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Anisotropic two-band α-model and its application to layered chalcogenide superconductor $NbSe_2$

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The generalized α-model for anisotropic two-band superconductivity is consistently constructed with the consideration of weak interband electron–electron interaction. Tailored from the two-band BCS theory, the developed framework can be applied to investigate thermodynamic properties of intraband strong-coupling superconductors. Accordingly, we perform a calculation on the temperature dependence of specific heat and obtain an analytic expression for specific heat jump at the superconducting critical temperature. Meanwhile, we also compute the superfluid density and the spin susceptibility with this formalism. Given the low-temperature superconducting gaps from experimental measurement, all of our theoretical results can fit the experimental data of the layered two-band superconductor $NbSe_2$ well.

Keywords: two-band superconductivity, anisotropic α-model, specific heat, $NbSe_2$

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1. Introduction

The hexagonal transition metal dichalcogenide $NbSe_2$, as a typical example of layered superconductors, has been extensively studied since its discovery in the 1960s.[1,2] This binary compound exhibits an incommensurate charge-density wave (CDW) order below 33.5 K[3] and enters the superconducting state at $T_c = 7.2$ K.[4] The high-resolution photoemission and magnetotransport measurements show that both orderings are driven by electron–phonon interaction and manifest an anisotropic feature of the layered material.[5,6] It is indicated from the scanning tunneling microscopy (STM) experiment that the formation of CDW induces small-amplitude atomic displacements and significantly alters the electron–phonon coupling, placing $NbSe_2$ in the strong-coupling regime.[7] Meanwhile, band structure calculations in $NbSe_2$ demonstrate that the electronic states around the Fermi level are dominated by two 4d orbitals of the Nb atoms, and the contribution from the Se 4p pocket is only about 5%.[8–10] Thereafter, the gap spectra from STM measurements show strong evidence of two-band superconductivity in $NbSe_2$,[11] and each superconducting gap function turns out to present an anisotropic distribution with six-fold symmetry over the Fermi surface.[12–14]

In principle, we should refer to the classical Eliashberg theory to study the superconductivity with strong electron–phonon interaction.[15] In 1973, Padamsee *et al.* proposed the α-model to avoid the difficulties of solving complex Eliashberg equations and interpret the deviation of electronic heat capacity data from the BCS prediction.[16] The α-model assumes that the normalized superconducting order parameter $\Delta(T)/\Delta(0)$ is the same as that in the BCS theory, but the ratio $\alpha = \Delta(0)/k_B T_c$ is treated as an adjustable parameter based on the experimental values.[17] In order to extend this formalism to multi-band superconductors, the usual procedure is a straightforward application of this model to each band regardless of the interband interaction. In fact, this oversimplified treatment is unsatisfactory since the smaller gap is highly dependent on the interband coupling and the anomalous variation of this gap with temperature will strongly affect the specific heat behavior near T_c. There is no doubt that the problem will become especially serious in anisotropic two-band superconductors.

In this paper, we will systematically develop a generalized α-model for anisotropic two-band superconductivity with weak interband electron–electron interaction. Based on the normalized gap functions from the anisotropic two-band BCS theory, we introduce two α-parameters in this formalism and calculate the temperature dependence of specific heat, superfluid density, and spin susceptibility for intraband strong-coupling superconductors. We then apply the two-band α-model to study thermodynamic properties of the layered chalcogenide superconductor $NbSe_2$. Given the low-temperature superconducting gaps from the experiment, our theoretical results agree well with the experimental data of this two-band material in a broad temperature range. Our theoretical results give the specific heat jump at the critical temperature as about 2.12, which is also consistent with the experimental measurement.[18,19]

The rest of this article is structured as follows. In the next

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section, we discuss the anisotropic two-band BCS theory and derive the equations for normalized energy gaps in the presence of weak interband interaction. In Section 3, we construct the generalized α-model and calculate the temperature dependence of specific heat for intraband strong-coupling superconductors. In Sections 4 and 5, we also compute the superfluid density and the spin susceptibility with this formalism. In Section 6, we apply this approach to study thermodynamic properties of the anisotropic two-band superconductor $NbSe_2$. In Section 7, we generalize this framework to include the interband pairing interaction. Finally, we conclude this article in Section 8.

2. Anisotropic two-band BCS theory

Following the previous works on the multi-band superconductivity,[20–22] we can write the Hamiltonian of an anisotropic two-band superconductor as

$$H=\sum_{ip\sigma}\xi_{ip}c^{\dagger}_{ip\sigma}c_{ip\sigma}-\sum_{ipi'p'}V_{ipi'p'}c^{\dagger}_{ip\uparrow}c^{\dagger}_{i-p\downarrow}c_{i'-p'\downarrow}c_{i'p'\uparrow}, \quad (1)$$

where $i,i'=1,2$ are the band indices and $\sigma=\uparrow,\downarrow$ is the spin index. ξ_{ip} represents the single-particle Hamiltonian of the normal metal with the wave vector $\boldsymbol{p}$. $V_{ipi'p'}$ corresponds to the attractive interaction between electrons with momenta $\boldsymbol{p}$ and $\boldsymbol{p}'$.

We can introduce the gap function

$$\Delta_{ip}(T)=-\sum_{i'p'}V_{ipi'p'}\langle\langle c_{i'-p'\downarrow}c_{i'p'\uparrow}\rangle\rangle \quad (2)$$

with the symbol $\langle\langle\cdots\rangle\rangle$ representing the thermodynamic ensemble average, and transform the Hamiltonian Eq. (1) into the mean-field form

$$H_{\rm eff}=\sum_{ip\sigma}\xi_{ip}c^{\dagger}_{ip\sigma}c_{ip\sigma}+\sum_{ip}\left[\Delta_{ip}(T)c^{\dagger}_{ip\uparrow}c^{\dagger}_{i-p\downarrow}+{\rm H.c.}\right]. \quad (3)$$

This effective Hamiltonian can be diagonalized by means of the Bogoliubov transformation with $b_{ip\sigma}$ and $b^{\dagger}_{ip\sigma}$ the annihilation and creation operators of quasi-particle excitations

$$c_{ip\uparrow}=u_{ip}b_{ip\uparrow}-v^{*}_{ip}b^{\dagger}_{i-p\downarrow}, \quad (4)$$

$$c_{i-p\downarrow}=u_{ip}b_{i-p\downarrow}+v^{*}_{ip}b^{\dagger}_{ip\uparrow}. \quad (5)$$

As a result, the effective Hamiltonian can be rewritten as

$$H_{\rm eff}=E_{\rm g}+\sum_{ip\sigma}E_{ip}b^{\dagger}_{ip\sigma}b_{ip\sigma}. \quad (6)$$

Here $E_{\rm g}$ is the groundstate energy and $E_{ip}=\sqrt{\xi^2_{ip}+\Delta^2_{ip}}$ stands for the quasi-particle excitation. From Eq. (6), we can compute $\langle\langle b^{\dagger}_{ip\sigma}b_{ip\sigma}\rangle\rangle=f_{ip}$ with $f_{ip}=1/\left[1+\exp\left(E_{ip}/k_{\rm B}T\right)\right]$ the Fermi distribution function. Then plugging Eqs. (4) and (5) into Eq. (2), we can transform the self-consistent gap equation into the form

$$\Delta_{ip}(T)=\sum_{i'p'}V_{ipi'p'}\frac{\Delta_{i'p'}(T)}{2E_{i'p'}}\left(1-2f_{i'p'}\right). \quad (7)$$

Now we try to employ the separability ansatz to obtain the general formulae formally exact for factorizable kernels in the problem.[23–26] We first assume that the pairing interaction can be written as $V_{ipi'p'}=g_{ii'}\chi_{ip}\chi_{i'p'}$ where χ_{ip} represents the angular dependence of the anisotropic interaction. Then due to the separable form of $V_{ipi'p'}$, the order parameter can also be decomposed into the following form:

$$\Delta_{ip}(T)=Q_i(T)\chi_{ip} \quad (8)$$

with $Q_i(T)$ the temperature-dependent part of the superconducting gap function. We then substitute the factorizable $V_{ipi'p'}$ and $\Delta_{ip}(T)$ into Eq. (7), and convert the summation over momentum $\boldsymbol{p}$ to an integration on the (ξ_i,θ,φ) in three dimensions. This allows us to transfer the anisotropic gap equation (7) to

$$Q_i(T)=\sum_{i'}\lambda_{ii'}Q_{i'}(T)\left\langle\chi^2_{i'p'}\int_0^{\hbar\omega_{\rm D}}\left(1-2f_{i'p'}\right)\frac{{\rm d}\xi_{i'}}{E_{i'p'}}\right\rangle, \quad (9)$$

where $\lambda_{ii'}=g_{ii'}N_{i'}$ with $N_{i'}$ is the density of states at the Fermi level for each band and $\omega_{\rm D}$ is the Debye frequency. Noting that χ_{ip} is a function of θ and φ, and the symbol $\langle\cdots\rangle$ denotes the average over these two spherical angles on the Fermi surface here. With some algebraic manipulations, we can also transform Eq. (9) into the form

$$\left\langle\chi^2_{1p}\int_0^{\hbar\omega_{\rm D}}(1-2f_{1p})\frac{{\rm d}\xi_1}{E_{1p}}\right\rangle=\tilde{\lambda}_{22}-\tilde{\lambda}_{12}\kappa(T), \quad (10)$$

$$\left\langle\chi^2_{2p}\int_0^{\hbar\omega_{\rm D}}(1-2f_{2p})\frac{{\rm d}\xi_2}{E_{2p}}\right\rangle=\tilde{\lambda}_{11}-\tilde{\lambda}_{21}/\kappa(T). \quad (11)$$

Here we define the gap ratio $\kappa(T)=Q_2(T)/Q_1(T)$ and the effective coupling constant $\tilde{\lambda}_{ii'}=\lambda_{ii'}/(\lambda_{11}\lambda_{22}-\lambda_{12}\lambda_{21})$.

At $T=0$, we have the Fermi distribution function $f_{ip}=0$. Then we can rewrite Eqs. (10) and (11) as

$$\left\langle\chi^2_{1p}\ln[2\hbar\omega_{\rm D}/Q_1(0)]-\chi^2_{1p}\ln\chi_{1p}\right\rangle=\tilde{\lambda}_{22}-\tilde{\lambda}_{12}\kappa(0), \quad (12)$$

$$\left\langle\chi^2_{2p}\ln[2\hbar\omega_{\rm D}/Q_2(0)]-\chi^2_{2p}\ln\chi_{2p}\right\rangle=\tilde{\lambda}_{11}-\tilde{\lambda}_{21}/\kappa(0). \quad (13)$$

From Eqs. (12) and (13), we obtain the expression for the gap function Q_i at zero temperature

$$Q_1(0)=2\hbar\omega_{\rm D}\exp\left[\frac{2\tilde{\lambda}_{12}\kappa(0)-2\tilde{\lambda}_{22}-\left\langle\chi^2_{1p}\ln\chi^2_{1p}\right\rangle}{2\left\langle\chi^2_{1p}\right\rangle}\right],$$

$$Q_2(0)=\kappa(0)Q_1(0), \quad (14)$$

where $\kappa(0)$ is determined by the following condition:

$$\frac{\tilde{\lambda}_{21}\left\langle\chi^2_{1p}\right\rangle}{\kappa(0)}-\ln\kappa(0)\left\langle\chi^2_{1p}\right\rangle\left\langle\chi^2_{2p}\right\rangle-\tilde{\lambda}_{12}\kappa(0)\left\langle\chi^2_{2p}\right\rangle$$

$$=\tilde{\Lambda}_0+\frac{1}{2}\left\langle\chi^2_{2p}\ln\chi^2_{2p}\right\rangle\left\langle\chi^2_{1p}\right\rangle-\frac{1}{2}\left\langle\chi^2_{1p}\ln\chi^2_{1p}\right\rangle\left\langle\chi^2_{2p}\right\rangle \quad (15)$$

with $\tilde{\Lambda}_0 = \tilde{\lambda}_{11}\langle\chi^2_{1\boldsymbol{p}}\rangle - \tilde{\lambda}_{22}\langle\chi^2_{2\boldsymbol{p}}\rangle$.

At $T = T_c$, we have the quasi-particle gap $\Delta_{i\boldsymbol{p}} = 0$. Performing the integrations in Eqs. (10) and (11), we can get $\int_0^{\hbar\omega_D}[(1-2f_{i\boldsymbol{p}})/E_{i\boldsymbol{p}}]\,\mathrm{d}\xi_i = \ln[2\hbar\omega_D\,\mathrm{e}^{\gamma}/(\pi k_B T_c)]$ with $\gamma \approx 0.58$ the Euler constant. This result enables us to easily compute the critical temperature

$$\begin{aligned} k_B T_c = {} & \frac{2\mathrm{e}^{\gamma}}{\pi}\hbar\omega_D \\ & \times \exp\left[\frac{1}{2\langle\chi^2_{1\boldsymbol{p}}\rangle\langle\chi^2_{2\boldsymbol{p}}\rangle}\left(\sqrt{\tilde{\Lambda}_0^2 + 4\tilde{\lambda}_{12}\tilde{\lambda}_{21}\langle\chi^2_{1\boldsymbol{p}}\rangle\langle\chi^2_{2\boldsymbol{p}}\rangle}\right.\right. \\ & \left.\left. - \tilde{\lambda}_{11}\langle\chi^2_{1\boldsymbol{p}}\rangle - \tilde{\lambda}_{22}\langle\chi^2_{2\boldsymbol{p}}\rangle\right)\right] \end{aligned} \tag{16}$$

and the gap ratio at critical temperature

$$\kappa(T_c) = \frac{1}{2\tilde{\lambda}_{12}\langle\chi^2_{2\boldsymbol{p}}\rangle}\left(\sqrt{\tilde{\Lambda}_0^2 + 4\tilde{\lambda}_{12}\tilde{\lambda}_{21}\langle\chi^2_{1\boldsymbol{p}}\rangle\langle\chi^2_{2\boldsymbol{p}}\rangle} - \tilde{\Lambda}_0\right) \tag{17}$$

from Eqs. (10) and (11).

At this point, we would like to define the dimensionless parameter $\alpha_i = Q_i(0)/k_B T_c$ in the frame of the BCS theory. According to Eqs. (14) and (16), we can represent α_i as follows:

$$\alpha_1 = \frac{Q_1(0)}{k_B T_c} \approx 1.76\,\mathrm{e}^{\tilde{\Lambda}_1}, \quad \alpha_2 = \frac{Q_2(0)}{k_B T_c} = \alpha_1\kappa(0) \tag{18}$$

with

$$\begin{aligned} \tilde{\Lambda}_1 = {} & \frac{1}{2\langle\chi^2_{1\boldsymbol{p}}\rangle\langle\chi^2_{2\boldsymbol{p}}\rangle} \\ & \times [\tilde{\Lambda}_0 + 2\tilde{\lambda}_{12}\kappa(0)\langle\chi^2_{2\boldsymbol{p}}\rangle - \langle\chi^2_{1\boldsymbol{p}}\ln\chi^2_{1\boldsymbol{p}}\rangle\langle\chi^2_{2\boldsymbol{p}}\rangle \\ & - \sqrt{\tilde{\Lambda}_0^2 + 4\tilde{\lambda}_{12}\tilde{\lambda}_{21}\langle\chi^2_{1\boldsymbol{p}}\rangle\langle\chi^2_{2\boldsymbol{p}}\rangle}]. \end{aligned} \tag{19}$$

To obtain a system of equations that allows for the direct calculation of the normalized gap function $\tilde{Q}_i(t) = Q_i(t)/Q_i(0)$ at a reduced temperature $t = T/T_c$, we take the difference between the zero-temperature and finite-temperature forms of Eqs. (10) and (11). Then these equations can be transformed into the following form:

$$\begin{aligned} & \left\langle \chi^2_{1\boldsymbol{p}}\int_0^{\infty}\left(\frac{1}{\sqrt{\tilde{\xi}_1^2+\chi^2_{1\boldsymbol{p}}}} - \frac{1-2f_{1\boldsymbol{p}}}{\tilde{E}_{1\boldsymbol{p}}}\right)\mathrm{d}\tilde{\xi}_1\right\rangle \\ = {} & -\tilde{\lambda}_{12}\kappa(0)\left[1-\frac{\tilde{Q}_2(t)}{\tilde{Q}_1(t)}\right], \end{aligned} \tag{20}$$

$$\begin{aligned} & \left\langle \chi^2_{2\boldsymbol{p}}\int_0^{\infty}\left(\frac{1}{\sqrt{\tilde{\xi}_2^2+\chi^2_{2\boldsymbol{p}}}} - \frac{1-2f_{2\boldsymbol{p}}}{\tilde{E}_{2\boldsymbol{p}}}\right)\mathrm{d}\tilde{\xi}_2\right\rangle \\ = {} & -\frac{\tilde{\lambda}_{21}}{\kappa(0)}\left[1-\frac{\tilde{Q}_1(t)}{\tilde{Q}_2(t)}\right]. \end{aligned} \tag{21}$$

Here we define $\tilde{\xi}_i = \xi_i/Q_i(0)$ and $\tilde{E}_{i\boldsymbol{p}} = E_{i\boldsymbol{p}}/Q_i(0)$. The Fermi distribution function for each band can also be written as $f_{i\boldsymbol{p}} = 1/[1+\exp(\alpha_i\tilde{E}_{i\boldsymbol{p}}/t)]$. It is straightforward to verify the convergence of the integrations after such technical treatment, as a result the upper limit of integrals has been extended to infinity in Eqs. (20) and (21). Given the weak interband coefficients $\tilde{\lambda}_{12}$ and $\tilde{\lambda}_{21}$, we can calculate the temperature dependence of $\tilde{Q}_1(t)$ and $\tilde{Q}_2(t)$ from Eqs. (20) and (21), which is the main result in this section.

3. Generalized two-band α-model and specific heat calculations

In this section, we will extend the anisotropic BCS theory to the so-called two-band α-model and derive specific heat formulae based on this new formalism. In the α-model, we first introduce new dimensionless parameter $\alpha_i^{\mathrm{E}} = Q_i^{\mathrm{E}}(0)/k_B T_c$, with $Q_i^{\mathrm{E}}(0)$ the zero-temperature gap obtained from the experiment. In close analogy with the BCS theory, we assume that the excitations above the superconducting ground state may still be treated as the well-defined fermions, but the quasi-particle energy is given by $\sqrt{\xi^2_{i\boldsymbol{p}} + (\Delta^{\mathrm{E}}_{i\boldsymbol{p}})^2}$ with $\Delta^{\mathrm{E}}_{i\boldsymbol{p}}(t) = Q_i^{\mathrm{E}}(0)\tilde{Q}_i(t)\chi_{i\boldsymbol{p}}$. Meanwhile, we suppose that the temperature dependence of $\tilde{Q}_1(t)$ and $\tilde{Q}_2(t)$ derived from the BCS theory will still be applicable in the study of intraband strong-coupling superconductors.

In statistical mechanics, the free energy for this free fermion system can be computed from the partition function Z as[27]

$$\frac{F}{k_B T_c} = -t\ln Z = -\sum_i 2N_i Q_i^{\mathrm{E}}(0)\left\langle\int_0^{\infty}\left[t\ln\left(1+\exp\left(-\alpha_i^{\mathrm{E}}\tilde{E}_{i\boldsymbol{p}}/t\right)\right)\right]\mathrm{d}\tilde{\xi}_i\right\rangle. \tag{22}$$

Here a rescaling $\tilde{\xi}_i \to [Q_i(0)/Q_i^{\mathrm{E}}(0)]\tilde{\xi}_i$ is performed in the integration and the factor of 2 is due to the spin degeneracy. Then, the internal energy U of this system takes the form

$$\frac{U}{k_B T_c} = t^2\frac{\partial\ln Z}{\partial t} = \sum_i 2N_i Q_i^{\mathrm{E}}(0)\left\langle\int_0^{\infty}\alpha_i^{\mathrm{E}}\tilde{E}_{i\boldsymbol{p}}f^{\mathrm{E}}_{i\boldsymbol{p}}\,\mathrm{d}\tilde{\xi}_i\right\rangle \tag{23}$$

with the Fermi distribution function $f^{\mathrm{E}}_{i\boldsymbol{p}} = 1/[1+\exp(\alpha_i^{\mathrm{E}}\tilde{E}_{i\boldsymbol{p}}/t)]$. According to the basic statistical relation $F = U - TS$, the entropy S can be expressed as

$$S = \frac{k_B}{t}\left(\frac{U}{k_B T_c} - \frac{F}{k_B T_c}\right) = \sum_i 2k_B N_i Q_i^{\mathrm{E}}(0)\left\langle\int_0^{\infty}\left[\alpha_i^{\mathrm{E}}\tilde{E}_{i\boldsymbol{p}}f^{\mathrm{E}}_{i\boldsymbol{p}}/t + \ln\left(1+\exp\left(-\alpha_i^{\mathrm{E}}\tilde{E}_{i\boldsymbol{p}}/t\right)\right)\right]\mathrm{d}\tilde{\xi}_i\right\rangle. \tag{24}$$

From Eq. (24), we can calculate the specific heat $C_{\rm es}$ in the superconducting phase as

$$\frac{C_{\rm es}}{k_{\rm B}T_{\rm c}}=t\left(\frac{\partial S}{\partial t}\right)=\sum_i 4k_{\rm B}N_i(\alpha_i^{\rm E})^3\left\langle\int_0^\infty f_{i\boldsymbol{p}}^{\rm E}\left(1-f_{i\boldsymbol{p}}^{\rm E}\right)\left[\frac{\tilde{E}_{i\boldsymbol{p}}^2}{t^2}-\frac{\chi_{i\boldsymbol{p}}^2}{2t}\frac{{\rm d}\tilde{Q}_i^2(t)}{{\rm d}t}\right]{\rm d}\tilde{\xi}_i\right\rangle. \tag{25}$$

We can see from Eq. (25) that the heat capacity $C_{\rm es}$ is composed of two parts, one is from the contribution of quasiparticle energy and the other is from the change rate of energy gaps with temperature. In the normal state, we have $\tilde{Q}_i(t)$=0 and ${\rm d}\tilde{Q}_i^2(t)/{\rm d}t=0$. In this case, we can perform the integration $\int_0^\infty f_{i\boldsymbol{p}}^{\rm E}\left(1-f_{i\boldsymbol{p}}^{\rm E}\right)\tilde{E}_{i\boldsymbol{p}}^2{\rm d}\tilde{\xi}_i=\pi^2t^3/[6(\alpha_i^{\rm E})^3]$. It allows us to obtain the well-known result for the specific heat of normal metal

$$\frac{C_{\rm en}}{k_{\rm B}T_{\rm c}}=\frac{2}{3}\pi^2k_{\rm B}(N_1+N_2)t. \tag{26}$$

Combining Eqs. (25) and (26), the specific heat ratio $C_{\rm es}/C_{\rm en}$ can be written as

$$\frac{C_{\rm es}}{C_{\rm en}}=\sum_i\frac{6N_i(\alpha_i^{\rm E})^3}{\pi^2(N_1+N_2)}\times\left\langle\int_0^\infty f_{i\boldsymbol{p}}^{\rm E}\left(1-f_{i\boldsymbol{p}}^{\rm E}\right)\left[\frac{\tilde{E}_{i\boldsymbol{p}}^2}{t^3}-\frac{\chi_{i\boldsymbol{p}}^2}{2t^2}\frac{{\rm d}\tilde{Q}_i^2(t)}{{\rm d}t}\right]{\rm d}\tilde{\xi}_i\right\rangle. \tag{27}$$

Based on Eq. (27), which is the first main result in this section, we will plug in the parameter $\alpha_i^{\rm E}$ from the experiment and numerically calculate the dependence of specific heat on temperature in the superconducting state.

At this stage, we would also like to obtain an analytic expression for the specific heat jump $\Delta C=C_{\rm es}-C_{\rm en}$ at the superconducting critical temperature. At $t=1$, we have $\int_0^\infty f_{i\boldsymbol{p}}^{\rm E}\left(1-f_{i\boldsymbol{p}}^{\rm E}\right){\rm d}\tilde{\xi}_i=1/(2\alpha_i^{\rm E})$. Then from Eqs. (26) and (27), the heat capacity jump can be expressed as

$$\left.\frac{\Delta C}{C_{\rm en}}\right|_{t=1}=-\sum_i\frac{3N_i(\alpha_i^{\rm E})^2}{2\pi^2(N_1+N_2)}\left[\left\langle\chi_{i\boldsymbol{p}}^2\right\rangle\left.\frac{{\rm d}\tilde{Q}_i^2(t)}{{\rm d}t}\right|_{t=1}\right]. \tag{28}$$

In order to compute ${\rm d}\tilde{Q}_i^2/{\rm d}t$, we need to take the derivative of t on both sides of Eqs. (20) and (21). In terms of the integral $\int_0^\infty[\tanh(\tilde{\xi}_i)/\tilde{\xi}_i^3-{\rm sech}^2(\tilde{\xi}_i)/\tilde{\xi}_i^2]{\rm d}\tilde{\xi}_i=7\zeta(3)/\pi^2$ where $\zeta(3)$ is the Riemann zeta function of argument 3, the detailed calculations will give us

$$\begin{aligned}&\frac{7\zeta(3)\alpha_1^2\left\langle\chi_{1\boldsymbol{p}}^4\right\rangle}{8\pi^2}\left.\frac{{\rm d}\tilde{Q}_1^2(t)}{{\rm d}t}\right|_{t=1}+\left\langle\chi_{1\boldsymbol{p}}^2\right\rangle\\&=\tilde{\lambda}_{12}\kappa(0)\left.\frac{\rm d}{{\rm d}t}\left[\frac{\tilde{Q}_2(t)}{\tilde{Q}_1(t)}\right]\right|_{t=1},\end{aligned} \tag{29}$$

$$\begin{aligned}&\frac{7\zeta(3)\alpha_2^2\left\langle\chi_{2\boldsymbol{p}}^4\right\rangle}{8\pi^2}\left.\frac{{\rm d}\tilde{Q}_2^2(t)}{{\rm d}t}\right|_{t=1}+\left\langle\chi_{2\boldsymbol{p}}^2\right\rangle\\&=-\frac{\tilde{\lambda}_{21}\tilde{Q}_1^2(t)}{\kappa(0)\tilde{Q}_2^2(t)}\left.\frac{\rm d}{{\rm d}t}\left[\frac{\tilde{Q}_2(t)}{\tilde{Q}_1(t)}\right]\right|_{t=1}\end{aligned} \tag{30}$$

from Eqs. (20) and (21), respectively. Based on Eqs. (29) and (30), we can obtain the first relation between ${\rm d}\tilde{Q}_i^2/{\rm d}t$ as

$$\begin{aligned}&\frac{7\zeta(3)\alpha_1^2\left\langle\chi_{1\boldsymbol{p}}^4\right\rangle}{8\pi^2}\left.\frac{{\rm d}\tilde{Q}_1^2(t)}{{\rm d}t}\right|_{t=1}+\left\langle\chi_{1\boldsymbol{p}}^2\right\rangle\\&=-\kappa^2(0)\frac{N_2\tilde{Q}_2^2(t)}{N_1\tilde{Q}_1^2(t)}\left[\frac{7\zeta(3)\alpha_2^2\left\langle\chi_{2\boldsymbol{p}}^4\right\rangle}{8\pi^2}\left.\frac{{\rm d}\tilde{Q}_2^2(t)}{{\rm d}t}\right|_{t=1}+\left\langle\chi_{2\boldsymbol{p}}^2\right\rangle\right].\end{aligned} \tag{31}$$

Meanwhile, the gap function close to the critical temperature can be approximated as[25]

$$\tilde{Q}_i^2(t)=(t-1)\left.\frac{{\rm d}\tilde{Q}_i^2(t)}{{\rm d}t}\right|_{t=1}. \tag{32}$$

From Eq. (32), we can derive the second relation between ${\rm d}\tilde{Q}_i^2/{\rm d}t$ as

$$\left.\frac{{\rm d}\tilde{Q}_1^2(t)}{{\rm d}t}\right|_{t=1}:\left.\frac{{\rm d}\tilde{Q}_2^2(t)}{{\rm d}t}\right|_{t=1}=\tilde{Q}_1^2(t):\tilde{Q}_2^2(t), \tag{33}$$

where the limit $t\to1$ is taken for the ratio of the two gap functions and $\tilde{Q}_1^2(t):\tilde{Q}_2^2(t)$ will be abbreviated as $\tilde{Q}_1^2:\tilde{Q}_2^2$ henceforth. Solving Eqs. (31) and (33), we can get

$$\left.\frac{{\rm d}\tilde{Q}_i^2(t)}{{\rm d}t}\right|_{t=1}=-\frac{8\pi^2\tilde{Q}_i^2}{7\zeta(3)\alpha_1^2}\frac{N_1\tilde{Q}_1^2\left\langle\chi_{1\boldsymbol{p}}^2\right\rangle+N_2\kappa^2(0)\tilde{Q}_2^2\left\langle\chi_{2\boldsymbol{p}}^2\right\rangle}{N_1\tilde{Q}_1^4\left\langle\chi_{1\boldsymbol{p}}^4\right\rangle+N_2\kappa^4(0)\tilde{Q}_2^4\left\langle\chi_{2\boldsymbol{p}}^4\right\rangle}. \tag{34}$$

Then plugging Eq. (34) into Eq. (28), the specific heat jump at the superconducting phase transition can be expressed analytically as

$$\begin{aligned}\left.\frac{\Delta C}{C_{\rm en}}\right|_{t=1}=&\frac{N_1\tilde{Q}_1^2\left\langle\chi_{1\boldsymbol{p}}^2\right\rangle+N_2\kappa^2(0)\tilde{Q}_2^2\left\langle\chi_{2\boldsymbol{p}}^2\right\rangle}{N_1\tilde{Q}_1^4\left\langle\chi_{1\boldsymbol{p}}^4\right\rangle+N_2\kappa^4(0)\tilde{Q}_2^4\left\langle\chi_{2\boldsymbol{p}}^4\right\rangle}\\&\times\sum_i\frac{12}{7\zeta(3)}\left(\frac{\alpha_i^{\rm E}}{\alpha_1}\right)^2\frac{N_i\tilde{Q}_i^2\left\langle\chi_{i\boldsymbol{p}}^2\right\rangle}{N_1+N_2},\end{aligned} \tag{35}$$

which is the second main result in this section.

For the weak-coupling superconductor, we have $\alpha_i^{\rm E}=\alpha_i$. Then we can simplify Eq. (35) and reduce the formula to the form

$$\left.\frac{\Delta C}{C_{\rm en}}\right|_{t=1}=\frac{12}{7\zeta(3)}\frac{\left[N_1\tilde{Q}_1^2\left\langle\chi_{1\boldsymbol{p}}^2\right\rangle+N_2\kappa^2(0)\tilde{Q}_2^2\left\langle\chi_{2\boldsymbol{p}}^2\right\rangle\right]^2}{(N_1+N_2)\left[N_1\tilde{Q}_1^4\left\langle\chi_{1\boldsymbol{p}}^4\right\rangle+N_2\kappa^4(0)\tilde{Q}_2^4\left\langle\chi_{2\boldsymbol{p}}^4\right\rangle\right]}, \tag{36}$$

which is consistent with previous results on isotropic ($\chi_{i\boldsymbol{p}}=1$) BCS superconductors.[21,25] Noting that due to the Cauchy inequality, the specific heat jump shown in Eq. (36) is always smaller than the single-band BCS prediction $\Delta C/C_{\rm en}=12/7\zeta(3)\approx1.43$ at $t=1$.

4. Superfluid density calculations in the α-model

In this section, we will perform the calculations on the superflid density based on the anisotropic two-band α-model. According to Refs. [28,29], the supercurrent $\boldsymbol{j}(\boldsymbol{r})$ is related locally to the vector potential $\boldsymbol{A}(\boldsymbol{r})$ through a tensor equation

$$\boldsymbol{j} = \mathcal{R}\cdot\boldsymbol{A} \tag{37}$$

and the symmetric response tensor $\mathcal{R}$ takes the form

$$\begin{aligned}\mathcal{R}_{\mu\mu'}(T) &= \frac{e^2}{4\pi^3\hbar c}\sum_{i=1,2}\oint_{\mathrm{FS}}\mathrm{d}S_i\left(\frac{v_i^{\mu}v_i^{\mu'}}{v_i}\right)\\ &\quad\times\left[1+2\int_{\Delta_{i\boldsymbol{p}}}^{\infty}\frac{\partial f_{i\boldsymbol{p}}}{\partial E_{i\boldsymbol{p}}}\left(\frac{E_{i\boldsymbol{p}}}{\sqrt{E_{i\boldsymbol{p}}^2-\Delta_{i\boldsymbol{p}}^2}}\right)\mathrm{d}E_i\right]\\ &= \frac{e^2}{4\pi^3\hbar c}\sum_{i=1,2}\oint_{\mathrm{FS}}\mathrm{d}S_i\left(\frac{v_i^{\mu}v_i^{\mu'}}{v_i}\right)\\ &\quad\times\left[1-\left(\frac{1}{2k_{\mathrm{B}}T}\right)\int_0^{\infty}\cosh^{-2}\left(\frac{E_{i\boldsymbol{p}}}{2k_{\mathrm{B}}T}\right)\mathrm{d}\xi_i\right]\end{aligned} \tag{38}$$

with $\mu,\mu'=a,b,c$ (a, b, and c are the crystal axes). Here v_i and v_i^{μ} are the magnitude of Fermi velocity and its μ-component for each band. $\mathrm{d}S_i$ is Fermi surface (FS) element and $S_i/v_i\propto N_i$. Then we can map the form of the tensor $\mathcal{R}$ in Eq. (38) to

$$\begin{aligned}\mathcal{R}_{\mu\mu'}(t) &= \frac{e^2}{4\pi^3\hbar c}\sum_{i=1,2}\oint_{\mathrm{FS}}\mathrm{d}S_i\frac{v_i^{\mu}v_i^{\mu'}}{v_i}\\ &\quad\times\left[1-\left(\frac{\alpha_i^{\mathrm{E}}}{2t}\right)\int_0^{\infty}\cosh^{-2}\left(\frac{\alpha_i^{\mathrm{E}}\tilde{E}_{i\boldsymbol{p}}}{2t}\right)\mathrm{d}\tilde{\xi}_i\right]\end{aligned} \tag{39}$$

in the α-model.

With the coordinate system defined by the principle axes of $\mathcal{R}_{\mu\mu}$, we have from Eq. (37)

$$j_{\mu}(\boldsymbol{r}) = \frac{c}{4\pi}\frac{A_{\mu}(\boldsymbol{r})}{\lambda_{\mu\mu}^2}, \tag{40}$$

where the penetration depth is given by

$$\lambda_{\mu\mu}^2 = \frac{c}{4\pi\mathcal{R}_{\mu\mu}(t)}. \tag{41}$$

Then the normalized superfluid density can be obtained from

$$\rho_{\mu}(t) = \left[\frac{\lambda_{\mu\mu}(0)}{\lambda_{\mu\mu}(t)}\right]^2 = \frac{\mathcal{R}_{\mu\mu}(t)}{\mathcal{R}_{\mu\mu}(0)}. \tag{42}$$

In the case of two-dimensional (2D) cylindrical Fermi surface, which can be employed as a simple approximation for the $NbSe_2$ bulk sample, the detailed calculations give the superfluid density in the a-direction as[29]

$$\rho_a(t) = \omega\rho_{1a}(t)+\left(1-\omega\right)\rho_{2a}(t) \tag{43}$$

with

$$\omega = \frac{N_1v_1^2}{N_1v_1^2+N_2v_2^2}, \tag{44}$$

$$\rho_{ia}(t) = 1-\frac{\alpha_i^{\mathrm{E}}}{t}\left\langle\int_0^{\infty}\cos^2\varphi\cosh^{-2}\left(\frac{\alpha_i^{\mathrm{E}}\tilde{E}_{i\boldsymbol{p}}}{2t}\right)\mathrm{d}\tilde{\xi}_i\right\rangle. \tag{45}$$

Similarly, we can also obtain the normalized superfluid density in the b-direction

$$\rho_b(t) = \omega\rho_{1b}(t)+(1-\omega)\rho_{2b}(t) \tag{46}$$

with

$$\rho_{ib}(t) = 1-\frac{\alpha_i^{\mathrm{E}}}{t}\left\langle\int_0^{\infty}\sin^2\varphi\cosh^{-2}\left(\frac{\alpha_i^{\mathrm{E}}\tilde{E}_{i\boldsymbol{p}}}{2t}\right)\mathrm{d}\tilde{\xi}_i\right\rangle. \tag{47}$$

Based on Eqs. (43) and (46), we can calculate the temperature dependence of superfluid density in the ab-plane for the superconducting state.

5. Spin susceptibility calculations in the α-model

In this section, we will perform the calculations on the spin susceptibility based on the anisotropic two-band α-model. In the experiment, the Knight shift in the resonance frequency will give a direct measure of the behavior of spin susceptibility for the superconducting state.

When an external magnetic field $\boldsymbol{H}$ is applied to the two-band superconductor, the Zeeman energy of the electron spin system is given by

$$H_z = \mu_{\mathrm{B}}\boldsymbol{H}\cdot\mathcal{G}\cdot\sum_{i\boldsymbol{p}\sigma\sigma'}c_{i\boldsymbol{p}\sigma}^{\dagger}\tau_{\sigma\sigma'}c_{i\boldsymbol{p}\sigma'} \tag{48}$$

with μ_{B} the Bohr magneton and τ the Pauli matrices. We have the Landé tensor $\mathcal{G}_{\mu\mu'}=\delta_{\mu\mu'}g_{\mu}$ for $\mu,\mu'=a,b,c$. According to Refs. [30,31], in the absence of spin–orbit coupling, the spin susceptibility tensor $\chi_{\mu\mu'}$ in the superconducting state can be expressed as

$$\begin{aligned}\chi_{\mu\mu'} &= -\frac{1}{4}g_{\mu}g_{\mu'}\mu_{\mathrm{B}}^2k_{\mathrm{B}}T\sum_{i\boldsymbol{p}\omega_n}\mathrm{Tr}\big[\tau_{\mu}G_i(\boldsymbol{p},\omega_n)\,\tau_{\mu'}G_i(\boldsymbol{p},\omega_n)\\ &\quad-\tau_{\mu}F_i(\boldsymbol{p},\omega_n)\,\tau_{\mu'}^{\mathrm{T}}F_i^{\dagger}(\boldsymbol{p},\omega_n)\big]\end{aligned} \tag{49}$$

with $\omega_n=(2n+1)\pi k_{\mathrm{B}}T$ ($n\in Z$). The superconducting electron Green's functions are defined by

$$G_i(\boldsymbol{p},\omega_n) = -\frac{\mathrm{i}\omega_n+\xi_{i\boldsymbol{p}}}{\omega_n^2+E_{i\boldsymbol{p}}^2}\tau_0, \tag{50}$$

$$F_i(\boldsymbol{p},\omega_n) = -F_i^{\dagger}(\boldsymbol{p},\omega_n) = \frac{\mathrm{i}\Delta_{i\boldsymbol{p}}}{\omega_n^2+E_{i\boldsymbol{p}}^2}\tau_2 \tag{51}$$

with τ_0 the 2D identity matrix. Algebraic manipulations on Eq. (49) will give $\chi_{\mu\mu'}=\chi_{\mu}\delta_{\mu\mu'}$, and the spin susceptibility in the μ-direction can be cast into the form

$$\chi_{\mu} = -\frac{1}{2}g_{\mu}^2\mu_{\mathrm{B}}^2k_{\mathrm{B}}T\sum_{i\boldsymbol{p}\omega_n}\left[\frac{(\mathrm{i}\omega_n+\xi_{i\boldsymbol{p}})^2}{\left(\omega_n^2+E_{i\boldsymbol{p}}^2\right)^2}+\frac{\Delta_{i\boldsymbol{p}}^2}{\left(\omega_n^2+E_{i\boldsymbol{p}}^2\right)^2}\right]$$

$$= \frac{1}{2} g_\mu^2 \mu_{\rm B}^2 k_{\rm B} T \sum_{i\boldsymbol{p}\omega_n} \frac{\omega_n^2 - E_{i\boldsymbol{p}}^2}{\left(\omega_n^2 + E_{i\boldsymbol{p}}^2\right)^2}. \tag{52}$$

With the identity

$$k_{\rm B} T \sum_{\omega_n} \frac{\omega_n^2 - E_{i\boldsymbol{p}}^2}{\left(\omega_n^2 + E_{i\boldsymbol{p}}^2\right)^2} = \frac{1}{4k_{\rm B}T} \cosh^{-2}\left(\frac{E_{i\boldsymbol{p}}}{2k_{\rm B}T}\right), \tag{53}$$

we can rewrite the spin susceptibility in Eq. (52) as

$$\chi_\mu = \frac{g_\mu^2 \mu_{\rm B}^2}{8k_{\rm B}T} \sum_{i\boldsymbol{p}} \cosh^{-2}\left(\frac{E_{i\boldsymbol{p}}}{2k_{\rm B}T}\right) \tag{54}$$

in the framework of the BCS theory.

Then we can map the form of spin susceptibility χ_μ in Eq. (54) to

$$\chi_\mu = \frac{g_\mu^2 \mu_{\rm B}^2}{8t} \sum_i N_i \alpha_i^{\rm E} \left\langle \int_0^\infty \cosh^{-2}\left(\frac{\alpha_i^{\rm E} \tilde{E}_{i\boldsymbol{p}}}{2t}\right) {\rm d}\tilde{\xi}_i \right\rangle \tag{55}$$

in the α-model. At $T = T_{\rm c}$, we can perform the integration with $\tilde{Q}_i = 0$ and get the spin susceptibility for the normal state from Eq. (55)

$$\chi_{n,\mu} = \frac{1}{4} g_\mu^2 \mu_{\rm B}^2 \left(N_1 + N_2\right). \tag{56}$$

Then the normalized spin susceptibility can be expressed as

$$\chi(t) = \frac{\chi_\mu}{\chi_{n,\mu}} = \sum_i \frac{N_i \alpha_i^{\rm E}}{2t\left(N_1 + N_2\right)} \times \left\langle \int_0^\infty \cosh^{-2}\left(\frac{\alpha_i^{\rm E} \tilde{E}_{i\boldsymbol{p}}}{2t}\right) {\rm d}\tilde{\xi}_i \right\rangle. \tag{57}$$

Based on Eq. (57), we can calculate the temperature dependence of spin susceptibility in the superconducting state.

6. Application to anisotropic two-band superconductor $NbSe_2$

In this section, we will compute the temperature dependence of specific heat, superfluid density and spin susceptibility for the layered chalcogenide superconductor $NbSe_2$. The 2H polytype of niobium diselenide has a hexagonal crystal structure with the space group $P6_3/mmc$. The primitive unit cell of $NbSe_2$ contains two niobium and four selenium atoms, and the electronic states around the Fermi level are dominated by two 4d orbitals of the Nb atoms as shown in Fig. 1(a). The Fermi surface of $NbSe_2$ is mainly determined by the bonding and antibonding combinations of these two orbitals, leading to double-walled barrel-shaped pockets around the Γ and K points of the hexagonal Brillouin zone, see Fig. 1(b).

For $NbSe_2$, first-principle calculations give the elements of the interaction matrix $g_{11} = 0.60$ eV, $g_{22} = 0.30$ eV, and $g_{12} = g_{21} = 0.056$ eV, and the density of states at the Fermi level $N_1 = 1.37$ eV^{-1} and $N_2 = 0.84$ eV^{-1}.[32] Then according to the definition of $\lambda_{ii'} = g_{ii'} N_{i'}$, we can obtain the effective coupling constants $\tilde{\lambda}_{11} = 4.04$, $\tilde{\lambda}_{22} = 1.24$, $\tilde{\lambda}_{21} = 0.38$, and $\tilde{\lambda}_{12} = 0.23$. Since each Nb band of this compound exhibits a gap function with six-fold symmetry, the superconducting order parameter can be expressed as $\Delta_{i\boldsymbol{p}}^{\rm E}(0) = Q_i^{\rm E}(0)\chi_{i\boldsymbol{p}}$ with the angular distribution $\chi_{i\boldsymbol{p}} = 1 + \varepsilon_i \cos(6\varphi)$.[12–14] We take $Q_1^{\rm E}(0) = 1.74$ meV, $Q_2^{\rm E}(0) = 0.57$ meV, and the anisotropy parameters $\varepsilon_1 = \varepsilon_2 = 0.41$ to fit the angle-resolved photoemission data in Ref. [14]. From the inset of Fig. 2, we can see that our fitting curves are in agreement with the experimental gaps measured at 1 K. Now we try to compute the temperature dependence of the reduced gap function $\tilde{Q}_i(t)$ based on the anisotropic BCS theory. With the effective interaction coefficient $\tilde{\lambda}_{ij}$, we can first obtain $\kappa(0) = 0.27$ from Eq. (15) and $\alpha_1 = 1.61$ and $\alpha_2 = 0.43$ from Eq. (18). Then $\tilde{Q}_i$ as a function of temperature can be numerically calculated with Eqs. (20) and (21). From Fig. 2, we can see that $\tilde{Q}_i$ decreases with the increase of t and eventually approaches to zero at the critical temperature. We can also observe that the behavior of the small gap $\tilde{Q}_2$ close to $T_{\rm c}$ is strongly deviated from the standard BCS form, which manifests the crucial role played by the interband interaction.

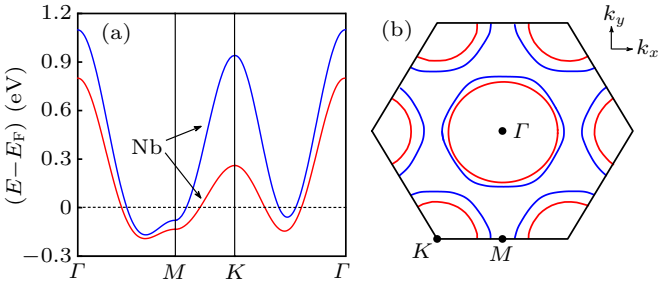


Fig. 1. (a) The band structure and (b) the Fermi surface of the $NbSe_2$ crystal. Inner pockets (red) around Γ and K points derive from one band, while the outer pockets (blue) derive from the second band.[14]

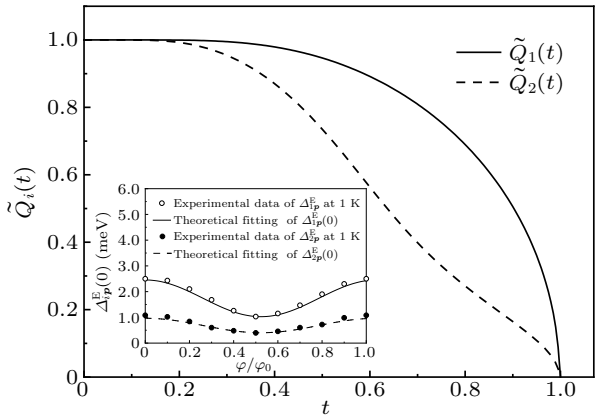


Fig. 2. The temperature dependence of normalized gap function $\tilde{Q}_i$ for the $NbSe_2$ crystal. Inset: The angular dependence of anisotropic superconducting gap $\Delta_{i\boldsymbol{p}}^{\rm E}$ with $\varphi_0 = \pi/3$. The experimental points measured at 1 K are extracted from Ref. [14].

Based on the discussions above, we first calculate the temperature dependence of specific heat with the anisotropic

two-band α-model. On account of $\alpha_i^{\mathrm{E}} = Q_i^{\mathrm{E}}(0)/k_{\mathrm{B}}T_{\mathrm{c}}$, we can get $\alpha_1^{\mathrm{E}} = 2.80$ and $\alpha_2^{\mathrm{E}} = 0.92$ from the $\Delta_{i\boldsymbol{p}}^{\mathrm{E}}(0)$ data. With the normalized gap $\tilde{Q}_i(t)$ from the BCS theory, we can compute the specific heat as a function of temperature with Eq. (27) and plot the numerical results in Fig. 3. From Fig. 3, we can see that our theoretical curve is in good agreement with the experimental points in the whole temperature range. Meanwhile, we can read out $\tilde{Q}_1 : \tilde{Q}_2 \approx 1.98$ close to T_{c} from the numerical data of the normalized gap function $\tilde{Q}_i(t)$ in Fig. 2. Then according to Eq. (35), the two-band α-model will give the specific heat jump $\Delta C/C_{\mathrm{en}}|_{t=1} = 2.12$ as shown in Fig. 3, which is consistent with the experimental measurement and much better than the two-band weak-coupling BCS value ($\leqslant 1.43$).

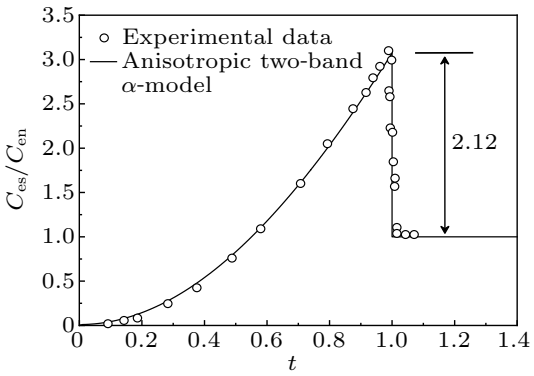


Fig. 3. The temperature dependence of specific heat for the $NbSe_2$ crystal. The experimental points are taken from Ref. [19].

Meanwhile, we calculate the temperature dependence of superfluid density for $NbSe_2$. From the first-principle calculations,[9] we can obtain the Fermi velocity as $v_1 = 0.21 \times 10^8$ cm/s and $v_2 = 0.19 \times 10^8$ cm/s. Given the above parameters, we can compute the average superfluid density in the basal plane $\rho(t) = (\rho_a + \rho_b)/2$ from Eqs. (43) and (46). The numerical result is plotted in Fig. 4. From Fig. 4, we can see that our theoretical result can fit the experimental data very well in a broad temperature range.

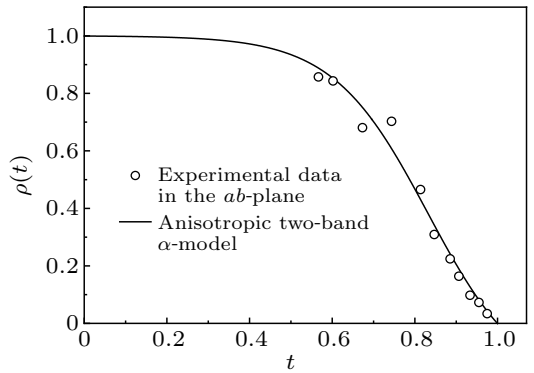


Fig. 4. The temperature dependence of normalized superfluid density for the $NbSe_2$ crystal. The experimental points are taken from Ref. [33].

Furthermore, we also calculate the temperature dependence of spin susceptibility for the centrosymmetric $NbSe_2$ crystal. From the tunneling spectroscopy data, we have the Landé factor $g_a = g_b = 1.67$ and $g_c = 1.94$ for $NbSe_2$.[34] Since the normalized gap function $\tilde{Q}_i$ as a function of temperature can be numerically calculated from the anisotropic two-band BCS theory, we can then compute the normalized spin susceptibility $\chi(t)$ from Eq. (57). The numerical result is plotted in Fig. 5. From Fig. 5, we can see that with the increase of temperature the normalized spin susceptibility increases gradually and then remains constant at $t > 1$. Up to now the experimental value of χ for $NbSe_2$ bulk sample to our knowledge has not been reported yet, we thus hope that future NMR measurements could serve to verify our theoretical investigation.

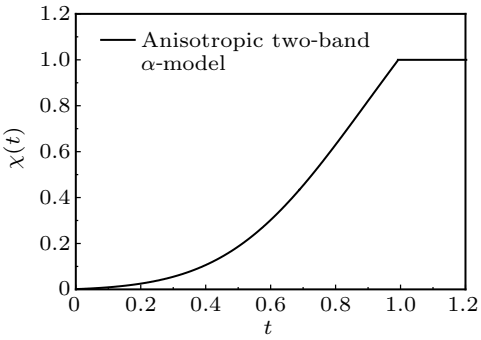


Fig. 5. The temperature dependence of normalized spin susceptibility for the $NbSe_2$ crystal.

7. Generalization to the interband pairing case

In this section, we examine the interplay between intraband and interband pairing and the generalization of our anisotropic α-model in this case. The full Hamiltonian which describes all of these pairing interactions can be written as

$$H = \sum_{i\boldsymbol{p}\sigma} \xi_{i\boldsymbol{p}} c^{\dagger}_{i\boldsymbol{p}\sigma} c_{i\boldsymbol{p}\sigma} - \sum_{ij\boldsymbol{p},i'j'\boldsymbol{p}'} V_{ij\boldsymbol{p},i'j'\boldsymbol{p}'} c^{\dagger}_{i\boldsymbol{p}\uparrow} c^{\dagger}_{j-\boldsymbol{p}\downarrow} c_{i'-\boldsymbol{p}'\downarrow} c_{j'\boldsymbol{p}'\uparrow}. \quad (58)$$

Here $i, j, i', j' = 1, 2$ are the band indices and $V_{ij\boldsymbol{p},i'j'\boldsymbol{p}'}$ corresponds to the interband pairing interaction between electrons with momenta $\boldsymbol{p}$ and $\boldsymbol{p}'$. From the symmetric consideration, we also have $V_{ij\boldsymbol{p},i'j'\boldsymbol{p}'} = -V_{ji\boldsymbol{p},i'j'\boldsymbol{p}'} = -V_{ij\boldsymbol{p},j'i'\boldsymbol{p}'} = V_{i'j'\boldsymbol{p}',ij\boldsymbol{p}}$.

Now we can introduce the gap function

$$\Delta_{ij\boldsymbol{p}}(T) = -\sum_{i'j'\boldsymbol{p}'} V_{ij\boldsymbol{p},i'j'\boldsymbol{p}'} \left\langle\left\langle c_{i'-\boldsymbol{p}'\downarrow} c_{j'\boldsymbol{p}'\uparrow}\right\rangle\right\rangle. \quad (59)$$

Then we can transform the Hamiltonian (58) into the mean-field form

$$H_{\mathrm{eff}} = \sum_{i\boldsymbol{p}\sigma} \xi_{i\boldsymbol{p}} c^{\dagger}_{i\boldsymbol{p}\sigma} c_{i\boldsymbol{p}\sigma} + \sum_{ij\boldsymbol{p}} \left[\Delta_{ij\boldsymbol{p}}(T)\, c^{\dagger}_{i\boldsymbol{p}\uparrow} c^{\dagger}_{j-\boldsymbol{p}\downarrow} + \mathrm{H.c.}\right]. \quad (60)$$

After setting $\Delta_{11\boldsymbol{p}} = \Delta_{1\boldsymbol{p}}$, $\Delta_{22\boldsymbol{p}} = \Delta_{2\boldsymbol{p}}$, and $\Delta_{12\boldsymbol{p}} = \Delta_{21\boldsymbol{p}} = \Delta_{3\boldsymbol{p}}$, we diagonalize the Hamiltonian (60) and get the quasi-particle

excitations explicitly as

$$E_{\pm \boldsymbol{p}} = \sqrt{A_{\boldsymbol{p}} \pm B_{\boldsymbol{p}}} \tag{61}$$

with

$$A_{\boldsymbol{p}} = \frac{1}{2}\left(E_{1\boldsymbol{p}}^2 + E_{2\boldsymbol{p}}^2\right) + \Delta_{3\boldsymbol{p}}^2, \tag{62}$$

$$B_{\boldsymbol{p}} = \sqrt{\left(E_{1\boldsymbol{p}}^2 - E_{2\boldsymbol{p}}^2\right)^2 + 4\Delta_{3\boldsymbol{p}}^2\left[\left(\xi_{1\boldsymbol{p}} - \xi_{2\boldsymbol{p}}\right)^2 + \left(\Delta_{1\boldsymbol{p}} + \Delta_{2\boldsymbol{p}}\right)^2\right]}. \tag{63}$$

We can see that with the inclusion of the interband pairing, the form of the quasi-particle energy $E_{\pm \boldsymbol{p}}$ is more complicated than $E_{i\boldsymbol{p}} = \sqrt{\xi_{i\boldsymbol{p}}^2 + \Delta_{i\boldsymbol{p}}^2}$.

With the definition of

$$\begin{aligned} &V_{11\boldsymbol{p},11\boldsymbol{p}'} = V_{1\boldsymbol{p}1\boldsymbol{p}'}, \quad V_{22\boldsymbol{p},22\boldsymbol{p}'} = V_{2\boldsymbol{p}2\boldsymbol{p}'}, \\ &V_{11\boldsymbol{p},22\boldsymbol{p}'} = V_{1\boldsymbol{p}2\boldsymbol{p}'}, \end{aligned} \tag{64}$$

$$\begin{aligned} &2V_{11\boldsymbol{p},12\boldsymbol{p}'} = V_{1\boldsymbol{p}3\boldsymbol{p}'} = V_{3\boldsymbol{p}1\boldsymbol{p}'}, \\ &2V_{22\boldsymbol{p},12\boldsymbol{p}'} = V_{2\boldsymbol{p}3\boldsymbol{p}'} = V_{3\boldsymbol{p}2\boldsymbol{p}'}, \\ &2V_{12\boldsymbol{p},12\boldsymbol{p}'} = V_{3\boldsymbol{p}3\boldsymbol{p}'}, \end{aligned} \tag{65}$$

we try to employ the separability ansatz to simplify the self-consistent gap equation (59). We first assume that the pairing interaction can be written as $V_{\mu\boldsymbol{p}\mu'\boldsymbol{p}'} = g_{\mu\mu'}\chi_{\mu\boldsymbol{p}}\chi_{\mu'\boldsymbol{p}'}$ with $\chi_{\mu\boldsymbol{p}}$ the angular dependence of the anisotropic pairing interaction and $\mu, \mu' = 1, 2, 3$. Then due to the separable form of $V_{\mu\boldsymbol{p}\mu'\boldsymbol{p}'}$, the order parameter can also be decomposed as $\Delta_{\mu\boldsymbol{p}}(T) = Q_\mu(T)\chi_{\mu\boldsymbol{p}}$ with $Q_\mu(T)$ the temperature-dependent part of the superconducting gap function. Substituting the factorizable forms of $V_{\mu\boldsymbol{p}\mu'\boldsymbol{p}'}$ and $\Delta_{\mu\boldsymbol{p}}(T)$ into Eq. (59), the detailed calculations give the self-consistent equations for Q_μ as

$$\begin{aligned} Q_\mu(T) = &\sum_{\mu'} g_{\mu\mu'} Q_{\mu'}(T) \int \frac{\mathrm{d}^3\boldsymbol{p}'}{(2\pi)^3} \chi_{\mu'\boldsymbol{p}'}^2 \\ &\times \left[\frac{\gamma_{\mu'\boldsymbol{p}'}^+}{2E_{+\boldsymbol{p}'}}\left(1 - 2f_{+\boldsymbol{p}'}\right) + \frac{\gamma_{\mu'\boldsymbol{p}'}^-}{2E_{-\boldsymbol{p}'}}\left(1 - 2f_{-\boldsymbol{p}'}\right)\right]. \end{aligned} \tag{66}$$

Here we define the Fermi distribution function $f_{\pm\boldsymbol{p}} = 1/\left[1 + \exp\left(E_{\pm\boldsymbol{p}}/k_\mathrm{B}T\right)\right]$ and $\gamma_{\mu\boldsymbol{p}}^\pm = 1 \pm \gamma_{\mu\boldsymbol{p}}/B_{\boldsymbol{p}}$ with $\gamma_{1\boldsymbol{p}} = E_{1\boldsymbol{p}}^2 - E_{2\boldsymbol{p}}^2 + 2\Delta_{3\boldsymbol{p}}^2 + 2\Delta_{3\boldsymbol{p}}^2\Delta_{2\boldsymbol{p}}/\Delta_{1\boldsymbol{p}}$, $\gamma_{2\boldsymbol{p}} = E_{2\boldsymbol{p}}^2 - E_{1\boldsymbol{p}}^2 + 2\Delta_{3\boldsymbol{p}}^2 + 2\Delta_{3\boldsymbol{p}}^2\Delta_{1\boldsymbol{p}}/\Delta_{2\boldsymbol{p}}$, and $\gamma_{3\boldsymbol{p}} = \left(\xi_{1\boldsymbol{p}} - \xi_{2\boldsymbol{p}}\right)^2 + \left(\Delta_{1\boldsymbol{p}} + \Delta_{2\boldsymbol{p}}\right)^2$. Noting that the three-dimensional integration over the momentum in Eq. (66) will be confined in the first Brillouin zone. Given the intraband and interband coefficients $g_{\mu\mu'}$, we can therefore numerically calculate the temperature dependence of $Q_\mu(t)$ and then $\tilde{Q}_\mu(t) = Q_\mu(t)/Q_\mu(0)$ from the two-band BCS theory.

Now we can extend our anisotropic two-band α-model with the inclusion of the interband pairing interaction. In this circumstance, we will introduce three dimensionless parameters $\alpha_\mu^\mathrm{E} = Q_\mu^\mathrm{E}(0)/k_\mathrm{B}T_\mathrm{c}$ with $Q_\mu^\mathrm{E}(0)$ the zero-temperature gap function obtained from the fitting of angle-resolved experimental measurements. In close analogy with the BCS theory, we assume that the excitations above the superconducting ground state may still be treated as the well-defined fermions, but the quasi-particle energy $E_{\pm\boldsymbol{p}}(\Delta_{\mu\boldsymbol{p}})$ in Eq. (61) will be substituted by $E_{\pm\boldsymbol{p}}\left(\Delta_{\mu\boldsymbol{p}}^\mathrm{E}\right)$ with $\Delta_{\mu\boldsymbol{p}}^\mathrm{E}(t) = Q_\mu^\mathrm{E}(0)\tilde{Q}_\mu(t)\chi_{\mu\boldsymbol{p}}$. Meanwhile, we suppose that the temperature dependence of $\tilde{Q}_\mu(t)$ derived from the multi-band BCS theory will still be applicable in the study of intraband strong-coupling superconductors. These two ingredients constitute the basic formalism for the anisotropic two-band α-model in the presence of interband pairing interaction.

8. Conclusion

In summary, we have proposed a generalized α-model for anisotropic two-band superconductors with weak interband interaction. Adapted from the two-band BCS theory, this model provides a framework to investigate thermodynamic properties of intraband strong-coupling superconductors. With this approach, we calculate the temperature dependence of specific heat and obtain an analytical formula for heat capacity jump at the critical temperature. Meanwhile, we also compute the superfluid density and the spin susceptibility with this formalism. We then apply this approach to analyze thermodynamic behaviors of the layered chalcogenide superconductor $NbSe_2$. Our theoretical results show good agreement with the experimental data for this two-band material, and the specific heat jump beyond the weak-coupling BCS limit can also be naturally explained in this frame. We hope that our theoretical work will inspire further research on better understanding microscopic pairing mechanisms and physical properties of multi-band strong-coupling superconductors.

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