Predicted giant magnetic moment on non-{$n0m$} surfaces of *d*-wave superconductors

Chia-Ren Hu
Department of Physics, Texas A&M University, College Station, Texas 77843-4242

Xin-Zhong Yan
Department of Physics, Texas A&M University, College Station, Texas 77843-4242
*and Institute of Physics, Chinese Academy of Sciences, P. O. Box 603, Beijing 100080, China**

(Received 1 June 1999; revised manuscript received 14 July 1999)

It has been noted that the sizable areal density of midgap states which must exist on any non-{$n0m$} surface of a *d*-wave superconductor can lead to a giant magnetic moment. Here we show that this effect is observable, and discuss two precise ways to observe it: (i) by directly measuring magnetic moment in a system with a large density of internal {110} surfaces, or (ii) by performing spin-polarized tunneling on a {110} surface. In both cases, a sufficiently large magnetic field should be applied in the $[1\bar{1}0]$ direction. Observing these predictions in high-T_c superconductors can provide a strong confirmation of the *d*-wave scenario for such materials. [S0163-1829(99)50942-9]

One of us has noted previously[1] that the sizable areal density of midgap states (MS's) which must exist on any non-{$n0m$} surface of a *d*-wave superconductor (DWSC) (with n and m integers or zero) can lead to a giant magnetic moment (GMM). The MS's are topological signatures of unconventional pairing symmetry. They are nearly dispersionless quasiparticle states, characterized by momenta along the surface ranging from $-k_F$ to k_F (k_F being the Fermi momemtum), but all with the same ''zero'' energy as measured from the Fermi energy (in the WKBJ approximation). These states can lead to a narrow density of states (DOS) peak at the Fermi energy, where the integrated bulk DOS dips to zero. One of the observable consequences of these MS's is therefore a zero bias conductance peak (ZBCP) in single-particle tunneling,[1–3] which has been observed ubiquitously in high-T_c superconductors (HTSC's) for more than a decade. (See Ref. 3 for a review.) Several carefully controlled experiments performed recently strongly supported the conclusion that the ZBCP's observed in them are due to such MS's.[4] Many other consequences of the MS's have been predicted,[5] including a contribution to Josephson tunneling,[6] a paramagnetic Meissner effect,[7,8] and a low-temperature anomaly in the penetration depth,[9] etc. The GMM is also a consequence of the MS's, which has not yet been looked for experimentally, perhaps because no detailed analysis has been made on whether and how it can be observed. Thus here we perform such an analysis.

An applied magnetic field B can have two simultaneous effects on the surface MS's:[1,7,9] (1) *Spin shift:* The MS's are spin eigenstates. The field B can cause the MS's of one spin to shift above the Fermi surface, and those of the other spin to shift below. If the orbital shift (described below) can be neglected, then, when the magnitude of the spin shifts grows past (i) the width of the MS's peak in the DOS, (ii) any small nonzero energies $\sim\Delta_0^2/E_F$ of the MS's, and (iii) the thermal energy k_BT, a measurement of the total magnetic moment of the system should exhibit a saturation phenomenon of a magnitude proportional to the total number of MS's on the surface. This is referred to as GMM in Ref. 1. (2) *Orbital shift* (including screening current effects): In the gauge in which the pair-potential order parameter Δ is real, this effect is due to a vector potential $\mathbf{A}$ alone. The MS's acquire energy shifts proportional to their momenta k along $\mathbf{A}$. At sufficiently low T all occupied MS's have the same sign of k (in the WKBJ approximation and neglecting the spin shift) implying a paramagnetic equilibrium current. Higashitani[7] thus proposed that this effect could account for the observed ''paramagnetic Meissner effect.''[8] Another predicted consequence is a low-temperature anomaly in the ab-plane penetration depth λ_{ab} which has been observed.[9]

Both types of energy shifts are really present at the same time. Thus it is important to estimate their relative magnitudes. We find that the conclusion depends crucially on the direction of B. Consider a thick single-crystal slab with a {110} surface, and with B applied parallel to the surface. If B is along [001], the screening current is along $[1\bar{1}0]$, which is denoted as the y axis, with the x axis perpendicular to the surface at $x=0$. The spin shift has essentially the magnitude $\mu_0 B$. (μ_0 is the Bohr magneton.) The orbital shift follows from first-order perturbation theory, giving $-(1/c)\langle\hat{\mathbf{j}}\cdot\mathbf{A}(x)\rangle$, where $\hat{\mathbf{j}}$ is the current density operator. In the gauge in which Δ is real, $\mathbf{A}(x)=-B\lambda_{ab}\exp(-x/\lambda_{ab})\hat{e}_y \simeq\mathbf{A}(0)=-B\lambda_{ab}\hat{e}_y$, because the MS's are localized within roughly one coherence length $\xi_{ab}\sim 15$ Å from the surface, which is much smaller than $\lambda_{ab}\sim 1500$ Å. (For the same reason the spin shift sees simply the applied field B.) Thus the orbital shift is $\simeq(e/m_{ab}c)kB\lambda_{ab}$. The ratio between the magnitudes of the orbital and spin shifts is $2(m_e/m_{ab})(|k|\lambda_{ab})$. The mass ratio m_e/m_{ab} is probably less than unity by a factor larger than 0.2.[10] k ranges essentially from $-k_F$ to k_F, and k_F should be somewhat less than $\pi/2a$, where a is the lattice parameter in the ab plane. Thus this ratio is around 200, showing that with B along [001] the spin shift is negligible in comparison with the orbital shift, and the previous analyses of the consequences of the orbital shift without considering the spin shift[7,9] is justified.

Next, let B be along $[1\bar{1}0]$. The screening current is then along [001]. The same ratio in the simplest estimate is now $2(m_e/m_c)(k_z\lambda_c)$. The London penetration-depth formula implies that $m_c \propto \lambda_c^2$. Thus this energy-shift ratio is reduced from the previous one by a factor (λ_{ab}/λ_c), which is $\sim 1/50$ for Hg-1201.[11] A more careful estimate, taking into account (i) the tight-binding nature in the c direction, and (ii) a k_z range from $-\pi/c$ to π/c with $c/a \sim 3$, reduces the energy-shift ratio to $\lesssim 2$. We shall see that this is quite sufficient to allow the GMM to be observed. On the other hand, by forming *NS* superlattices, it should be possible to increase λ_c by another factor of 10 or larger, then one can even explore the regime where the orbital shift is negligible. Below, we first consider the effects of a spin shift alone, and then comment later on the effects of a simultaneous orbital shift of a comparable magnitude. We shall discuss the spin magnetization first, and then the spin polarized tunneling conductance. We believe that the latter is a very promising way to see this effect.

Consider first the spin magnetization M (which we define as the magnetic moment per unit area per CuO_2 plane). With

$$M(\mathbf{x}) \equiv -\mu_0[\langle \psi_\uparrow^\dagger(\mathbf{x})\psi_\uparrow(\mathbf{x})\rangle - \langle \psi_\downarrow^\dagger(\mathbf{x})\psi_\downarrow(\mathbf{x})\rangle], \tag{1}$$

where $\psi_s(\mathbf{x})$ is the field operator of spin-s electrons, its main contribution from the MS's follows easily from a perturbative treatment of the Bogoliubov–de Gennes (BdG) equations,[2,3] which gives

$$M(x) = \mu_0 g(\mu_0 B) f(x), \tag{2}$$

with

$$g(E) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \tanh(\beta\omega/2)\,\mathrm{Im}\left(\frac{1}{\omega + E + i\delta} - \frac{1}{\omega - E + i\delta}\right), \tag{3}$$

$$f(x) = \int_{-k_F}^{k_F} \frac{dk}{2\pi}[|u_k(\mathbf{x})|^2 + |v_k(\mathbf{x})|^2], \tag{4}$$

where $\beta = 1/k_B T$; $u_k(\mathbf{x})$ and $v_k(\mathbf{x})$ are the electron and hole components of the wave function of the MS of momentum k along y; and $\delta > 0$ takes into account a finite lifetime due to surface and/or bulk scatterings. In the limit $\delta \to 0^+$, $g(E) \to \tanh(\beta E/2)$. In general, g is a function of both $\beta\mu_0 B$ and $\beta\delta$, and is a monotonically decreasing function of T at any given B and δ. The largest value for g is unity, corresponding to $\mu_0 B \gg \{\delta \text{ and } k_B T\}$. Then the total magnetic moment per CuO_2 plane, associated with the MS's on one {110} edge of the plane, obtained by integrating $M(x)$ over x and y, is equal to $(2L_y/\lambda_F)\mu_0$. That is, for every Fermi wavelength on each {110} edge of a CuO_2 plane, there are two MS electrons contributing to the GMM. This is the maximum magnitude of the saturation phenomenon mentioned earlier. To observe it directly, however, one needs to drastically increase the surface to volume ratio in the sample. The approach adopted in Ref. 9, where a sample is irradiated with ions along [110] in order to create a large number of straight tracks, might offer some hope.

Next we consider tunneling between a spin-polarized normal metal (N_{sp}) (i.e., a ferromagnetic metal or a half-metallic magnet[12]) and a DWSC (S_d) with a {110} surface. With B along $[1\bar{1}0]$ and the orbit shift neglected, the ZBCP should split into two peaks at nonzero voltages where the Fermi level of each spin species in N_{sp} matches the shifted energy of the MS's in S_d *of the same spin*. The relative heights of these two peaks should depend directly on the spin polarization in N_{sp}. Below we make these statements more quantitative by considering the effects of finite peak width and temperature.

We assume, for simplicity, that both sides of the junction have the same carrier type and density, and the same *two-dimensional* band dispersion (with HTSC's in mind). We also assume that the carriers are electrons with charge $-e < 0$ and a gyromagnetic ratio $\gamma = -ge/2m_e c$ with $g = 2$. Later we will comment on the effects of replacing these assumptions by more realistic ones, such as a three-dimensional band dispersion for N_{sp}, and different carrier types and densities in the two sides of the junction.

The zero-field polarization in N_{sp} is defined to be

$$P \equiv (n_\uparrow - n_\downarrow)/(n_\uparrow + n_\downarrow), \tag{5}$$

where n_s is the density of spin-s electrons at $B = 0$. We consider $P > 0$. The zero-field Fermi energies for spin-s electrons in N_{sp} can then be expressed as $E_{F,s}^{(0)}/\overline{E_F^{(0)}} = 1 + sP$ [$s = 1(-1)$ for spin $\uparrow(\downarrow)$], where $\overline{E_F^{(0)}} = (E_{F,\uparrow}^{(0)} + E_{F,\downarrow}^{(0)})/2$, and is equal to the Fermi energy E_F in S_d due to our simplifying assumptions. The single-particle excitations in this system are governed by the BdG equations,[13]

$$\begin{pmatrix} \hat{H}_\uparrow & \Delta \\ \Delta^* & -\hat{H}_\downarrow \end{pmatrix}\begin{pmatrix} u \\ v \end{pmatrix} = \epsilon \begin{pmatrix} u \\ v \end{pmatrix}, \tag{6}$$

where $\hat{H}_s(x)$ is equal to $p^2/2m + s\mu_0 B - E_{F,s}^{(0)}$ for $x < 0$ (i.e., in N_{sp}, valid for $E_{F,\uparrow}^{(0)} > \mu_0 B$ only), and to $p^2/2m + s\mu_0 B(x) - E_F$ for $x > 0$ [i.e., in S_d, $B(x) \simeq B$ for the MS's]. The pair potential Δ vanishes in N_{sp}, and is assumed to be x independent in S_d. (Its self-consistency need not be considered, for the MS's are topological.) ϵ is the quasiparticle energy measured from the chemical potential, which is $= E_F$ because we take the bottom of the conduction band in S_d to be zero. The bottom of the conduction band of each spin in N_{sp} is then not zero, and has been absorbed in the definition of $E_{F,s}^{(0)}$. In momentum space, the d-wave pair potential $\Delta(\mathbf{k}_F)$ is taken to be $\Delta_0 \cos(2\theta - 2\alpha)$, where θ and α are the angles that $\mathbf{k}_F$ and the crystal a axis make with the x axis. We consider $\alpha = \pi/4$. At $x = 0$ a δ-function barrier, $H\delta(x)$, is assumed. All wave vectors are two dimensional due to our assumptions. In N_{sp}, the two-component quasiparticle wave function is, aside from a factor $\exp(iq_y y)$,

$$\Psi_s = \psi_{s,q_x} - a_s \psi_{-s,k_x} - b_s \psi_{s,-q_x}, \tag{7}$$

where $\psi_{s,q_x} = \psi_s \exp(iq_x x)/\sqrt{|v_{q_x}|}$ with $\psi_\uparrow = \binom{1}{0}$ for a spin-up electron, and $\psi_\downarrow = \binom{0}{1}$ for a spin-down hole, and $v_{q_x} = d\epsilon/dq_x$ is the qroup velocity. The first term in the right-hand side of Eq. (7) expresses the incoming quasiparticle with spin s and wave number q_x normal to the interface. The other two terms correspond to Andreev and ordinary reflections, respectively, with a_s and b_s their respective coefficients. Equaion (6) gives $\hbar^2 q_x^2/2m = E_{F,s}^{(0)} - s\mu_0 B + s\epsilon$

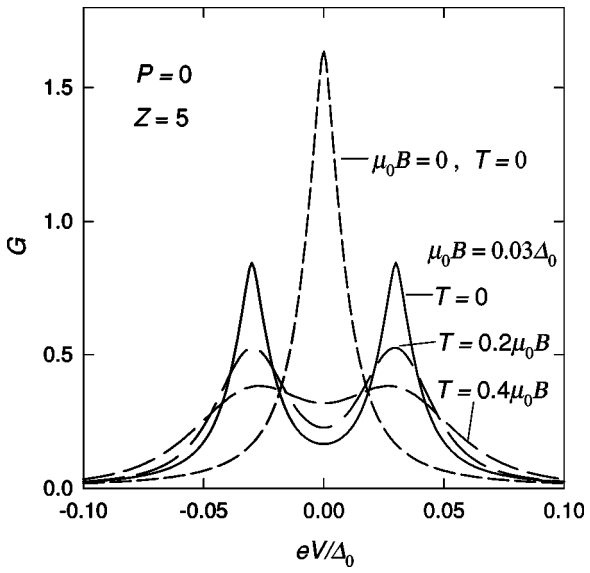

FIG. 1. Normalized tunneling conductance G between an unpolarized ($P=0$) normal metal and a d-wave superconductor with a {110} surface, as a function of voltage V, for $B=0$, $T=0$, and $B=0.03\Delta_0/\mu_0$ at three values of T. The interfacial barrier parameter $Z=5$. Only the contributions from the midgap states are included.

$-\hbar^2 q_y^2/2m$, and $\hbar^2 k_x^2/2m = E_{F,-s} + s\mu_0 B - s\epsilon - \hbar^2 q_y^2/2m$. The transmitted wave in S_d is a linear combination of outgoing waves (from the interface) that are solutions of the BdG equations for a bulk DWSC. Matching the wave function at the interface gives a_s, b_s, and other coefficients in the transmitted waves.

The tunneling conductance G (normalized to unity at $E_F \gg eV \gg \Delta_0$ when T, P, and B are all 0) is calculated using the Blonder-Tinkham-Klapwijk formalism:[14,15]

$$G = -\frac{\hbar^2}{4q_F}\int_0^\infty q\,dq \int_{-\pi/2}^{\pi/2} d\phi \frac{q\cos\phi}{m} \times \left\{ \sum_{s=\uparrow,\downarrow} f'(s\epsilon + eV)[1 + A_s(\epsilon,\phi) - B_s(\epsilon,\phi)] \right\}, \tag{8}$$

where ϕ is the angle between $\mathbf{q}$ and the x axis, $\epsilon(s,q,\phi)$ is given in the previous paragraph, $q_F \equiv (2mE_F)^{1/2}/\hbar$, $f(\epsilon) \equiv 1/[\exp(\epsilon/k_BT)+1]$, and $A_s \equiv |a_s|^2$, $B_s \equiv |b_s|^2$. For numerical calculation, we take $\Delta_0/E_F = 0.08$ as a typical value for HTSC's. The dimensionless barrier parameter is $Z = H/\hbar\sqrt{m/2E_F}$.[14] Figure 1 gives G as a function of V at $Z=5$, for $B=T=0$ and for $\mu_0 B = 0.03\Delta_0$, $k_BT = (0, 0.2, \text{and } 0.4)\mu_0 B$, for a nonmagnetic N_{sp}, $P=0$. At $B=0$, we get the ZBCP as observed in many experiments. At $B\neq 0$, the conductance peak splits into two peaks at $eV = \pm\mu_0 B$ which correspond to the energy levels of the surface states of different spins in the superconductor (SC).

At $\mu_0 B \gg (k_BT$ and the peaks' width), the spin-down surface states with energy $\epsilon = -\mu_0 B$ are occupied with electrons, whereas the spin-up surface states at energy $+\mu_0 B$ are empty. As a voltage $V>0$ is applied between N_{sp} and S_d, the chemical potential in N_{sp} is lowered by eV. The spin-down electrons in the surface states in S_d will tunnel into N_{sp} only when eV increases past $\mu_0 B$, leading to a steplike increase in the tunneling current, or a conductance peak. If a negative voltage V is applied between N_{sp} and S_d, the chemical potential in N_{sp} is increased by $e|V|$. When it exceeds $\mu_0 B$, The spin-up electrons in N_{sp} can then tunnel into the empty spin-up MS's in S_d, leading also to a peak in G.

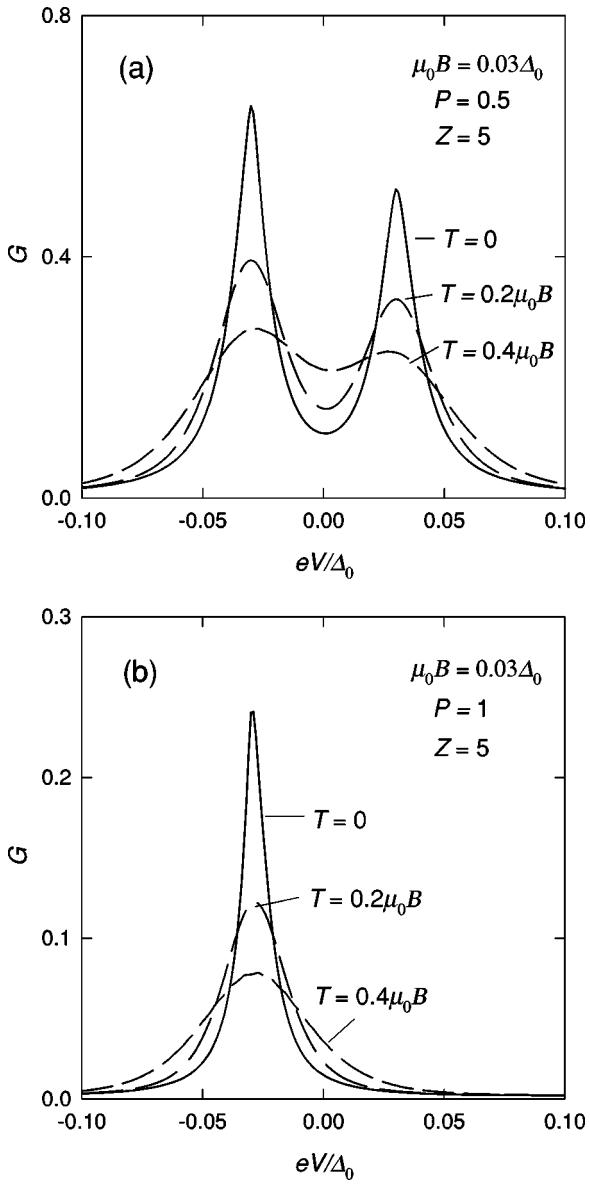

FIG. 2. Similar plots for G except that the normal metal is (a) 50% ($P=0.5$), (b) 100% ($P=1$), spin polarized. Only the $B\neq 0$ case is plotted since the $B=0$ case is practically independent of P.

Figure 2(a) gives a similar plot for G at $P=0.5$ (without the $B=0$ case, which does not change with P). The two conductance peaks at $eV = \pm\mu_0 B$ now have different heights. The peak associated with tunneling of spin-down electrons is lower, because their Fermi velocity in N_{sp} is smaller. (The DOS in two dimensions is a constant of energy, otherwise there would be another source for the height difference.) Figure 2(b) gives G when N_{sp} is fully polarized, $P=1$, as found in some half-metallic magnets.[12] In this case only one peak appears, which is associated with the tunneling of spin-up electrons.

The absolute heights of these peaks have meaning, as G has been normalized. Note that the conductance peaks are

higher for larger Z. At the same time, they become narrower. This is because, for higher barriers, the lifetimes of the surface states in S_d become longer, and there is a sharper resonance between the particles from N_{sp} and the MS's in S_d. Therefore, to detect the GMM this way, it is preferable to work in the ''tunneling limit,'' i.e., when the interfacial barrier is high.

A typical value for Δ_0 in HTSC's is about 16.5 meV. Then to reach the energy $0.03\Delta_0$, the magnetic field needs to be around 8.6 Tesla. In addition, $0.03\Delta_0$ in temperature is about 5.7 K. To measure such an energy shift, the experiment should be performed at liquid helium or lower temperatures.

If an orbital shift of the same order as the spin shift is present in the system, then each peak will become wider and approximately rectangularly shaped. But the effects predicted here are still observable, even if the maximum orbital shift is, say, three times larger than the spin shift. Correction to the WKBJ approximation has been neglected, otherwise $\mu_0 B$ might have to be larger to see this effect. (Accurate estimate of this correction is difficult, but it is of the order Δ_0^2/E_F.)

If the carrier density in N_{sp} is different from that in S_d, or if the band dispersion relations of the two sides are different, then the main effects, as far as we can see, are (i) a change in the absolute magnitude of the tunneling conductance which does not affect the normalized conductance; (ii) a stronger P dependence due to the energy dependence of the DOS in N_{sp} (without changing the limiting behavior at $P=1$); and (iii) a change in the ordinary reflection coefficient at the interface, which can be simulated with an effective Z. Even when the carriers in S_d are holes, and those in N_{sp} are electrons, we still find no essential change in our predictions.

In summary, we have analyzed in detail the giant magnetic moment that can result from the midgap states on the {110} surface of a d-wave superconductor. With high-T_c superconductors most likely having d-wave pairing, this predicted giant magnetic moment should be observable either directly in samples with a high concentration of internal {110} surfaces generated by ion irradiation, or, with better promise, by measuring the tunneling conductance between a spin-polarized normal metal and a high-T_c superconductor with a {110} surface. At a large enough external magnetic field applied along $[1\bar{1}0]$, and low enough temperature, the ZBCP is shown to split into two peaks, with their relative heights determined by the polarization of the normal metal because each peak is associated with a single spin. Since these predicted effects are rather difficult to simulate with other physics [such as the Appelbaum-Anderson mechanism[16] as an alternative possible explanation of the observed ZBCP (Ref. 3)], observing these predictions can provide a particularly strong confirmation on the existence of the midgap states and unconventional pairing, and remove any remaining suspicion that the observed ZBCP's might not be due to the midgap states.[17]

This work was supported by the Texas Higher Education Coordinating Board (Grant No. 1997-010366-029), and by the Texas Center for Superconductivity at the University of Houston.

*Permanent address.

[1] C.-R. Hu, Phys. Rev. Lett. **72**, 1526 (1994); J. Yang and C.-R. Hu, Phys. Rev. B **50**, 16 766 (1994).

[2] Y. Tanaka and S. Kashiwaya, Phys. Rev. Lett. **74**, 3451 (1995); S. Kashiwaya *et al.*, Phys. Rev. B **53**, 2667 (1996); J.-H. Xu *et al.*, *ibid.* **53**, 3604 (1996).

[3] C.-R. Hu, Phys. Rev. B **57**, 1266 (1998).

[4] M. Covington *et al.*, Phys. Rev. Lett. **79**, 277 (1997); L. Alff *et al.*, Phys. Rev. B **55**, 14 757 (1997); S. Sinha and K.-W. Ng, Phys. Rev. Lett. **80**, 1296 (1998); J.Y.T. Wei *et al.*, *ibid.* **81**, 2542 (1998).

[5] For a review, see C.-R. Hu, Int. J. Mod. Phys. B **12**, 3002 (1998).

[6] Yu.S. Barash, H. Burkhardt, and D. Rainer, Phys. Rev. Lett. **77**, 4070 (1996); M.P. Samanta and S. Datta, Phys. Rev. B **55**, R8689 (1997); X.-Z. Yan and C.-R. Hu, Phys. Rev. Lett. **83**, 1656 (1999).

[7] S. Higashitani, J. Phys. Soc. Jpn. **66**, 2556 (1997). See also, A.P. Niersen *et al.*, Bull. Am. Phys. Soc. **44**, 1697 (1999).

[8] W. Braunisch *et al.*, Phys. Rev. Lett. **68**, 1908 (1992).

[9] H. Walter *et al.*, Phys. Rev. Lett. **80**, 3598 (1998).

[10] A. Ino *et al.*, Phys. Rev. Lett. **81**, 2124 (1998). This reference gives $m_{ab}/M_b \simeq 1-3$ for $La_{2-x}Sr_xCuO_4$, where M_b is the band mass, which we estimate to be comparable to the free electron mass m_e, based on L.F. Mattheiss, *ibid.* **58**, 1028 (1987).

[11] J.R. Kirtley *et al.*, Phys. Rev. Lett. **81**, 2140 (1998).

[12] J.H. Park *et al.*, Nature (London) **392**, 794 (1998); C.T. Tanaka and J.S. Moodera, J. Appl. Phys. **79**, 6265 (1996).

[13] M.J.M. de Jong and C.W.J. Beenakker, Phys. Rev. Lett. **74**, 1657 (1995).

[14] G.E. Blonder, M. Tinkham, and T.M. Klapwijk, Phys. Rev. B **25**, 4515 (1982).

[15] I. Žutić and O. T. Valls, Phys. Rev. B **60**, 6320 (1999).

[16] P.W. Anderson, Phys. Rev. Lett. **17**, 95 (1966); J.A. Appelbaum, *ibid.* **17**, 91 (1966); Phys. Rev. **154**, 633 (1967).

[17] Charge/spin-density waves (CDW/SDW's) can potentially also give rise to ZBCP's [cf., J.H. Miller, Bull. Am. Phys. Soc. **44**, 1758 (1999)], MS's with similar spin and orbital shifts, and GMM if due to soliton-antisoliton formation in simple CDW/SDW's involving full one-dimensional nesting bands. Such MS's are not associated with surfaces and interfaces. Higher-dimensional CDW/SDW's may have k-dependent gaps which vanish at points, lines, or even regions of the Fermi surface. Whether they can lead to surface/interface MS's remains to be investigated. But, not being bound by Andreev reflections, such MS's cannot transport charge in the bound direction. Thus experimentally distinguishing the two sources of MS's should be possible.