Effect of Phase Fluctuations on the Low-Temperature Penetration Depth of High-T_c Superconductors

Eric Roddick and David Stroud
Department of Physics, Ohio State University, Columbus, Ohio 43210
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We describe a simple model to estimate the effects of order parameter phase fluctuations on the penetration depth $\lambda(T)$ of high-T_c superconductors. When treated classically, such fluctuations are found to produce a linear temperature dependence of $\lambda(T)$, which may be comparable to the experimentally observed magnitude. This dependence persists when the combined effects of charging interactions and dissipation are included in the model. Hence, such a dependence may not be a unique signature of a superconductor with line nodes at the Fermi surface.

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It is widely believed that one probe of the symmetry of the pairing state in high-T_c superconductors is the temperature dependence of the London penetration depth $\lambda(T)$ at low temperatures T [1–5]. For example, s-wave pairing produces a nodeless energy gap with the full crystal symmetry. In this case $\lambda(T)$ should have the characteristic BCS temperature dependence $\lambda(T)/\lambda(0) - 1 \propto (2\pi\Delta_0/k_BT)^{1/2}e^{-\Delta_0/k_BT}$, where Δ_0 is the zero-temperature BCS energy gap. On the other hand, in superconductors with orthorhombic symmetry, such as low-temperature $La_2CuO_{4-\delta}$ and $YBa_2Cu_3O_{6.95}$, and superconductors with tetragonal symmetry, such as electron-doped Nd_2CuO_4 and some Tl-based materials, there are many possible singlet pairing states, in addition to s-wave states. All such states, other than s-wave states, lead to energy gaps with line nodes at the Fermi surface (assuming a spherical or cylindrical Fermi surface). Hence, they produce a $\lambda(T)$ which is *linear* rather than exponential in T, at low temperatures, i.e., $\lambda(T) = \lambda(0) + CT$. Nuclear magnetic resonance measurements on $YBa_2Cu_3O_{6.95}$ and other CuO-based high-temperature superconductors [6] have found a drop in the Knight shift consistent with singlet, rather than triplet, pairing.

The temperature dependence of $\lambda_{ab}(T)$ (for a field $\mathbf{H}\|\mathbf{c}$) has been measured by Hardy *et al.* [1] in untwinned single crystals of $YBa_2Cu_3O_{6.95}$. They reported a linear temperature dependence and interpreted it as implying a singlet superconducting order parameter with d-wave pairing. A similar temperature dependence was obtained in experiments in (not necessarily single-crystal) $YBa_2Cu_3O_{6.95}$.

In this Letter, we show that order parameter phase fluctuations produce a linear T dependence in $\lambda_{ab}(T)$ in the classical limit. We also present a variational calculation showing that this linear T dependence persists even when quantum effects due to charging and dissipation are included in a simple model. Thus, the presence of a linear T dependence is not sufficient, by itself, to demonstrate an unconventional order parameter in the high-T_c superconductors.

We first give a simple general argument suggesting that classical phase fluctuations in a nodeless order parameter could produce a low-temperature penetration depth $\lambda(T)$ varying *linearly* with T in an isotropic, three-dimensional (3D) material. Denote the (complex scalar) order parameter by $\psi(\mathbf{x}) = \psi_0(\mathbf{x})\exp[i\theta(\mathbf{x})]$ and assume, as in the BCS theory, that the *amplitude* $\overline{\psi}_0 \equiv \langle\psi_0\rangle$ (where $\langle\cdots\rangle$ is a canonical average) is approximately T independent at low T. [The actual exponential T dependence will not produce a linear variation in $\lambda(T)$.] The dominant thermal effects at low T are therefore due to phase fluctuations.

For an isotropic superconductor, the energy associated with phase fluctuations will be of the form

$$H = \int \frac{\hbar^2}{2m^*}|\nabla\psi|^2\,d^3x \approx \frac{\hbar^2\overline{\psi}_0^2}{2m^*}\int |\nabla\theta|^2\,d^3x\,. \qquad (1)$$

We Fourier transform this to obtain $H = (\hbar^2\overline{\psi}_0^2/2m^*)\times\sum_{\mathbf{k}} k^2|\theta_{\mathbf{k}}|^2$ and use the equipartition theorem to get $\langle|\theta_{\mathbf{k}}|^2\rangle = k_BT/\overline{\psi}_0^2\epsilon_{\mathbf{k}}$, where $\epsilon_{\mathbf{k}} = \hbar^2k^2/2m^*$. There is an upper cutoff wave vector in the sum of order $1/\xi_0$, where ξ_0 is the zero-temperature coherence length.

Now $\lambda(T)$ is related to the Helmholtz free energy F by

$$c\left(\frac{\partial^2F}{\partial A_\alpha^2}\right)_{\mathbf{A}=0} \equiv -\left(\frac{\partial J_\alpha}{\partial A_\alpha}\right)_{\mathbf{A}=0} = \frac{c}{4\pi\lambda^2(T)}\,, \qquad (2)$$

where J_α is the αth Cartesian component of current density. In the presence of a vector potential $\mathbf{A}$, $-i\hbar\nabla$ is replaced by the gauge-invariant operator $-i\hbar\nabla - e^*\mathbf{A}/c$. Substituting this relation into (1), and using (2) gives

$$\frac{1}{\lambda^2(0)} = 4\pi\overline{\psi}_0^2\frac{(e^*)^2}{m^*c^2}\,. \qquad (3)$$

Equation (2) shows that $1/\lambda^2(T)$ is proportional to the helicity modulus, $\gamma \equiv (\partial^2F/\partial A_\alpha^2)_{\mathbf{A}=0}$, of the superconductor [7], which measures the stiffness of the superconductor against phase twists, and is analogous to the spin-wave

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stiffness in a ferromagnet. In the classical limit, this helicity modulus *decreases linearly with* T at low T in both 2D and 3D, leading to a linear increase in $\lambda(T)$ with T.

We can make a crude estimate of this slope in 3D, by considering the variation of $\langle\psi\rangle$, which is analogous to the magnetization [this approach would not work in 2D, since the magnetization there is zero, but $\gamma(T)$ would still depend linearly on T at low T]. At low T, the dominant T dependence of $\langle\psi\rangle$ arises from phase fluctuations, so that $\langle\psi\rangle \approx \overline{\psi}_0|\langle\exp(i\theta)\rangle|$. Expanding the exponential to second order in θ, we obtain $\langle\exp(i\theta)\rangle \approx 1 - \langle\theta^2\rangle/2$, where $\langle\theta^2\rangle = \sum_{\mathbf{k}}\langle|\theta_{\mathbf{k}}|^2\rangle = [1/(2\pi)^3\overline{\psi}_0^2]\int_{|\mathbf{k}|<1/\xi_0} d^3k(k_BT/\epsilon_{\mathbf{k}})$. This shows that, in 3D, $\langle\psi\rangle$ decreases linearly with T. We can estimate the effect of this decrease on $1/\lambda^2(T)$, using Eq. (3) but with $\overline{\psi}_0$ replaced by $\langle\psi\rangle$. The result is

$$\Delta\lambda(T) \equiv \lambda(T) - \lambda(0) \approx CT\,, \tag{4}$$

where $C = k_B[8\pi\lambda^3(0)]/\xi_0\Phi_0^2$ and $\Phi_0 = |hc/e^*|$ is the flux quantum. If we take $e^* = 2e$, $\lambda(0) = 2000$ Å, and $\xi_0 = 10$ Å, we obtain $C \approx 1$ Å/K. This is somewhat smaller than the value observed by Hardy *et al.* but these are intended only as a very rough estimate.

Next, we attempt a more quantitative estimate of the expected linear T coefficient, and also introduce a simplified description of the expected quantum corrections. We again consider only *phase* fluctuations of the order parameter. We also use a discrete representation, in which the superconductor crystal is described as many small "grains," each comparable in size to ξ_0 and coupled together by a Josephson-like interaction. Such a representation has frequently been used to represent *granular* [7–9] and even single-crystal [10] superconductors.

These assumptions lead to a description of the superconductor in terms of an *anisotropic x-y model:*

$$H = J_1 \sum_{\{ij\},ab}[1 - \cos(\theta_i - \theta_j)] + J_2 \sum_{\{ij\},c}[1 - \cos(\theta_i - \theta_j)]. \tag{5}$$

Here the sums run over all nearest-neighbor bonds in the a-b plane and in the c direction of a simple cubic lattice, which we take to have lattice constant ξ_0. The relation between the parameters of this model and those of the original superconductor are described below.

$\lambda(T)$ in the two principal directions can now be estimated using a "self-consistent phase phonon" (SCPP) approximation previously used to treat isotropic granular superconductors [8]. To allow for quantum corrections, we use a more general Hamiltonian than Eq. (5), which includes a diagonal charging energy $H_Q = (U_0/2)\sum_i n_i^2$. U_0 is an effective "grain charging energy," proportional to the inverse of the effective "grain self-capacitance." n_i is the Cooper pair number operator for grain i; it is quantum-mechanically conjugate to θ_i, and has the representation $n_i = -i\partial/\partial\theta_i$. Possible forms other than the assumed diagonal charging energy are discussed below. Besides being required to insure zero entropy as $T \to 0$, these charging effects may be of measurable significance in some high-T_c materials [11]. The total Hamiltonian is the sum of these two terms, i.e., $H_{\rm tot} = H_Q + H$.

In the SCPP approximation, one approximates $H_{\rm tot}$ by "best" harmonic Hamiltonian of the form

$$H_h = \frac{U_0}{2}\sum_i n_i^2 + \frac{K_1}{2}\sum_{\{ij\},ab}(\theta_i - \theta_j)^2 + \frac{K_2}{2}\sum_{\{ij\},c}(\theta_i - \theta_j)^2. \tag{6}$$

$F_{\rm tot}$ is evaluated using the true Hamiltonian $H_{\rm tot}$ but the eigenstates of the harmonic Hamiltonian:

$$F_{\rm tot} = F_h + \langle H_{\rm tot} + H_h\rangle_h\,, \tag{7}$$

where the angular brackets denote canonical averages in an ensemble corresponding the harmonic Hamiltonian (6), and F_h is the harmonic free energy. According to the Gibbs-Bogolyubov inequality [12], the right-hand side of (7) represents an upper bound to F for any K_1 and K_2. Substituting $H_{\rm tot}$ and Eq. (6) into Eq. (7), we find that the quantity to be minimized is

$$F_{\rm tot} = F_h + \sum_{\{ij\},ab}\left\{J_1\left[1 - \exp\left(-\frac{D_{ij}}{2}\right)\right] - \frac{1}{2}K_1D_{ij}\right\} + \sum_{\{ij\},c}\left\{J_2\left[1 - \exp\left(-\frac{D_{ij}}{2}\right)\right] - \frac{1}{2}K_2D_{ij}\right\}. \tag{8}$$

Here we have used the identity, valid for a Gaussian Hamiltonian, that $\langle\cos(\theta_i - \theta_j)\rangle = \exp[-\frac{1}{2}\langle(\theta_i - \theta_j)^2\rangle]$, and $D_{ij} \equiv \langle(\theta_i - \theta_j)^2\rangle$.

On Fourier transforming, one obtains $D_{ij} = (4/N)\times\sum_{\mathbf{q}}\langle|\theta_{\mathbf{q}}|^2\rangle\sin^2(\frac{1}{2}\mathbf{q}\cdot\mathbf{R}_{ij})$, and $H_h = (U_0/2)\sum_{\mathbf{q}}[n_{\mathbf{q}}n_{-\mathbf{q}} + \omega_{\mathbf{q}}^2(\hbar/2U_0)^2\theta_{\mathbf{q}}\theta_{-\mathbf{q}}]$. Here $\omega_{\mathbf{q}}^2 = (16U/\hbar^2)\{K_1[\sin^2(q_xa/2) + \sin^2(q_ya/2)] + K_2\sin^2(q_za/2)\}$, a being the lattice constant, which is taken to be the same in all three directions. At finite temperatures, $\langle|\theta_{\mathbf{q}}|^2\rangle = (2U_0/\hbar\omega_q)\coth(\beta\hbar\omega_q/2)$. For given parameters J_1 and J_2, the values of K_1 and K_2 which minimize the free energy can now be determined as functions of temperature.

In the presence of a vector potential $\mathbf{A}$ in the αth direction, $\theta_i - \theta_j$ is to be replaced by the *gauge-invariant phase difference,* $\theta_i - \theta_j - A_{ij}$, where $A_{ij} = (2\pi/\Phi_0)\int_i^j \mathbf{A}\cdot d\mathbf{l} = 2\pi A_\alpha a/\Phi_0$ in the α direction and zero in the other two directions. This vector potential induces a current in the α direction even at zero phase difference. The resulting current density will be

$$-(2e/a^2\hbar)K_\alpha A_{ij} = -(2e/a^2\hbar)K_\alpha(2\pi A_\alpha a)/\Phi_0\,. \tag{9}$$

From the coefficient of A_α in (9), we can deduce the penetration depth via the first London equation. The result is

$$K_\alpha = \frac{c}{4\pi\lambda_\alpha^2}\frac{\hbar}{2e}\frac{a\Phi_0}{2\pi}\,. \tag{10}$$

This equation connects K_α to the temperature-dependent penetration depth λ_α and the lattice constant $a \equiv \xi_0$.

We can use these relationships to estimate the T dependence of λ_{ab} and λ_c. The $T = 0$ value of J_1 [$\equiv K_1(T = 0)$ in the classical limit] can be determined from the measured value $\lambda_{ab}(T = 0)$, i.e., from Eq. (10). The anisotropy at any temperature J_1/J_2 is taken as the mass ratio, m_c/m_{ab}, a quantity whose value can range from 25 for $YBa_2Cu_3O_{6.95}$ [13] to $\approx$3000 for $Bi_2Sr_2CaCu_2O_{8+\delta}$ [14]. We obtain the temperature dependence of J_1 by assuming the relation $J_1(T) = J_1(0)[\lambda_{BCS}(0)/\lambda_{BCS}(T)]^2$, where $\lambda_{BCS}(T)$ is the BCS form, a quantity which varies exponentially slowly at low T.

We turn now to variational results, considering first $U_0 = 0$. In this case, both K_1 and K_2 are linear in temperature at low temperatures, as expected from the qualitative arguments given earlier. For $J_1/J_2 = 25$, $J_1(0) = 90.9$ K, and $\xi_0 = 10$ Å (values roughly appropriate to $YBa_2Cu_3O_{6.95}$), we estimate $\lambda_{ab}(0) = 2600$ Å and $d\lambda_{ab}/dT = 3.5$ Å/K. In Fig. 1 we plot $K_1(T)$ and $K_2(T)$ for these parameters. The low-temperature slopes of these curves are $dK_1/dT = 0.245$, $dK_2/dT = 0.018$. The corresponding $\Delta\lambda(T) \equiv \lambda_{ab}(T) - \lambda_{ab}(0)$ obtained from these data is shown in the inset.

The slopes $d\lambda_c/dT$ and $d\lambda_{ab}/dT$ depend on the assumed values of $J_1(0)$ and $J_2(0)$, and hence on $\lambda_c(0)$ and $\lambda_{ab}(0)$. Figure 2 exhibits this dependence for three choices of parameters, assuming $\xi_0 = 10$ Å. From top to bottom, these correspond to the (2D) limit of infinite anisotropy, the $YBa_2Cu_3O_{6.95}$ mass anisotropy of 25, and the isotropic 3D case. The ξ_0 dependence enters only as an overall scaling of the abscissa and ordinate—that is, $\xi_0^{-1/2}(d\lambda_{ab}/dT)_{T=0}$ has a *universal* dependence on $\xi_0^{-1/2}\lambda_{ab}(T = 0)$, independent of ξ_0, as indicated in the figure. Evidently, even in this simple model, the SCPP approximation can produce slopes of the order of the experimental values of 3.5–4.3 Å/K [1], depending on the assumed values of $\lambda(0)$ and of ξ_0.

Figure 3 shows the influence of charging effects. The parameters here are chosen purely for illustrative purposes, and are not intended to apply to specific real materials. For the cases shown, we use $J_1 > U_0 \simeq J_2$. The extra term adds a low-temperature curvature to $\Delta\lambda(T)$, which we expect to vary as T^3 for this assumed form of the charging energy. This temperature dependence is anticipated because the diagonal form of the charging energy allows for acoustic phase phonons, which would lead to a T^3 term in the specific heat, and also in $\Delta\lambda(T)$. The "Debye temperature" corresponding to these excitations may be extremely small, allowing the linear T dependence to persist to very low T.

If the Coulomb energy were *long range*, e.g., if $H_Q = [(e^*)^2/2]\sum_{ij} n_i n_j/|\mathbf{r}_i - \mathbf{r}_j|$, where $\mathbf{r}_i$ is the position of the ith grain, then the "acoustic phase phonons" would be driven up to a finite "Einstein" frequency, $\omega_E \equiv k_B T_E/\hbar$. The corresponding low-temperature thermodynamic properties, including the penetration depth, would have a dominant exponential temperature dependence below T_E, destroying, for sufficiently large T_E, the linear T dependence of $1/\lambda^2$.

This outcome can be avoided, and the low-temperature linear T dependence restored, by including Ohmic dissipation. Using a variational approach similar to ours, Chakravarty *et al.* [9] have shown that if an isotropic $H_{tot} = H + H_Q$ is coupled to an Ohmic heat bath, the transition to a phase coherent state occurs at a critical value of the intergranular shunt resistance R (of order $R_0 \equiv \hbar/e^2$, irrespective of the magnitude of the charging energy).

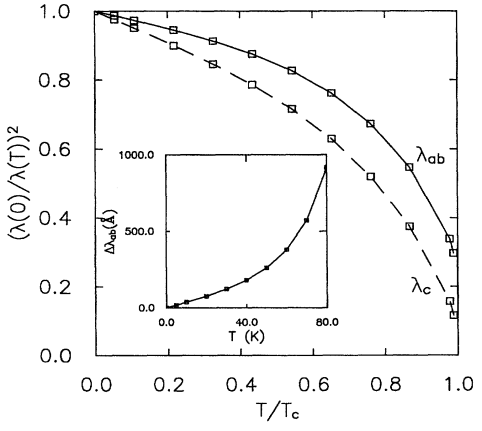

FIG. 1. Plot of $K_1(T)/K_1(0) \equiv [\lambda_{ab}(T)]^2$. Solid line corresponds to an in-plane penetration depth ($\mathbf{H}\|\mathbf{c}$) assuming $\lambda_{ab}(0) = 2600$ Å. Dashed line corresponds to $\lambda_c(\mathbf{H}\perp\mathbf{c})$ assuming anisotropy $[\lambda_{ab}(0)/\lambda_c(0)]^2 = 1/25$. Inset: plot of $\Delta\lambda(T) \equiv \lambda_{ab}(T) - \lambda_{ab}(0)$. At low temperatures, there is a linear temperature dependence with slope $d\lambda_{ab}/dT = 3.5$ K/Å.

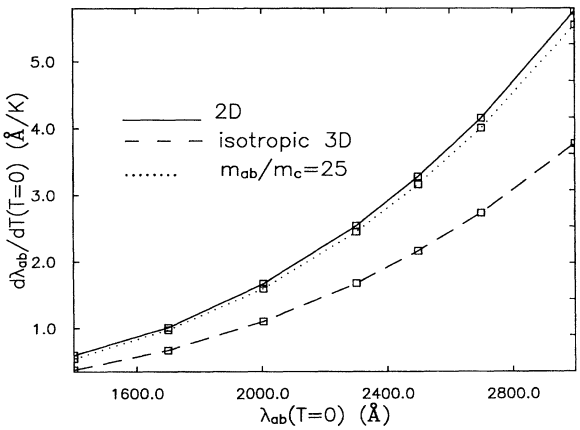

FIG. 2. Plot of $(d\lambda_{ab}/dT)_{T=0}$ as a function of $\lambda_{ab}(0)$ for three cases: 2D limit ("infinite anisotropy"), mass anisotropy approximately equal to that of $YBa_2Cu_3O_{6.95}$, and isotropic 3D limit. Right hand and top scales also show the "universal" dependence of $\xi_0^{-1/2}(d\lambda_{ab}/dT)_{T=0}$ upon $\xi_0^{-1/2}\lambda_{ab}(T = 0)$.

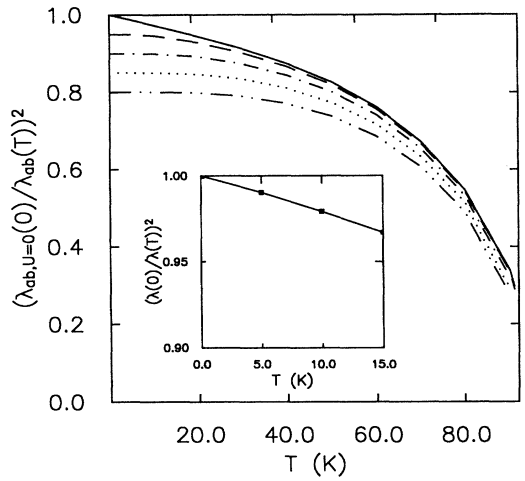

FIG. 3. Plots of $[\lambda_{ab}(0)/\lambda_{ab}(T)]^2$ for several different charging energies U_0 and zero dissipation: from top down, curves correspond to $U_0 = 0$, 1, 4, 9, and 16 K. Inset shows the combined effects of long-range Coulomb interaction and dissipation for dissipation parameter $\alpha = \pi\hbar/2e^2R = 8$ in an isotropic model, as described in the text.

We have extended these calculations to long-range Coulomb interactions, assuming that such a model, with dissipation, is properly applied to single-crystal high-T_c superconductors. Whenever R is small enough to allow a transition to phase coherence at $T = 0$, for both short-range and long-range Coulomb interactions of any strength, we find that at low T, $1/\lambda^2(T)$ varies *linearly* with T, the classical behavior is restored. As an illustration, the inset of Fig. 3 shows $1/\lambda^2(T)$ as calculated for an isotropic 3D superconductor with long-range charging energy and a dissipation coefficient, $\alpha \equiv (\pi/2)(\hbar/e^2)/R = 8$. This value is obtained by arbitrarily choosing $R \approx \xi_0^{-1}\rho_{ab}(T = T_c)$, where we take the grain size as $\xi_0 \approx 10$ Å and $\rho_{ab}(T = T_c) \approx 80\ \mu\Omega$ cm as the normal-state a-b resistivity of $YBa_2Cu_3O_{6.95}$ just above T_c. Note that this choice gives roughly the experimentally observed $d\lambda/dT = 3.5$ Å/K.

In conclusion, we have shown that phase fluctuations in a scalar order parameter produce a linear T dependence in $\lambda(T)$ in the classical limit. If quantum effects can be neglected, the slope can reach an order of magnitude comparable to the experimental value of 3.5 Å/K, when reasonable estimates of the zero-temperature penetration depth and anisotropy are incorporated. This T dependence remains when the combined influence of (short- or long-range) Coulomb interactions and shunt dissipation are variationally included in the calculation. Thus, these simple calculations suggest that thermodynamic phase fluctuations cannot be ignored in considering the low-temperature behavior of $\lambda_{ab}(T)$. Their effects should be ruled out before the behavior of $\lambda_{ab}(T)$, by itself, is used to infer conclusions regarding the symmetry of the order parameter in high-T_c superconductors.

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Note added.—Emery and Kivelson [15] have shown that a model mathematically resembling that of [9] can be derived for superconductivity in a bad metal *without* invoking a heat bath, yet still producing a linear T dependence of $1/\lambda(T)^2$ at low T for an isotropic or anisotropic material.

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