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COHERENCE LENGTH AND PENETRATION DEPTH OF CLEAN ANISOTROPIC SUPERCONDUCTORS CLOSE TO T_C.

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Within weak-coupling BCS theory, we have derived the Ginzburg-Landau equations of a clean superconductor with anisotropic single-particle dispersion and order parameter, at a temperature close to the superconducting transition temperature T_c. The resulting expressions for the coherence length and penetration depth close to T_c are discussed.

The superconducting order parameter of the high temperature superconductors (HTS) is highly anisotropic [1]. Another source of anisotropy in the cuprates is their single-particle dispersion in the normal state. The layered structure of HTS causes the nearly two-dimensional character of the electrons; moreover, the closeness of the Van Hove points to the Fermi energy discovered in recent photoemission experiments [2] leads to a substantial in-plane anisotropy of the low-lying electron states. The purpose of this paper is to determine the basic parameters of the superconducting state (coherence length ξ and penetration depth λ) close to T_c from microscopic parameters allowing for both types of anisotropy.

The Ginzburg-Landau equations for a clean anisotropic superconductor were derived from the microscopic theory by Gorkov and Melik-Barkhudarov [3] by making use of the Green's function technique. We sketch first a simpler derivation of their results. We consider electrons described by the Hamiltonian

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c^{\dagger}_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} - \sum_{\mathbf{k},\mathbf{k}',\mathbf{p}} V_{\mathbf{k},\mathbf{k}'} c^{\dagger}_{\mathbf{k}+\mathbf{p},\uparrow} c^{\dagger}_{-\mathbf{k}+\mathbf{p},\downarrow} c_{-\mathbf{k}'+\mathbf{p},\downarrow} c_{\mathbf{k}'+\mathbf{p},\uparrow}, \qquad (1)$$

where the effective electron-electron interaction $V_{\mathbf{k},\mathbf{k}'}$ is acting on electrons in a shell of width $2\hbar\omega_D$ around the Fermi surface. We assume $|\mathbf{p}| \ll k_F$ where $k_F^3 = 3\pi^2 n$ and n is the density of electrons. We do not specify the origin of the energy scale $\hbar\omega_D$ but we require that $\hbar\omega_D \ll E_F$ where E_F is the Fermi energy. We introduce the order parameter $\Delta_{\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \langle c_{-\mathbf{k}'+\mathbf{q},\downarrow} c_{\mathbf{k}'+\mathbf{q},\uparrow} \rangle$ in order to describe a spatially varying

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condensate $\Delta e^{2i\mathbf{q}\cdot\mathbf{r}}$. The mean field Hamiltonian reads (we omit additional c-number terms)

$$H = \sum_{\mathbf{k}} \alpha^\dagger_{\mathbf{k}} \begin{pmatrix} \varepsilon_{\mathbf{k+q}} & -\Delta_{\mathbf{k}} \\ -\Delta^*_{\mathbf{k}} & -\varepsilon_{\mathbf{k-q}} \end{pmatrix} \alpha_{\mathbf{k}}, \tag{2}$$

where $\alpha^\dagger_{\mathbf{k}} = (c^\dagger_{\mathbf{k+q},\uparrow}, c_{-\mathbf{k+q},\downarrow})$. This Hamiltonian is diagonalized by standard techniques and the resulting gap equation is

$$\Delta_{\mathbf{k}} = \sum_{\mathbf{k}'} V_{\mathbf{k},\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \left[1 - f(E_{\mathbf{k}',+}) - f(E_{\mathbf{k}',-})\right], \tag{3}$$

where $E_{\mathbf{k}} = \sqrt{(\varepsilon_{\mathbf{k+q}} + \varepsilon_{\mathbf{k-q}})^2/4 + \Delta^2_{\mathbf{k}}}$ and $E_{\mathbf{k},\pm} = E_{\mathbf{k}} \pm (\varepsilon_{\mathbf{k+q}} - \varepsilon_{\mathbf{k-q}})/2$. Let us assume now that $\Delta_{\mathbf{k}} = \Delta\Phi_{\mathbf{k}}$ with $|\Phi_{\mathbf{k}}| \leq 1$ so that $\Delta > 0$ is the maximal gap. We assume further that $V_{\mathbf{k},\mathbf{k}'}$ takes a separable form, $V_{\mathbf{k},\mathbf{k}'} = V\Phi_{\mathbf{k}}\Phi_{\mathbf{k}'}$. Expanding $\varepsilon_{\mathbf{k}\pm\mathbf{q}}$ to second order in $\mathbf{q}$ we have $E_{\mathbf{k}} = |\varepsilon_{\mathbf{k}} + \hbar^2 q^i q^j/2m^{i,j}|$ and $\varepsilon_{\mathbf{k+q}} - \varepsilon_{\mathbf{k-q}} = \hbar\mathbf{v}_{\mathbf{k}}\cdot\mathbf{q}$, where $\mathbf{v}_{\mathbf{k}} = (1/\hbar)\partial\varepsilon_{\mathbf{k}}/\partial\mathbf{k}$ and $1/m_{i,j} = (1/\hbar^2)\partial^2\varepsilon_{\mathbf{k}}/\partial k_i\partial k_j$ are the group velocity and the inverse effective mass tensor in the point $\mathbf{k}$, respectively; summation over repeated indices i,j is understood. Since the sum over $\mathbf{k}'$ in the gap equation is restricted to the neighborhood $\hbar\omega_D \ll E_F$ of the Fermi surface, we can split the integration into directions parallel and perpendicular to the Fermi surface and the latter can be transformed to an integral over energy: $\sum_{\mathbf{k}} = \oint d\mathbf{K} N_{\mathbf{K}} \int d\varepsilon$, where $N_{\mathbf{K}} = 1/(2\pi)^3\hbar v_{\mathbf{K}}$ is the density of states per spin in the point $\mathbf{K}$ of the Fermi surface. Let us expand the gap equation in powers of Δ and make use of the equation for T_c [4], $T_c = (2\gamma/\pi)\hbar\omega_D e^{-1/\lambda}$, where $\ln\gamma = C \approx 0.577$ is Euler's constant and $\lambda = V\overline{N(0)} = V\oint d\mathbf{K} N_{\mathbf{K}}\Phi^2_{\mathbf{K}}$ is a dimensionless coupling constant. After a Fourier transformation to real space we find

$$\alpha\psi + \beta|\psi|^2\psi + \frac{1}{2m^*_{i,j}}(-i\hbar\nabla_i)(-i\hbar\nabla_j)\psi = 0, \tag{4}$$

where $\alpha = (8\pi^2/7\zeta(3))(\overline{N(0)}T_c/n)(T - T_c)$, $\beta = (8\pi^2/7\zeta(3))\langle\Phi^2_{\mathbf{K}}\rangle\overline{N(0)}T_c^2/n^2$, and the effective mass tensor of the superconducting condensate is given by $1/m^*_{i,j} = (\overline{N(0)}/n)\langle v^i_{\mathbf{K}} v^j_{\mathbf{K}}\rangle$. We have introduced in Eq.4 a macroscopic wavefunction $\psi = \sqrt{7\zeta(3)n/8\pi^2T_c^2}\Delta$. ζ is the zeta function: $\zeta(3) \approx 1.20$ and $\langle A_{\mathbf{K}}\rangle$ denotes the following average of $A_{\mathbf{K}}$ along the Fermi surface:

$$\langle A_{\mathbf{K}}\rangle = \frac{\oint d\mathbf{K} N_{\mathbf{K}}\Phi^2_{\mathbf{K}} A_{\mathbf{K}}}{\oint d\mathbf{K} N_{\mathbf{K}}\Phi^2_{\mathbf{K}}}. \tag{5}$$

Note that Eq.4 is not explicitly gauge invariant. We shall assume that a correct way to remove this deficiency is to replace $-i\hbar\nabla_i$ with $D_i = -i\hbar\nabla_i - 2eA_i$, where e is the elementary charge and $\mathbf{A}$ is the vector potential. After this replacement, Eq.4 agrees with the result of Gorkov and Melik-Barkhudarov [5].

It is seen that the Ginzburg-Landau coherence length is, in general, a tensor: $\xi^2_{i,j} = \hbar^2/2m^*_{i,j}|\alpha|$. In what follows we will work in a coordinate system where $\xi_{i,j}$ is diagonal. Since the maximal zero-temperature gap $\Delta(0)$ is given by $2\Delta(0)/T_c = (2\pi/\gamma)\exp\langle\ln|1/\Phi_{\mathbf{K}}|\rangle$ [4] where $2\pi/\gamma \approx 3.5$, we can write

$$\xi^i = B\frac{\xi^i_0}{\sqrt{1-\Theta}}, \tag{6}$$

where $B = (\pi/4\gamma)\sqrt{7\zeta(3)/3} \approx 0.74$, $\Theta = T/T_c$, and we have introduced

$$\xi^i_0 = \frac{\hbar\sqrt{3\langle(v^i_{\mathbf{K}})^2\rangle}}{\pi\exp\langle\ln|\Delta_{\mathbf{K}}|\rangle}. \tag{7}$$

Eq.7 reduces in the isotropic case to the standard BCS result and we take it as a definition of the BCS coherence length in the general case.

As an example, let us consider electrons with the dispersion $\varepsilon_{\mathbf{k}} = \hbar^2(k_x^2 + k_y^2)/2m$. The Fermi surface is cylindrical with k_F being the radius of its circular cross-section. We will assume further that $\Phi_{\mathbf{K}}$ does not depend on k_z. Thus we have $\xi^z_0 = 0$ and $\xi^x_0 = \xi^y_0 = \xi_0$ depends on the symmetry of the order parameter. Consider first $\Phi_{\mathbf{K}} = 1$ (isotropic s-wave pairing). We find $\xi_0/\xi_{BCS} = \sqrt{3/2} \approx 1.22$, where $\xi_{BCS} = \hbar v_F/\pi\Delta$ and $v_F = \hbar k_F/m$. This is consistent with the results obtained in Ref.[6]. For $\Phi_{\mathbf{K}} = \cos 2\varphi$ where $\tan\varphi = k_y/k_x$ (d-wave pairing) we find $\xi_0/\xi_{BCS} \approx 1.49$. Both types of anisotropy are seen to enhance the coherence length compared to its BCS value. We emphasize that the sign of $\Phi_{\mathbf{K}}$ is irrelevant for the whole of the present paper. Both for $\Phi_{\mathbf{K}} = \cos 2\varphi$ and $\Phi_{\mathbf{K}} = |\cos 2\varphi|$ ("extended s-wave") we obtain identical results.

As an example of an anisotropy which shortens the coherence length, let us consider a cylindrical Fermi surface as before but with a modulation of the Fermi velocity with φ: $v_{\mathbf{K}} = v_F - u\cos 4\varphi$, $|u| < v_F$ ($l = 4$ is chosen as the lowest nontrivial harmonic allowed by tetragonal symmetry). For $\Phi_{\mathbf{K}} = 1$ we find $\xi_0/\xi_{BCS} = \sqrt{3/2}(1 - u^2/v_F^2)^{1/4}$ and thus $\xi_0 < \xi_{BCS}$ occurs for $u/v_F > \sqrt{5}/3 \approx 0.75$, i.e., substantial modulation of the Fermi velocity is necessary. Note that our analysis does not apply for $u \to v_F$ since in that case the Fermi velocity and effective mass of the electrons close to the Fermi level can not be taken as independent of energy any more. For an estimate of ξ_0 of a superconductor with isotropic pairing in this regime, see Ref.[7]. [The result of Ref.[7] should be multiplied by $\sqrt{3/2}$ as appropriate for a two-dimensional system.]

It is interesting that although anisotropic pairing alone increases the coherence length, when suitably combined with a modulation of the Fermi velocity, it can give a coherence length which is shorter than for isotropic pairing and the same modulation of the Fermi velocity. In fact, consider $\Phi_{\mathbf{K}} = \cos 2\varphi$ and $v_{\mathbf{K}} = v_F - u\cos 4\varphi$. For $u/v_F > 0$, the maxima of $|\Phi_{\mathbf{K}}|$ coincide with the minima of $v_{\mathbf{K}}$, whereas for $u/v_F < 0$, the reverse is true. We have calculated ξ_0/ξ_{BCS} in the whole range $-1 < u/v_F < 1$. The result is presented in Fig.1 as a solid line. For comparison, the same quantity is plotted also for the isotropic s-wave solution $\Phi_{\mathbf{K}} = 1$ as a dashed line. Two features are worth mentioning: (i) for d-wave pairing, ξ_0/ξ_{BCS} depends strongly on the sign of

u/v_F and (ii) for $u/v_F > 0.31$, the coherence length is in fact shorter for d-wave pairing. The latter feature is due to the fact that the gap in the d-wave solution has most of its "weight" in the regions with a high density of states.

It is well known that the other characteristic length of a superconductor, the penetration depth $\lambda(T)$, also depends on the modulation of the gap. In fact, the linear response coefficient $K^{i,j}$ relating the current density j_i and the local magnetic field described by a vector potential A_j in the transverse gauge $\nabla \cdot \mathbf{A} = 0$, $j_i = -K^{i,j}A_j$, is given by $K^{i,j} = 2\sum_{\mathbf{k}}[f(\epsilon_{\mathbf{k}})/m^{i,j}_{\mathbf{k}} + v^i_{\mathbf{k}} v^j_{\mathbf{k}} \partial f(E_{\mathbf{k}})/\partial E_{\mathbf{k}}]$ where $f(\varepsilon)$ is the Fermi distribution function [8]. Integrating the first term by parts and making use of the Matsubara representation we find

$$K^{i,j} = e^2 \oint d\mathbf{K} N_{\mathbf{K}} v^i_{\mathbf{K}} v^j_{\mathbf{K}} 2\pi T \sum_n \frac{\Delta^2_{\mathbf{K}}}{(\hbar^2\omega_n^2 + \Delta^2_{\mathbf{K}})^{3/2}}. \tag{8}$$

After diagonalization of the matrix $K^{i,j}$ we have $K^{i,i} = \epsilon_0 c^2/\lambda_i^2$, where ϵ_0 and c are the permittivity of vacuum and speed of light, respectively, and λ_i is the penetration depth in the direction i. In what follows we assume again that the coordinates are chosen so that this is the case. At $T = 0$, we find from Eq.8

$$\frac{1}{\lambda_i^2(0)} = \frac{g^2}{\pi^2 c} \oint \frac{d\mathbf{K}}{v_{\mathbf{K}}} (v^i_{\mathbf{K}})^2, \tag{9}$$

where $g^2 \approx 1/137$ is the fine-structure constant. It is thus seen that the ground-state penetration depth does not depend on the symmetry of the pairing state and is completely determined by the normal-state dispersion at the Fermi level. For instance, the 'in-plane' penetration depth of a superconductor with a cylindrical Fermi surface is $1/\lambda^2 = ne^2/m\epsilon_0 c^2$ for all pairing states $\Phi_{\mathbf{K}}$. [We neglect variations of $\mathbf{v_k}$ and $1/m^{i,j}_{\mathbf{k}}$ on the energy scale Δ.] However, depending on the pairing state, the function $\lambda_i(T)$ is expected to exhibit qualitatively different behavior for $0 < T \ll T_c$. There exists large literature on this aspect of anisotropic pairing [1]. We would like to point out here that one can extract information on the pairing state of a weak-coupling superconductor also from the knowledge of $\lambda_i(T)$ close to T_c. In that case we have

$$\lambda_i(T) = \sqrt{\frac{\langle \Phi^2_{\mathbf{K}} \rangle \langle (v^i_{\mathbf{K}})^2/\Phi^2_{\mathbf{K}} \rangle}{\langle (v^i_{\mathbf{K}})^2 \rangle}} \frac{\lambda_i(0)}{\sqrt{2(1-\Theta)}}. \tag{10}$$

For isotropic pairing, $\Phi_{\mathbf{K}} = 1$, we recover the standard BCS result. The first factor on the right-hand side represents therefore a measure of the effects of the pairing-state anisotropy on the penetration depth. For instance, for a d-wave superconductor with a cylindrical Fermi surface discussed above, the normalized slope of the inverse penetration depth squared close to T_c is $-d(\lambda^2(0)/\lambda^2(T))/d\Theta = 2x(2-x)/(3x+1-\sqrt{1-x^2})$ where $x = u/v_F$, see Fig.1. The importance of bandstructure effects for the slope of $\lambda^2(0)/\lambda^2(T)$ has been noted previously in Ref.[8].

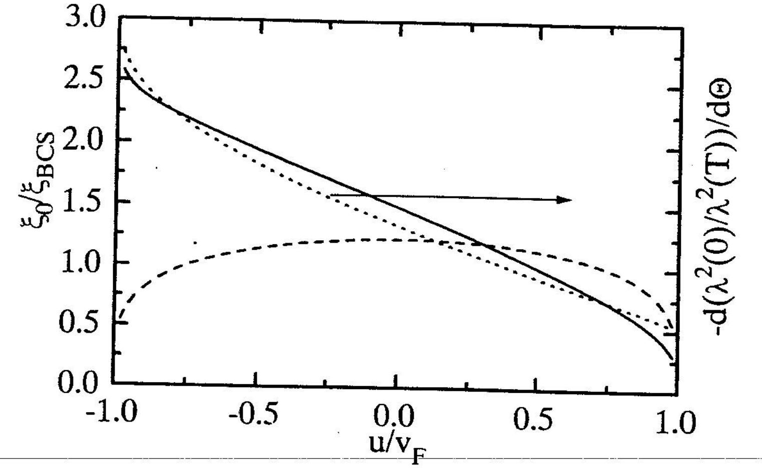

Fig.1. Normalized coherence length ξ_0/ξ_{BCS} of a weak-coupling BCS superconductor with a cylindrical Fermi surface as a function of u/v_F. The Fermi velocity varies as $v_{\mathbf{K}} = v_F - u\cos 4\varphi$. Solid line: $\Phi_{\mathbf{K}} = \cos 2\varphi$ (d-wave pairing). Dashed line: $\Phi_{\mathbf{K}} = 1$ (isotropic s-wave pairing). Dotted line: The normalized slope $-d(\lambda^2(0)/\lambda^2(T))/d\Theta$ of the inverse penetration depth squared close to T_c for $\Phi_{\mathbf{K}} = \cos 2\varphi$. The vertical scale is the same as for ξ_0/ξ_{BCS}. For $\Phi_{\mathbf{K}} = 1$, $-d(\lambda^2(0)/\lambda^2(T))/d\Theta = 2$.

The generalized Ginzburg-Landau equation for the superconducting current can be obtained from $j_i = -K^{i,j}A_j$ for T close to T_c by requiring that the theory is gauge invariant. We find

$$j_i(\mathbf{r}) = \frac{e}{m^*_{i,j}} \left[-i\hbar(\psi^* \nabla_j \psi - \psi \nabla_j \psi^*) - 4eA_j(\mathbf{r})|\psi|^2\right]. \tag{11}$$

For completeness, let us mention that Eqs.4 and 11 can be derived from a free energy functional with the local free energy density in the superconducting state f_S given by

$$f_S = f_N + \alpha|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \frac{1}{2m^*_{i,j}}(D_i\psi)^* D_j\psi + \frac{\epsilon_0 c^2}{2}(\nabla \times \mathbf{A})^2. \tag{12}$$

In Eq.12, f_N is the free energy density in the normal state. The normalization of the last term on the right-hand side is known from the theory of electromagnetism and this is sufficient to determine the free energy density in a unique way. For the specific heat jump at T_c, one finds from Eq.12 $(c_S - c_N)/c_N = (12/7\zeta(3))/\langle \Phi^2_{\mathbf{K}} \rangle \langle 1/\Phi^2_{\mathbf{K}} \rangle \le 12/7\zeta(3) \approx 1.43$, in agreement with Ref.[4].

In conclusion, we have derived expressions for the coherence length and penetration depth of anisotropic superconductors close to T_c. Our calculation should be relevant to clean anisotropic weak-coupling materials. An analysis of the results of point-contact spectroscopy on HTS based on the present work has been attempted in Ref.[9]. It was argued there that it is crucial to take into account not only the anisotropy of the cuprates, but also the strong-coupling effects, short quasiparticle lifetime, and the critical fluctuations close to T_c. Further work is needed to clarify the interplay of these effects.

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