

## Phase fluctuations and spectral properties of underdoped cuprates

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We consider the effect of classical phase fluctuations on the quasiparticle spectra of underdoped high- $T_c$  cuprate superconductors in the pseudogap regime above  $T_c$ . We show that photoemission and tunneling spectroscopy data are well accounted for by a simple model in which mean-field  $d$ -wave quasiparticles are semiclassically coupled to supercurrents induced by fluctuating unbound vortex-antivortex pairs. We argue that the data imply that transverse phase fluctuations are important at temperatures above  $T_c$ , while longitudinal fluctuations are unimportant at all temperatures.

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### I. INTRODUCTION

It is now a well established experimental fact that the underdoped cuprate superconductors exhibit a ‘‘pseudogap’’ behavior above the superconducting critical temperature  $T_c$ , which is characterized by a vanishing superfluid density as obtained by transport measurements, but persistence of a gap in the quasiparticle excitation spectrum as measured by various spectroscopies.<sup>1</sup> Recent angle-resolved photoemission spectroscopy<sup>2-5</sup> (ARPES) and scanning-tunneling spectroscopy<sup>6,7</sup> (STS) experiments indicate that in the underdoped cuprates the gap evolves smoothly as the temperature is increased through  $T_c$ . Although the gap begins to fill in and the sharp quasiparticle peaks are lost above  $T_c$ , the position of the gap edge changes only slightly. This is in sharp contrast to the behavior of overdoped cuprates and conventional superconductors where the gap *closes* at  $T=T_c$ . It is further found that the gap *increases* as the doping concentration is reduced from its optimum value, while at the same time  $T_c$  decreases. This results in highly anomalous ratios  $2\Delta/k_B T_c$  that were reported to attain values of 12 or more in  $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$  (BiSCCO), compared to the weak coupling BCS value of 3.54. ARPES results also indicate that the angular dependence of the gap function on the Fermi surface, which below  $T_c$  follows the  $\Delta_{\mathbf{k}}=\Delta_d \cos(2\theta)$  shape expected for a  $d_{x^2-y^2}$  order parameter, develops extended gapless regions around the nodes above  $T_c$  whose size increases with  $T$ . Although a number of important experimental issues remains to be settled, such as the temperature at which the pseudogap closes and its possible persistence in optimally and even overdoped cuprates suggested by the recent STS results,<sup>6</sup> the basic picture of a superconducting quasiparticle gap persisting over a wide range of  $T>T_c$  in underdoped materials is well established.

Many theoretical concepts, including spin fluctuations,<sup>8</sup> condensation of preformed pairs,<sup>9</sup> SO(5) symmetry,<sup>10</sup> and spin-charge separation,<sup>11</sup> have been invoked to explain the pseudogap behavior. In this paper we study the implications of a scenario put forward by Emery and Kivelson<sup>12</sup> who, following earlier work of Uemura *et al.*,<sup>13</sup> proposed that the underdoped material above  $T_c$  is in a state with a nonzero *local* amplitude of superconducting pairing, but is not truly superconducting due to thermal fluctuations in the phase of the order parameter. Within such a scenario the transition at

$T_c$  is of the Kosterlitz-Thouless (KT) type, slightly rounded by the weak coupling between the copper-oxygen planes along the  $c$ -axis. In a strictly 2D system the KT transition is associated with proliferation of unbound vortex-antivortex pairs. Weak coupling between the planes leads to correlated motion between vortices in adjacent planes that form three dimensional (3D) vortex loops close to the critical temperature. The transition to the disordered phase is then characterized by the appearance of vortex loops with arbitrarily large radii.<sup>14</sup>

In the present paper we study the spectral properties of a superconductor in the incoherent state above the phase-disordering transition but below the mean-field transition at which the local gap forms. We find that fluctuating currents arising from unbound vortex-antivortex pairs can contribute significantly to the ARPES and STS line-shape broadening in the low-energy region of the spectrum. By analyzing the experimental data we estimate the strength of these superconducting phase fluctuations and we deduce the vortex core energy.

We model the underdoped cuprate superconductor as a set of independent 2D superconducting layers, each undergoing a KT transition at a temperature  $T_{KT}$  that we identify with the superconducting critical temperature  $T_c$ . The weak inter-plane coupling, which we neglect, will affect the very long length-scale physics (changing, e.g., the universality class of the transition from KT to 3D XY), but should not affect the shorter length-scale fluctuations that contribute to the electron spectral functions of interest here. The disordered state above  $T_{KT}$  can be thought of as a ‘‘soup’’ of fluctuating vortices with positive and negative topological charges and with total vorticity constrained to zero. Each of these vortices is surrounded by a circulating supercurrent which decays as  $1/r$  with the distance from the core. Such supercurrents, within a semiclassical approximation, lead to a Doppler-shifted local quasiparticle excitation spectrum of the form<sup>15,16</sup>

$$E_{\mathbf{k}}=E_{\mathbf{k}}^0+\hbar\mathbf{k}\cdot\mathbf{v}_s(\mathbf{r}), \quad (1)$$

where  $\mathbf{v}_s(\mathbf{r})$  is the local superfluid velocity and  $E_{\mathbf{k}}^0=\sqrt{\epsilon_{\mathbf{k}}^2+|\Delta_{\mathbf{k}}|^2}$  is the usual BCS spectrum. The change in the local excitation spectrum will affect the spectral properties of

the superconductor in that the physically relevant spectral function must be averaged over the positions of fluctuating vortices.

This effect will be particularly pronounced in a  $d$ -wave superconductor since Eq. (1) implies formation of a region on the Fermi surface with  $E_{\mathbf{k}} < 0$  around a nodal point for arbitrarily small  $\mathbf{v}_s(\mathbf{r})$ . Physically this corresponds to a region of gapless excitations on the Fermi surface that leads to a finite density of states (DOS) at the Fermi level. As first discussed by Volovik,<sup>17</sup> a similar situation arises in the *mixed* state of a  $d$ -wave superconductor where the superflow around the field-induced vortices leads to the residual DOS proportional to  $\sqrt{H}$ . This unusual field dependence arises because the distance between vortices in the vortex lattice  $d_v \sim H^{-1/2}$  and the average superfluid velocity projected onto a gap-node direction is proportional to  $d_v^{-1}$ . At low  $T$  and high field this implies a  $\sim T\sqrt{H}$  contribution to the electronic specific heat that was indeed observed in the measurements on  $\text{YBa}_2\text{Cu}_3\text{O}_{6.95}$  single crystals.<sup>18,19</sup> In the present case, instead of a regular Abrikosov lattice of field-induced vortices, we consider a fluctuating plasma of thermally induced vortices and antivortices. The essential physics however remains the same.

## II. THEORY: QUASIPARTICLE EXCITATIONS COUPLED TO PHASE FLUCTUATIONS

We shall be interested in how the supercurrents induced by phase fluctuations affect the spectral function of a superconductor  $A(\mathbf{k}, \omega) = -\pi^{-1} \text{Im} \mathcal{G}(\mathbf{k}, \omega)$ , which may be measured by ARPES and STS experiments. Here  $\mathcal{G}(\mathbf{k}, \omega)$  is the diagonal part of the full superconducting Green's function that solves the Gorkov equations for a  $d$ -wave superconductor, given in the Appendix. In the mean-field approximation (neglecting, among other things, phase fluctuations) the diagonal Green's function may be written as

$$\mathcal{G}_0^{-1}(\mathbf{k}, \omega) = \omega - \epsilon_{\mathbf{k}} + i\Gamma_1 - \frac{\Delta_{\mathbf{k}}^2}{\omega + \epsilon_{\mathbf{k}}}, \quad (2)$$

where, following Ref. 5, we have added to the usual mean-field solution a single-particle scattering rate  $\Gamma_1$ . Note that this form of the scattering rate in  $\mathcal{G}_0$  constitutes a nontrivial assumption. It is not pair breaking, in the sense that it is ineffective at small  $\omega$ ,  $\epsilon_{\mathbf{k}}$ , i.e., in the region  $\omega < E_{\mathbf{k}} \sim \sqrt{\epsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$ . By contrast, in a  $d$ -wave superconductor, a conventional scattering rate enters via the replacement  $\omega \rightarrow \omega + i\Gamma$ , leading to a broadening that is effective even at low  $\omega$ ,  $\epsilon_{\mathbf{k}}$ . As shown by Norman *et al.*<sup>5</sup> the form given in Eq. (2) agrees with the ARPES data at  $T < T_c$ . We demonstrate below that it also agrees with STS.

At  $T > T_c$  Norman *et al.*<sup>5</sup> showed that additional *pair-breaking* scattering is needed to account for the ARPES data, which they modeled phenomenologically by introducing another scattering rate  $\Gamma_0 \neq \Gamma_1$ , making a replacement  $\omega \rightarrow \omega + i\Gamma_0$  in the last term of Eq. (2). They suggested that  $\Gamma_0$  could arise from exchange of pair fluctuations; we find, by explicitly evaluating the corresponding propagator,<sup>20</sup> that this proposed mechanism does not account for the observed magnitude of  $\Gamma_0$ . This conclusion is supported by the results of Vilk and Tremblay.<sup>21</sup>

We now discuss what we believe to be a more likely source of the pair-breaking scattering, namely, supercurrents induced by phase fluctuations. In order to determine how  $\mathcal{G}_0$  is changed in the presence of superflow it is useful to recall the origin of the energy shift in Eq.(1). This can be derived<sup>15,16</sup> by assuming a state of *uniform* superflow with  $\mathbf{v}_s = \hbar \mathbf{q}/m$  (Ref. 22) induced by an order parameter of the form  $e^{2iq \cdot \mathbf{r}} \Delta_{\mathbf{k}}$ . By solving the appropriate set of Bogoliubov–de Gennes equations and retaining only terms to linear order in  $\mathbf{q}$ , one finds that the energy is modified as indicated in Eq. (1) while the coherence factors are to the same order unchanged. This result is then semiclassically extended to nonuniform situations by assuming slow spatial variations of  $\mathbf{v}_s(\mathbf{r})$ .

One can follow this exact procedure and solve the appropriate Gorkov equations for  $\mathcal{G}_{\mathbf{q}}$  in the presence of superflow. One finds (see Appendix) the following intuitively plausible result, which is exact for uniform flow up to terms linear in  $\mathbf{q}$ :<sup>23</sup>

$$\mathcal{G}_{\mathbf{q}}(\mathbf{k}, \omega) = \mathcal{G}_0(\mathbf{k} - \mathbf{q}, \omega - \eta), \quad (3)$$

where  $\eta \equiv \hbar \mathbf{v}_F(\mathbf{k}) \cdot \mathbf{q} \approx \hbar \mathbf{k} \cdot \mathbf{v}_s$ . Here  $\mathbf{v}_F(\mathbf{k}) = (\partial \epsilon_{\mathbf{k}} / \partial \mathbf{k})_{k=k_F} \approx \hbar \mathbf{k}_F / m$  is the Fermi velocity and the last equality holds when the Fermi surface is approximately isotropic. In the following we shall assume that Eq. (3) can be applied locally when  $\mathbf{v}_s(\mathbf{r})$  varies slowly in space. Applying the above prescription to Eq. (2) one finds, again to the leading order in  $\mathbf{q}$ ,

$$\mathcal{G}_{\mathbf{q}}^{-1}(\mathbf{k}, \omega) = \omega - \epsilon_{\mathbf{k}} + i\Gamma_1 - \frac{(\Delta_{\mathbf{k}} - \zeta)^2}{\omega + \epsilon_{\mathbf{k}} - 2\eta}, \quad (4)$$

where  $\zeta \equiv \mathbf{v}_{\Delta}(\mathbf{k}) \cdot \mathbf{q}$  with  $\mathbf{v}_{\Delta}(\mathbf{k}) = (\partial \Delta_{\mathbf{k}} / \partial \mathbf{k})_{k=k_F}$ . One can easily estimate  $v_{\Delta} / v_F \sim (\xi_0 k_F)^{-1} \sim \Delta_d / \epsilon_F$ , which is typically a small number in a superconductor. We therefore expect that  $\zeta \ll \eta$ . A more detailed numerical analysis indeed shows that, as long as  $\Delta_d / \epsilon_F$  is small compared to unity, the effect of  $\zeta$  on the spectral line shape is negligible compared to that of  $\eta$ , and will be dropped in the following.

A typical experimentally measured quantity, such as the ARPES or STS line shape, will provide information on  $\mathcal{G}_{\mathbf{q}}$  averaged over the phase fluctuations. Thus, we need to evaluate

$$\bar{\mathcal{G}}_{\mathbf{q}}(\mathbf{k}, \omega) = \int d\eta P(\eta) \mathcal{G}_{\mathbf{q}}(\mathbf{k}, \omega), \quad (5)$$

where  $P$  is the probability distribution of  $\eta$  given by

$$P(\eta) = \langle \delta[\eta - \hbar \mathbf{k} \cdot \mathbf{v}_s(\mathbf{r})] \rangle. \quad (6)$$

The angular brackets indicate thermodynamic averaging over the phase fluctuations in the ensemble specified by the 2D XY Hamiltonian<sup>12</sup>

$$\frac{\mathcal{H}_{XY}}{k_B T} = \frac{1}{2} V \left( \frac{2m}{\hbar} \right)^2 \int \mathbf{v}_s^2(\mathbf{r}) d^2 r, \quad (7)$$

where  $\mathbf{v}_s(\mathbf{r})$  is understood to contain both longitudinal (spin-wave-like) and transverse (vortexlike) excitations.  $V = V_0 / k_B T$  is a dimensionless coupling constant and  $V_0$  is related to the superfluid density  $n_s$  by  $V_0 = \hbar^2 n_s / 4m$ . In the nearest-neighbor XY model,  $k_B T_{KT} \approx 0.9 V_0$ ;<sup>12</sup> more gener-

ally  $k_B T_{\text{KT}} = (\pi/2) V_0 (T = T_{\text{KT}})$ .<sup>26</sup> Longitudinal phase fluctuations result in the spatial modulation of charge density and will be therefore suppressed by Coulomb interaction at long wavelengths. This interaction is not explicitly included in the XY Hamiltonian (7) but we return to it shortly.

The last term in Eq. (2) can be thought of as a superconducting self-energy  $\Sigma_s(\omega, \mathbf{k})$ . Equations (4) and (5) then imply that the primary effect of the phase fluctuations is to smear the functional dependence of  $\Sigma_s(\omega, \mathbf{k})$  on the energy variable, broadening the spectral line shape. A more detailed analysis shows that  $\eta$  acts primarily to fill in the gap, in a way similar to the inverse pair lifetime  $\Gamma_0$  introduced by phenomenological considerations in Ref. 5.  $\Gamma_1$ , on the other hand, does not affect the line shape at low energies: notice that  $\mathcal{G}_0(\mathbf{k}_F, \omega = 0) = 0$  for any  $\Gamma_1$ .

We now give a quantitative description of this broadening by explicitly evaluating  $P(\eta)$  and the resulting line shapes as a function of temperature. Making use of the identity  $\delta(x) = (2\pi)^{-1} \int ds e^{isx}$ , Eq. (6) becomes

$$P(\eta) = \frac{1}{2\pi} \int_{-\infty}^{\infty} ds e^{is\eta} \langle e^{-is\hbar\mathbf{k}\cdot\mathbf{v}_s(\mathbf{r})} \rangle. \quad (8)$$

To the leading order in cumulant expansion one can write  $\langle e^{-is\hbar\mathbf{k}\cdot\mathbf{v}_s(\mathbf{r})} \rangle = \exp[-\frac{1}{2}s^2\hbar^2 k_\alpha k_\beta \langle v_s^\alpha v_s^\beta \rangle]$ , where summation over repeated indices is implied and the spatial variable has been suppressed. This statement becomes exact when the transverse fluctuations can be represented by Gaussian degrees of freedom, as is done in the Debye-Hückel approximation employed below. The  $s$  integral in Eq. (8) can now be explicitly carried out, yielding a Gaussian distribution

$$P(\eta) = (2\pi W)^{-1/2} e^{-\eta^2/2W}, \quad (9)$$

with  $W = \hbar^2 k_\alpha k_\beta \langle v_s^\alpha v_s^\beta \rangle$ . We have thus reduced the problem of finding the probability distribution  $P$  to evaluation of a correlator  $\langle v_s^\alpha v_s^\beta \rangle$ . For a 2D system described by the Hamiltonian (7), this correlator has been considered by Halperin and Nelson.<sup>27</sup> They found, using a Debye-Hückel approximation valid for  $T$  well above  $T_{\text{KT}}$ ,

$$\langle v_s^\alpha(\mathbf{p}) v_s^\beta(-\mathbf{p}) \rangle = \frac{\hbar^2}{2m^2 V} \left[ \frac{p_\alpha p_\beta}{p^2} + \frac{\delta_{\alpha\beta} - p_\alpha p_\beta / p^2}{1 + c_3 \xi_c^2 p^2 / 4\pi^2 V} \right], \quad (10)$$

where  $\mathbf{v}_s(\mathbf{p}) = \int d\mathbf{r} e^{-i\mathbf{p}\cdot\mathbf{r}} \mathbf{v}_s(\mathbf{r})$ . The first term in brackets comes from the longitudinal and the second from the transverse fluctuations.  $c_3 = (2E_c - \pi^2 V_0) / k_B T$  is a dimensionless quantity related to the density of vortices,  $E_c$  is the vortex core energy, and  $\xi_c$  is the core cutoff.

Upon averaging over fluctuations the translational invariance is restored and we may evaluate the real-space correlator at  $\mathbf{r} = 0$ :

$$\langle v_s^\alpha(0) v_s^\beta(0) \rangle = \frac{1}{(2\pi)^2} \int d^2 p \langle v_s^\alpha(\mathbf{p}) v_s^\beta(-\mathbf{p}) \rangle. \quad (11)$$

Explicit integration finally yields, for  $|\mathbf{k}| = k_F$ ,

$$W = \frac{\pi^3 \Delta_d^2}{8V} \left[ 1 + \frac{V}{c_3} \ln \left( 1 + \frac{c_3}{V} \right) \right]. \quad (12)$$

The short wavelength divergence in Eq. (11) has been cut off at  $q_c = 2\pi / \xi_c$  and we used the BCS relation  $\xi_c = \hbar v_F / \pi \Delta_d$ . The first term in brackets comes from longitudinal fluctuations and would be suppressed in realistic models in which the Coulomb interaction is important. The second term,  $\alpha_v \equiv (V/c_3) \ln(1 + c_3/V)$ , comes from transverse fluctuations due to vortices, and is always positive and smaller than 1 (this follows since  $c_3 > 0$  is required by the stability of the system). To the extent that  $E_c$  is independent of temperature, the ratio  $c_3/V$ , and therefore  $\alpha_v$ , is  $T$  independent. The primary  $T$  dependence of  $W$  therefore comes from  $V$  in the prefactor. After expressing  $V_0$  in terms of  $T_{\text{KT}}$ ,  $W$  may be written as

$$W \approx 3.48(1 + \alpha_v)(T/T_{\text{KT}}) \Delta_d^2. \quad (13)$$

Equations (4), (5), and (9) describe the effect of classical phase fluctuations on the spectral function of a superconductor. From the knowledge of such a spectral function one can compute the respective ARPES and STS line shapes, extract the parameter  $W$ , and compare it with the prediction given by Eq. (13). This will be done in the next section, but we first discuss the validity and some qualitative aspects of the results presented above.

Our results depend on three assumptions; that the electron Green's function may be calculated using semiclassical methods, that the phase fluctuations are quasistatic, and that there is a sufficiently wide KT temperature regime in which reasonably well-defined vortex-antivortex plasma exists. The first of these assumptions applies when the coherence length is sufficiently larger than the inter electron spacing (i.e.,  $k_F \xi \gg 1$ ) and is the same assumption as underlies Volovik's prediction<sup>17</sup> of a  $\sim T\sqrt{H}$  dependence of the specific heat in the mixed state of a  $d$ -wave superconductor. As this behavior is observed in  $\text{YBa}_2\text{Cu}_3\text{O}_7$  (Refs. 18 and 19), we believe that this assumption is well justified. The second assumption, of quasistatic phase fluctuations, has two parts. The transverse fluctuations come from vortices, so for them the essential assumption is that vortices move slowly compared to electrons. This is justified by Bardeen-Stephen results, which imply that vortex motion is overdamped and thus diffusive, and so surely slower than the ballistic motion of the electrons. For longitudinal fluctuations the situation is less clear. If the hypothesis of Emery and Kivelson that they are classical (i.e., that at  $q \sim \xi_c^{-1}$  we have  $\omega_q \ll T$ ) (Ref. 12) is accepted, then Eq. (10) applies. However, as we shall see, the data contradict this. A more likely scenario is that Coulomb interaction pushes the longitudinal fluctuations up to the plasma frequency, in which case the coupling to electrons is very weak and one should simply remove the longitudinal fluctuations from the theory. We shall see that the data are consistent with this picture. If (for some as yet unknown reason) the longitudinal fluctuations are collective modes with a velocity of the order of the Fermi velocity, then our results do not apply. The final assumption, of a wide temperature regime between the mean-field and KT transitions, is the most difficult to justify, except on empirical grounds. This hypothesis was proposed in Ref. 12 and our results are consistent with it. The theoretical justification for the existence of a wide intermediate regime in a clean system must involve proximity to a Mott insulating phase, which sup-

presses the superfluid stiffness and hence  $T_{KT}$ , but does not suppress the pairing. A detailed theoretical treatment in two dimensions has not been given.

As mentioned above,  $W$  given by Eq. (13) describes both longitudinal and transverse fluctuations of the phase and can be written accordingly as  $W = W_L + W_T$ , where

$$W_L \approx 3.48(T/T_{KT})\Delta_d^2, \quad (14)$$

$$W_T \approx 3.48\alpha_v(T/T_{KT})\Delta_d^2. \quad (15)$$

The expression for  $W_T$  is valid at temperatures well above  $T_{KT}$ , where all pairs can be thought of as unbound and thermal energy dominates over the intervortex interaction.<sup>26</sup> Well below  $T_{KT}$ , on the other hand, we expect  $W_T = 0$  since the vortices appear only in tightly bound pairs that contribute negligible supercurrent beyond the lengthscale set by the pair size and the pair density is exponentially small  $\sim e^{-2E_c/k_B T}$ . By numerically integrating the appropriate scaling relations<sup>27</sup> one could in fact obtain  $W_T$  at all temperatures. However, such level of detail is beyond the scope of this paper and we shall confine ourselves to the limiting cases stated above and note that  $W_T$  has nonsingular monotonic behavior across  $T_{KT}$ .

The expression, Eq. (14), for  $W_L$  is expected to be valid down to low temperatures, provided quantum fluctuations and the Coulomb interaction can be neglected. In a  $d$ -wave superconductor the temperature dependence of  $W_L$  will be modified by the  $T$ -linear temperature dependence of the superfluid density<sup>28</sup>  $n_s \sim \lambda^{-2}(T)$  that enters the definition of  $V_0$  in the  $XY$  Hamiltonian (7). It is interesting to note that at temperatures below  $T_c$ , say at  $T = T_c/2$ , Eq. (14) implies  $W_L \approx \Delta_d^2$ , i.e., large broadening of the spectral function by longitudinal fluctuations. Such a large broadening, comparable to the gap itself, would completely obliterate any signature of the gap in the excitation spectrum. Clearly, this is not observed experimentally.<sup>2,3,6</sup> As shown below and in Ref. 5, experimental data are consistent with  $W = 0$  below  $T_c$ . We must therefore conclude that longitudinal fluctuations are strongly suppressed by the Coulomb interaction as suggested in Ref. 29. On the same grounds we may argue that the observed linear temperature dependence of the magnetic penetration depth<sup>28</sup> is not due to phase fluctuations, as suggested by some authors,<sup>30,31</sup> but due to thermally excited quasiparticles in the nodes of the  $d$ -wave gap.<sup>32</sup> Transverse fluctuations, on the other hand, result in no net charge displacement and are thus unaffected by Coulomb interaction.

### III. COMPARISON TO EXPERIMENTAL DATA

#### A. Photoemission

As shown by Norman *et al.*,<sup>3</sup> a particularly simple relationship exists between the spectral function of a superconductor and a *symmetrized* ARPES spectrum at the Fermi surface,

$$I_S(\omega) \propto \bar{A}(\mathbf{k}_F, \omega), \quad (16)$$

where  $I_S(\omega) = I(\omega) + I(-\omega)$  and  $I(\omega)$  is the measured ARPES line shape. The advantage of this symmetrized representation is that the thermal broadening due to the Fermi functions is automatically subtracted out. The proportionality

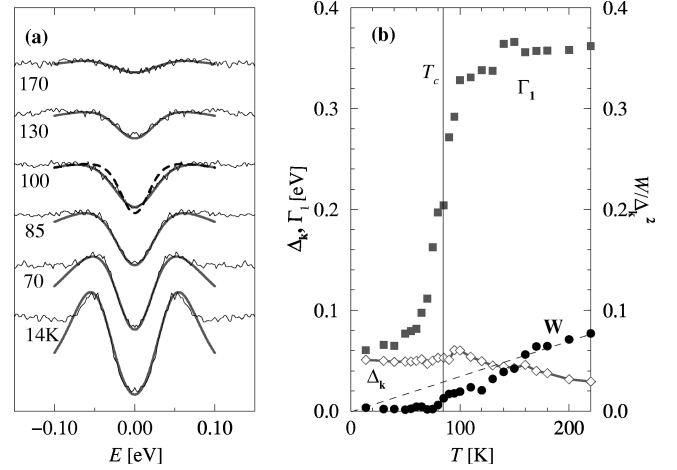


FIG. 1. (a) Symmetrized ARPES line shapes  $I_S(\omega)$  at momentum near  $(\pi, 0)$  from Ref. 5 (thin line) and our fits to the spectral function (thick line) at selected temperatures. The dashed line illustrates fit with  $W = 0$ . Region of the fit is  $|\omega| < 80$  meV. (b) Parameters of the fit as a function of  $T$ .

(16) is expected to hold for  $|\omega|$  less than a few tens of meV and remains valid in the presence of a symmetric energy-resolution function. We first discuss qualitative features of our predicted line shape and the experimental data, and then present results of a detailed fitting procedure.

The symmetrized experimental ARPES line shapes for the 83-K underdoped BiSCCO sample of Ref. 5 for the  $\mathbf{k} = \mathbf{k}_F$  vector along the  $(0, 0) \rightarrow (0, \pi)$  direction at selected temperatures are shown in Fig. 1(a). Below  $T_c$  we wish to model these line shapes by the spectral function corresponding to Eq. (2), which for  $\mathbf{k} = \mathbf{k}_F$ ,  $\epsilon_{\mathbf{k}_F} = 0$  becomes

$$I_S(\omega) \propto A_0(\mathbf{k}_F, \omega) = \frac{1}{\pi} \frac{\Gamma_1}{(\omega - \Delta_{\mathbf{k}}^2/\omega)^2 + \Gamma_1^2}. \quad (17)$$

As noted in Ref. 5, this functional form indeed describes the data below  $T_c$  well, after it is convolved in  $\omega$  with a Gaussian of width  $\sigma = 13.5$  meV representing the estimated experimental resolution. Qualitatively,  $\Delta_{\mathbf{k}}$  sets the position of the quasiparticle peaks and  $\Gamma_1$  (together with  $\sigma$ ) sets their width. Note that for  $\Gamma_1 = \sigma = 0$  the above line shape consists of two  $\delta$  functions at  $\omega = \pm \Delta_{\mathbf{k}}$ . It is thus clear that fairly large values of  $\Gamma_1$  in Eq. (17) are needed in order to obtain quasiparticle peaks of the correct width. Even for large  $\Gamma_1$  the theoretical line shape  $I(\omega)$  tends to zero for  $|\omega|$  larger than several  $\Delta_{\mathbf{k}}$ , while the experimental line shape saturates to a finite value. Understanding this large- $\omega$  background presents a challenge for any theory of ARPES in the cuprates and is beyond the scope of this paper. Here we focus on the low-energy region of the spectrum where we may reasonably expect the present simple model to be valid.

For  $\sigma \ll \Gamma_1$  one can easily estimate  $I_S(0) \approx I_0(\Gamma_1 \sigma^2 / \Delta_{\mathbf{k}}^4)$  and  $I_S(\Delta_{\mathbf{k}}) \approx I_0 \Gamma_1^{-1}$ . The peak to valley ratio

$$\kappa \equiv \frac{I_S(\Delta_{\mathbf{k}})}{I_S(0)} \approx \frac{\Delta_{\mathbf{k}}^4}{\Gamma_1^2 \sigma^2} \quad (18)$$

is independent of the unknown prefactor  $I_0$  and can be easily extracted from the raw data. Assuming fixed  $\Delta_{\mathbf{k}}$  one can thus

obtain reliable estimates of  $\Gamma_1$  without performing detailed fits. In particular, application of Eq. (18) to the data in Fig. 1(a) implies that  $\Gamma_1$  grows by about a factor of 6 between  $T=14$  K and 100 K. The above analysis also implies that at low  $\omega$  the line shape depends crucially on the experimental resolution  $\sigma$ . For instance, decreasing  $\sigma$  by a factor of 2 the ratio  $\kappa$  should grow by a factor of 4. Confirming this prediction experimentally would be a valuable test of the present model.

Above  $T_c$  Eq. (17) no longer provides a good fit for the data. The reason for this is the persistence (up to  $\sim 200$  K) of a well-defined edgeline feature around  $\omega = \Delta_{\mathbf{k}}$  along with a pronounced increase in the low- $\omega$  density of states. This behavior cannot be modeled by further increasing  $\Gamma_1$  since the values needed to fix  $I(0)$  would rapidly smear the edge. Inclusion of the phase fluctuations, i.e., finite  $W$  in the averaged spectral function (5), rectifies this problem. Analytically it is somewhat difficult to discuss the combined effect of  $W$ ,  $\Gamma_1$ , and  $\sigma$  on the line shape. Qualitatively one can show that the primary effect of increasing  $W$  is to ‘‘fill in’’ the gap. This is precisely what is needed to describe the ARPES data above  $T_c$ .

Figure 1(a) shows our fit to the symmetrized ARPES line shapes for the underdoped sample for a momentum near  $(0, \pi)$  (zone face) using a numerical computation of the full spectral function extracted from Eq. (5). Least-square fits in which  $\Delta_{\mathbf{k}}$ ,  $\Gamma_1$ , and  $W$  were taken as free parameters, were performed after convolving the spectral function  $\bar{A}(\mathbf{k}_F, \omega)$  with experimental resolution  $\sigma = 13.5$  meV. In the low-energy region  $|\omega| \leq 80$  meV, where the simple model Green’s function approach with  $\omega$ -independent scattering rate  $\Gamma_1$  is expected to be valid, the fits are excellent for all temperatures. The extracted parameters are displayed in Fig. 1(b). Both  $\Delta_{\mathbf{k}}$  and  $\Gamma_1$  behave in the way expected for an underdoped cuprate: the gap is approximately constant across  $T_c$  while the scattering rate rises sharply below  $T_c$  and saturates at higher temperatures. In the present model the large increase in  $\Gamma_1$  is required to wipe out the quasiparticle peaks.  $W$  also behaves as anticipated from the above considerations. At low temperatures  $W \approx 0$  indicating that below  $T_c$  the phase fluctuations are negligible; vortices appear only in tightly bound pairs and longitudinal fluctuations are suppressed by the Coulomb interaction. Above  $T_c$  fluctuations become important (pairs unbind) and  $W$  approaches the  $T$ -linear behavior consistent with Eq. (13). We stress here that a good fit to the data *requires*  $W > 0$  above  $T_c$ . This is illustrated by the dashed line in Fig. 1(a) that represents the fit to the 100-K line shape with  $W = 0$  and the gap value restricted to  $\Delta_{\mathbf{k}} \leq \Delta_{\mathbf{k}}(T=0)$ .<sup>33</sup> We note, however, that in this model much of the observed low- $\omega$  density arises from the large value of  $\Gamma_1$  in combination with the instrumental resolution. It is possible (and is indeed suggested by the analysis of the STS data in the next section) that the large  $\Gamma_1$  contribution is an artifact, arising from a combination of experimental resolution in the photoemission experiments and inadequacies of our theoretical model. We therefore regard the values of  $W$  obtained here as underestimates.

From the slope of  $W(T)$ , assuming that transverse fluctuations are dominant, we estimate  $\alpha_v \approx 0.009$  implying the vortex core energy  $E_c/V_0 \approx 360$ . This value is much larger

than the usual condensation energy in the vortex core  $E_c \approx 2V_0$ .<sup>16</sup> Within the Debye-Hückel approximation the vortex density can be estimated as  $\rho_v = \xi_c^{-2}(\pi/c_3)(1 - \alpha_v) \approx \xi_c^{-2}(T/T_{KT})(V/c_3)$ , for  $\alpha_v \ll 1$  and  $k_B T_{KT} \approx V_0$ . This implies, for the parameters extracted from ARPES data,  $\rho_v \approx 4.3 \times 10^{-3} \xi_c^{-2}(T/T_{KT})$ . It is remarkable that such a small density of vortices leads to significant broadening of the line shape. We should also remark that for such a small density of vortices one may question the validity of Debye-Hückel approximation at temperatures in consideration. We emphasize, however, that only our interpretation of  $W$  and in particular the estimates of  $E_c$  and  $\rho_v$  depend on the validity of this approximation. Our analysis of the line shapes is quite general, since we treat  $W$  as a free parameter of the model.

We have performed similar fits for an overdoped 82-K BiSCCO sample of Ref. 5. Our results are consistent with  $\Delta_{\mathbf{k}}$  vanishing close to  $T_c$  and, within statistical noise,  $W = 0$  at all temperatures. This indicates that phase fluctuations are unimportant in overdoped cuprates and the transition is essentially mean field-like.

We now consider ARPES data at the Fermi crossing close to the gap node direction  $(\pi, \pi)$ . These indicate extended regions of gapless excitations above  $T_c$  that grow in size with temperature.<sup>2,3,5</sup> This is not reproduced by the simple model we have considered so far. The reason is that adding the  $\hbar \mathbf{v}_s \cdot \mathbf{k}$  term to the quasiparticle energy [cf. Eq. (3)] effectively depletes the local spectral function for  $\mathbf{v}_s$  parallel to  $\mathbf{k}$  but enhances it by equal amount for opposite  $\mathbf{v}_s$ . Upon averaging over all directions of  $\mathbf{v}_s$  (for fixed  $\mathbf{k}$ ) the net effect is to broaden the mean-field line shapes as seen in Fig. 1(a). Phase fluctuations cause no net depletion of the spectral weight near the gap nodes.

In order to account for the ARPES data the form of  $\Delta_{\mathbf{k}}$  must change. Since the supercurrent flowing around individual vortices is pair breaking, it is in principle possible that it will alter the internal structure of the self-consistent gap function in addition to usual suppression of the order parameter in the core. A similar scenario has been proposed by Haas *et al.*<sup>35</sup> who considered the effect of nonmagnetic impurities on a  $d$ -wave gap function. They found that it was possible to construct a gap function such that with increasing disorder nodes indeed expanded into finite gapless arcs. Intuitively this effect can be understood on the grounds that a smaller gap near the nodes is more susceptible to the pair breaking. In the present case pair breaking is caused by supercurrents rather than impurities, but the physics remains the same.

In order to substantiate this idea we have solved the self-consistent gap equation for a  $d$ -wave superconductor in the presence of *uniform* superflow. We considered a model gap function of the form  $\Delta_{\mathbf{k}} = \Delta_d \cos(2\theta) + \Delta'_d \cos(6\theta)$  with the appropriately generalized pairing interaction.<sup>35</sup> We found that, for a system with  $\Delta'_d < 0$  in the absence of superflow, a transition to  $\Delta'_d > 0$  occurs when sufficiently strong supercurrent flows in the direction close to the nodal vector  $\mathbf{k}_n$ ; i.e., when  $|\mathbf{v}_s \cdot \hat{\mathbf{k}}_n| > b \Delta_d / \hbar k_F$ , with  $b \approx 0.7$  a model dependent constant. The state with  $\Delta'_d > 0$  exhibits extended gapless regions (cf. Fig. 2) while that with  $\Delta'_d < 0$  only the usual point nodes. Extrapolating this behavior to the supercurrent flowing around the vortex we argue that a region of extended

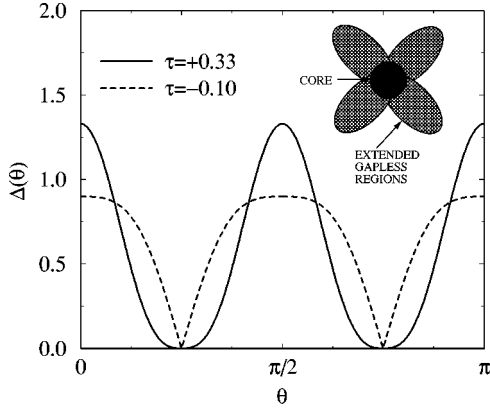


FIG. 2. Model gap function  $\Delta(\theta) = \Delta_d \cos(2\theta) + \Delta'_d \cos(6\theta)$  with  $\tau \equiv \Delta'_d/\Delta_d$  positive (extended nodes) and negative (point nodes). Inset illustrates the proposed real-space electronic structure of the vortex in a  $d$ -wave superconductor.

gapless excitations may form in the vicinity of the core. Such a region would have the shape of a four-leaf clover (schematically depicted in the inset of Fig. 2) and a spatial extent of several  $\xi_c$ . A truly quantitative treatment of this effect is complicated because it involves self-consistently solving the  $d$ -wave vortex problem, which is a highly nontrivial task.<sup>36</sup> We note, however, that recent STS data on vortices in BiSCCO (Ref. 37) show a peculiar pseudogap behavior near the vortex core, which may be indicative of a formation of the gapless regions around a vortex proposed above.

Assuming that this picture is correct, it is clear that in the vortex-antivortex plasma above  $T_c$ , upon averaging over fluctuations, ARPES will detect a gap function strongly suppressed for  $\mathbf{k}$  close to the nodes. Furthermore, with increasing temperature the volume fraction of gapless regions will grow (since the vortex density grows) leading to larger gapless areas on the Fermi surface in agreement with experimental observation.

### B. Tunneling

Tunneling conductance, the quantity measured by STS, is related to the spectral function of the superconductor by

$$g(E) = - \int_{-\infty}^{\infty} d\omega f'(\omega - E) \sum_{\mathbf{k}} |M_{\mathbf{k}}(\omega)|^2 \bar{A}(\mathbf{k}, \omega), \quad (19)$$

where  $f$  is the Fermi function and  $M_{\mathbf{k}}(\omega)$  is the tunneling matrix element, usually approximated by a constant. Tunneling conductance reflects the spectral function averaged over the entire Brillouin zone and broadened in the energy variable by the Fermi function. Thus, unlike in the ARPES line-shape function  $I_S(E)$ , quasiparticle peaks in  $g(E)$  will be broadened even in the absence of scattering and at  $T=0$ . For measurements performed on similar samples one would thus expect ARPES spectra to be much sharper than STS spectra, at any temperature. Figure 3(a) displays  $g(E)$  as measured by STS on the 83-K underdoped BiSSCO sample of Ref. 6. Surprisingly, we observe that at lowest available temperatures the STS line is in fact *sharper* than the ARPES line. As discussed in the previous section the broadening of the ARPES line comes exclusively from the scattering and ex-

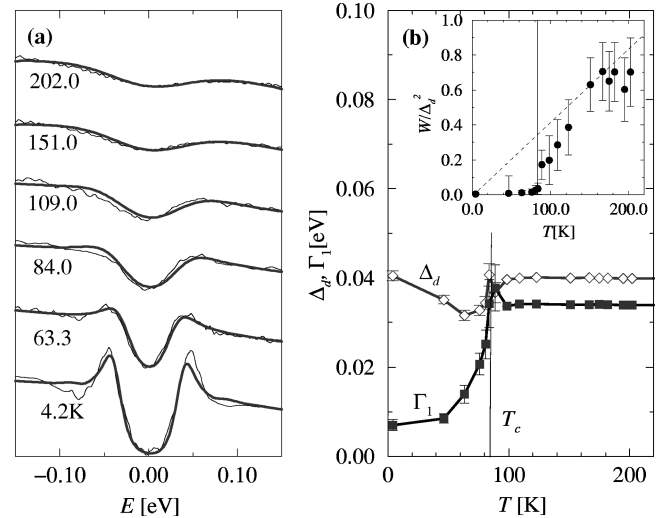


FIG. 3. (a) Fit to the STS data of Ref. 6 at selected temperatures. (b) Parameters of the fit as a function of  $T$ . Above  $T_c$  both  $\Delta_d$  and  $\Gamma_1$  are fixed to their values at 84 K.

perimental resolution. Therefore, inspection of the raw data suggests that the scattering rate  $\Gamma_1^{\text{STS}}$  will be much smaller than  $\Gamma_1^{\text{ARPES}}$ . This conclusion is indeed borne out by the detailed fitting procedure carried out below. This is a rather surprising result that we discuss more fully in the next section.

As seen from Eq. (19), modeling of the tunneling conductance requires knowledge of the band structure away from the Fermi surface and is therefore somewhat more involved than that of ARPES. Nevertheless, we find that assuming a simple free-electron dispersion with cylindrical Fermi surface and  $\Delta_{\mathbf{k}} = \Delta_d \cos(2\theta)$ , provides a reasonable fit for the data at low temperatures, provided that one compensates for the asymmetric background conductance and assumes a  $\theta$ -dependent matrix element  $M_{\mathbf{k}}(\omega) \propto |\cos(2\theta)|$ . The latter assumption is motivated by band-structure calculations<sup>38</sup> that indicate that tunneling between layers is dominated by the regions on the Fermi surface close to the  $(0, \pi)$  points. As shown in Fig. 3(a), this  $\theta$  dependence allows one to simultaneously account for the sharp quasiparticle peak and the wide gap in the STS line. Assuming  $M_{\mathbf{k}}(\omega) = \text{const}$  leads to broader peaks and sharper V-shaped gap structure, inconsistent with experimental data. We further remark that our simple model does not (and is not expected to) explain the pronounced dip feature appearing in the spectrum at higher energies, whose origin is at present unknown. Over the range  $T < T_c$ ,  $\Gamma_1^{\text{STS}}$  has similar qualitative behavior as  $\Gamma_1^{\text{ARPES}}$  [compare Figs. 1(b) and 3(b)], but remains about one order of magnitude smaller. We have attempted to reconcile the two sets of data by considering a more realistic band structure and  $\theta$ -dependent scattering rate in Eq. (19). However, even under the most favorable conditions  $\Gamma_1^{\text{STS}}$  remains a factor of 5–6 smaller than  $\Gamma_1^{\text{ARPES}}$ .

Above  $T_c$  the STS line does not have enough features to permit a meaningful three-parameter fit. In particular the sharp gap edge completely disappears above 100 K, which leads to ambiguity in defining  $\Delta_d$  from the data. Based on our previous finding (from the ARPES data) that both  $\Delta_d$  and  $\Gamma_1$  exhibit only weak  $T$  dependence above  $T_c$ , we fix

these two parameters at their respective values at 84 K (40 meV and 34 meV) and extract the temperature dependence of  $W$ . This appears to us as a reasonable procedure, which we further check by performing two-parameter fits with  $\Delta_d$  held constant or slowly decreasing with temperature as implied by Fig. 1(b).  $W$  is shown in the inset to Fig. 3(b). Its qualitative behavior is similar to that of  $W^{\text{ARPES}}$  but the amplitude is roughly factor of 10 *larger*. The difference is caused in part by the much smaller value of  $\Gamma_1$  discussed above. Part of the discrepancy between  $W^{\text{ARPES}}$  and  $W^{\text{STS}}$  can presumably be attributed to differences in material and experimental uncertainties, as well as the failure of our fit to account for the temperature variation of  $\Gamma_1$ , which according to Fig. 1(b) grows by another factor of 2 between 80 K and 200 K. Nevertheless, after accounting for these factors, considerable discrepancy remains in place, which is not understood at present. We estimate  $\alpha_v \approx 0.097$  which implies the vortex core energy  $E_c \approx 22V_0$  and vortex density  $\rho_v \approx 8.7 \times 10^{-2} \xi_c^{-2} (T/T_{\text{KT}})$ . The value of  $E_c/V_0$  is still large compared to the conventional estimate of the condensation energy in the core  $E_c \approx 2V_0$ ,<sup>16</sup> but is consistent with large core energy  $E_c \approx 26V_0$  deduced from lower critical field measurements of  $\text{YBa}_2\text{Cu}_3\text{O}_{6.95}$  at  $T=0$ .<sup>34</sup> We note that  $E_c$  is a cutoff-dependent quantity and therefore the precise numerical value quoted here should be accepted with that in mind. It is also possible that the large value of the ratio  $E_c/V_0$  is due to an unusually small  $V_0$  rather than unusually large  $E_c$ . Indeed, the vortex core energy is typically of the order of Fermi energy. An estimate of  $V_0$  given in Ref. 29,  $5 < V_0 < 10$  meV, implies  $E_c \sim 0.1\text{--}0.2$  eV, in reasonable agreement with many theories of underdoped cuprates, which suggest a Fermi energy of the order of the exchange constant  $J \sim 0.15$  eV.

#### IV. DISCUSSION

The qualitative behavior of ARPES and STS line shapes in underdoped BiSCCO clearly establishes the existence of a scattering mechanism that becomes operative at  $T > T_c$  and that acts primarily to fill in the gap at low energies. We have shown that transverse phase fluctuations associated with proliferation of unbound vortex-antivortex pairs in the system provide a reasonable explanation for this scattering. Our analysis also indicates that longitudinal (spin-wave) fluctuations are almost completely suppressed, above and below  $T_c$ . It has been proposed<sup>30,31</sup> that in high- $T_c$  materials, longitudinal phase fluctuations governed by the XY Hamiltonian (7) are important in that they significantly contribute to the observed temperature dependence of the magnetic penetration depth.<sup>28</sup> We have calculated the broadening of the spectral function that would be caused by these fluctuations, and found it to be much greater than the experimental data would permit. We therefore conclude that longitudinal fluctuations are suppressed, perhaps by the Coulomb interaction as suggested in Ref. 29.

Quantitatively there exists considerable discrepancy between the parameters describing the ARPES and STS line shapes, in particular the single-particle scattering rate  $\Gamma_1$  and phase fluctuation broadening  $W$ . Since the discrepancy is apparent at low temperatures and in overdoped cuprates we are led to believe that the problem lies primarily in our lack

of detailed understanding of the line shapes rather than the physics of phase fluctuations above  $T_c$ . The most disturbing is almost an order of magnitude difference between  $\Gamma_1^{\text{ARPES}}$  and  $\Gamma_1^{\text{STS}}$  found below  $T_c$ , which is implied directly by the raw data. In view of the fact that both measurements pertain to underdoped BiSCCO crystals with similar critical temperatures, it appears unreasonable to attribute such a large discrepancy to the material differences. We speculate that the large scattering rate needed to fit the ARPES data is an artifact related to our incomplete understanding of the photoemission process in the superconductor, which is theoretically not completely understood even in simple metals.<sup>25</sup> Tunneling spectroscopy, on the other hand, is a technique well established in superconductors. We therefore surmise that parameters obtained from STS more directly reflect the underlying physics. Indeed  $\Gamma_1^{\text{STS}} \approx 8$  meV at 4.2 K is comparable to the scattering rates deduced from transport measurements<sup>39,40</sup> on underdoped cuprates, and  $E_c^{\text{STS}} \approx 22V_0$ , although large for a conventional superconductor, is perhaps not unreasonable in cuprates.<sup>34</sup> Consequently, ARPES line shapes appear to reflect significant extrinsic broadening of unknown origin. The puzzling aspect of this interpretation is that the additional physics in the ARPES spectra enters as a *multiplicative* rather than additive factor to the apparent scattering rate; cf.  $\Gamma_1^{\text{ARPES}} \approx 8\Gamma_1^{\text{STS}}$  over the entire temperature range below  $T_c$ , in which  $\Gamma_1$  changes by a factor of 6. It is also possible that in the cuprates the  $c$ -axis tunneling matrix element  $M_{\mathbf{k}}(\omega)$  introduced in Eq. (19) is itself anomalous. Improving the energy resolution  $\sigma$  of ARPES could shed some light on this issue. As noted below Eq. (18) the ARPES line shapes are strongly affected by experimental resolution at small  $\omega$ . If the model Green's function (2) is correct, a factor of 2 improvement in  $\sigma$  should lead to considerable decrease in the measured intensity at  $\omega=0$  but almost no change in the width or height of the quasiparticle peaks at  $|\omega| = \Delta_{\mathbf{k}}$ .

Finally we note that sizable transverse phase fluctuations implied by this work will also affect other properties of the underdoped systems, such as the electronic specific heat, fluctuation diamagnetism, and transport. Vortices existing above  $T_c$  should also generate local magnetic fields that are zero on average but have a nonvanishing variance. If such fields could be detected, e.g., by muon spin rotation experiment, this would constitute a direct evidence for the phase fluctuation model of the pseudogap phase.

#### ACKNOWLEDGMENTS

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#### APPENDIX: GORKOV EQUATIONS IN THE PRESENCE OF SUPERFLOW

Real-space Gorkov equations<sup>41</sup> generalized to anisotropic superconductors read

$$(\omega - \hat{\mathcal{H}}_e)\mathcal{G}(\mathbf{r}_1, \mathbf{r}_2; \omega) + \hat{\Delta}\mathcal{F}^+(\mathbf{r}_1, \mathbf{r}_2; \omega) = \delta(\mathbf{r}_1 - \mathbf{r}_2),$$

$$(\omega + \hat{\mathcal{H}}_e^*)\mathcal{F}^+(\mathbf{r}_1, \mathbf{r}_2; \omega) + \hat{\Delta}^*\mathcal{G}(\mathbf{r}_1, \mathbf{r}_2; \omega) = 0. \quad (\text{A1})$$

Here  $\hat{\mathcal{H}}_e = [i\nabla - (e/c)\mathbf{A}]^2/2m - \epsilon_F$  is the single-electron Hamiltonian and  $\hat{\Delta}$  is the gap operator for spin singlet superconductivity defined as

$$\hat{\Delta}\mathcal{F}^+(\mathbf{r}_1, \mathbf{r}_2; \omega) = \int d^2r' \Delta(\mathbf{r}_1, \mathbf{r}')\mathcal{F}^+(\mathbf{r}', \mathbf{r}_2; \omega). \quad (\text{A2})$$

$\Delta(\mathbf{r}_1, \mathbf{r}_2)$  is the gap function that is in general a nontrivial function of both electron coordinates in the anisotropic superconductor. We are interested in the state of uniform superflow induced by the gap function of the form

$$\Delta(\mathbf{r}_1, \mathbf{r}_2) = \Delta_0(\mathbf{r}_1 - \mathbf{r}_2)e^{i\mathbf{q}\cdot(\mathbf{r}_1 + \mathbf{r}_2)} \quad (\text{A3})$$

and  $\mathbf{A} = 0$ . The easiest way to solve Eq. (A1) for  $\mathcal{G}$  is to perform a gauge transformation to the gauge where the order parameter is real and independent of the center-of-mass coordinate  $\mathbf{R} = (\mathbf{r}_1 + \mathbf{r}_2)/2$ :

$$\Delta(\mathbf{r}_1, \mathbf{r}_2) \rightarrow \Delta(\mathbf{r}_1, \mathbf{r}_2)e^{-i\mathbf{q}\cdot(\mathbf{r}_1 + \mathbf{r}_2)},$$

$$\mathbf{A} \rightarrow \mathbf{A} - \frac{c}{e}\mathbf{q},$$

$$\mathcal{G}(\mathbf{r}_1, \mathbf{r}_2; \omega) \rightarrow \mathcal{G}(\mathbf{r}_1, \mathbf{r}_2; \omega)e^{-i\mathbf{q}\cdot(\mathbf{r}_1 - \mathbf{r}_2)}, \quad (\text{A4})$$

$$\mathcal{F}^+(\mathbf{r}_1, \mathbf{r}_2; \omega) \rightarrow \mathcal{F}^+(\mathbf{r}_1, \mathbf{r}_2; \omega)e^{i\mathbf{q}\cdot(\mathbf{r}_1 + \mathbf{r}_2)}.$$

It is easy to verify that under such transformation Eqs. (A1) remain invariant.<sup>41</sup> In the new gauge Gorkov equations are manifestly translationally invariant, i.e., independent of  $\mathbf{R}$ . Fourier transforming in the relative coordinate  $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$  leads to algebraic equations for  $\mathcal{G}$  and  $\mathcal{F}^+$  of the form

$$(\omega - \epsilon_{\mathbf{k}-\mathbf{q}})\mathcal{G}(\mathbf{k}, \omega) + \Delta_{\mathbf{k}}\mathcal{F}^+(\mathbf{k}, \omega) = 1, \quad (\text{A5})$$

$$(\omega + \epsilon_{\mathbf{k}+\mathbf{q}})\mathcal{F}^+(\mathbf{k}, \omega) + \Delta_{\mathbf{k}}\mathcal{G}(\mathbf{k}, \omega) = 0,$$

where  $\epsilon_{\mathbf{k}} = \mathbf{k}^2/2m - \epsilon_F$ . The solution for  $\mathcal{G}$  is

$$\mathcal{G}_{\mathbf{q}}^{-1}(\mathbf{k}, \omega) = \omega - \epsilon_{\mathbf{k}+\mathbf{q}} - \frac{\Delta_{\mathbf{k}}^2}{\omega + \epsilon_{\mathbf{k}-\mathbf{q}}}. \quad (\text{A6})$$

Expanding  $\epsilon_{\mathbf{k}\pm\mathbf{q}}$  to leading order in  $\mathbf{q}$  we obtain

$$\mathcal{G}_{\mathbf{q}}^{-1}(\mathbf{k}, \omega) = (\omega - \eta) - \epsilon_{\mathbf{k}} - \frac{\Delta_{\mathbf{k}}^2}{(\omega - \eta) + \epsilon_{\mathbf{k}}} = \mathcal{G}_0^{-1}(\mathbf{k}, \omega - \eta), \quad (\text{A7})$$

with  $\eta \equiv \mathbf{v}_F(\mathbf{k}) \cdot \mathbf{q} \approx \mathbf{k} \cdot \mathbf{v}_s$ . As a final step we transform  $\mathcal{G}$  back to the original gauge with  $\mathbf{A} = 0$ . According to Eq. (A4) this amounts to simply replacing  $\mathbf{k} \rightarrow \mathbf{k} - \mathbf{q}$  on the right-hand side of Eq. (A7). We thus obtain the desired expression (3). In deriving this result we have assumed for simplicity a free-particle form of the single-electron Hamiltonian  $\hat{\mathcal{H}}_e$ . Evidently, the calculation remains valid for more complicated Hamiltonians.

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- <sup>23</sup>Note that  $\mathcal{G}_{\mathbf{q}}(\mathbf{k}, \omega)$  is a gauge-dependent object. Expression (3) holds in the Coulomb gauge  $\nabla \cdot \mathbf{A} = 0$  and it therefore differs from the standard expression found, e.g., in Ref. 24, which uses a gauge where  $\Delta$  is real. ARPES line shape is proportional to the spectral function in the Coulomb gauge (Ref. 25).
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