Effects of Thermal Phase Fluctuations in a Two-Dimensional Superconductor: An Exact Result for the Spectral Function

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We consider the single particle spectral function for a two-dimensional clean superconductor in a regime of strong critical thermal phase fluctuations. In the limit where the maximum of the superconducting gap is much smaller than the Fermi energy we obtain an exact expression for the spectral function integrated over the momentum component perpendicular to the Fermi surface.

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In conventional BCS superconductors the amplitude of the complex order parameter $|\Delta|e^{i\Phi}$ vanishes at the transition temperature T_c. This is in contrast to the underdoped cuprates, where experimental evidence [1,2] suggests that the transition is instead driven by the disordering of the superconducting phase through thermal fluctuations, while leaving the magnitude $|\Delta|$ of the order parameter intact. A quantitative measure for the strength of phase fluctuations is provided by the ratio $Q = 2T_c/\pi\rho_s(0)$, where $\rho_s(0)$ is the zero temperature phase stiffness. This ratio determines how close the transition is to being mean-field like. In BCS superconductors $Q \ll 1$, while in the underdoped cuprates $Q \sim 1$ [3]. The effects of thermal phase fluctuations on d-wave superconductors have been investigated before, see, e.g., Refs. [4–10]. A key objective of these works is to identify clear signatures of thermal phase fluctuations in single particle properties such as the spectral function measured by ARPES and STS (scanning tunneling spectroscopy). The purpose of this Letter is to provide an exact result for the partially integrated spectral function of a phase fluctuating superconductor in a particular limit. The latter quantity is defined as

$$\rho_P(\omega, k_\perp) = \int dk_\parallel A(\omega, \mathbf{k}) \tag{1}$$

where $k_\parallel$, $k_\perp$ are the wave vector components parallel and perpendicular to the Fermi velocity at the point of observation. We start by summarizing the essential assumptions underlying the model proposed by one of the authors and M. Khodas in [7,11]. The starting point is a superconductor with a general order parameter that arises from pairing on a Fermi surface, the shape of which we keep general for now. In particular it could be open or consist of several pockets, as is believed to be the case in underdoped cuprates [12–15]. Our following analysis is based on the existence of well defined quasiparticles, which is a reasonable assumption for the nodal regions. The corresponding Bogoliubov–deGennes Hamiltonian is

$$H = \int \mathbf{dr}\,\mathbf{dr}'[\Psi^+(\mathbf{r})]^T\{\delta(\mathbf{r}-\mathbf{r}')\hat{\epsilon}(-i\nabla)\tau^3 + \frac{1}{2}\tilde{\Delta}(\mathbf{r},\mathbf{r}')\tau^+ + \text{H.c.}\}\Psi(\mathbf{r}'), \tag{2}$$

where we have defined Nambu spinors $\Psi^T = (\psi_\uparrow, \bar{\psi}_\downarrow)$, τ^a are Pauli matrices and the pairing amplitude can be cast in the form

$$\tilde{\Delta}(\mathbf{r},\mathbf{r}') = \Delta(\mathbf{r}-\mathbf{r}')e^{i\phi(\mathbf{R})}. \tag{3}$$

Here $\Delta(\mathbf{r})$ determines the symmetry of the order parameter and $\mathbf{R} = (\mathbf{r}+\mathbf{r}')/2$ is the center of mass coordinate. Following the standard assumptions we neglect quantum fluctuations of $\tilde{\Delta}$ and focus exclusively on thermal fluctuations of the phase ϕ. The key point is to choose an appropriate model for these phase fluctuations. The effects of fully three-dimensional fluctuations are well studied in the literature [16] and are found to be small. On the other hand, one would expect the spatial anisotropy of layered materials like the cuprates to strongly enhance the role of phase fluctuations. The extreme limit would be the purely two-dimensional case, on which we focus in what follows. We emphasize that even purely 2D models have a window of applicability to, e.g., thin films [17] and $La_{1.875}Ba_{0.125}CuO_4$, where the phase transition was found to be of Berezinskii-Kosterlitz-Thouless (BKT) type [18–20]. Similarly, the analyses of the temperature dependence of magnetization, London penetration [21] depth and terahertz conductivity [22] for high quality underdoped BiSCO crystals show that although the superconductivity below T_c is of a 3D nature, the superconducting transition in these systems is rather close to a BKT transition. In the latter case our theory will be applicable in a temperature regime above T_c, where the phase correlation length is exponentially large and the phase fluctuations can effectively be considered as critical.

In the mean-field approximation fluctuations of the order parameter $\tilde{\Delta}$ are ignored, and the resulting Green function takes the familiar BSC form

$$G_{\rm BCS}(\omega,\mathbf{k}) = \frac{\omega+\epsilon_{\mathbf{k}}}{(\omega+i0)^2-\epsilon_{\mathbf{k}}^2-\Delta^2(\mathbf{k})}. \qquad (4)$$

The corresponding spectral function $-\frac{1}{\pi}\,{\rm Im}G_{\rm BCS}$ consists of two delta function peaks centered at positive and negative frequencies. These peaks will be broadened by thermal phase fluctuations. The following facts are of crucial importance. (i) Since the long wavelength fluctuations are classical, the electron frequency is conserved. (ii) Since in the region of interest the amplitude $|\Delta|$ is assumed to be fixed, self-consistency between the electron Green function and the order parameter is not an issue. Hence, the calculation of the spectral function is reduced to solving the Bogoliubov–deGennes equations for a particle with pairing amplitude (3) and then averaging the result over a given distribution of phase fluctuations. (iii) Since we are interested only in long wavelength fluctuations, the distribution function $P(\phi) = e^{-F_\phi/T}$ can be fixed by symmetry considerations: as long as the discrete lattice symmetries include C_4, the group of in-plane rotations by 90 degrees, the distribution function must be spatially isotropic (apart from irrelevant higher gradient terms). This leads to

$$\frac{F_\phi}{T} = \frac{\rho_s}{2T}\int dxdy[(\partial_x\phi)^2+(\partial_y\phi)^2], \qquad (5)$$

where the prefactor T^{-1} results from the integration over imaginary time. In contrast to the phase fluctuations, the Green's function at low energies is very different in the directions perpendicular and tangential to the Fermi surface. In a process where an electron close to the Fermi surface changes its momentum from $\mathbf{k}$ to $\mathbf{k}+\mathbf{q}$ by scattering off the pairing potential its Green's function is

$$G_0^{-1}(\omega,\mathbf{k}+\mathbf{q}) = \omega-\epsilon(\mathbf{k}+\mathbf{q}) \approx \omega-\epsilon(\mathbf{k})-vq_\parallel-\frac{q_\perp^2}{2m}. \qquad (6)$$

Here $q_\parallel$ and $q_\perp$ are the components of the momentum, respectively, parallel and perpendicular to the Fermi velocity $\nabla\epsilon(\mathbf{k})$. As a result of the isotropy of the distribution F_ϕ of phase fluctuations the typical values of $q_\parallel$ and $q_\perp$ are the same and of order $\Delta_{\rm max}$ (the maximal gap). Therefore the last term in (6) is proportional to the small parameter Δ/ϵ_F. If we neglect such small corrections the electron propagates along a straight line in real space and the transverse momentum is conserved. The electron Green's function can then be calculated separately for each frequency ω and Fermi surface point $\mathbf{k}$. Under the assumptions summarized above, the initial problem (2) is recast as a field theory described by the Lagrangian $\mathcal{L} = F_\phi + \bar{\Psi}_{\omega_n}\mathcal{H}\Psi_{\omega_n}$ with

$$\mathcal{H} = -i\omega_n I - iv\tau^z\partial_x + \frac{\tilde{\Delta}(k_\perp,x)}{2}\tau^+ + \frac{\tilde{\Delta}^*(k_\perp,x)}{2}\tau^-, \qquad (7)$$

where $\tilde{\Delta}(k_\perp,x) = \Delta(k_\perp)e^{i\phi(x,0)}$ and we have introduced $\Psi_{\omega_n} = (\psi_{\omega_n,\uparrow}, \psi^\dagger_{-\omega_n,\downarrow})^T$. In (8) we have used coordinates as shown in Fig. 1. As was pointed out in Ref. [7], the model defined through Eqs. (7) and (5) is in fact equivalent to the anisotropic spin-1/2 Kondo problem. In terms of this impurity model the phase fluctuations play the role of the host, while a *single* Bogoliubov quasiparticle constitutes the magnetic impurity. The reduction of the underlying interacting electron model to a single-impurity problem is possible because the emergent low-energy degrees of freedom are noninteracting Bogoliubov quasiparticles. The many-body aspects of the problem enter the determination of $|\Delta|$, but as this is treated as a parameter of our model we can avoid the issue of its calculation. Under a field redefinition

$$\begin{pmatrix}\psi_{\omega_n,\uparrow}\\ \psi^\dagger_{-\omega_n,\downarrow}\end{pmatrix} = \begin{pmatrix}\chi_{\omega_n,\uparrow}\\ -i\chi^\dagger_{-\omega_n,\downarrow}\end{pmatrix}, \qquad \begin{pmatrix}\psi^\dagger_{\omega_n,\uparrow}\\ \psi_{-\omega_n,\downarrow}\end{pmatrix} = \begin{pmatrix}i\chi_{\omega_n,\uparrow}\\ \chi^\dagger_{-\omega_n,\downarrow}\end{pmatrix}, \qquad (8)$$

and subsequent analytic continuation $i\omega_n \to \omega + i0$ we obtain the Hamiltonian

$$H_{\rm eff} = v^{-1}i(\omega+i0)\hat{\tau}^3 + H_{\rm bulk}[\phi] + \frac{\Delta(k_\perp)}{2v}[\hat{\tau}^+e^{i\phi(y=0)} + \hat{\tau}^-e^{-i\phi(y=0)}], \qquad (9)$$

where $\hat{\tau}^a \equiv \chi^+\tau^a\chi$ is a shorthand notation for fermionic bilinears. In this setting the coordinate x plays the role of Matsubara time. It is dual to the momentum component $k_\parallel$ parallel to the Fermi velocity at the point of observation. We note that in the approximation underlying (7) the electron momentum parallel to the Fermi surface is conserved so that the fermions χ depend only on x, while the phase field ϕ is a function of both x and y. For convenience we assign χ the coordinate $y = 0$. Since the fermion number is conserved, the $\hat{\tau}$ operators are in fact components of a spin $S = 1/2$.

The Hamiltonian $H_{\rm bulk}$ arising from (5) describes the phase fluctuations. For temperatures below the BKT transition temperature $T_{\rm BKT} = \pi\rho_s/2$ only smooth field configurations contribute so that

$$H_{\rm bulk}[\phi] = \frac{1}{8\pi d}\int_{-\infty}^{\infty} dy[(4\pi d)^2\Pi^2 + (\partial_y\phi)^2], \qquad (10)$$

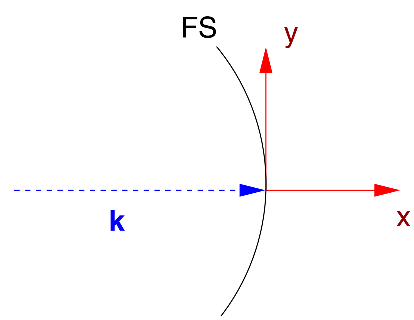

FIG. 1 (color online). Geometry defining the model in (8).

where Π is the momentum density conjugate to the field ϕ, with equal time commutator $[\Pi(y_1), \phi(y_2)]_- = -i\delta(y_1 - y_2)$. In order to be able to treat the temperature region $T > T_{\rm BKT}$ we need to allow singular (vortex) configurations of the ϕ field. The effects of vortices can be illustrated for the example of the two point correlation function of bosonic exponents. The latter takes the form

$$\langle e^{i\phi(\mathbf{r}_1)} e^{-i\phi(\mathbf{r}_2)}\rangle = \left|\frac{b}{\xi(T)}\right|^{2d} F\left(\frac{\mathbf{r}_{12}}{\xi(T)}\right), \tag{11}$$

where $d = T/(8T_{\rm BKT})$ is the scaling dimension of the order parameter, $\xi(T)$ is the correlation length and $b \sim (v/\epsilon_F)$ is the short distance cutoff. The short and long distance behavior of the scaling function is $F(\rho \ll 1) = \rho^{-2d}$ and $F(\rho > 1) \sim K_0(\rho)$, respectively (see also [23]). Below the transition (where $\xi = \infty$) the function (11) decays as a power law and above the transition where the vortices are relevant it decays exponentially with finite correlation length $\xi(T)$. We show below how to take this into account. It was shown in Ref [24] that (9) and (10) are equivalent to the anisotropic $S = 1/2$ Kondo model in the regime of extreme anisotropy $g_\parallel \gg g_\perp$

$$H_{\rm Kondo} = \sum_k v k a^+_{k\sigma} a_{k\sigma} + h\tau^z + \frac{J}{N}\sum_{p,k} g_\parallel a^+_{k\sigma}\tau^z_{\sigma\sigma'} a_{p\sigma'} + \frac{g_\perp}{2}[a^+_{k\sigma}\tau^+_{\sigma\sigma'}a_{p\sigma'} + \text{H.c.}], \tag{12}$$

where the magnetic field h is related to the real frequency ω in (9) by analytic continuation $h = i\omega + 0$. Our main result derives from the observation that the partial density of states (PDOS) defined by (1) is equal to the Green function of χ fermions at coinciding coordinates x. Taking into account the change of variables (8) we find that the PDOS is obtained by analytic continuation of the impurity magnetization of the Kondo model (12)

$$\rho_P(\omega)/\rho_0 = 2\,\text{Re}M(h = i\omega + 0). \tag{13}$$

Here ρ_0 is the bare density of states. This expression provides a link between spectral properties of the single electron problem (2) and thermodynamic properties of the many-body theory (12). In order to utilize the known exact expression for $M(h)$ in the Kondo problem [25] we need to relate the parameters $Jg_\parallel$, $Jg_\perp$ in (12) to d and $\Delta(k_\perp)$. The interactions in the Kondo model increase under renormalization and enter the strong coupling regime at a scale T_H which is known from the exact solution [25]

$$T_H \sim \epsilon_F (g_\perp/g_\parallel)^{2\pi/g_\parallel}. \tag{14}$$

On the other hand the usual scaling argument gives $T_H \sim \epsilon_F g_\perp^{1/(1-d)}$, which leads to the identification $g_\parallel/2\pi = 1 - d$ with $d = T/(8T_{\rm BKT})$. The expression for the impurity magnetization derived in [25] then reads (the parameter μ in [25] is related to d by $\mu = \pi(1-d)$):

$$M(h/T_H) = \frac{i}{4\pi^{3/2}}\int_{-\infty}^{\infty}\frac{dx}{x + i0}\frac{\Gamma(1 - i\frac{x}{1-d})\Gamma(\frac{1}{2} + ix)}{\Gamma(1 - i\frac{xd}{1-d})} \times \exp\{-2ix[\ln(h/T_H) + \pi a]\}, \tag{15}$$

where $\pi a = \frac{1}{2(1-d)}[d\ln d + (1-d)\ln(1-d)]$. As a function of a complex variable, $M(z)$ admits a power series expansion in odd powers of z for $|z| < 1$ and concomitantly is purely imaginary along the imaginary axis. By virtue of the identification (13) this implies that the PDOS vanishes at $|\omega| < T_H$. Thus there is a sharp gap equal to T_H in the density of states, which at $T \neq 0$ is always smaller than the mean-field gap $\Delta(k_\perp)$. On the other hand, for $|z| > 1$ the following expansion holds

$$\frac{\rho_P(\omega)}{\rho_0} = 1 + \sum_{n=1}^{\infty}\frac{\sin[2\pi n d]}{2\pi^{3/2}(n!)}\Gamma(nd)\Gamma\left(\frac{1}{2} + (1-d)n\right) \times\left[\frac{T_H e^{-\pi a}}{\omega}\right]^{2n(1-d)}, \qquad |\omega| > T_H. \tag{16}$$

We note that

$$\lim_{d\to 0}\frac{\rho_P(\omega)}{\rho_0} = \frac{|\omega|}{\sqrt{\omega^2 - \Delta^2}}\theta(|\omega| - \Delta), \tag{17}$$

which corresponds to the mean-field result. In order to establish the relation between the gap T_H and $\Delta(k_\perp)$, d we compare (16) to the perturbative expansion for the PDOS in the model (9). Second order perturbation theory gives

$$\frac{\delta\rho_P}{\rho_0} = \frac{\cos(\pi d)\Gamma(2 - 2d)2^{2d}\Delta^2 b^{2d}}{2\omega^{2(1-d)}}, \tag{18}$$

which yields the desired identification

$$T_H = \Delta(k_\perp)\sqrt{1-d}[\sqrt{d}b\Delta(k_\perp)]^{d/1-d}[\Gamma(1-d)]^{1/1-d}. \tag{19}$$

Given the result (16) for the PDOS we may calculate the full tunneling density of states. In the case of a d-wave superconductor this results in

$$\rho(\omega) \propto |b\omega|^{1-d}. \tag{20}$$

In Fig. 2 we show the PDOS (16) as a function of frequency for several different temperatures. The most noticeable feature is the persistence of a sharp gap. In addition we observe that the singularity characteristic of the BCS mean-field solution is strongly suppressed as T increases. This demonstrates that thermal phase fluctuations have a sizable effect on integrated spectral properties. In realistic materials the sharp gap will be smeared by both impurity scattering and the effects of Fermi surface curvature neglected in our analysis. In Fig. 3 we plot the temperature evolution of the gap T_H. We see that temperature effects are negligible. In particular this implies that the (d-wave) form of the gap remains robust through the transition, at least if vortices are ignored. As discussed above, the main effect of vortices is to induce a finite correlation length

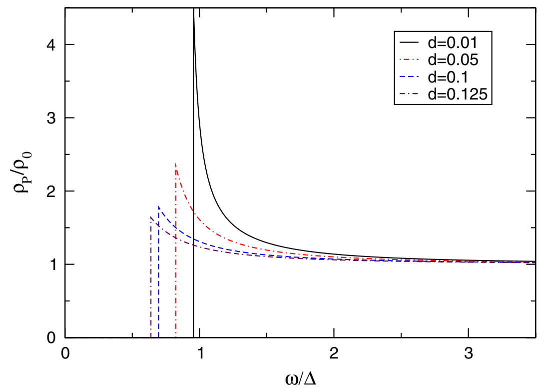

FIG. 2 (color online). Partial DOS as a function of frequency plotted for different temperatures $T = 8dT_{BKT}$. The ratio of $\Delta(k_\perp)$ to the cutoff $1/b$ is fixed as 0.1. Because of particle-hole symmetry $\rho_P(-\omega) = \rho_P(\omega)$.

$\xi(T)$. In the corresponding Kondo picture this translates to a gap in the excitation spectrum of the host. Exact results are available in this case as well [26]. On a qualitative level what happens in the Kondo picture is the following: as long as the correlation length $\xi(T)$ is larger than the inverse Kondo scale v/T_H the vortices have little effect on the physical properties. However, as soon as $\xi(T)$ falls below v/T_H the scaling terminates before the strong coupling regime is reached. As a consequence the gap in the PDOS is reduced for momenta close to the node $k_\perp < 1/[b\Delta\xi(T)]$. We have indicated this effect in the dotted curve in Fig. 3.

In this Letter we have considered a model for thermal phase fluctuations in a superconductor recently proposed in Ref. [7]. By exploiting a mapping to an effective spin-1/2 Kondo problem we have derived an *exact* result for the partially integrated spectral function (1). Our main result is that thermal fluctuations have a substantial effect on the single particle spectral function. The best candidate for comparing our theory to experiment is $La_{1.875}Ba_{0.125}CuO_4$. ARPES and STS measurements performed in [27] show that the d-wave gap is already well formed at the BKT transition. It would be interesting to map out the detailed temperature dependence of the spectral function by ARPES in the region of strong diamagnetic fluctuations $T < 40$ K and carry out a partial integration along the nodal direction.

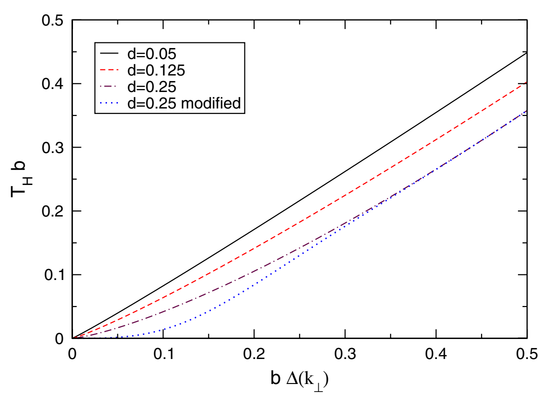

FIG. 3 (color online). The dimensionless gap $T_H b$ as a function of $q = \Delta(k_\perp)b$ for $d = 0.05, 0.125, 0.25$. The lowest curve, corresponding to $T = 2T_{BKT}$, has been modified to indicate the effects of vortices as described in the main text.

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