\begin{aligned}\Psi^{\ell}_{triplet} &= (d(k)\cdot\sigma)i\sigma_y = (d_x(k)\sigma_x, d_y(k)\sigma_y, d_z(k)\sigma_z)i\sigma_y \\ &= \begin{pmatrix} -d_x(k)+id_y(k) & d_z(k) \\ d_z(k) & d_x(k)+id_y(k)\end{pmatrix}.\end{aligned} \tag{2.12}$$

To summarize, the superconducting state can be characterized by its total spin $S = 0$ (spin-singlet) and $S = 1$ (spin-triplet). Thus, the superconducting gap functions for the singlet and triplet pairings are given by

$$\Delta^s_{k,\alpha\beta} = \Delta_0 g(k)(i\sigma_y)_{\alpha\beta}, \tag{2.13}$$

$$\Delta^t_{k,\alpha\beta} = \Delta_0 d(k)(i\sigma\sigma_y)_{\alpha\beta}, \tag{2.14}$$

where Δ_0 is the k-independent part of the gap. For the spin-singlet case, the energy of single particle excitation is given by

$$E_k = \sqrt{\xi_k^2 + \Delta_0^2|g(k)|^2}, \tag{2.15}$$

where ξ_k represents the band energy relative to the chemical potential. In the case of spin-triplet pairing state, if d is unitary it can be written as

$$E_k = \sqrt{\xi_k^2 + \Delta_0^2|d(k)|^2}. \tag{2.16}$$

If d is not-unitary, the excitation spectrum is given by

$$E_{k,\pm} = \sqrt{\xi_k^2 + \Delta_0^2(|d(k)|^2 \pm |d^*(k)\times d(k))|)}. \tag{2.17}$$

2.2 Superconducting Gap Structure and Quasiparticle Density of States

In this section, we focus on the quasiparticle density of states (QDOS) in a singlet superconducting state. The QDOS is defined as follows:

$$N(E) = \sum_k \delta(E - E_k). \tag{2.18}$$

From Eq. 2.15, if the superconducting order parameter Δ_k exhibits k-dependence, $\Delta_k \equiv \Delta_0 g(k)$, the quasiparticle energy in the spin-singlet state is given by

$$E_k = \sqrt{\xi_k^2 + \Delta_k^2}. \tag{2.19}$$

Using Eqs. 2.18 and 2.19, we obtain

$$N(E) = \int \frac{d^3k}{(2\pi)^3}\delta(E - E_k) = N_0 \int \frac{d\Omega}{4\pi} \frac{E}{\sqrt{E^2 - \Delta_k^2}}, \tag{2.20}$$

where N_0 is the density of states in the normal state and Ω is the solid angle. It follows from Eq. 2.20 that for a conventional isotropic s-wave superconductor ($\Delta_k = \Delta_0$),

$$N(E) = N_0 \begin{cases} 0 & (E < \Delta_0) \\ \frac{E}{\sqrt{E^2-\Delta_0^2}} & (E > \Delta_0). \end{cases} \tag{2.21}$$

The quasiparticle density of states for an s-wave superconductor drops abruptly to zero for $E < \Delta_0$. For a d-wave superconductor, $\Delta_k = \Delta_0 \cos(2\varphi)$, the quasiparticle density of states is given by

$$\frac{N(E)}{N_0} = \int_0^{2\pi} \frac{d\varphi}{2\pi} \frac{E}{\sqrt{E^2 - \Delta_k^2}} = \int_0^{2\pi} \frac{d\varphi}{2\pi} \frac{E}{\sqrt{E^2 - \Delta_0^2 \cos^2(2\varphi)}}. \tag{2.22}$$

The last integral of Eq. 2.22 can be calculated by a numerical analysis. The result is given by

$$\frac{N(E)}{N_0} = \begin{cases} \frac{2}{\pi}\frac{E}{\Delta_0}\kappa(\frac{E}{\Delta_0}) & (E < \Delta_0) \\ \frac{2}{\pi}\kappa(\frac{\Delta_0}{E}) & (E > \Delta_0). \end{cases} \tag{2.23}$$

For $E \ll \Delta_0$, $\kappa(\frac{E}{\Delta_0}) \approx \frac{\pi}{2}$. Therefore we obtain

$$\frac{N(E)}{N_0} \approx \frac{E}{\Delta_0} \quad (E \ll \Delta_0). \tag{2.24}$$

In general, for the fully gapped state and nodal states with line node and point nodes, we obtain the following energy dependence of the density of states for $E \ll \Delta_0$ in the clean limit:

$$\frac{N(E)}{N_0} \propto \begin{cases} 0 & \text{(full gap)} \\ E & \text{(line node)} \\ E^2 & \text{(point node).} \end{cases} \tag{2.25}$$

The entire energy dependence of the quasiparticle states is summarized in Fig. 2.1.

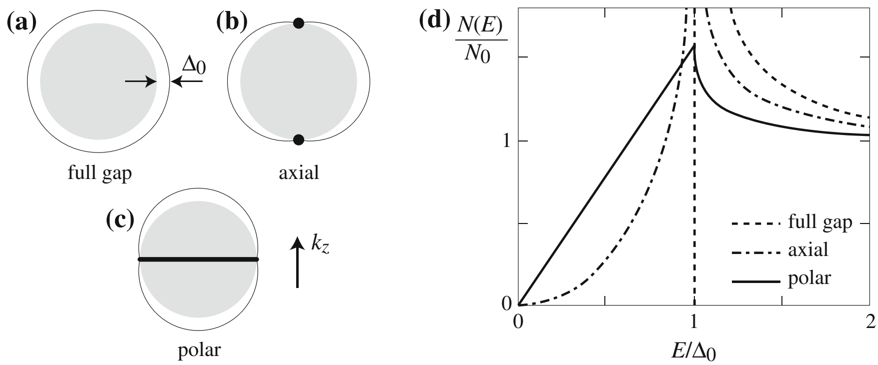

Fig. 2.1 Schematic pictures of the superconducting gap structure in a 3D spherical Fermi surface for **a** the fully gapped state and nodal state with **b** point nodes and **c** line node. The *shaded circles* represent the Fermi surface. The *thick line* and points represent the line node and point nodes, respectively. **d** The density of states of the quasiparticles $N(E)$ for the fully gapped state and nodal state with point nodes and line node in the clean limit. N_0 represents the normal state density of states

2.3 Magnetic Penetration Depth

2.3.1 London Penetration Depth

The Meissner effect, which is one of the most striking and fundamental properties of superconductors, is the exclusion of a magnetic field from a superconducting material below its transition temperature. In a weak applied magnetic field, a superconductor expels nearly all magnetic flux, because the magnetic field induced by the supercurrents near its surface cancels the applied magnetic field within the bulk of the superconductor. However, near the surface, within a distance of the order of Angstroms, the magnetic field is not completely cancelled. Each superconducting material has its own characteristic penetration depth, which is the so-called London penetration depth λ_L. Since the penetration depth is directly connected to the superfluid density, the measurement of the penetration depth is a powerful method to elucidate the superconducting gap structure, particularly the presence or absence of nodes.

In the normal-state of a conventional metal, electrical conduction is well described by the Ohm's law $j = \sigma E$. On the other hand, in the superconducting state, the current density j is proportional to the applied vector potential A (the so-called London equation):

$$\mu_0 j = -\frac{ne^2}{m^*} A. \tag{2.26}$$

By combining the London equation with the Maxwell's equations, we obtain

$$\nabla^2 B = \frac{\mu_0 n e^2}{m^*} B. \quad (2.27)$$

Let's discuss the penetration of a magnetic field into a superconductor by solving the London equation. Here we consider the simplest case, where the surface of the sample is defined by the xy plane, and the region of $z < 0$ is a vacuum [3]. We assume that the magnetic field is applied along the x direction. Since the field depends on only z, $B_x = B_x(z)$, we obtain

$$\frac{d^2 z}{dz^2} B_x = \frac{1}{\lambda_L^2} B_x, \quad (2.28)$$

where the London penetration depth is defined as

$$\lambda_L = \left(\frac{\mu_0 n e^2}{m^*} \right)^{-1/2}. \quad (2.29)$$

The solution of Eq. 2.28 gives the following form,

$$B_x(z) = B_x(0) \exp\left(-z/\lambda_L\right). \quad (2.30)$$

The most striking consequence of the London equation is that the magnetic fields are screened from the interior of a bulk superconductor within a characteristic penetration depth λ_L, from which we can estimate the ratio of the concentration of the superconducting carriers to the effective mass, n/m^*.

2.3.2 Semiclassical Approach

In this subsection, we will describe the penetration depth in the framework of a semiclassical model given by Chandrasekhar and Einzel [4]. Here we focus on the case of the spin-singlet superconducting state [5]. This approach provides a general formula for all three spatial components of the penetration depth. In the London limit, the supercurrent $j(r)$ is related to the vector potential $A(r)$ through a tensor equation:

$$j = -\mathbb{R} A, \quad (2.31)$$

where the response tensor is given by

$$\mathbb{R}_{ij} = \frac{e^2}{4\pi^3 \hbar} \oint_{\mathrm{FS}} dS_k \left[\frac{v_F^i v_F^j}{|v_F|} \left(1 + 2 \int_{\Delta_k}^{\infty} \frac{\partial f(E_k)}{\partial E_k} \frac{N(E_k)}{N(0)} dE_k \right) \right]. \quad (2.32)$$

Here f is the Fermi function and v_F^i is the i-axis component of Fermi velocity v_F. $N(E)/N(0) = E/\sqrt{E^2 - \Delta_k^2}$ is the density of states normalized by its value at the Fermi level in the normal state. If we define λ_{ij}^{-2} as a response tensor in the London equation, $\mu_0 j_i = -\lambda_{ij}^{-2} A_j$, we obtain

$$\lambda_{ij}^{-2} = \frac{\mu_0 e^2}{4\pi^3 \hbar} \oint_{\mathrm{FS}} dS_k \left[\frac{v_F^i v_F^j}{|v_F|} \left(1 + 2 \int_{\Delta(k)}^{\infty} \frac{\partial f(E_k)}{\partial E_k} \frac{N(E_k)}{N(0)} dE_k \right) \right]. \tag{2.33}$$

Here we note that the integral consists of two terms; the first term is diamagnetic and independent of temperature, while the second term is paramagnetic, temperature-dependent, and vanishes as the temperature goes to zero. If we assume that the effective mass m_{ii}^* is independent of temperature, then the normalized superfluid density are given by

$$\rho_{ii} = \frac{n_{ii}(T)}{n_{ii}(0)} = \left(\frac{\lambda_{ii}(0)}{\lambda_{ii}(T)} \right)^2 . \tag{2.34}$$

In the case of a 2D cylindrical Fermi surface, the normalized superfluid density is given by

$$\rho_{bb}^{aa} = 1 - \frac{1}{2\pi T} \int_0^{2\pi} \begin{pmatrix} \cos^2(\varphi) \\ \sin^2(\varphi) \end{pmatrix} \int_0^{\infty} \cosh^{-2} \left(\frac{\sqrt{\varepsilon^2 + \Delta^2(T, \varphi)}}{2T} \right) d\varepsilon \, d\varphi, \tag{2.35}$$

where $\Delta(\varphi)$ is an angle-dependent gap function. For a 3D spherical Fermi surface and an anisotropic gap function $\Delta(\theta, \varphi)$, we obtain

$$\begin{aligned} \rho_{bb}^{aa} = 1 - \frac{3}{4\pi T} \int_0^1 (1 - z^2) \int_0^{2\pi} \begin{pmatrix} \cos^2(\varphi) \\ \sin^2(\varphi) \end{pmatrix} \\ \int_0^{\infty} \cosh^{-2} \left(\frac{\sqrt{\varepsilon^2 + \Delta^2(T, \theta, \varphi)}}{2T} \right) d\varepsilon \, d\varphi \, dz, \end{aligned} \tag{2.36}$$

and

$$\rho_c = 1 - \frac{3}{2\pi T} \int_0^1 z^2 \int_0^{2\pi} \cos^2(\varphi) \int_0^{\infty} \cosh^{-2} \left(\frac{\sqrt{\varepsilon^2 + \Delta^2(T, \theta, \varphi)}}{2T} \right) d\varepsilon \, d\varphi \, dz, \tag{2.37}$$

where $z = \cos\theta$.

For an isotropic s-wave superconductor, both 2D and 3D expressions are given by [6]

$$\rho \approx 1 - \frac{1}{2T}\int_0^\infty \cosh^{-2}\left(\frac{\sqrt{\varepsilon^2 + \Delta^2(T)}}{2T}\right) d\varepsilon. \tag{2.38}$$

Then we obtain the normalized fluid density for $T \ll T_c$,

$$\rho(T) = 1 - \sqrt{\frac{2\pi\Delta_0}{k_B T}} \exp\left(-\frac{\Delta_0}{k_B T}\right), \tag{2.39}$$

where Δ_0 is the magnitude of the superconducting gap at $T = 0$ K. Hence, we obtain the penetration depth λ from Eq. 2.29,

$$\begin{aligned}\lambda(T) &= \left(\frac{\mu_0 n e^2}{m^*}\right)^{-1/2} \\ &\approx \lambda(0)\left[1 + \sqrt{\frac{\pi\Delta_0}{2k_B T}} \exp\left(-\frac{\Delta_0}{k_B T}\right)\right].\end{aligned} \tag{2.40}$$

For superconductors with line nodes, the normalized superfluid density ρ_s can be calculated as follows:

$$\rho_s \approx 1 - \frac{2\ln 2}{\Delta_0} T \quad (T \ll T_c), \tag{2.41}$$

which gives

$$\lambda(T) \approx \lambda(0)\left(1 + \frac{\ln 2}{\Delta_0} T\right). \tag{2.42}$$

For the fully gapped s-wave state, nodal state with line node and point nodes, we can summarize the temperature dependence of the penetration depth as follows:

$$\lambda(T) \propto \begin{cases} \exp(-\Delta_0/k_B T) & \text{(full gap)} \\ T & \text{(line node)} \\ T^2 & \text{(point node).} \end{cases} \tag{2.43}$$

Thus, we can distinguish types of the superconducting gap structure from the differences arising from the quasiparticle excitations.

2.3.3 Impurity Effect

The above discussion is restricted to pure systems without impurities. The introduction of controlled disorder has long been used as a probe of the gap structure of unconventional superconductors. For conventional superconductors disorder has relatively little effect, however for unconventional superconductors the effects can be dramatic. Besides driving down T_c, disorder affects the low energy quasiparticle dynamics, for example, changing a T-linear behavior of the penetration depth to a quadratic T^2 behavior at low temperatures [7].

In unconventional superconductors where the gap has significant anisotropy or especially where it changes sign on different parts of the Fermi surface, non-magnetic impurities act as pair breakers, similar to magnetic impurities in conventional s-wave superconductors. For nodal superconductors in the strong scattering limit (unitary limit), quasiparticle density of states are bound to the non-magnetic impurity level with an energy close to E_F [8], which is a consequence of the interference of particle-like and hole-like excitations that undergo Andreev scattering arising from the sign changing order parameter and the scattering due to the impurities. A finite number of impurities broadens the bound state to the impurity band with bandwidth γ. As a result, a finite density of state appears at zero energy.

For superconductors with line nodes, γ and the density of quasiparticle bound states at zero energy $N(0)$ become finite for any amount of impurity concentration. The energy dependence of the quasiparticle density of states is modified, as shown in Fig. 2.2. Due to the appearance of $N(0)$, the density of states near Δ_0 is reduced.

In a two-dimensional d-wave superconductor, $N(0)$ in the unitary limit is given by

$$\frac{N(0)}{N_0} = \frac{2\gamma}{\pi\Delta_0}\ln\left(\frac{\Delta_0}{\gamma}\right), \tag{2.44}$$

which is approximately given by $N(0)/N_0 \sim \gamma/\Delta_0$ at $\gamma \ll \Delta_0$. Therefore the impurity scattering modifies the temperature dependence of physical quantities at the

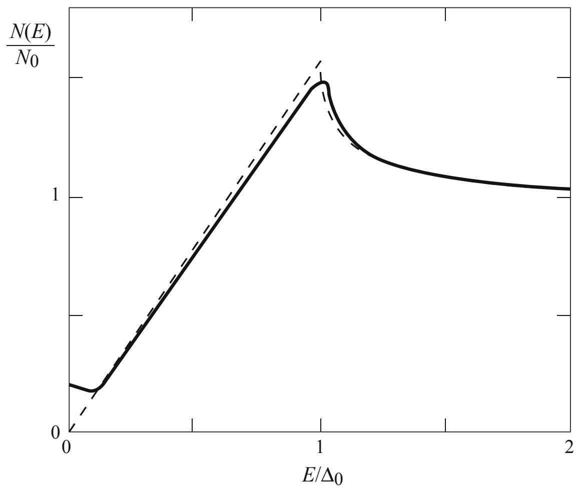

Fig. 2.2 $N(E)/N_0$ for an unconventional superconductor with line nodes in the superconducting gap. The *dashed line* represents the density of states in the absence of impurities. The *solid line* represents the density of states in the presence of dilute non-magnetic impurities ($\Gamma/\Delta_0 = 0.01$) in the strong scattering limit (unitary limit). A finite density of states at zero energy $N(0)$ appears

Table 2.1 Temperature dependence of several physical quantities in superconductors with line nodes in the superconducting gap in a clean limit and unitary limit

Quantity		Temperature dependence	
		Clean limit	Unitary limit
Specific heat	C	T^2	T
NMR relaxation rate	$1/T_1$	T^3	T
Penetration depth	λ	T	T^2

region of $k_B T < \gamma$, where the impurity-induced $N(0)$ dominates the transport and thermodynamic properties. For instance, the penetration depth changes from a T-linear behavior to a quadratic T^2 behavior at low temperatures. In Table 2.1, we summarize the power-law behaviors of the specific heat C, NMR relaxation rate $1/T_1$, and magnetic penetration depth λ for superconductors with line nodes in the superconducting gap, both in pure system and in the presence of impurities.

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