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Magnetic field dependence of T_c and temperature dependence of H_{c2} in layered superconductors with open normal state Fermi surface

SUDHANSHU S JHA and A K RAJAGOPAL*
Tata Institute of Fundamental Research, Bombay 400005, India
*Naval Research Laboratory, Washington DC 20375–5000, USA

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Abstract. A theoretical framework for treating the effects of magnetic field **H** on the pairing theory of superconductivity is considered, where the field is taken in an arbitrary direction with respect to crystal axes. This is applicable to closed, as well as open normal state Fermi surface (FS), including simple layered metals. The orbital effects of the magnetic field are treated semiclassically while retaining the full anisotropic paramagnetic contribution. Explicit calculations are presented in the limits $|\mathbf{H}| \to |\mathbf{H}_{c2}(T)|$, $T \sim 0$ and $T \to T_c(|\mathbf{H}|)$, $|\mathbf{H}| \sim 0$. Effects of weak nonmagnetic impurity scattering, without vertex corrections, have also been taken into account in a phenomenological way. The final results for the case of open FS and layered materials are found to differ considerably from those of the closed FS. For example, an important parameter, $h^*(T=0) \equiv |\mathbf{H}_{c2}(0)|/[-T\delta|H_{c2}(T)|/\delta T]_{T_{c0}}$ for the case of a FS open in k_z-direction with the k_z-bandwidth, $4t_3$, very small compared to the Fermi energy, E_F, is close to 0·5906, compared to 0·7273 for the closed FS, in the clean limit. Analytical results are given for the magnetic field dependence of T_c and the temperature dependence of H_{c2} for a model of layered superconductors with widely open FS. For a set of band structure parameters for $YBa_2Cu_3O_7$ used elsewhere, we find reasonable values for the upper critical field $\mathrm{H}_{c2}(0)$, the slope $(\mathrm{dH}_{c2}/\mathrm{d}T)_{T_{c0}}$, anisotropic coherence lengths $\xi_i(T=0)$, $i = x, y, z$, and $(\mathrm{d}T_c/\mathrm{d}|\mathbf{H}|)_{|\mathbf{H}| \to 0}$.

Keywords. Upper critical magnetic field; layered superconductors, open Fermi surface.

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1. Introduction

A reexamination of the superconducting transition in the presence of an applied homogeneous magnetic field has become important in the context of the new high-T_c layered materials. In the past such investigations for type-II supercounductors were mostly limited to spherical or closed anisotropic Fermi surface associated with the three-dimensonal electronic band energy in the normal state (Werthamer 1969; Fetter and Hohenberg 1969), with the exception of a recent work by Rieck and Scharnberg (1990). Since high-T_c materials are layered, with highly anisotropic Fermi surface, open in the direction perpendicular to the layer planes (i.e. open in the k_z-direction), the dependence of T_c on the magnetic field strength, **H**, the anisotropy of the upper critical field, $\mathbf{H}_{c2}$, and their variation with temperature, T, are expected to be quite different from those found in the isotropic case.

For the case of isotropic normal state Fermi surface, the linearized gap equation

*On sabbatical leave at Tata Institute of Fundamental Research, Bombay 400005, India was solved and a condition for the transition in the (T, H) plane was obtained by Helfand and Werthamer (1966) in a semiclassical approximation, ignoring the discrete Landau-level effects, and by Rajagopal and Vasudevan (1966a,b) in a fully quantum mechanical framework. Explicit analytical results for $T_c(H)$ and $H_{c2}(T)$ were obtained for such a case by Gruenberg and Gunther (1968) in the semiclassical approximation. More recently, a detailed numerical analysis of the above condition in the extreme quantum limit, determining the transition in the (T, H) plane was given by Rieck *et al* (1990). The Ginzburg–Landau theory with anisotropic effective mass tensor has been employed by several authors (Werthamer 1969; Rieck and Scharnberg 1990; Bulaevskii *et al* 1988) to investigate this problem which, of course, is valid only for $T \sim T_c$. A more general calculation for the case of a closed anisotropic Fermi surface has been done by Prohammer and Carbotte (1990) and Rieck and Scharnberg (1990). In this paper, we consider the linearized gap equation in the presence of nonmagnetic impurities and a homogeneous magnetic field for the case of layered systems with anisotropic open Fermi surface in the normal state. Our formulation of the problem is such that it can, in fact, be used for any general form of the single-particle energy dispersion and Fermi surface. Note that the self-consistent magnetic field **H** inside a type-II superconductor is spatially inhomogeneous. However, close to the transition, it is a good approximation to take it to be the constant applied magnetic field because of the large penetration depths. It should also be noted that in high-T_c materials the anisotropic superconducting coherence length is much smaller than the impurity scattering mean free path (ℓ) in most of the experimental situations. However, a much more general formulation including strong momentum dependent magnetic and nonmagnetic impurity scattering, anisotropy of FS and pairing interaction, and more accurate calculation of the spatial dependence of the order parameter has been given by Rieck *et al* (1991). Because of the complexity of the problem in all its generality, the actual application of the formalism has been confined to only a few simple forms of FS and special directions of the magnetic field (Rieck and Scharnberg 1990; Rieck *et al* 1991). Since the change in the superconducting pair wave function is known to be small in the limit of small coherence length, ξ, in comparison to the scattering mean free path ℓ, the formulation given here, without vertex corrections, is sufficient to treat the problem of high T_c layered superconductors.

Although, the Landau-level quantization effects in very high magnetic fields may be important to describe the nature of pairing explicitly (Rieck *et al* 1990; Tesanovic *et al* 1989, 1991; Rajagopal and Vasudevan 1991; Rajagopal and Ryan 1991), here we will restrict ourselves to a semiclassical approximation for calculating $T_c(\mathbf{H})$ and $\mathbf{H}_{c2}(T)$ within the usual spin-singlet pairing theory of superconductivity in layered materials (Rajagopal and Jha 1991a). This allows us to extend the analytic results of Gruenberg and Gunther (1968) to the case of anisotropic materials with closed or open Fermi surface (FS). This includes the limiting effects of the paramagnetic Zeeman term and broadening due to the nonmagnetic impurity scattering. We find that the anisotropy of $H_{c2}(0)$ is quite different for the case of open FS than in the usual case of closed FS with anisotropic effective mass. The variation of $|\mathbf{H}_{c2}|(T)|$ with T is also much more rapid for the open FS compared to the closed FS. These arise because of an additional factor $E_F/t_3 \gg 1$, apart from the large effective mass factor $m_z(k_z \simeq 0)$, where $4t_3$ is the width of the energy band in the k_z-direction and E_F is the Fermi energy. Also, the effects of impurity scattering on $\mathbf{H}_{c2}(T)$ and $T_c(\mathbf{H})$ are markedly different in the two cases.

In the second section, we set up the linearized gap equation for our problem, in the presence of a magnetic field, and solve it in the semiclassical approximation. Explicit analytical expressions for $T_c(\mathbf{H})$ and $\mathbf{H}_{c2}(T)$, both when $T \sim T_c$, with $\mathbf{H} \to 0$, and $\mathbf{H} \sim \mathbf{H}_{c2}$, with $T \to 0$, are derived in § 3. We discuss our results in § 4.

2. Linearized gap equation

In the presence of a magnetic field $\mathbf{H} = \text{Curl}\ \mathbf{A}$, where $\mathbf{A}(\mathbf{r})$ is the vector potential, the single-particle electron Hamiltonian can be described by

$$\begin{aligned} H_0 - \mu N &= \hbar K_0(\mathbf{r}, \mathbf{A}(\mathbf{r}))\boldsymbol{\sigma}_4 - \tfrac{1}{2}\mu_B \mathbf{H}\cdot\mathbf{g}\cdot\boldsymbol{\sigma} \\ &= \left[\frac{1}{2m}\left(-i\hbar\nabla + \frac{e}{c}\mathbf{A}(\mathbf{r})\right)^2 + V_p(\mathbf{r})\right]\sigma_4 - \hbar\boldsymbol{\Omega}_H\cdot\boldsymbol{\sigma} \end{aligned} \tag{1}$$

where V_p is the periodic potential $\boldsymbol{\sigma} = (\boldsymbol{\sigma}_x, \boldsymbol{\sigma}_y, \boldsymbol{\sigma}_z)$ are the usual Pauli-matrices, σ_4 is the (2×2) unit matrix and $\hbar\boldsymbol{\Omega}_H$ is equal to $\frac{1}{2}\mu_B\mathbf{H}\cdot\mathbf{g}$, in terms of the electronic g-tensor g_{ij} and the Bohr-magneton μ_B. Because of the last (paramagnetic) term in equation (1), the hamiltonian is a 2×2 matrix in the spin-space. The general single-particle Green function matrix $\mathbf{G}$ for the system (in the presence of interactions) is defined by its matrix elements $G_{\alpha\beta}(x_1, x_2) = -\langle T(\psi_\alpha(x_1)\psi_\beta^\dagger(x_2))\rangle$ where x stands for ($\mathbf{r}$, it). One also defines a corresponding Green function matrix $\mathbf{G}$ with its elements $\mathbf{G}_{\alpha\beta}(x_1, x_2) = -\langle T(\psi_\alpha^\dagger(x_1)\psi_\beta(x_2))\rangle = -G_{\beta\alpha}(x_2, x_1)$. For the unperturbed Hamiltonian (1), the Green function matrix $\mathbf{G}_0$ satisfies the equation

$$[i\omega_n - K_0(\mathbf{r}_1, \mathbf{A}(\mathbf{r}_1))\boldsymbol{\sigma}_4 + \boldsymbol{\Omega}_H\cdot\boldsymbol{\sigma}]\mathbf{G}_0(\mathbf{r}_1, \mathbf{r}_2, i\omega_n) = \delta(\mathbf{r}_1 - \mathbf{r}_2)\boldsymbol{\sigma}_4 \tag{2}$$

in the Matsubara-frequency representation. Note that $\mathbf{G}_0(\mathbf{r}_1, \mathbf{r}_2, i\omega_n) = -\mathbf{G}_0^{\text{tr}}(\mathbf{r}_2, \mathbf{r}_1, -i\omega_n)$, where the superscript tr stands for transposition of (α, β) indices.

When a general effective interaction $\mathbf{V}(\mathbf{r}_1, \mathbf{r}_2; i\omega_n - i\omega_m)$ is taken into account, there is a self-energy contribution, $-\boldsymbol{\Sigma}$, to $\mathbf{G}_0^{-1}$. We call this modified Green function in the normal state as $\mathbf{g}$, with the corresponding time-reversed counter part $\bar{\mathbf{g}}$. We shall assume that $\mathbf{g}$ is known approximately, and model it appropriately at a later stage. In the superconducting state, in addition to the single-particle Green functions $\mathbf{G}$, $\bar{\mathbf{G}}$, there appear non-vanishing (2×2) matrix Green functions $\mathbf{F}$ and $\bar{\mathbf{F}}$ defined by (Rajagopal and Jha 1991a)

$$\begin{aligned} F_{\alpha\beta}(x_1, x_2) &= -\langle P\dagger\ T(\psi_\alpha(x_1)\psi_\beta(x_2))\rangle; \\ \bar{F}_{\alpha\beta}(x_1, x_2) &= -\langle PT(\psi_\alpha^\dagger(x_1)\psi_\alpha^\dagger(x_2))\rangle. \end{aligned}$$

The corresponding self-energies are the gap functions $\boldsymbol{\Delta}$ and $\bar{\boldsymbol{\Delta}}$, with

$$\boldsymbol{\Delta}(\mathbf{r}_1, \mathbf{r}_2, i\omega_n) = \frac{1}{\beta}\sum_m \mathbf{V}(\mathbf{r}_1, \mathbf{r}_2, i\omega_n - i\omega_m)\mathbf{F}(\mathbf{r}_1, \mathbf{r}_2, i\omega_m); \text{ etc.} \tag{3}$$

where $\beta = \hbar/k_B T$ is the inverse temperature parameter. Then the full set of self-consistent generalized Gorkov equations are given by

$$\mathbf{G}(\mathbf{r}_1,\mathbf{r}_2,i\omega_n)=\mathbf{g}(\mathbf{r}_1,\mathbf{r}_2,i\omega_n)+\int d^3r_3\int d^3r_4\mathbf{g}(\mathbf{r}_1,\mathbf{r}_3,i\omega_n)$$
$$\Delta(\mathbf{r}_3,\mathbf{r}_4,i\omega_n)\bar{\mathbf{F}}(\mathbf{r}_4,\mathbf{r}_2,i\omega_n) \tag{4}$$

$$\bar{\mathbf{F}}(\mathbf{r}_1,\mathbf{r}_2,i\omega_n)=\int d^3r_3\int d^3r_4\bar{\mathbf{g}}(\mathbf{r}_1,\mathbf{r}_3,i\omega_n)\Delta(\mathbf{r}_3,\mathbf{r}_4,i\omega_n)\mathbf{G}(\mathbf{r}_4,\mathbf{r}_2,i\omega_n) \tag{5}$$

with similar equations for $\bar{\mathbf{G}}$ and $\bar{\mathbf{F}}$, where in (4) and (5), $\mathbf{g}\leftrightarrow\bar{\mathbf{g}}$, $\Delta\leftrightarrow\bar{\Delta}$, $\mathbf{G}\leftrightarrow\bar{\mathbf{G}}$, and $\mathbf{F}\leftrightarrow\bar{\mathbf{F}}$. These set of equations are generalizations of (25)–(27) of Rajagopal and Jha (1991a), and are sometimes written as a 4×4 matrix equation. These represent the possibilities of both spin-singlet and spin-triplet pairings.

In this paper, we restrict ourselves only to the possibility of spin-singlet pairing for which there is only one gap function $\Delta_s(\mathbf{r}_1,\mathbf{r}_2,i\omega_n)$. Close to the superconducting transition, this obeys a linearlized gap equation

$$\Delta_s(\mathbf{r}_1,\mathbf{r}_2,i\omega_n)=\frac{1}{\beta}\sum_m\int d^3r_3\int d^3r_4\, V(\mathbf{r}_1,\mathbf{r}_2,i\omega_n-i\omega_m)\Delta_s(\mathbf{r}_3,\mathbf{r}_1,i\omega_m)$$
$$\times[g_{\uparrow\uparrow}(\mathbf{r}_3,\mathbf{r}_1;-i\omega_m)g_{\downarrow\downarrow}(\mathbf{r}_4,\mathbf{r}_2,i\omega_m)$$
$$-g_{\downarrow\uparrow}(\mathbf{r}_3,\mathbf{r}_1,i\omega_m)g_{\uparrow\downarrow}(\mathbf{r}_4,\mathbf{r}_2,i\omega_m)]. \tag{6}$$

In the first approximation, the normal state $\mathbf{g}$ can be replaced by $\mathbf{G}_0$ of (2), which can be expressed in terms of the complete orthonormal set of states $\{\phi_\nu\}$ associated with the operator K_0, with a set of quantum numbers collectively denoted by ν:

$$K_0(\mathbf{r},\mathbf{A})\phi_\nu(\mathbf{r})=\varepsilon_\nu\phi_\nu(\mathbf{r}). \tag{7}$$

A further simplification of (6) involves using an effective short-range attractive potential in the form

$$V(\mathbf{r}_1,\mathbf{r}_2,\omega)\simeq-\bar{V}\delta(\mathbf{r}_1-\mathbf{r}_2),\text{ for }|\omega|<\omega_d\equiv k_B\Theta^*/\hbar$$
$$=0,\text{ elsewhere.} \tag{8}$$

However, before using this form of V, it should be noted that in the case of layered systems, (8) has to be replaced by

$$V(\mathbf{r}_1,\mathbf{r}_2,\omega)\simeq\delta^2(\boldsymbol{\rho}_1-\boldsymbol{\rho}_2)\,\bar{V}(z_1,z_2,\omega)\text{ for }|\omega|<\omega_d$$
$$=0,\text{ elsewhere} \tag{9}$$

as was discussed by Rajagopal and Jha (1991b). We will return to discuss this modification later at the end of § 3. For the present, with the condition (8), the gap function $\Delta_s(\mathbf{r}_1,\mathbf{r}_2,i\omega_n)$ has the form $\Delta(\mathbf{r}_1)\delta(\mathbf{r}_1-\mathbf{r}_2)$ with the same frequency cut-off as in (8). $\Delta(\mathbf{r}_1)$ then obeys the equation

$$\Delta(\mathbf{r}_1)=\int K(\mathbf{r}_1,\mathbf{r}_2)\Delta(\mathbf{r}_2)d^3r_2 \tag{10}$$

where

$$K(\mathbf{r}_1,\mathbf{r}_2)=\bar{V}\sum_{\nu_1}\sum_{\nu_2}\frac{\phi^*_{\nu_1}(\mathbf{r}_1)\phi_{\nu_1}(\mathbf{r}_2)\phi_{\nu_2}(\mathbf{r}_2)\phi^*_{\nu_2}(\mathbf{r}_1)}{2(\varepsilon_{\nu_1}+\varepsilon_{\nu_2})}$$
$$\times[\tanh[\beta(\varepsilon_{\nu_1}+\Omega_H)/2]+\tanh[\beta(\varepsilon_{\nu_2}-\Omega_H)/2]]. \qquad (11)$$

Here, $\Omega_H^2=\Sigma_i\Omega_{Hi}^2$ with $\Omega_{Hi}=(\mu_B/2\hbar)\Sigma_i H_j g_{ji}$, $(i,j=x,y,z)$. A nontrivial solution of (10) and (11) leads to the condition determining $T_c(\mathbf{H})$ for all $\mathbf{H}$ and $\mathbf{H}_{c2}(T)$ for all T.

To proceed further, we need to solve (7). For a magnetic field in an arbitrary direction, it is difficult to tackle this equation in the presence of a periodic potential, even for carriers in a single band but having an open Fermi-surface in the absence of the magnetic field. Of cource, for a closed Fermi surface, (7) can be solved analytically in the anisotropic effective-mass approximation. In any case, for most purposes, it suffices to treat the diamagnetic part of K_0 involving the vector potential $\mathbf{A}$, in a semiclassical approximation:

$$\mathbf{g}(\mathbf{r}_1,\mathbf{r}_2,i\omega_n)\simeq\exp\left(\frac{ie}{c\hbar}\int_{\mathbf{r}_2}^{\mathbf{r}_1}\mathbf{A}(\mathbf{s})\cdot\mathbf{d}s\right)\mathbf{g}_0(\mathbf{r}_1,\mathbf{r}_2,i\omega_n) \qquad (12)$$

where $\mathbf{g}_0$ is the Green function associated with unperturbed Hamiltonian (1), with $\mathbf{A}$ in K_0 set equal to zero. Then ϕ_ν and ε_ν in (7) are just Bloch functions $\phi_{b\mathbf{k}}(\mathbf{r})$ and energy $\hbar\varepsilon_{b\mathbf{k}}$, respectively, with band index b and wave vector $\mathbf{k}$. With $\mathbf{A}=(1/2)\mathbf{H}\times\mathbf{r}$, for a single band the linearized gap equation then takes the simpler form

$$\Delta(\mathbf{r}_1)=\int d^3r_2\,L(\mathbf{r}_1,\mathbf{r}_2)[\exp(i(\mathbf{r}_1\times\mathbf{r}_2)\cdot\hat{n}/r_c^2)]\Delta(\mathbf{r}_2) \qquad (13)$$

where $\hat{n}$ is the unit vector along the magnetic field, $\mathbf{H}$, $r_c^2=c\hbar/e|H|$, and in which, employing usual simplifying assumptions near the Fermi surface, L can be reduced to the from

$$L(\mathbf{r}_1,\mathbf{r}_2)=\bar{V}N(0)\int_{-\omega_d+\Omega_H}^{\omega_d+\Omega_H}\frac{d\xi}{2}\tanh(\beta\xi/2)\int\frac{d^3\mathbf{Q}}{(2\pi)^3}\exp[i\mathbf{q}\cdot(\mathbf{r}_1-\mathbf{r}_2)]P_H(\mathbf{Q},\xi), \qquad (14a)$$

$$P_H(\mathbf{Q},\xi)=\int\frac{dS_{kF}}{4\pi}\frac{1}{2\xi-2\Omega_H-\mathbf{V}_{kF}\cdot\mathbf{Q}}. \qquad (14b)$$

While obtaining the above equation, the Bloch functions are taken approximately to be plane waves. Here, $N(0)$ is the density of states (per spin) at the Fermi surface (FS), $\omega_d=k_B\Theta^*/\hbar$ is the energy cut-off, dS_{kF} represents the element of solid angle at FS, and $V_\mathbf{k}\equiv\nabla_\mathbf{k}\varepsilon_\mathbf{k}$ is the carrier velocity.

For a given form of $\varepsilon_\mathbf{k}$ and the shape of FS, if the function $P_H(\mathbf{Q},\xi)$ depends on $\mathbf{Q}$ in the form $\tilde{P}_H(a_x^2Q_x^2+a_y^2Q_y^2+a_z^2Q_z^2,\xi)$, then the resulting gap equation (13) can be solved in a straightforward manner by making a simple scale transformation on $\mathbf{Q}$ and the reciprocal transformation on $\mathbf{r}_1$ and $\mathbf{r}_2$. This leads to a self-consistent condition for determining $T_c(\mathbf{H})$ and $\mathbf{H}_{c2}(T)$. For explicit forms of the band energy $\hbar\varepsilon_\mathbf{k}$ and the orientation of the magnetic field $\mathbf{H}$, the corresponding solutions will be obtained and analysed in the next section. However, before closing this section, we must mention here the modifications required in the above formulation if we would like to investigate the effects of weak nonmagnetic impurity scattering phenomenologically. In such a case, it is more convenient to perform the discrete summation over $\omega_n = (2n+1)\pi/\beta$ at the end of the calculation, i.e. after integration over ξ, etc. For weak scattering it can be shown that this effect can be included approximately by changing $i\omega_n$ to $i\omega_n + i\Gamma$ sign ω_n in the normal state Green's function g_0 of (12). This essentially means that in (14), one replaces the integral over ξ as follows:

$$\int \frac{d\xi}{2} \tanh(\beta\xi/2) P_H(\mathbf{Q}, \xi) \to \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \int \frac{d\xi}{2} \frac{2\xi}{\xi^2 + (|\omega_n| + \Gamma)^2} P_H(\mathbf{Q}, \xi)$$

$$= -\frac{2\pi \operatorname{Im}}{\beta} \sum_{n=0}^{n_{\max}} P_H(\mathbf{Q}, i\omega_n + i\Gamma) \tag{15}$$

where the cut-off $n_{\max}$ corresponds to $\omega_n^{\max} \approx \omega_d$, for $\Omega_H \ll \omega_d$. The phenomenological Γ is related to the mean free path, $\langle \ell \rangle$, by $\Gamma = \langle V_F \rangle / 2\langle \ell \rangle$.

3. Calculations of T_c(H) and $H_{c2}(T)$

We now consider two specific forms of ε_k near the FS, which represent situations of physical interest. For the case of a closed anisotropic FS, we take

(a) $$\hbar\varepsilon_k = \frac{\hbar^2 k_x^2}{2m_x} + \frac{\hbar^2 k_y^2}{2m_y} + \frac{\hbar^2 k_z^2}{2m_z} - E_F \tag{16}$$

where as for a FS open in the k_z-direction, we use the form

(b) $$\hbar\varepsilon_k = \frac{\hbar^2 k_x^2}{2m_x} + \frac{\hbar^2 k_y^2}{2m_y} + 2t_3(1 - \cos k_z d) - E_F;$$

$$4t_3 < E_F, \quad -\pi/d \leqslant k_z \leqslant \pi/d. \tag{17}$$

The second form of the band structure is appropriate for the case of quasi-two dimensional high-T_c superconductors. The ensuing analysis of the solutions etc. in the above two cases will be given first, before considering, in subsection (c), the case of layered superconductors having more than one layer per unit cell.

3.1 *Closed Fermi surface*

In this case, $\mathbf{V}_{kF}$ of (14b) is given by

$$V_{Fx} = V_F^*(m^*/m_x)^{1/2} \sin\theta \cos\phi, \quad V_{Fy} = V_F^*(m^*/m_y)^{1/2} \sin\theta \sin\phi,$$
$$V_{Fz} = V_F^*(m^*/m_z)^{1/2} \cos\theta \tag{18}$$

where $V_F^* = (2E_F/m^*)^{1/2}$ and $m^{*^3} = m_x m_y m_z$. Then, $P_H(\mathbf{Q}, \xi)$ is found to be

$$P_H(\mathbf{Q}, \xi) = \frac{\operatorname{Re}}{2V_F^* q} \ln\left(\frac{2(\xi - \Omega_H) + qV_F^*}{2(\xi - \Omega_H) - qV_F^*}\right) \tag{19}$$

where

$$\mathbf{q} = \left(\left(\frac{m^*}{m_x}\right)^{1/2} Q_x, \left(\frac{m^*}{m_y}\right)^{1/2} Q_y, \left(\frac{m^*}{m_z}\right)^{1/2} Q_z\right). \tag{20}$$

Introducing $\mathbf{R}_1$, $\mathbf{R}_2$ by scaling the vectors $\mathbf{r}_1, \mathbf{r}_2$ as

$$\mathbf{R} = \left(\left(\frac{m_x}{m^*}\right)^{1/2} x,\ \left(\frac{m_y}{m^*}\right)^{1/2} y,\ \left(\frac{m_z}{m^*}\right)^{1/2} z\right), \tag{21}$$

and

$$\mathbf{H}^* = \left(\left(\frac{m_x}{m^*}\right)^{1/2} H_x,\ \left(\frac{m_y}{m^*}\right)^{1/2} H_y,\ \left(\frac{m_z}{m^*}\right)^{1/2} H_z\right), \tag{22}$$

$$r_c^{*^2} = c\hbar/eH^*, \tag{23}$$

we find that the gap equation (13) reduces to

$$\Delta(\mathbf{R}_1) = N(0)\,\bar{V}\int d^3R_2 \int_{-\omega_d+\Omega_H}^{\omega_d+\Omega_H} \frac{d\xi}{2}\tanh(\beta\xi/2)\int\frac{d^3q}{(2\pi)^3}$$
$$\times \exp[i\mathbf{q}\cdot(\mathbf{R}_1-\mathbf{R}_2)]P_H(\mathbf{q},\xi)(\exp[i(\mathbf{R}_1\times\mathbf{R}_2)\cdot\hat{H}^*/r_c^{*^2}])\Delta(\mathbf{R}_2) \tag{24}$$

where

$$N(0) = m^*k_F/2\pi^2\hbar^2 = 3n/4E_F \tag{25}$$

n being the number density $k_F^3/3\pi^2$, and $\hat{H}^*$ is a unit vector along $\mathbf{H}^*$. In this new frame, this gap equation is the same as for the spherical Fermi surface so that the general solution for arbitrary orientation of the magnetic field can then be written (Rajagopal and Vasudevan 1966a, b; Prohammer and Carbotte 1990):

$$\Delta(\mathbf{r}) = \Delta_0\exp[-(\mathbf{r}\times\hat{H}^*)^2/2r_c^{*^2}] \tag{26}$$

with the condition

$$\frac{1}{g} \equiv \frac{1}{N(0)\,\bar{V}} = \frac{r_c^{*^2}}{V_F^*}\int_{-\omega_d+\Omega_H}^{\omega_d+\Omega_H}\frac{d\xi}{2}\tanh\beta\xi/2$$
$$\times\int_0^\infty dq[\exp(-q^2r_c^{*^2}/2)]\,\mathrm{Re}\ln\left(\frac{\xi-\Omega_H+V_F^*q/2}{\xi-\Omega_H-V_F^*q/2}\right). \tag{27}$$

For $\mathbf{H}\to\mathbf{H}_{c2}$, $T\to 0$, with $\omega_d \gg k_B T/\hbar$, Ω_H, we can use the standard low temperature expansion of the ξ-integral involving $\tanh\beta\xi/2$. However, when impurity scattering is included, we follow the procedure given by (15). In that more general case, we use the following low temperature expansion in performing the summation over n,

$$\frac{2\pi}{\beta}\sum_{n=0}^{n_{max}} F(\omega_\nu) \simeq \int_0^{\omega_d} F(\omega)d\omega + \frac{\pi^2}{6}(k_B T)^2\left(\frac{\partial F}{\partial\omega}\right)_{\omega=0} \tag{28}$$

We thus obtain

$$\frac{1}{g} \equiv \ln\frac{2\hbar\omega_d}{\Delta_0} = 1 + \ln(\sqrt{2}\omega_d r_c^*/V_F^*) + \frac{\gamma}{2}$$
$$+\frac{\pi^2}{3}\frac{(k_B T)^2 r_c^{*^2}}{\hbar^2 V_F^{*^2}}\mathrm{Re}\left[\gamma + \ln\left[\frac{2r_c^{*^2}}{\hbar V_F^{*^2}}(\Omega_H - i\Gamma)^2\right]\right] \tag{29}$$

where $\gamma = 0{\cdot}5772$ is Euler's constant. Equivalently, this condition can be rewritten as

$$0 = \frac{1}{2}\ln\left(\frac{H^*}{H_{c2}^{(0)}}\right) + \frac{1}{2}a\frac{T^2}{T_{c0}^2} \tag{30}$$

where

$$H_{c2}^{(0)} = \frac{e^{2+\gamma}\Delta_0^2 c}{2V_F^{*2} e\hbar}, \quad \Delta_0 = \pi e^{-\gamma} k_B T_{c0}, \quad T_{c0} = \frac{2e^\gamma}{\pi}\theta^* e^{-1/g}$$

$$\mu_B H_p = \Delta_0/\sqrt{2}, \quad a = 0{\cdot}6456\left\{1 - \frac{1}{2}\ln\left[2\left(\frac{|\mathbf{H}\cdot\mathbf{g}|^2}{4H_p^2} + \frac{\Gamma^2}{\mu_B^2 H_p^2}\right)\right]\right\}. \tag{31}$$

Equation (30) represents the superconducting transition line in the (H, T) plane. Thus at low temperatures, we have

$$|\mathbf{H}_{c2}^*(T)| = H_{c2}^{(0)}\exp(-T^2/T_{c0}^2) \simeq H_{c2}^{(0)}[1 - aT^2/T_{c0}^2] \tag{32}$$

and

$$T_c(\mathbf{H}) = a^{-1/2}T_{c0}(-\ln(|\mathbf{H}^*|/H_{c2}^{(0)}))^{1/2} \simeq a^{-1/2}T_{c0}\left[1 - \frac{|\mathbf{H}^*|}{H_{c2}^{(0)}}\right]^{1/2} \tag{33}$$

where $H_{c2}^{(0)}$ and $\mathbf{H}^*$ are given explicitly by (31) and (22) respectively. These lead to the expected relations

$$H_{c2x}(0) = \left(\frac{m^*}{m_x}\right)^{1/2} H_{c2}^{(0)}, \quad H_{c2y}(0) = \left(\frac{m^*}{m_y}\right)^{1/2} H_{c2}^{(0)},$$

$$H_{c2z}(0) = \left(\frac{m^*}{m_z}\right)^{1/2} H_{c2}^{(0)} \tag{34}$$

and

$$T_c(\mathbf{H}) = a^{-1/2}T_{c0}\left[1 - \left(\frac{H_x^2}{H_{c2x}^2(0)} + \frac{H_y^2}{H_{c2y}^2(0)} + \frac{H_z^2}{H_{c2z}^2(0)}\right)^{1/2}\right]^{1/2}. \tag{35}$$

We can also calculate in the Ginzburg-Landau regime the behavior of the system as $H \to 0$, near $T \sim T_{c0}$ by changing the variable q to $\bar{Q} = qr_c^*$ in (27) and expanding the log term in powers of $\bar{Q}/r_c^*$. In this limit, with $\Gamma \to 0$, we find in agreement with Rieck and Scharnberg (1990) and Prohammer and Carbotte (1990),

$$\frac{1}{g} = \ln\left(\frac{T_{c0}}{T}\right) + \frac{1}{g} - \frac{|\mathbf{H}^*|}{h_c^{(0)}}\left(\frac{T_{c0}}{T}\right)^2 \tag{36}$$

where

$$h_c^{(0)} = \frac{24\pi^2(k_B T_{c0})^2}{7\zeta(3)V_F^{*2}}\left(\frac{c}{e\hbar}\right) \tag{37}$$

with $\zeta(3) \simeq 1{\cdot}202$. Hence,

$$|\mathbf{H}_{c2}^*(T)| = h_c^{(0)}\frac{T^2}{T_{c0}^2}\ln\left(\frac{T_{c0}}{T}\right) \simeq h_c^{(0)}\left(1 - \frac{T}{T_{c0}}\right), \quad T \sim T_{c0} \tag{38}$$

$$T_c(\mathbf{H}) \simeq T_{c0}\left[1 - \frac{1}{h_{c0}^{(0)}}\left\{\frac{m_x}{m^*}H_x^2 + \frac{m_y}{m^*}H_y^2 + \frac{m_z}{m^*}H_z^2\right\}^{1/2}\right], \quad H^* \ll h_c^{(0)}. \tag{39}$$

For the magnetic field in any arbitrary direction, one obtains the familiar clean limit result in this case for the ratio

$$h^* \equiv \frac{|\mathbf{H}_{c2}(T=0)|}{-T_{c0}[\mathrm{d}|\mathbf{H}_{c2}(T)|/\mathrm{d}T]_{T_{c0}}} = \frac{7\zeta(3)}{48e^{\gamma-2}} = 0{\cdot}7273. \tag{40}$$

3.2 *Open Fermi surface*

The analysis in this case, with $\hbar\varepsilon_{\mathbf{k}}$ given by (19), is quite different because at the Fermi surface there is now a cut-off in the integration over the polar angle θ with respect to the k_z-axis, and k_z-integration is over the whole range $-\pi/d$ to π/d. In fact, for $4t_3/E_F \ll 1$, $\sin\theta$ at FS $\simeq 1$. The relevant transformation which we employ in this case can be written as

$$k_x = \left(\frac{2m_x}{\hbar^2}\right)^{1/2}(\hbar\xi + E_F)^{1/2}\sin\theta\cos\phi, \quad k_y = \left(\frac{2m_y}{\hbar^2}\right)^{1/2}(\hbar\xi + E_F)^{1/2}\sin\theta\sin\phi,$$
$$k_z = (1/\mathrm{d})\cos^{-1}\left[1 - \left(\frac{\hbar\xi + E_F}{2t_3}\right)\cos^2\theta\right] \tag{41}$$

where $\xi = \varepsilon_k - E_F/\hbar$. For a widely open FS, with $4t_3 \ll E_F$, the density of states $N(0)$ at FS becomes

$$N(0) = n/2E_F = (m_x m_y)^{1/2}/(2\pi\hbar^2\mathrm{d}). \tag{42}$$

Also, in this case, $\mathbf{V}_{kF}$ of (14b) is given by

$$V_{Fx} = V_{FL}\left(\frac{m_L}{m_x}\right)^{1/2}\sin\theta_F\cos\phi \simeq V_{FL}\left(\frac{m_L}{m_x}\right)^{1/2}\cos\phi,$$
$$V_{Fy} = V_{FL}\left(\frac{m_L}{m_y}\right)^{1/2}\sin\theta_F\sin\phi \simeq V_{FL}\left(\frac{m_L}{m_y}\right)^{1/2}\sin\phi, \tag{43}$$
$$V_{Fz} = \frac{2t_3 d}{\hbar}\sin k_z d = V_{FL}\left(\frac{m_L}{m_3}\right)^{1/2}\sin k_z d,$$

with

$$m_3(n) = E_F\hbar^2/2t_3^2d^2 \equiv m_z(0)E_F/t_3, \quad m_L^3 = m_x m_y m_3, \quad V_{FL} = (2E_F/m_L)^{1/2} \tag{44}$$

where $m_z(0)$ is the effective mass in the k_z-direction at $k_z \simeq 0$. Then $P_H(\mathbf{Q},\xi)$ of (14) is of the form

$$P_H(\mathbf{Q},\xi) \simeq \int_0^{2\pi}\frac{\mathrm{d}\phi}{2\pi}\int_{-\pi/d}^{\pi/d}\frac{\mathrm{d}k_z}{(2\pi/\mathrm{d})}\mathrm{Re}\left[\frac{1}{2(\xi-\Omega_H) - V_{FL}(q_x\cos\phi + q_y\sin\phi + q_z\sin k_z\mathrm{d})}\right] \tag{45}$$

where

$$q_x = Q_x\left(\frac{m_L}{m_x}\right)^{1/2}, \quad q_y = Q_y\left(\frac{m_L}{m_y}\right)^{1/2}, \quad q_z = Q_z\left(\frac{m_L}{m_3}\right)^{1/2}. \tag{46}$$

The above integral can be evaluated easily when $Q_z = 0$ or when $Q_x = Q_y = 0$ (i.e. $Q_t = 0$). In general, we will take

$$P_H(\mathbf{Q}, \xi) = \mathrm{Re}\left[\frac{1}{[4(\xi - \Omega_H)^2 - V_{FL}^2|\mathbf{q}|^2]^{1/2}}\right] \tag{47}$$

which reduces to the exact expressions in the two opposite limits mentioned. Note that the form (47) is different from the logarithmic form found in the case (a) for Closed FS. Introducing $\mathbf{R}_1$, $\mathbf{R}_2$ by scaling $\mathbf{r}_1$, $\mathbf{r}_2$, as

$$\mathbf{R} = \left[\left(\frac{m_x}{m_L}\right)^{1/2} x,\ \left(\frac{m_y}{m_L}\right)^{1/2} y,\ \left(\frac{m_3}{m_L}\right)^{1/2} z\right], \tag{48}$$

and

$$\mathbf{H}^{(L)} = \left[\left(\frac{m_x}{m_L}\right)^{1/2} H_x,\ \left(\frac{m_y}{m_L}\right)^{1/2} H_y,\ \left(\frac{m_3}{m_L}\right)^{1/2} H_z\right], \tag{49}$$

$$r_L^2 = c\hbar/eH^{(L)},\quad H^{(L)} = |\mathbf{H}^{(L)}|, \tag{50}$$

one finds that the solution of the resulting gap equation has the same structure as (26), with the unit vector $\hat{H}^*$ replaced by the unit vector $\hat{H}^{(L)}$ and r_c^* replaced by r_L. However, the self-consistency condition condition has now a new form given by

$$\frac{1}{g} \equiv \frac{1}{N(0)\,\bar{V}} = r_L^2 \int_{-\omega_d+\Omega_H}^{\omega_d+\Omega_H} \frac{\mathrm{d}\xi}{2} \tanh \beta\xi/2 \int_0^\infty q\mathrm{d}q \exp(-q^2 r_L^2/2) \times \mathrm{Re}\left[\frac{1}{[(\xi - \Omega_H)^2 - q^2 V_{FL}^2/4]^{1/2}}\right]. \tag{51}$$

In the low temperature limit ($T \to 0$), with $H \sim H_{c2}$, we obtain

$$\frac{1}{g} = \ln 2 + \ln(\sqrt{2}\omega_d r_L/V_{FL}) + \gamma/2 - \frac{2\pi^2 (k_B T)^2 r_L^2}{3\hbar^2 V_{FL}^2}\left[1 - \frac{\sqrt{2\pi} r_L \Gamma}{V_{FL}} - \frac{4r_L^2}{V_{FL}^2}(\Omega_H^2 - \Gamma^2)\right]. \tag{52}$$

As before, this may be rewritten as

$$0 = \frac{1}{2}\ln\left(\frac{H^{(L)}}{H_{c2L}^{(0)}}\right) + \frac{1}{2} a_L \frac{T^2}{T_{c0}^2} \tag{53}$$

where

$$H_{c2L}^{(0)} = \frac{2e^\gamma \Delta_0^2}{V_{FL}^2}\left(\frac{c}{e\hbar}\right) \tag{54}$$

$$a_L \simeq 1{\cdot}1874\left\{1 - \left(\frac{\pi e^{-\gamma}}{2}\right)^{1/2}\left(\frac{\Gamma}{\mu_B H_p}\right) + e^{-\gamma}\left(\frac{\Gamma}{\mu_B H_p}\right)^2 - \frac{e^{-\gamma}}{4}\frac{|\mathbf{H}\cdot\mathbf{g}|^2}{H_p^2}\right\} \tag{55}$$

and where T_{c0}, Δ_0, H_p are defined in the same usual way as in (31). Thus at low temperatures, with $H^{(L)}$ near $H^{(0)}_{c2L}$, we have

$$\left[\frac{m_x}{m_L}H^2_{c2x}(T)+\frac{m_y}{m_L}H^2_{c2y}(T)+\frac{m_z(0)E_F}{m_L t_3}H^2_{c2x}(T)\right]^{1/2}\simeq H^{(0)}_{c2L}[1-a_L\,T^2/T^2_{c0}] \tag{56}$$

$$T_c(\mathbf{H})\simeq a_L^{-1/2}\,T_{c0}\left[1-\left(\frac{H_x^2}{H^2_{c2x}(0)}+\frac{H_y^2}{H^2_{c2y}(0)}+\frac{H_z^2}{H^2_{c2z}(0)}\right)^{1/2}\right]^{1/2} \tag{57}$$

where

$$H_{c2x}(0)=\left(\frac{m_L}{m_x}\right)^{1/2}H^{(0)}_{c2L},\quad H_{c2y}(0)=\left(\frac{m_L}{m_y}\right)^{1/2}H^{(0)}_{c2L},$$

$$H_{c2z}(0)=\left(\frac{m_L}{m_z(0)}\frac{t_3}{E_F}\right)^{1/2}H^{(0)}_{c2L}. \tag{58}$$

In the Ginzburg-Landau regime ($T\sim T_{c0}$, $H\to 0$), we now find

$$\frac{1}{g}=\ln\left(\frac{T_{c0}}{T}\right)+\frac{1}{g}-\frac{|\mathbf{H}^{(L)}|}{h^{(0)}_{cL}}\left(\frac{T_{c0}}{T}\right)^2 \tag{59}$$

where

$$h^{(0)}_{cL}=\frac{16\pi^2(k_B\,T_{c0})^2}{7\zeta(3)\,V^2_{FL}}\left(\frac{c}{e\hbar}\right). \tag{60}$$

This leads to

$$\left[\frac{m_x}{m_L}H^2_{c2x}(T)+\frac{m_y}{m_L}H^2_{c2y}(T)+\frac{m_z(0)E_F}{m_L t_3}H^2_{c2z}(T)\right]^{1/2}\simeq h^{(0)}_{cL}\left(1-\frac{T}{T_{c0}}\right),\quad T\sim T_{c0} \tag{61}$$

and

$$T_c(\mathbf{H})\simeq T_{c0}\left[1-\frac{1}{h^{(0)}_{cL}}\left\{\frac{m_x}{m_L}H_x^2+\frac{m_y}{m_L}H_y^2+\frac{m_z(0)E_F}{m_L t_3}H_z^2\right\}^{1/2}\right]. \tag{62}$$

Note that for the magnetic field in any arbitrary direction,

$$h^*_L(0)\equiv\frac{|\mathbf{H}_{c2}(T=0)|}{-T_{c0}[\mathrm{d}|\mathbf{H}_{c2}(T)|/\mathrm{d}T]_{T=T_{c0}}}=\frac{H^{(0)}_{c2L}}{h^{(0)}_{cL}}=\frac{7\zeta(3)}{8\mathrm{e}^{\gamma}}=0{\cdot}5906 \tag{63}$$

which differs considerably from the clean limit value of 0·7273, obtained for the closed anisotropic Fermi surface. Because of our assumption $4t_3\ll E_F$, this coincides with the 2-*D* result (Rieck and Scharnberg 1990). Corrections to these results as a function of $4t_3/E_F$ can be calculated explicitly by relaxing the approximation $\sin\theta_F\simeq 1$ in (43), and obtaining the corresponding $P_H(\mathbf{Q},\xi)$.

3.3 *Layered superconductors*

Based on the pairing theory for layered systems (Rajagopal and Jha 1991a), a preliminary examination of the nature of the solution of the linearized gap equation in such materials, in the presence of a constant magnetic field perpendicular to the layers, was made earlier by us (Rajagopal and Jha 1991b). With an approximate form of interaction $V(\mathbf{r}_1, \mathbf{r}_2, \omega)$ given by (9) and the assumption

$$\Delta_{J_1J_2}(\boldsymbol{\rho}_1, \boldsymbol{\rho}_2) = \Delta_{J_1J_2} \exp(-\rho_1^2/2r_c^2)\delta^{(2)}(\boldsymbol{\rho}_1 - \boldsymbol{\rho}_2) \tag{64}$$

for the gap function in the layer-representation (Rajagopal and Jha 1991a), where $\boldsymbol{\rho} = (\mathbf{x}, \mathbf{y})$ is the position vector in the plane of the layers and J is the label for the conducting layer in the unit cell of the crystal, the linearized gap equation reduces to

$$\Delta_{J_1J_2} = -\sum_{J_3J_4} V_{J_3J_4, J_1J_2} M_{J_3J_4} \Delta_{J_3J_4}. \tag{65}$$

Here, $\Delta_{J_1J_2}$ describes spin-singlet pairing of carriers in layers J_1 and J_2, V is the matrix-element of the interaction (9) in the layer-representation,

$$M_{J_3J_4}(T, H_z) = \frac{1}{2\pi r_c^2} \sum_{n_3, n_4} \left[\frac{(n_3 + n_4)!}{n_3! n_4!} \frac{1}{2^{n_3 + n_4 + 1}} \right] \int_{-\pi/d}^{\pi/d} \mathrm{d}k_z \times \left[\frac{\tanh[\beta(\varepsilon_{n_3J_3k_z} + \Omega_H)/2] + \tanh[\beta(\varepsilon_{n_4J_4k_z} - \Omega_H)/2]}{\varepsilon_{n_3J_3k_z} + \varepsilon_{n_4J_4k_z}} \right] \tag{66}$$

and $r_c^2 = c\hbar/eH_z$, $\hbar\varepsilon_{nJk_z} = \hbar(n + \frac{1}{2})eH_z/cm_J + \hbar\varepsilon_J(k_z) - E_{FJ}$ is the one electron energy associated with layer J, having planar effective mass m_J, $\hbar\varepsilon_J(k_z)$ describes the energy dispersion in the k_z-direction, and $\hbar\Omega_H$ is the Zeeman energy defined earlier. For the sake of simplicity, we consider here only intralayer pairing for which $\Delta_{J_1J_2} \to \Delta_{J_1}\delta_{J_1,J_2}$. If we introduce the dimensionless coupling constants $\lambda_{JJ'} = N_{J'}^{1/2} V_{J'J',JJ} N_J^{1/2}$ where $N_J = m_J/2\pi\hbar^2 d$ is the density of states for the layer J, the gap equation (66) simplifies to a simultaneous linear set of equations for Δ_J which has a nontrivial solution only if

$$\det|I_J(T, H_z)\delta_{JJ'} + \lambda_{JJ'}| = 0 \tag{67}$$

where

$$\frac{1}{I_J} \equiv \frac{1}{N_J} M_{JJ}(T, H_z). \tag{68}$$

We may now employ the semiclassical approximation for M_{JJ} defined in (63) by taking (Gruenberg and Gunther 1968)

$$\left(\frac{1}{2}\right)^{n_3+n_4} \frac{(n_3 + n_4)!}{n_3! n_4!} \simeq \frac{1}{(n_3 n_4 \pi^2)^{1/4}} \exp - [(n_3 - n_4)^2 (n_3 + n_4)/8 n_3 n_4] \tag{69}$$

$$\frac{n_3 eH_z}{cm_J} \to \frac{\hbar k_t^2}{2m_J}, \quad \frac{n_4 eH_z}{cm_J} \to \hbar k_t'^2/2m_J \tag{70}$$

$$(n_3 - n_4)^2 (n_3 + n_4)/8 n_3 n_4 \simeq (k_t - k_t')^2 r_c^2/2 \tag{71}$$

$$\left(\frac{k_t k_t' r_c^2}{2\pi}\right)^{1/2} \int_0^{2\pi} \mathrm{d}\phi \exp[-(|\mathbf{k}_t - \mathbf{k}_t'|^2 r_c^2/2)] \simeq \exp[-(k_t - k_t')^2 r_c^2/2] \tag{72}$$

where $\mathbf{k}_t, \mathbf{k}_t'$ are 2-dimensional vectors in the (k_x, k_y) plane. Using the standard Poisson-Sum formula over n_3, n_4 sums and ignoring the oscillatory contributions, we then obtain

$$1/I_J = N_J^{-1} M_{JJ}(T,H_z) \simeq \frac{r_c^2}{N_J} \mathrm{Re} \int \frac{\mathrm{d}^2\mathbf{k}_t}{(2\pi)^2} \int_{-\pi/d}^{\pi/d} \frac{dk_z}{2\pi} \int \frac{\mathrm{d}^2\mathbf{Q}_t}{(2\pi)} \exp[-(|\mathbf{Q}_t|^2 r_c^2/2)]$$
$$\times \frac{\left[\tanh\frac{\beta}{2}(\varepsilon_{J\mathbf{k}_t,k_z} + \Omega_H) + \tanh\frac{\beta}{2}(\varepsilon_{J\mathbf{k}_t-\mathbf{Q}_t,k_z} - \Omega_H)\right]}{[\varepsilon_{J\mathbf{k}_t,k_z} + \varepsilon_{J\mathbf{k}_t-\mathbf{Q}_t,k_z}]}. \tag{73}$$

Here,

$$\hbar\varepsilon_{J\mathbf{k}_t,k_z} = \hbar^2 k_t^2/2m_J + \hbar\varepsilon_J(k_z) - E_{FJ}. \tag{74}$$

If we take $\hbar\varepsilon_J = 2t_{3J}(1-\cos k_z \mathrm{d})$ as in (17), then the analysis given in § 2(b) is applicable to (70) so that

$$\frac{1}{I_J} \simeq \frac{r_c^2}{2} \int_{-\omega_d+|\Omega|}^{\omega_d+|\Omega|} \mathrm{d}\xi \tanh\frac{\beta}{2}\xi \int_0^\infty q\,\mathrm{d}q \exp[-(q^2 r_c^2/2)]$$
$$\times \mathrm{Re}\{(\xi - |\Omega_H|)^2 - q^2 V_{FJ}^2\}^{-1/2} \tag{75}$$

where $V_{FJ} = (2E_{FJ}/m_J)^{1/2}$. For the case when all the conducting layers in the unit cell are equivalent so that all the m_J's and I_J's are the same, with $\lambda_{11} = \lambda_{22} = \cdots = -\lambda$ and nearest neighbour interlayer coupling $\lambda_{12} = \lambda_{23} = \cdots = \lambda'$, the solution of (64) for the highest T_c reduces to the condition

$$\frac{1}{g_N} = I_J^{-1}(T,H_z), \quad g_N = \lambda + 2|\lambda'|\cos[\pi/(N+1)] \tag{76}$$

where N is the number of conducting layers per unit cell. For $H_z = 0$, this gives $T_{c0} = (2e^\gamma/\pi)\Theta^* e^{-1/g_N}$. The rest of the analysis is exactly similar to those in § 2(b) for the case of open FS. Thus except for the scaling of the coupling constant and hence T_{c0}, the behavior of $T_c(H_z)$ and $H_{c2z}(T)$ are similar to those given in §(2b).

When the magnetic field is in the plane of the layers, the problem is much more complex unless the electron orbit radius in the presence of the magnetic field is less than the inter-layer separation. However, for only one layer per unit cell, the results of §(2b) should be a good approximation for general directions of **H** also. Near $T \to T_{c0}$, this is consistent with the results derived by Lawrence and Doniach (1971) who obtained a difference equation based on a generalization of the Ginzburg-Landau approach to layered materials. In the case of materials like $YBaCu_2O_7$, to apply the results obtained in §(2b), we have to assume that all the three Cu–O layers are approximately equivalent with the corresponding parameter, d, in (17), taken to be $L/3$, where L is the unit cell dimension along the Z-axis.

In the next section, we discuss these results.

4. Discussion of the results and conclusions

In table 1, we have summarized the list of parameters of our calculations. The major differences arising from the shapes of the two Fermi surfaces (closed and open) are found in the densities of states, $N(0)$, the equivalent mass-parameters m_z and $m_3(n)$

Table 1. Model parameters and upper critical magnetic field.

Nature of parameters	Anisotropic closed FS (effective mass)	Anisotropic open FS (layer)
$\hbar\varepsilon_k$	$\hbar^2\left(\frac{k_x^2}{2m_x}+\frac{k_y^2}{2m_y}+\frac{k_z^2}{2m_z}\right)-E_F$	$\hbar^2\left(\frac{k_x^2}{2m_x}+\frac{k_y^2}{2m_y}\right)+2t_3(1-\cos k_z d)-E_F$ $4t_3 \ll E_F,\quad \frac{-\pi}{d}\leqslant k_z\leqslant\frac{\pi}{d}.$
Band structure parameters	$m^*=(m_x m_y m_z)^{1/3}$ $E_F=\frac{\hbar^2}{2m^*}(3\pi^2 n)^{2/3}$ $V_F^*=(2E_F/m^*)^{1/2}$ $N(0)=3n/4E_F=\frac{m^*(3\pi^2 n)^{1/3}}{2\pi^2\hbar^2}$	$m_z(0)=\frac{\hbar^2}{2t_3 d^2};\, m_3(n)\equiv m_z(0)\frac{E_F}{t_3}.$ $E_F=\frac{\pi\hbar^2 d}{(m_x m_y)^{1/2}}n$ $V_{FL}=(2E_F/m_L)^{1/2},\, m_L=[m_x m_y m_3]^{1/3}$ $N(0)=n/2E_F=(m_x m_y)^{1/2}/2\pi\hbar^2 d$
Magnetic field parameters	$\mathbf{H}^*=\left(\left(\frac{m_x}{m^*}\right)^{1/2}H_x,\left(\frac{m_y}{m^*}\right)^{1/2}H_y,\left(\frac{m_z}{m^*}\right)^{1/2}H_z\right)$ $r_c^{*2}=c\hbar/e\lvert\mathbf{H}^*\rvert$ $\mathbf{\Omega}_H=\frac{1}{2\hbar}\mu_B\mathbf{H}\cdot\mathbf{g}$	$\mathbf{H}^{(L)}=\left(\left(\frac{m_x}{m_L}\right)^{1/2}H_x,\left(\frac{m_y}{m_L}\right)^{1/2}H_y,\left(\frac{m_3}{m_L}\right)^{1/2}H_z\right)$ $r_L^2=c\hbar/e\lvert\mathbf{H}^{(L)}\rvert$ $\mathbf{\Omega}_H=\frac{1}{2\hbar}\mu_B\mathbf{H}\cdot\mathbf{g}$
$H_{c2}(T=0)$	$H_{c2i}(0)=\left(\frac{m^*}{m_i}\right)^{1/2}H_{c2}^{(0)},(i=x,y,z)$ $H_{c2}^{(0)}=\frac{e^{2+\gamma}\Delta_0^2 c}{2V_F^{*2}e\hbar}$ $\gamma\simeq 0.5772$	$H_{c2i}(0)=\left(\frac{m_L}{m_i}\right)^{1/2}H_{c2L}^{(0)},(i=x,y)$ $H_{c2z}(0)=\left(\frac{m_L}{m_z(0)}\frac{t_3}{E_F}\right)^{1/3}H_{c2L}^{(0)}$ $H_{c2L}^{(0)}=\frac{2e^{\gamma}\Delta_0^2 c}{V_{FL}^2 e\hbar}$
$h^*(0)=\frac{\lvert H_{c2}(T=0)\rvert}{-T_{c0}\left[\frac{d\lvert H_{c2}(T)\rvert}{\mathrm{d}T}\right]_{T_{c0}}}$ (clean limit)	$\frac{7\zeta(3)}{48e^{\gamma-2}}\simeq 0{\cdot}7273$	$\frac{7\zeta(3)}{8e^{\gamma}}\simeq 0{\cdot}5906,\quad 4t_3\ll E_F$

respectively, in the z-direction, and in the structure of the function, $P_H(\mathbf{Q}, \xi)$, appearing in the kernel of the linearized gap equation, (13). For the closed, anisotropic FS, P_H, given by (19), is of the logarithmic form, whereas that for the widely open FS, P_H is given by (47), with a square-root structure. These differences show up most prominently in the expressions for the upper critical field $\mathbf{H}_{c2}(T=0)$ and $(\mathrm{d}|\mathbf{H}_{c2}(T)|/\mathrm{d}T)_{T_{c0}}$. The numerical parameter $h^*(0)$ defined in table 1 is often used in estimating $|\mathbf{H}_{c2}(T=0)|$ from an experimental knowledge of $-T_{c0}(\mathrm{d}|\mathbf{H}_{c2}(T)|/\mathrm{d}T)_{T_{c0}}$. In the clean limit, we find that for the case of a widely open FS considered here (applicable to layered superconductors, with $4t_3 \ll E_F$), $h^*(0) = 0{\cdot}5906$ instead of $0{\cdot}7273$ for the three-dimensional closed FS. To obtain a lower extrapolated values of $|\mathbf{H}_{c2}(0)|$, experimentalists have often used (Lan *et al* 1991) the dirty-limit result, $0{\cdot}69$, for this parameter, although coherence lengths in high-T_c superconductors are much smaller than the mean free path to justify such an assumption. For extreme layered systems, our value of $0{\cdot}5906$ for $h^*(0)$ in the clean limit ought to be used in such extrapolations. From our calculation, we can, of course, obtain directly the value of $\mathbf{H}_{c20}(0)$, for single-crystal materials like $YBa_2Cu_3O_3$(YBCO) where estimates of band structure parameters are more reliable. Even for YBCO, one can obtain more than one set of consistent parameters from experimental observations (Batlogg 1990; Kresin and Wolf 1990; Press and Jha 1991a, b). The observed anisotropy of the d.c. resistivity ρ_c/ρ_{ab} in YBCO ranges from 25 to 300, with larger values at lower temperatures. Consistent with Hall measurements and other data for single crystals of YBCO, we may assume the following set of values of relevant parameters: $n = 4 \times 10^{21}\,\mathrm{cm}^{-3}$, $(m_z(0)/(m_x m_y)^{1/2})(E_F/t_3) = m_3(n)/(m_x m_y)^{1/2} = 27$; $(m_x m_y)^{1/2} = 4{\cdot}5\,\mathrm{m}$, $E_F \simeq 0{\cdot}1\,\mathrm{eV}$, and $T_{c0} = 90\,\mathrm{K}$. These lead to $m_L = (m_x m_y m_3)^{1/3} \simeq 13{\cdot}5\,\mathrm{m}$, $V_{\mathrm{Fab}} = 8{\cdot}83 \times 10^6\,\mathrm{cm\,sec^{-1}}$, $V_{F3} = 1{\cdot}7 \times 10^6\,\mathrm{cm\,sec^{-1}}$ and $V_{FL} = 5{\cdot}1 \times 10^6\,\mathrm{cm\,sec^{-1}}$. We thus obtain $H_{cL}^{(0)} \simeq 124{\cdot}5$ Tesla, $H_{c2}^{ab}(0) = (m_L/(m_x m_y)^{1/2})^{1/2}\; H_{cL}^{(0)} \simeq 216$ Tesla, $H_{c2}^{c}(0) = (m_L/m_3)^{1/2} H_{cL}^{(0)} \simeq 42$ Tesla, $(\mathrm{d}H_{c2}^{ab}/\mathrm{d}T)_{T_{c0}} \simeq -4$ Tesla/K and $(\mathrm{d}H_{c2}^{c}/\mathrm{d}T)_{T_{c0}} \simeq -0{\cdot}8$ Tesla/K. Because of the broadening of the resistivity transition curve when a magnetic field is applied, it has been difficult to get reliable experimental estimates (Worthington *et al* 1987) of the derivatives and H_{c2}. Also, estimates based on magnetization measurements (Welp *et al* 1989 and 1991) differ considerably from the measurements based on resistivity. Our results fall within the range of the observations, and can be classified as good, keeping in mind our simplifying assumptions in ignoring the differences between chain and plane layers in YBCO, and strong coupling effects. In fact, if instead of the weak coupling value of Δ_0, given by (31), the actual experimental value of the average gap parameter for YBCO is used in (54) for determining $\mathbf{H}_{c2}$, etc., their values increase by factor of about 2, with (Batlog 1990) $E_F \simeq 0{\cdot}25\,\mathrm{eV}$.

The effects of weak, nonmagnetic impurity scattering and the paramagnetic interaction are manifested in fixing the parameter a_{eff} in the condition

$$\ln(|H_{\mathrm{eff}}|/H_{c2\mathrm{eff}}^{(0)}) + a_{\mathrm{eff}} T^2/T_{c0}^2 = 0 \tag{77}$$

for determining the low-temperature transition in the (H, T) plane. As shown explicitly in (30) and (31) for the closed FS, and in (53)–(55) for the open FS, the dependence of respective a_{eff}, on the impurity scattering parameter, Γ, and the paramagnetic energy $\hbar|\Omega_H|$ are quite different. For the closed FS, the parameter $a(\mathbf{H}, \Gamma)$ has an addition of a logarithmic term, whereas for the widely open FS, the corrections are linear in Γ and quadratic in $|\Omega_H|$. This implies that at low temperatures, the variation of $|\mathbf{H}_{c2\text{eff}}(T)|$ as a function of T and that of $T_c(\mathbf{H})$ as a function of $\mathbf{H}$ differ considerably in these two cases. In the dimensionless parameter $h^*(T)$, defined by,

$$h^*(T) = |\mathbf{H}_{c2}(T)| \Big/ \left[-T_c \left(\frac{\mathrm{d}|\mathbf{H}_{c2}(T)|}{\mathrm{d}T} \right)_{T=T_{c0}} \right]$$
$$= h^*(0)(1 - a_{\text{eff}}\, T^2/T_{c0}^2) \tag{78}$$

where $a_{\text{eff}} = a$ is given by (31) for the closed FS, and $a_{\text{eff}} = a_L$ is given by (55) for widely open FS. Note that the numerical prefactor in this parameter is 1.1874 for the widely open FS, compared to 0.4645 for closed FS. In fact, for the open FS, $a_L(\mathbf{H}, \Gamma)$ is well-behaved in the limit $\mathbf{H} \to 0$ and $\Gamma \to 0$ while $a(\mathbf{H}, \Gamma)$ is well known (Gruenberg and Gunther 1968) to be nonanalytic there. Also, the behavior of $T_c(\mathbf{H})$ for $\mathbf{H}$ near $\mathbf{H}_{c2}$ is governed by the coefficients $a^{-1/2}(\mathbf{H}, \Gamma)$ and $a_L^{-1/2}(\mathbf{H}, \Gamma)$, respectively, in these two cases, via (33) and (57).

The spatial coherence length in the superconductor may be estimated either from the BCS approach or from the Ginzburg-Landau theory. At $T = 0$, the BCS coherence lengths are given by

$$\xi_{ab}^{\text{BCS}}(0) = \hbar V_{Fi}/1{\cdot}76\pi k_B\, T_{c0} \quad (i = x, y, z). \tag{79}$$

Using the parameters for single crystal YBCO given earlier, we obtain

$$\xi_{ab}^{\text{BCS}}(0) \simeq 13{\cdot}5\,\text{Å}, \quad \xi_c^{\text{BCS}}(0) \simeq 2{\cdot}6\text{Å}.$$

These are consistent with the oft-quoted experimental numbers, 15 Å and 3 Å respectively. The anisotropic coherence lengths ξ_i, defined in the Ginzburg–Landau scheme, are given by the relations

$$H_{c2z} = \Phi_0/2\pi\xi_x\xi_y, (x, y, z, \text{ cyclic}); \; \Phi_0 = c\hbar/2e. \tag{80}$$

For the case of a widely open FS (extreme layered system), near $T \sim T_{c0}$, we find

$$\xi_z(T) = \left[\frac{\Phi_0}{2\pi} \right]^{1/2} \frac{[m_L/m_z(0)]^{1/2}(t_3/E_F)^{1/2}}{[h_{cL}^{(0)}(1 - T/T_{c0})]^{1/2}}, \tag{81}$$

$$\xi_i(T) = \left[\frac{\Phi_0}{2\pi} \right]^{1/2} \frac{(m_L/m_i)^{1/2}}{[h_{cL}^{(0)}(1 - T/T_{c0})]^{1/2}}, i = x, y \tag{82}$$

where m_L and $m_z(0)E_F/t_3 \equiv m_3(n)$ are same as in table 1, and $h_{cL}^{(0)}$ is defined by (60). For YBCO, the ratio of the coherence lengths is found to be $\xi_z^{GL}(0)/\xi_{ab}^{GL}(0) \sim 1/5{\cdot}2$, with $\xi_z^{GL}(0) \simeq 4$ Å, for the parameters discussed earlier.

In conclusion, we have presented the conditions for the superconducting transition in the $(\mathbf{H}, T)$ plane for an anisotropic, layered, type II superconductor with open normal state FS. We have treated the orbital effects of the magnetic field semiclassically, but we have included the effects of anisotropic paramagnetic interaction and weak nonmagnetic impurity scattering. Numerical estimates for $\mathbf{H}_{c2}(0)$ and $\xi_i(T)$ in YBCO are in reasonable agreement with experimental data. It may be necessary to include the effects of spin-orbit interaction and magnetic impurity scattering in a more general situation in which the high-T_c superconductors are doped with nonmagnetic ions, using the more general formulation of Rieck *et al* (1991). Usually these effects reduce $h^*(0)$ to values much lower than its value, 0·69, in the extreme dirty limit. However, we have shown that for the case of anisotropic widely open FS considered here, the parameter is already reduced to 0·59 in the clean limit. This is of importance in finding the extrapolated values of $\mathbf{H}_{c2}(0)$ from measurements. Although, we have presented here the analytical results for two specific forms for the single particle energies and FS's, we should emphasize that our formulation is such that it can be used for any general single particle dispersion, $\hbar\varepsilon(\mathbf{k})$, if we resort to numerical evaluation of (14). We should however point out that in the above analysis, we have not considered the high field Landau level quantization effects, and, the possible inhomogeneity of the fields inside the superconductor arising from the formation of vortex lattice structures (Rieck and Scharnberg 1990; Prohammer and Carbotte 1990; Rieck *et al* 1991). From the work of Prohammer and Carbotte (1990), for T near T_c the corrections to the Gaussian form of the gap function, are expected to be small in the weak scattering limit treated here. For the more general case, some of these questions will be considered in a future communication.

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