RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 52, NUMBER 6 1 AUGUST 1995-II

Mixed-state quasiparticle spectrum for d-wave superconductors

Yong Wang and A. H. MacDonald
Department of Physics, Indiana University, Bloomington, Indiana 47405
(Received 26 May 1995)

Controversy concerning the pairing symmetry of high-T_c materials has motivated an interest in those measurable properties of superconductors for which qualitative differences exist between the s-wave and d-wave cases. We report on a comparison between the microscopic electronic properties of d-wave and s-wave superconductors in the mixed state. Our study is based on self-consistent numerical solutions of the mean-field Bogoliubov–de Gennes equations for phenomenological BCS models which have s-wave and d-wave condensates in the absence of a magnetic field. We discuss differences between the s-wave and the d-wave local density of states, both near and away from vortex cores. Experimental implications for both scanning-tunneling-microscopy measurements and specific-heat measurements are discussed.

Since shortly after the discovery of high-temperature superconductors (HTSC), there has been great interest in determining the pairing symmetry of the order parameter.[1] In the absence of disorder, low-temperature electronic properties in the Meissner state of a d-wave superconductor differ qualitatively from those of a conventional s-wave superconconductor because of the existence of nodes in the gap function. These differences can in principle be used to identify the pairing symmetry, although strong anisotropy and the complicated nature of the materials have conspired to make conclusive experiments difficult. (Recent work is strongly suggestive of $d_{x^2-y^2}$ pairing.) It is also of interest to study differences between the mixed states of d-wave and s-wave type-II superconductors. In the mixed-state magnetic flux will penetrate the superconductor and form an Abrikosov vortex lattice. Low-lying quasiparticle excitations will then exist for both pairings, although in the conventional case they must be bound to the vortex core where the order parameter vanishes. The existence of bound quasiparticle states was first predicted by Caroli, de Gennes, and Matricon[2] when they studied an isolated vortex line in a conventional superconductor. Experimentally, these quasiparticles have been observed in scanning-tunneling-microscopy (STM) measurements.[3] For the d-wave case, progress has recently been made on both experimental and theoretical fronts. Volovik has used semiclassical approximations,[4,5] valid when the coherence length is much larger than the mean particle spacing, to calculate the spatially averaged density of states (DOS) at the Fermi energy $N(0)$ for the mixed state of a $d_{x^2-y^2}$ superconductor in a weak magnetic field $H \ll H_{c2}$. He found a finite $N(0)$ in the absence of disorder proportional to $H^{1/2}$ compared to the H^1 behavior expected for conventional superconductors in the same approximation. This prediction appears to be in accord with recent measurements of the magnetic-field dependence of the low-temperature specific heat[6,7] in high-T_c materials. However, the short coherence length of high-T_c materials raises some uncertainty about the detailed applicability of a semiclassical analysis and motivates a fully microscopic study of the same problem. In this Rapid Communication we report on such a study.

Application of microscopic mean-field theory to inhomogeneous states of superconductors gives rise to the Bogoliubov–de Gennes (BdG) equations.[8] Motivated by the STM experiments of Hess,[3] numerical solutions of the BdG equations have been obtained for both continuum[9,10] and lattice[11] models of a superconductor containing an isolated vortex. This work has recently been generalized to the case of isolated vortex in a d-wave superconductor.[12] According to Volovik, the DOS in the mixed state of a d-wave superconductor is dependent on the typical distance between vortices so that for the present study it is necessary to solve the BdG equations for the vortex-lattice state of a d-wave superconductor.

To model decoupled CuO_2 layers we consider single-band Hamiltonians on a two-dimensional (2D) square lattice with nearest-neighbor hopping and both on-site and nearest-neighbor interactions:

$$H = H^0 + H', \tag{1a}$$

$$H^0 = -\sum_{\langle ij\rangle\sigma} (t_{ij} c^\dagger_{j\sigma} c_{i\sigma} + t_{ji} c^\dagger_{i\sigma} c_{j\sigma}) - \sum_{i\sigma} \mu \hat{n}_{i\sigma}, \tag{1b}$$

$$H' = U \sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} + \frac{V}{2} \sum_{\langle ij\rangle\sigma\sigma'} \hat{n}_{i\sigma}\hat{n}_{j\sigma'}. \tag{1c}$$

Here i and j are site labels, the angle brackets in Eq. (1a) imply the restriction to neighboring sites, $\hat{n}_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ is the electron number operator on site i, and μ is the chemical potential. We will assume that the screened magnetic field inside the superconductor can be taken to be constant; for high-T_c materials this is a good approximation except for external fields extremely close to H_{c1}. In a one-band lattice model the magnetic field (perpendicular to the 2D plane) appears in the hopping amplitudes:

$$t_{ij} = t e^{-i \frac{e}{\hbar c} \int_{\vec{r}_i}^{\vec{r}_j} d\vec{r} \cdot \vec{A}(\vec{r})}, \tag{2}$$

where t is the nearest-neighbor hopping amplitude in zero field and $\nabla \times \vec{A}(\vec{r}) = \vec{h}(\vec{r})$. We report results below for two different models. The "s-wave" model has on-site attraction $U<0$, and no nearest-neighbor interaction. For the "d-wave" model, we set $U>0$ and $V<0$. When the magnetic field is set to zero the mean-field BCS gap equations are readily solved for either model by using translational invariance on the lattice. For the "s-wave" case the pairing self-energy in the ordered state is proportional to the order parameter

$$\Phi_i^s=\langle c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger\rangle, \tag{3}$$

while for the "d-wave" model it is proportional to

$$\Phi_i^d=\frac{1}{4}\sum_\delta (-1)^{\delta_y}\langle c_{i\uparrow}^\dagger c_{i+\delta\downarrow}^\dagger\rangle, \tag{4}$$

where the sum is over the nearest neighbors of site i, represented by the unit vectors $\hat\delta\equiv(\delta_x,\delta_y)=(\pm\hat e_x,\pm\hat e_y)$. (In the homogeneous zero-field states Φ_i^s and Φ_i^d are independent of i.) For both models the numerical values of the interaction parameters have been chosen to give a zero-temperature coherence length (estimated from the pair wave function) $\sim 4a$, as in high-T_c materials. The results reported below were calculated for the case of a band filling factor $\langle n\rangle=0.8$. For the s-wave model, we set $U=-3.5t$ and $V=0.0$ while for the d-wave model we choose $U=2.1t$, and $V=-2.1t$. For layer separations and bandwidths appropriate for models of high-temperature superconductors, the penetration depths (at $T=0$) for these models are several hundred times larger than the coherence lengths so that the models do indeed describe strongly type-II superconductors.

To study vortex lattice states, we introduce magnetic unit cells, each containing two superconducting flux quanta: $\Phi_0=hc/2e$. The size of a unit cell is $N_xa\times N_ya$ in general, where a is the lattice constant. We then define magnetic Bloch states labeled by a magnetic wave vector $\vec k$, a site index i within the magnetic unit cell, and a spin index σ and denote the corresponding creation and annihilation operators by $c_{\vec k i\sigma}^\dagger$ and $c_{\vec k i\sigma}$. In mean-field theory these are related to the quasiparticle creation and annihilation operators by

$$c_{\vec k i\uparrow}^\dagger=\sum_\alpha u_i^\alpha(\vec k)\gamma_{\vec k\alpha\uparrow}^\dagger-\sum_\alpha v_i^{\alpha *}(\vec k)\gamma_{\vec k\alpha\downarrow}, \tag{5a}$$

$$c_{-\vec k i\downarrow}=\sum_\alpha v_i^\alpha(\vec k)\gamma_{\vec k\alpha\uparrow}^\dagger+\sum_\alpha u_i^{\alpha *}(\vec k)\gamma_{\vec k\alpha\downarrow}, \tag{5b}$$

where $u^\alpha(\vec k)$ and $v^\alpha(\vec k)$ are determined by solving the BdG equations:

$$\begin{pmatrix} H^0(\vec k) & UF_1(\vec k)+VF_2(\vec k)\\ UF_1^*(\vec k)+VF_2^*(\vec k) & -H^{0*}(\vec k)\end{pmatrix}\begin{pmatrix}u^\alpha(\vec k)\\ v^\alpha(\vec k)\end{pmatrix}=E^\alpha(\vec k)\begin{pmatrix}u^\alpha(\vec k)\\ v^\alpha(\vec k)\end{pmatrix}, \tag{6}$$

where H^0, F_1, and F_2 are $N_xN_y\times N_xN_y$ matrices. The off-diagonal blocks in Eq. (6) are the pairing self-energies and these can be expressed in terms of quasiparticle amplitudes. The on-site interaction contribution is diagonal in site indices with

$$[F_1(\vec k)]_{ii}\equiv\langle c_{\vec k i\uparrow}^\dagger c_{-\vec k i\downarrow}^\dagger\rangle=-\sum_\alpha \tanh\frac{\beta E^\alpha(\vec k)}{2}\, u_i^\alpha(\vec k)v_i^{\alpha *}(\vec k), \tag{7}$$

while the nearest-neighbor interaction contribution is

$$[F_2(\vec k)]_{ij}\equiv\langle c_{\vec k i\uparrow}^\dagger c_{-\vec k j\downarrow}^\dagger\rangle\Delta_{j,i+\delta}$$
$$=-\frac{1}{2}\sum_\alpha \tanh\frac{\beta E^\alpha(\vec k)}{2}[u_i^\alpha(\vec k)v_j^{\alpha *}(\vec k)+u_j^\alpha(\vec k)v_i^{\alpha *}(\vec k)]\Delta_{j,i+\delta}. \tag{8}$$

Here $\beta=1/k_BT$ and

$$\Delta_{j,i+\delta}=\begin{cases}\delta_{j,i+\delta}, & \text{if site } i+\delta \text{ and site } i \text{ are in the same cell;}\\ \delta_{j,i-N_\delta\delta}, & \text{if site } i+\delta \text{ and site } i \text{ are in different cells,}\end{cases}$$

where N_δ is the number of sites along δ direction in a cell. Equations (6), (7), and (8) constitute a set of self-consistent equations, whose solutions can be obtained numerically by iteration.

Typical[14] self-consistent results for the order parameter of the d-wave model in the vortex lattice state at $T=0$ are shown in Fig. 1. The size of the cell is $28a\times 56a$, corresponding to a field of $H=\Phi_0/(28a)^2$; if we associate a with the typical Cu-Cu distance in high-T_c materials this corresponds to a magnetic field ~ 10 T. The value of the order parameter at the midpoint between neighboring vortices is $\Phi_{i,\max}^d(H)=0.063$, which may be compared with the value $\Phi^d=0.065$ obtained at $T=0$ for the Meissner state of the same model. The magnetic field suppresses superconductivity everywhere in the system; numerical calculations at stronger fields are consistent[15] with upper critical fields $H_{c2}\sim 100$ T for the model we study, as expected from the zero-temperature coherence length. We remark that the extended s-wave component of the order parameter, permitted by symmetry[4,12,13] in the vortex lattice state and possibly of experimental relevance[16,17] in high-T_c materials, is smaller than the d-wave component by about two orders of magnitude for the model parameters we have chosen.

We define the local density of states (LDOS) on site i by

$$N_i(E)=-\frac{1}{N_c}\sum_{\vec k,\alpha}[|u_i^\alpha(\vec k)|^2 f'(E^\alpha(\vec k)-E)+|v_i^\alpha(\vec k)|^2 f'(E^\alpha(\vec k)+E)], \tag{9}$$

where $f(E)=[\exp(\beta E)+1]^{-1}$, and N_c is the number of the magnetic cells in the system. $N_i(E)$ is proportional to the

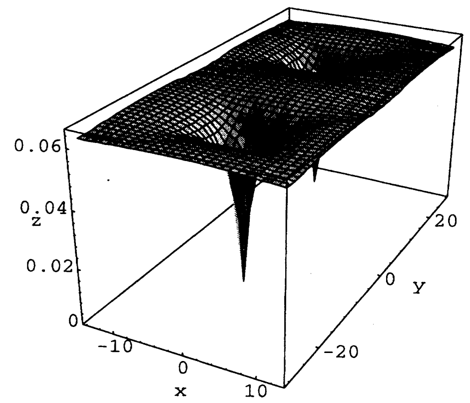

FIG. 1. The amplitude of a d-wave order parameter Φ_i^d (z axis) in a unit cell for the square lattice solution at $T=0$. The size of the cell is $28a\times 56a$ (intervortex spacing $28a$), corresponding to a field $H=\Phi_0/(28a)^2$.

differential tunneling conductance[9,18] which is measured in an STM experiment. We show in Fig. 2 $N_i(E)$ at a site midway between two neighboring vortices for both s-wave and d-wave superconductors at zero field and at several different finite field strengths. Although at first sight the s-wave and d-wave cases appear quite similar, closer inspection reveals important differences for the density of states near the Fermi level. Most importantly, the density of states at the Fermi level, $N_i(0)$, is much larger for the d-wave case than for the s-wave case as predicted by Volovik. (We are unable to solve the BdG equations at weak enough fields to verify the expected $H^{1/2}$ behavior, although as seen in the inset our results are consistent with this prediction.) It is presumably this density of states away from the d-wave vortex cores which is responsible for the enhancement of the low-temperature specific heat of high-T_c superconductors in a field seen by Moler *et al.*[6,20] In the s-wave case, the zero-field gap remains quite well defined out to fairly strong magnetic-field strengths although, in contrast with the semiclassical result, the density of states is not strictly zero at any energy. The size of the gap decreases with increasing field as expected. The sharp peaks in zero-field DOS are of different origins. The peak closest to the Fermi energy is due to superconductivity while the second peak reflects the Van Hove singularity in the band structure. These peaks are smeared out in finite field. In Fig. 3 we show $N_i(E)$ for a site at the center of a vortex core. In both s-wave and d-wave cases, we find large peaks near the Fermi energy, reflecting resonances which will evolve into quasiparticle bound states in the limit of isolated vortices. The positions of the peaks are distinctly different in two cases. In the d-wave model, the LDOS peak is not as strong and is clearly centered at the Fermi energy. In the s-wave case two quasiparticle LDOS peaks are visible and the lowest energy of these is clearly located away from the Fermi energy. The scale of the separation between s-wave bound-state peaks is $\sim 0.2t$, in accord with expectations based on the size of the gap and the bandwidth. For these short coherence length models, the separation between quasiparticle bound states is large enough to be resolved[19] so

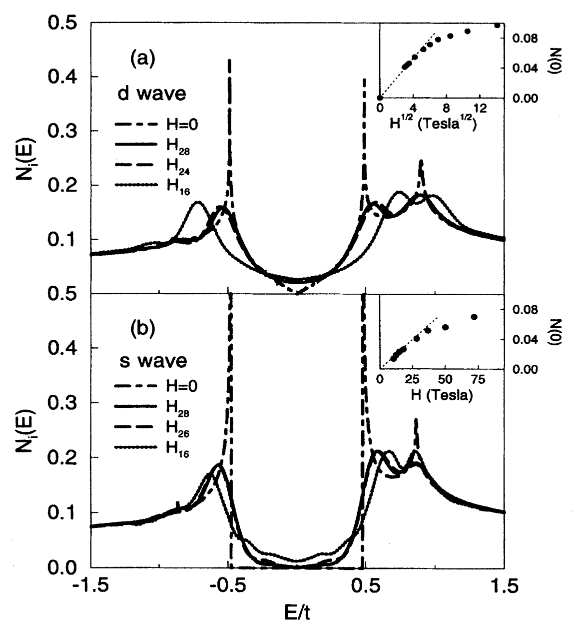

FIG. 2. Quasiparticle LDOS profiles at $T=0$ away from vortex cores for different magnetic fields are plotted in (a) for the d-wave model and in (b) for the s-wave model. H_n represents the field corresponding to the intervortex spacing of na. For typical Cu-Cu distance in high-T_c materials, H_{28}, H_{26}, H_{24}, and H_{16} are 9.2, 10.7, 12.5, and 28.1 T, respectively. The $H=0$ limits are also plotted. Energies are in units of t and measured from the Fermi energy. The insets are the spatially averaged DOS $N(0)$. The dotted lines here are guides for the eye; in the s-wave case $N(0)$ vanishes more rapidly than H^1 when averaged over intervals smaller than the separation between vortex-core bound states energies.

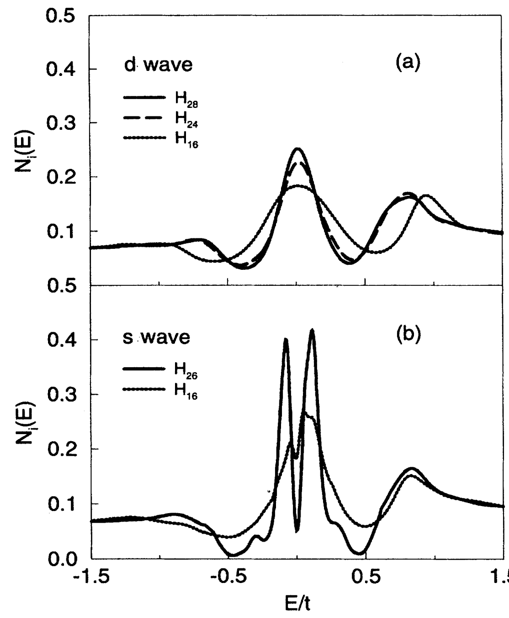

FIG. 3. Quasiparticle LDOS profiles at $T=0$ at the center of the vortex cores are plotted in (a) for the d-wave model and (b) for the s-wave model. Energies are in units of t and measured from the Fermi energy.

that low-temperature STM experiments would see a double-peak structure in high-T_c materials if they had s-wave symmetry, rather than the zero-bias peak observed[3] in conventional superconductors.

This work was supported by the National Science Foundation under Grant No. DMR-9416906. The authors are grateful to D. Arovas, A.J. Berlinsky, C. Kallin, and M. Norman for helpful conversations.

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[1] For recent reviews, see R.C. Dynes, Solid State Commun. **92**, 53 (1994); J.R. Schrieffer, *ibid.* **92**, 129 (1994); D.J. Scalapino, Phys. Rep. **250**, 329 (1995).

[2] C. Caroli, P.G. de Gennes, and J. Matricon, Phys. Lett. **9**, 307 (1964).

[3] H.F. Hess *et al.*, Phys. Rev. Lett. **62**, 214 (1989); **64**, 2711 (1990).

[4] G.E. Volovik, Sov. Phys. JETP **58**, 469 (1993).

[5] See also Kazumi Maki, Nils Schopohl, and Hyekyung Won, Physica B **204** 214 (1995); Nils Schopohl and Kazumi Maki (unpublished).

[6] K.A. Moler *et al.*, Phys. Rev. Lett. **73**, 2744 (1994).

[7] For review, see N.E. Phillips *et al.*, in *Progress in Low Temperature Physics XIII*, edited by D.F. Brewer (North-Holland, Amsterdam, 1992); A. Junod, in *Physical Properties of HTSC II*, edited by D. Ginsberg (World Scientific, Singapore, 1990).

[8] See, e.g., P.G. de Gennes, *Superconductivity of Metals and Alloys* (Addison-Wesley, Reading, MA, 1989).

[9] F. Gygi and M. Schluter, Phys. Rev. Lett. **65**, 1820 (1990); Phys. Rev. B **41**, 822 (1990); **43**, 7609 (1991).

[10] J.D. Shore, M. Huang, A.T. Dorsey, and J.P. Sethna, Phys. Rev. Lett. **62**, 3089 (1989).

[11] Yu-Dong Zhu, Fu Chun Zhang, and Manfred Sigrist, Phys. Rev. B **51**, 1105 (1995).

[12] P.I. Soininen, C. Kallin, and A.J. Berlinsky, Phys. Rev. B **50**, 13 883 (1994).

[13] Yong Ren, Ji-Hai Xu, and C.S. Ting, Phys. Rev. Lett. **74**, 3680 (1995).

[14] We have obtained solutions for both square and triangular vortex lattices. For the models considered the triangular lattice always has lower energy. However, the dependence of the quasiparticle density of states on the vortex lattice structure is not of importance for the issues addressed here and all the results reported here were calculated for the square vortex lattice state.

[15] We remark that for very low temperatures and strong fields, quantum corrections due to Landau quantization become important in our gap equations. These effects lead, within mean-field theory, to superconductivity at arbitrarily strong magnetic fields. For detail, see M.R. Norman, A.H. MacDonald, and Hiroshi Akera, Phys. Rev. **51**, 5927 (1995); H. Akera, A.H. MacDonald, and M.R. Norman, Physica B **184**, 337 (1993); M. Rasolt and Z. Tešanović, Rev. Mod. Phys. **64**, 709 (1992); and work therein.

[16] A.J. Berlinsky, A.L. Fetter, M. Franz, C. Kallin, and P.I. Soininen (unpublished).

[17] B. Keimer *et al.*, J. Appl. Phys. **76**, 6778 (1994).

[18] See, e.g., Michael Tinkham, *Introduction to Superconductivity* (McGraw-Hill, New York, 1975).

[19] It is known that the local density of states for a particular material can depend sensitively on its disorder content; Ch. Renner *et al.*, Phys. Rev. Lett. **67**, 1650 (1991) and U. Klein, Phys. Rev. B **41**, 4819 (1990). Our results apply only for clean materials.

[20] Further details of these calculations, along with detailed results for the temperature dependence of the specific heat will be published elsewhere. Yong Wang and A.H. MacDonald (unpublished).