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Spontaneous Magnetic Field near a Time-Reversal Symmetry Broken Surface State of YBCO

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Spatial distributions of spontaneous magnetic fields near a surface of cuprate high- T_C superconductor YBCO with broken time-reversal symmetry are calculated using the Ginzburg-Landau theory derived from the $t - J$ model. It is found that the magnetic field exists in a narrow region inside the superconductor, and it decays quickly outside the surface. Experimental approaches possible to detect such spontaneous magnetic fields are discussed.

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More than two decades ago, the peak splitting of zero bias conductance in *ab*-oriented YBCO/insulator/Cu tunnel junction was observed,¹⁾ and it has been considered as a sign of spontaneous violation of time-reversal symmetry (\mathcal{T}).²⁾ To interpret this experiment, superconducting (SC) states with a second SC order parameter (OP) that has symmetry different from that in the bulk ($d_{x^2-y^2}$ wave) have been proposed.³⁻⁵⁾ In these states, spontaneous currents and magnetic fields would occur near the surface. However, their existence is still controversial.^{6,7)}

The present author studied (110) surface states of YBCO that has two CuO_2 planes in a unit cell, using a bilayer $t - J$ model and the Bogoliubov de Gennes (BdG) method.^{8,9)} Near the (110) surface, where the $d_{x^2-y^2}$ -wave SCOP (Δ_d) is strongly suppressed, flux phase appears locally leading to a \mathcal{T} -breaking surface state. Flux phase is a mean-field solution to the $t - J$ model in which staggered currents flow and the flux penetrates a plaquette in a square lattice.¹⁰⁾ Although this state is only a metastable solution, its free energy is close to that of $d_{x^2-y^2}$ -wave SC state, because the former also has $d_{x^2-y^2}$ symmetry.^{11,12)} (On the contrary, on the basis of the $t - J$ model, *s*-wave SC state is not favored when the *d*-wave state is realized.) Then, the flux phase can occur once the *d*-wave SC order is suppressed. In the surface state with local flux phase order, the current is oscillating as a function of the distance from the surface. Moreover, in the bilayer model the fluxes in two layers are opposite.^{8,13)} Thus the spontaneous magnetic field near the surface is expected to be small.

In this short note, we study the spatial distributions of spontaneous magnetic fields near the (110) surface of YBCO, using the Ginzburg-Landau (GL) free energy derived from the $t - J$ model.¹⁴⁾ The purpose is to show that it will be difficult to observe the spontaneous field outside the sample even when \mathcal{T} is broken, while it may be detected inside the superconductor. The GL theory in this work is derived from the microscopic model and the parameters are chosen to represent the electronic structure of YBCO. This is the difference from other theories that have been proposed to explain the absence of spontaneous magnetic fields.^{15,16)}

First we consider the single layer case. GL free energy F_{GL} derived from the $t - J$ model consists of SCOPs (Δ_d and Δ_s), flux phase OP (Π), and the vector potential. Coefficients of all terms in F_{GL} can be calculated as functions of the first- (t), second- (t'), and third- (t'') neighbor transfer integrals, the superexchange interaction (J), the doping rare (δ), and the temperature (T). We take x (y) axis perpendicular (parallel) to the (110) surface. The region $x > 0$ ($x < 0$) is a superconductor (vacuum), and we assume that the system is uniform along the y direction. Numerical solutions are obtained by applying a quasi-Newton method to F_{GL} under the constraint that Δ_d vanishes at $x = 0$.

In Fig. 1, the spatial variations of the OPs are shown. Here we take $t/J = 2.5$ ($J = 0.1\text{eV}$), $t'/t = -0.3$, $t''/t = 0.15$, $\delta = 0.13$, and $T = 0.45T_C$ ($T_C = 0.131J$ being the SC transition temperature) and ξ_d is the coherence length of Δ_d . (For the parameters used here and the lattice constant of the square lattice $a = 3.8 \text{ \AA}$, $\xi_d \sim 9.4 \text{ \AA}$.) It is seen that the flux phase OP becomes finite near the surface where the d -wave SCOP is suppressed. In this region spontaneous staggered currents J_y and magnetic fields appear.

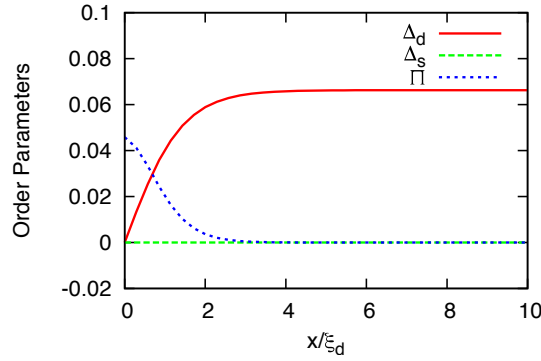


Fig. 1. (Color online) Spatial variations of the d -wave (Δ_d) and s -wave (Δ_s) SCOPs, and the OP for the flux phase (Π) near the (110) surface. Note that all OPs are non dimensional.

Next we treat a bilayer system by stacking the single-layer systems in such a way that the fluxes (and the currents) point oppositely in neighboring layers. The c axis lattice constant and the distance between a bilayer are taken to be $c = 11.7 \text{ \AA}$ and $c_1 = 3.4 \text{ \AA}$, respectively, to represent the structure of YBCO. We take the origin of the z axis at the center of a bilayer, and consider infinite stacking of CuO_2 planes. (Distance between neighbor currents in a plane is $a/\sqrt{2}$.^{9,17)}) We calculate magnetic fields \mathbf{B} by using the Biot-Savart law with the spontaneous currents obtained in the GL solutions to the single layer case. In this approach the screening effects in superconductors are neglected, so that the results should be taken as an upper limit of the absolute value of B .

Now we show the spatial variations of the magnetic fields in Fig.2. It is seen that both in-plane (B_x) and vertical (B_z) components occur near the surface, $x \lesssim \xi_d$, and they are oscillating as functions of x . (For $z = 0$, B_z vanishes due to symmetry.)

In fig.3, B_z and B_x are presented as functions of z for two choices of x (< 0). (The points $z = 0$ and $z = \pm c$ are the center of a bilayer in neighboring unit cell.) Outside the surface, both $|B_z|$ and $|B_x|$ are quite small. For $x = -0.2c$, B_x and B_z are already $\sim 1\%$ compared to those inside the superconductor, and they almost vanish for $x = -c$. For the sake of comparison,

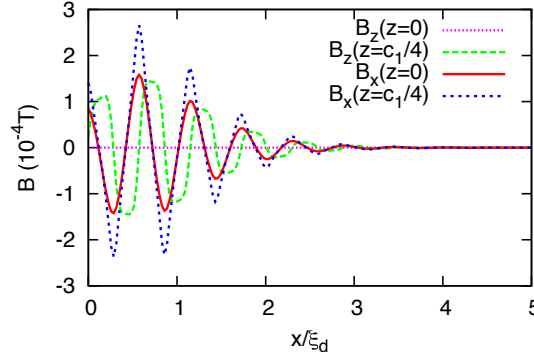


Fig. 2. (Color online) Spatial variations of B_z and B_x as functions of the distance from the surface, x , for $z = 0$ and $z = c_1/4$.

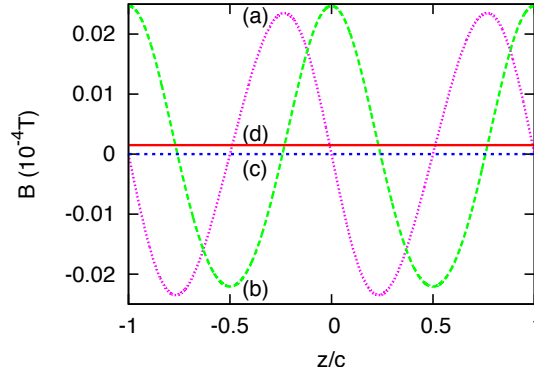


Fig. 3. (Color online) z dependence of B_z and B_x outside the superconductor. (a) $B_z(x = -0.2c, z)$, (b) $B_x(x = -0.2c, z)$, (c) $B_z(x = -c, z) \times 10^2$, and (d) $B_x(x = -c, z) \times 10^2$.

we show the results for the system where the currents in all layers are parallel. (Fig.4) In this case B_z stays constant when $x \gg c$, while B_x becomes zero. This is because the situation is equivalent to uniform currents flowing in an infinite plane ((110) plane), if one looks from a point far away from the surface. In the case of antiparallel currents, however, cancellation among contributions from staggered currents forces \mathbf{B} to vanish. Then the typical length scale for the decay of \mathbf{B} is of the order of c_1 , i.e., the distance between bilayer, or, antiparallel currents.

The difference between the cases of parallel and antiparallel currents is crucial to explain the apparent absence of spontaneous fields at the (110) surface of YBCO, where the peak spilling of the zero bias conductance was observed and \mathcal{T} breaking has been expected. Since the spontaneous magnetic field exists essentially inside the sample, it would be difficult to detect it using, e.g., SQUID microscope. Experimental approaches possible to measure it may be μ SR or polarized neutron scattering.

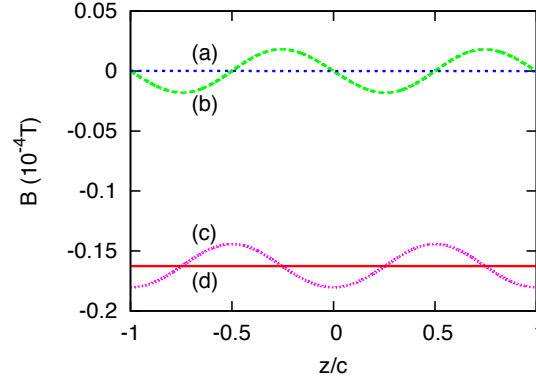


Fig. 4. (Color online) z dependence of B_z and B_x outside the superconductor, when the currents in neighboring layers are parallel. (a) $B_x(x = -100c, z)$, (b) $B_x(x = -0.2c, z)$, (c) $B_z(x = -0.2c, z)$, and (d) $B_z(x = -100c, z)$.

In the scenario to explain \mathcal{T} violation using the second SCOP, e.g., $(d \pm is)$ -wave state, spontaneous currents on different layers would be parallel, because Josephson coupling between layers should favor the phase difference to be zero. Thus \mathbf{B} may be observable outside the system in this case.

In this work, we obtained the absolute value of B (inside the superconductor) of the order of 1 G. However, it could be larger if T is lowered. Since the GL theory cannot handle the temperature region $T \ll T_C$, other approach, e.g., the BdG method has to be employed to examine this issue. We will study this problem separately.

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