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Spontaneous Magnetic Field and Local Density of States near a Time-Reversal Symmetry Broken Surface State of YBCO

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We study theoretically the spatial distribution of spontaneous magnetic fields near a (110) surface of cuprate high- T_C superconductor YBCO by treating a bilayer $t - J$ model with the Bogoliubov-de Gennes method. Near a (110) surface where $d_{x^2-y^2}$ -wave superconductivity is strongly suppressed, flux phase order occurs locally leading to a time-reversal symmetry broken surface state. Since the spontaneous currents flowing in the flux phase in two layers are antiparallel, resulting spontaneous magnetic fields are quite small. They exist in a narrow region inside the superconductor, and essentially vanish outside irrespective of the temperature. This result, together with the splitting of zero-energy peak of the local density of states, can provide consistent explanations for several experiments on YBCO.

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Spontaneous breaking of time-reversal symmetry (\mathcal{T}) near a surface or grain boundary of superconductors attracts much attention, because it is closely related to the symmetry of superconducting (SC) states and the mechanism of superconductivity. In the case of cuprate high- T_C superconductors, splitting of zero-bias conductance peak in YBCO/insulator/Cu junction was observed,¹⁾ and it has been regarded as a sign of spontaneous violation of time-reversal symmetry.²⁾ This experimental finding has been theoretically interpreted as due to the appearance of a second SC order parameter (OP) that has symmetry different from that in the bulk ($d_{x^2-y^2}$ wave). Since the $d_{x^2-y^2}$ -wave SC (d SC) state is strongly suppressed near a (110) surface, \mathcal{T} -breaking SC states with $(d \pm is)$ -wave symmetry may occur near the surface.³⁻⁶⁾ In these states, spontaneous currents and magnetic fields are expected to arise, but their existence is still controversial.^{7,8)} (Also, the splitting of the peak is not always observed in experiments in similar situations.⁹⁾)

In order to explain these phenomena, Håkansson et al.¹⁰⁾ considered the edge state of a d -wave superconductor where neighboring vortices have opposite current circulation. This state breaks \mathcal{T} , and gives rise to split peaks in the local density of states (LDOS) and a relatively small spontaneous magnetic field. Potter and Lee¹¹⁾ discussed ferromagnetism induced at the edge of d -wave superconductor that also leads to the splitting of the zero-energy peak.

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.^{12,13)} Near the (110) surface where the $d_{x^2-y^2}$ -wave SC state is strongly suppressed, a flux phase appears locally leading to a \mathcal{T} -violating surface state. The flux phase is a metastable mean-field solution to the $t - J$ model in which staggered currents flow and a flux penetrates a plaquette on a square lattice.¹⁴⁾ (The d -density wave state, which was introduced in a different context, have similar properties.¹⁵⁾) Mean-field calculations¹⁶⁻²¹⁾ and variational Monte Carlo (VMC) study²²⁻²⁴⁾ have shown that free energy of the flux state is higher than that of d SC state except very near half filling, so that it is only a next-to-leading (metastable) state in uniform systems. (Inclusion of nearest-neighbor repulsive interactions to the model may lead to the appearance of the flux phase for small doping rates.²⁵⁾) VMC calculations for the Hubbard model have shown that coexistence of flux phase and superconductivity is not possible in uniform systems,²⁶⁾ in agreement with the results for the $t - J$ model.

When the shape of the Fermi surface is favorable to the d SC state, other kind of ordered states that has the same symmetry may have free energy close to that of the former. This is because self-consistency equations in both states have the same form factor $(\cos k_x - \cos k_y)^2$, where $\mathbf{k} = (k_x, k_y)$ is a wave vector in the Brillouin zone, and it is large on the Fermi surface.

On the contrary, the s -wave SC (s SC) state has higher free energy, since the corresponding form factor $(\cos k_x + \cos k_y)^2$ is small on the same Fermi surface.²⁷⁾ (For an onsite pairing SC state, the form factor is a \mathbf{k} -independent constant, but this pairing is not allowed in the strongly correlated systems.) The flux phase has $d_{x^2-y^2}$ -wave symmetry, so that its free energy is close to that of d SC state compared with the s SC state. Thus, once the d SC order is suppressed, the flux phase can be a leading candidate of the local ordered state near the surface.

When the flux phase arises, spontaneous currents flow along the surface as in $(d \pm is)$ -wave SC state. However, the current in this case is oscillating as a function of the distance from the surface. Thus the spontaneous magnetic field generated by this current is expected to be smaller compared with that in the surface $(d \pm is)$ -wave SC state. Moreover in the bilayer $t - J$ model that describes the low-energy electronic states of YBCO, the directions of both fluxes and currents in the flux phase are opposite in two layers^{12,19)} This should further reduce the absolute values of spontaneous magnetic fields. We have investigated this problem using the Ginzburg-Landau (GL) theory derived from the $t - J$ model,^{28,29)} and showed that magnetic fields are actually very small. They almost vanish outside the superconductor, although they are finite inside the sample within a narrow region of SC coherence length, ξ_d , from the surface. However, the temperature (T) region in which the GL theory is quantitatively reliable is limited to that near T_C , i.e., the SC transition temperature.

In this letter, we study the spatial distribution of the spontaneous magnetic field near the (110) surface of YBCO, using the BdG method applied to the bilayer $t - J$ model. We examine their temperature dependence, and show that even at lowest T the spontaneous magnetic fields are measurable only in a narrow region inside the superconductor (with a width of the order of ξ_d), and in a quite narrow region outside. By measuring these magnetic field distributions experimentally, it will be possible to decide whether the present theory correctly describes the surface state of YBCO. We also study the temperature dependence of the LDOS near the surface, which can also be tested experimentally.

We treat the bilayer $t - J$ model whose Hamiltonian is given by $H = H_1 + H_2 + H_T$ with

$$H_i = - \sum_{j,\ell,\sigma} t_{j\ell} e^{i\phi_{j\ell}} \tilde{c}_{j\sigma}^{(i)\dagger} \tilde{c}_{\ell\sigma}^{(i)} + J \sum_{\langle j,\ell \rangle} \mathbf{S}_j^{(i)} \cdot \mathbf{S}_\ell^{(i)} \quad (i = 1, 2) \quad (1)$$

$$H_\perp = - \sum_{j,\ell,\sigma} t_{j\ell}^\perp (\tilde{c}_{j\sigma}^{(1)\dagger} \tilde{c}_{\ell\sigma}^{(2)} + h.c.) + J_\perp \sum_j \mathbf{S}_j^{(1)} \cdot \mathbf{S}_j^{(2)}, \quad (2)$$

where H_1 and H_2 are the Hamiltonian for each layer (with a square lattice) and H_T describes interlayer couplings. $\tilde{c}_{j\sigma}^{(i)}$ is the electron operator at a site j on the i -th plane with spin σ in Fock space without double occupancy, and we treat this condition using the slave-

boson (SB) method.^{30,31)} Here \mathbf{S}_j denotes the spin operator. (For the detail of SB mean-field calculation, see Ref. 13.) The in-plane transfer integrals $t_{j\ell}$ are finite for the first- (t), second- (t'), and third-nearest-neighbor bonds (t''), or zero otherwise. J (J_\perp) is the inplane (interplane) antiferromagnetic superexchange interaction, and $\langle j, \ell \rangle$ denotes nearest-neighbor bonds. The interplane transfer integrals $t_{j\ell}^\perp$ are chosen to reproduce the dispersion in k space,³²⁾ $t_k^\perp = -t_0^\perp(\cos k_x - \cos k_y)^2$, namely, "on-site" (t_0^\perp), second- ($t_2^\perp = -t_0^\perp/2$), and third-nearest-neighbor bonds ($t_3^\perp = t_0^\perp/4$) are taken into account. The magnetic field is taken into account using the Peierls phase $\phi_{j,\ell} \equiv \frac{\pi}{\phi_0} \int_j^\ell \mathbf{A} \cdot d\mathbf{l}$, with \mathbf{A} and $\phi_0 = \frac{h}{2e}$ being the vector potential and flux quantum, respectively. Following Ref. 33, we take $t/J = 2.5$ ($J = 0.1\text{eV}$), $t'/t = -0.3$, $t''/t = 0.15$, $t_0^\perp/t = 0.15$, and $J_\perp/J = 0.1$. These parameters were chosen to reproduce experimental results for YBCO. We take $\delta = 0.15$ for the doping rate throughout in this work. The results for other values of δ are qualitatively the same; for larger value of δ , $\text{Im } \chi$ becomes smaller and so the absolute value of B . In mean-field calculations for uniform systems, the flux phase with opposite directions of fluxes in two layers persists only up to $\delta \sim 0.15$.¹²⁾ However in the BdG calculation it can occur up to $\delta \sim 0.3$, because the incommensurate solution that is not taken into account in the former can arise, and it has free energy lower than that of the flux phase with the same direction of fluxes.¹³⁾

We consider a system with a (110) surface, and denote the direction perpendicular (parallel) to the surface as x (y), where the region $x > 0$ ($x < 0$) is a superconductor (vacuum). We assume that the system is uniform along the y direction, and the periodic boundary condition is used for this direction. For the system size, $N_x = 200$ and $N_y = 100$ are used. Following the procedure presented in Refs. 13 and 34, we perform BdG calculations to study spatial variations of the d SC (Δ_d) and s SC (Δ_s) OPs, and the bond OP (χ). The imaginary part of χ corresponds to the OP for the flux phase.

In Fig.1, we show the spatial variations of the OP for the flux phase, $\text{Im } \chi$, for several temperatures. Surface flux phase appears below $T = 0.19T_C$ ($T_C = 0.1164J$), and $\text{Im } \chi$ becomes larger as T is lowered. The spontaneous current along the surface in the i -th layer, $J_y^{(i)}$, is proportional to $\text{Im } \chi^{(i)}$ as^{13,34)}

$$J_y^{(i)}(x) = \frac{\sqrt{2}\pi t \delta}{\phi_0} \text{Im } \chi^{(i)}(x) \quad (i = 1, 2). \quad (3)$$

The currents in two layers are antiparallel: $J_y^{(1)}(x) = -J_y^{(2)}(x)$.

Next we calculate spontaneous magnetic fields generated by these currents. We model the actual system by considering the infinite stacking of bilayer systems. Assuming the tetragonal structure, c -axis lattice constant and the distance between a bilayer are taken to be $c = 11.7$

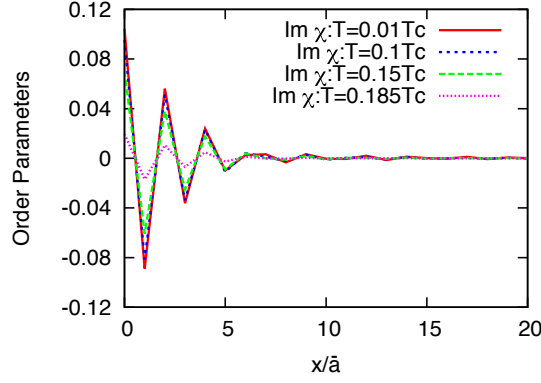


Fig. 1. (Color online) Spatial variations of the imaginary part of the bond order parameter, $\text{Im } \chi$, on the first layer ($i = 1$). Note that χ is nondimensional.

\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. (Distance between neighbor currents in a plane is $\bar{a} \equiv a/\sqrt{2}$,^{13,34}) where $a = 3.8 \text{ \AA}$ is the a -axis lattice constant.) Magnetic fields \mathbf{B} are estimated by using the Biot-Savart law

$$B_x(x, z) = \frac{\mu_0}{2\pi} \sum_{j=1}^{N_x-1} \sum_{n=-\infty}^{\infty} \left[\frac{(z - z_n^{(+)})J_y^{(2)}(x_j)}{(x - x_j)^2 + (z - z_n^{(+)})^2} + \frac{(z - z_n^{(-)})J_y^{(1)}(x_j)}{(x - x_j)^2 + (z - z_n^{(-)})^2} \right] \quad (4)$$

$$B_z(x, z) = -\frac{\mu_0}{2\pi} \sum_{j=1}^{N_x-1} \sum_{n=-\infty}^{\infty} \left[\frac{(x - x_j)J_y^{(2)}(x_j)}{(x - x_j)^2 + (z - z_n^{(+)})^2} + \frac{(x - x_j)J_y^{(1)}(x_j)}{(x - x_j)^2 + (z - z_n^{(-)})^2} \right], \quad (5)$$

where $x_j = (j - 1/2)\bar{a}$ and $z_n^{(\pm)} = cn \pm c_1/2$. The expression for B_z can be simplified as

$$B_z(x, z) = \frac{\mu_0}{2\pi c} \sum_{j=1}^{N_x-1} [G^{(+)}(x, z, j) - G^{(-)}(x, z, j)]J_y^{(1)}(x_j), \quad (6)$$

where

$$G^{(\pm)}(x, z, j) = \frac{\pi \sinh\left(\frac{2\pi}{c}(x - x_j)\right)}{\cosh\left(\frac{2\pi}{c}(x - x_j)\right) - \cos\left(\frac{2\pi}{c}(z \mp \frac{c_1}{2})\right)}. \quad (7)$$

In this approach the screening effects in superconductors are neglected, so that the results should be taken as upper limits of the absolute values of B .

We show the x dependence of the magnetic fields inside the superconductor for two choices of z in Fig.2. Here the temperature is $T = 0.01T_C$. It is seen that both in-plane (B_x) and vertical (B_z) components occur near the surface and they are oscillating as functions of x . (For $z = 0$, B_z vanishes due to symmetry.) The important feature is that the magnetic fields decay quite rapidly as functions of x . This is because contributions from antiparallel currents cancel each other at a site where $J_y \sim 0$. Actually, we can see from Eqs. (6) and (7) that the

typical length scale of the decay of B_z is $c/2\pi$. The amplitude of the magnetic field is large near the surface where J_y is finite. These large magnetic fields existing in a narrow region of $x \lesssim \xi_d$ may be detected by experimental approaches such as μ SR or polarized neutron scattering, although the values of B will be reduced if one treats the screening effect correctly. (Surface roughness, which is inevitable in real materials, would also reduce the value of B .) If $J_y(x)$ does not oscillate and has definite sign, B will be finite for $x \lesssim \lambda$ (λ being the penetration depth), even when we treat the screening effect properly.

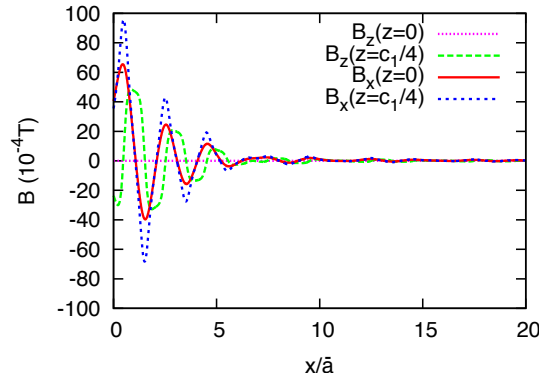


Fig. 2. (Color online) Spatial variations of B_x and B_z as functions of the distance from the surface, x , for $z = 0$ and $c_1/4$. The temperature is $T = 0.01T_C$.

In Fig.3, B_x and B_z are presented as functions of z for two choices of x (< 0), i.e., outside the superconductor. Here the points $z = 0$ and $\pm c$ are the center of a bilayer in neighboring unit cells. Outside the sample B decays quickly in a manner similar to the case of $x \gtrsim \xi_d$ (i.e., inside the superconductor) due to cancellation among contributions from antiparallel currents. Although the values of B outside the superconductor are quite small, we may expect that the spin polarized scanning tunneling microscopy (STM) could measure the spatial distribution of the magnetic field.

In order to examine the temperature dependence of the magnetic field, we plot their variations along the x (z) direction for $T = 0.185T_C$ in Fig. 4 (Fig. 5). As the temperature is raised, the OP for the flux phase decreases as shown in Fig.1. Then the amplitudes of the magnetic fields are expected to decrease in proportion to it. This is actually the case as we can see by comparing Fig.4 (Fig.5) with Fig.2 (Fig.3).

In the scenario to explain \mathcal{T} violation using the second SCOP, e.g., $(d \pm is)$ -wave SC states, spontaneous currents on different layers would be parallel, since Josephson coupling between layers would favor phase difference of the s SC OPs to be zero. Thus \mathbf{B} should be

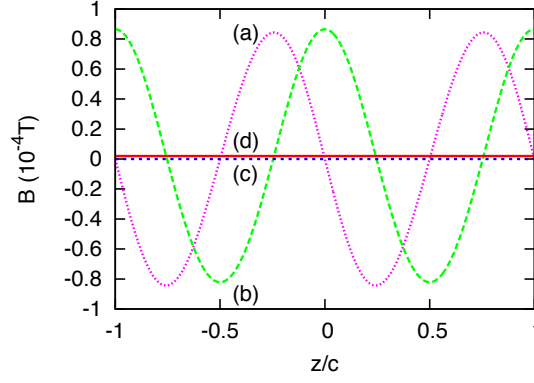


Fig. 3. (Color online) z dependence of B_x and B_z outside the superconductor for $T = 0.01T_C$. (a) $B_z(x = -0.2c, z)$, (b) $B_x(x = -0.2c, z)$, (c) $B_z(x = -c, z) \times 10$, and (d) $B_x(x = -c, z) \times 10$.

observable outside the sample in this case.

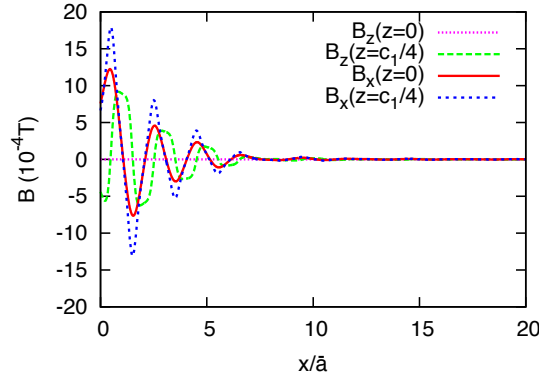


Fig. 4. (Color online) Spatial variations of B_x and B_z as functions of the distance from the surface, x , for $z = 0$ and $c_1/4$. The temperature is $T = 0.185T_C$.

Next we calculate the LDOS by employing the prescription described in Ref. 13. (In numerical calculations, we replace the δ function by a Lorentzian with the width $0.005J$.) In Fig.6, the LODS at the surface site is shown for several temperatures. At $T = 0.19T_C$, where $\text{Im } \chi = 0$, a zero-energy peak due to Andreev bound state appears. For $T < 0.19T_C$, flux phase order occurs and then the splitting of the peak takes place. When the temperature is decreased, $\text{Im } \chi$ becomes larger, and the splitting broadens as $T \rightarrow 0$. The theoretical result for the splitting at $T = 0.01T_C$ ($\sim 1\text{K}$) is large in comparison to the experiment.¹⁾ This discrepancy could be due to the neglect of fluctuations around the mean-field solution. Also, for the comparison to the experiment, it should be noted that the LDOS at the surface directly corresponds to the tunneling conductance only when the interface is flat and clean and the

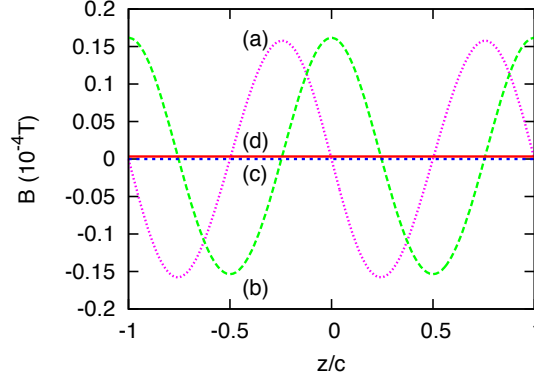


Fig. 5. (Color online) z dependence of B_x and B_z outside the superconductor for $T = 0.185T_c$. (a) $B_z(x = -0.2c, z)$, (b) $B_x(x = -0.2c, z)$, (c) $B_z(x = -c, z) \times 10$, and (d) $B_x(x = -c, z) \times 10$.

transparency is low.^{35,36)}

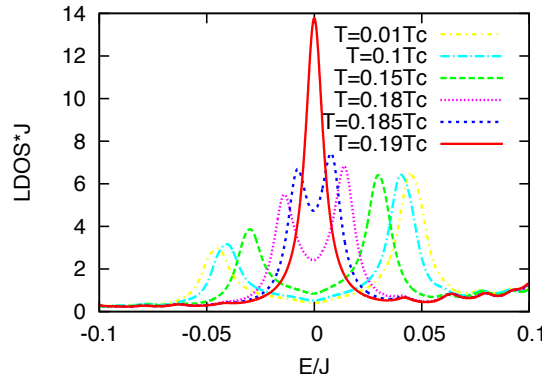


Fig. 6. (Color online) LDOS at the (110) surface for several temperatures.

In summary, we have studied the spontaneous magnetic field and the LDOS near the (110) surface of YBCO, where the time-reversal symmetry is spontaneously broken, by using the BdG method applied to the bilayer $t - J$ model. It is found that in the superconductor spontaneous magnetic fields can arise, but only in a narrow region with a width of the order of ξ_d from the surface. Outside the sample, the region in which B is finite is much narrower; B decays within a few \AA from the surface. These magnetic fields may be difficult to detect experimentally, but we expect μSR , polarized neutron scattering, and the spin polarized STM could detect them. We have also investigated the temperature dependence of the LDOS at the surface, and found that the splitting of the zero-energy peak decreases as the temperature is increased.

For the values of B , our estimates give the upper bound, because we did not take into

account the screening effect in superconductors (due to the use of Biot-Savart law), surface roughness, and the fluctuations around the mean-field solution. These effects will reduce not only the flux phase OP and the values of B , but also the splitting of the peak in the LDOS. The latter could make the theoretical results get closer to the experimental values.

There have been many other mechanisms aimed to explain the splitting of zero-energy peak observed by Covington et al.¹⁾ Effects of impurity scattering,³⁷⁾ coexistence of spin-density wave^{38,39)} and d -density wave order³⁹⁾ with d -wave SC states near the surface have been proposed. Also, p -wave SC order near the surface has been predicted.^{38,40)} Since a large zero-energy DOS due to Andreev bound state exists near a (110) surface of d -wave superconductor, the system has a tendency toward ferromagnetism if an on-site repulsive interaction is present.^{11,41)} This can lead to edge ferromagnetic order with split peak.

In the present work, the BdG equations are 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 both the apparent absence of spontaneous magnetic fields and the splitting of the zero-energy peak in the LDOS. The results for the distribution of spontaneous magnetic fields calculated in this work may be tested experimentally, and it will decide whether the present theory correctly describes the surface state of YBCO.

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References

- 1) M. Covington, M. Aprili, E. Paraoanu, L. H. Greene, F. Xu, J. Zhu, and C. A. Mirkin, Phys. Rev. Lett. **79**, 277 (1997).
- 2) M. Sigrist, Prog. Theor. Phys. **99**, 899 (1998).
- 3) M. Matsumoto and H. Shiba, J. Phys. Soc. Jpn. **64**, 3384 (1995).
- 4) M. Matsumoto and H. Shiba, J. Phys. Soc. Jpn. **64**, 4867 (1995).
- 5) M. Fogelström, D. Rainer, and J. A. Sauls, Phys. Rev. Lett. **79**, 281 (1997).
- 6) Y. Tanuma, Y. Tanaka, M. Ogata, and S. Kashiwaya, Phys. Rev. B **60** 9817 (1999).
- 7) R. Carmi, E. Polturak, G. Koren, and A. Auerbach, Nature **404**, 853 (2000).
- 8) H. Saadaoui, Z. Salman, T. Prokscha, A. Suter, H. Huhtinen, P. Paturi, and E. Morenzoni, Phys. Rev. B **88**, 180501(R) (2013).
- 9) H. Kashiwaya, S. Kashiwaya, B. Prijamboedi, A. Sawa, I. Kurosawa, Y. Tanaka, and I. Iguchi, Phys. Rev. B **70**, 094501 (2004).
- 10) M. Håkansson, T. Löfwander, and M. Fogelström, Nature Physics **11**, 755 (2015).
- 11) A. C. Potter and P. A. Lee, Phys. Rev. Lett. **112**, 117002 (2014).
- 12) K. Kuboki, J. Phys. Soc. Jpn. **83**, 125001 (2014).
- 13) K. Kuboki, J. Phys. Soc. Jpn. **84**, 064706 (2015).
- 14) I. Affleck and J. B. Marston, Phys. Rev. B **37**, 3774 (1988).
- 15) S. Chakravarty, R. B. Laughlin, D. K. Morr, and C. Nayak, Phys. Rev. B **63**, 094503 (2001).
- 16) F. C. Zhang, Phys. Rev. Lett. **64**, 974 (1990).
- 17) M. U. Ubbens and P. A. Lee, Phys. Rev. B **46**, 8434 (1992).
- 18) K. Hamada and D. Yoshioka, Phys. Rev. B **67**, 184503 (2003).
- 19) H. Zhao and J. R. Engelbrecht, Phys. Rev. B **71**, 054508 (2005).
- 20) M. Bejas, A. Greco, and H. Yamase, Phys. Rev. B **86**, 224509 (2012).
- 21) K. Kuboki, J. Phys. Soc. Jpn. **83**, 015003 (2014).
- 22) H. Yokoyama and M. Ogata, J. Phys. Soc. Jpn. **65**, 3615 (1996).
- 23) T. K. Lee and L. N. Chang, Phys. Rev. B **42**, 8720 (1990).
- 24) D. A. Ivanov and P. A. Lee, Phys. Rev. B **68**, 132501 (2003).
- 25) S. Zhou and Z. Wang, Phys. Rev. B **70**, 020501(R) (2004).

- 26) H. Yokoyama, S. Tamura, and M. Ogata, J. Phys. Soc. Jpn. **85**, 124707 (2016).
- 27) K. Kuboki, J. Phys. Soc. Jpn. **70**, 2698 (2001).
- 28) K. Kuboki, J. Phys. Soc. Jpn. **87**, 024703 (2018).
- 29) K. Kuboki, J. Phys. Soc. Jpn. **88**, 095002 (2019).
- 30) M. Ogata and H. Fukuyama, Rep. Prog. Phys. **71**, 036501 (2008).
- 31) P. A. Lee, N. Nagaosa, and X. G. Wen, Rev. Mod. Phys. **78**, 17 (2006).
- 32) O. K. Andersen, A. I. Lichtenstein, O. Jepsen, and F. Paulsen, J. Phys. Chem. Solids **56**, 1573 (1995).
- 33) H. Yamase and W. Metzner, Phys. Rev. B **73**, 214517 (2006).
- 34) K. Kuboki, J. Phys. Soc. Jpn. **83**, 054703 (2014).
- 35) S. Kashiwaya, Y. Tanaka, M. Koyanagi, and K. Kajimura, Phys. Rev. B **53**, 2667 (1996).
- 36) Y. Tanuma, Y. Tanaka, and S. Kashiwaya, Phys. Rev. B **64**, 214519 (2001).
- 37) Y. Asano and Y. Tanaka, Phys. Rev. B **65**, 064522 (2002).
- 38) C. Honerkamp, K. Wakabayashi, and M. Sigrist, EPL **50**, 368 (2000).
- 39) Y. Asano, Y. Tanaka, H. Tsuchiura, and S. Kashiwaya, J. Phys. and Chem. of Solids **67**, 186 (2006).
- 40) S. Matsubara and H. Kontani, arXiv:2002.06891.
- 41) S. Matsubara and H. Kontani, Phys. Rev. B **101**, 075114 (2020)