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Kuboki, Kazuhiro

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Ginzburg-Landau Theory for Flux Phase and Superconductivity in $t - J$ Model

Kazuhiro Kuboki *

Department of Physics, Kobe University, Kobe 657-8501, Japan

Ginzburg-Landau (GL) equations and GL free energy for flux phase and superconductivity are derived microscopically from the $t - J$ model on a square lattice. Order parameter (OP) for the flux phase has direct coupling to a magnetic field, in contrast to the superconducting OP which has minimal coupling to a vector potential. Therefore, when the flux phase OP has unidirectional spatial variation, staggered currents would flow in a perpendicular direction. The derived GL theory can be used for various problems in high-T_c cuprate superconductors, e.g., states near a surface or impurities, and the effect of an external magnetic field. Since the GL theory derived microscopically directly reflects the electronic structure of the system, e.g., the shape of the Fermi surface that changes with doping, it can provide more useful information than that from phenomenological GL theories.

*kuboki@kobe-u.ac.jp

1. Introduction

Spontaneous violation of time-reversal symmetry $\mathcal{T}$ in superconductors has been discussed intensively. Especially, in high-T_c cuprate superconductors, a sign of spontaneous $\mathcal{T}$ violation was detected two decades ago. Covington *et al.* observed the peak splitting of zero bias conductance in ab-oriented YBCO/insulator/Cu junction,[1] and this has been interpreted as evidence of $\mathcal{T}$ violation induced by a second superconducting (SC) order parameter (OP) near the surface, with the symmetry different from that in the bulk.[2–4] In the literature, surface (or interface) $\mathcal{T}$-breaking states with $(d \pm is)$-, $(d \pm id')$-, and $(d \pm ig)$-wave symmetry have been discussed.[2–8] However, existence of spontaneous current which would flow along the surface and an accompanying magnetic field is still controversial.[9,10]

The present author has studied (110) surface states of high-T_C cuprates based on the Bogoliubov-de Gennes (BdG) method by employing single-layer and bilayer $t-J$ models, and found that a different kind of $\mathcal{T}$-breaking surface state, flux phase, can occur.[11–14] 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.[15] (The d-density wave state, which has been introduced in a different context, have similar properties.[16]) Mean-field[17–21] and variational Monte Carlo[22–25] calculations have shown that free energy of the flux state is higher than that of a $d_{x^2-y^2}$-wave 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.[26]) Besides the $t-J$ model, variational Monte Carlo calculations for the Hubbard model have shown that coexistence of flux phase and superconductivity cannot occur in uniform systems,[27] and this feature is consistent with the results for the $t-J$ model. However, near the (110) surface, the $d_{x^2-y^2}$-wave SC state is strongly suppressed, and the flux phase may arise locally leading to a $\mathcal{T}$-breaking surface state. Since the spontaneous current in this state is a staggered one, accompanying magnetic fields will be smaller compared to those induced in surface states with the second SCOP.

The peak splitting of zero bias conductance was observed in systems composed of YBCO cuprates that has two CuO_2 planes in a unit cell. In the case of a bilayer $t-J$ model, which is a model to describe bilayer cuprates such as YBCO, there may be two types of flux phase in which the directions of the flux in two layers are the same or opposite. Mean-field approximation (MFA) and BdG calculations have shown that the latter state has lower energy than that of the former.[13,14] Then the spontaneous currents and magnetic fields in two layers have opposite signs, and so the observed field near the surface will be smaller compared to the single-layer systems. The theoretically obtained magnetic field is, however, still comparable or larger than the upper bound set by experiments. In order to determine whether or not the peak splitting can be explained in terms of the flux state, we have to evaluate the magnetic field strength in a self-consistent manner, which is difficult to carry out in BdG calculations.

In this paper, we derive Ginzburg-Landau (GL) equations and GL free energy microscopically from the two-dimensional $t - J$ model on a square lattice, in order to provide a tool to investigate the distribution of magnetic fields more accurately. The method of deriving GL equations is essentially the same as that used in previous studies which treat the coexistence of magnetic order and superconductivity in the extended Hubbard model[28] and the $t - J$ model.[29] The resulting GL theory can be used for various problems, e.g., investigation of the magnetic field distribution near the surface, states near impurities, and the effect of an external magnetic field. Although the GL theory is reliable only qualitatively except near T_C, it can give simple and intuitive description of the coexistence and competition of multiple OPs. Thus, it is complementary to more sophisticated methods such as the BdG and quasiclassical Green's function theory.

This paper is organized as follows. In Sect. 2 we present the model and treat it by a mean-field approximation. GL equations and GL free energy are derived in Sect. 3. Sect. 4 is devoted to summary.

2. Model and Mean-Field Approximation

We consider the $t - J$ model on a square lattice whose Hamiltonian is given by

$$H = -\sum_{j,\ell,\sigma} t_{j\ell}\tilde{c}^{\dagger}_{j\sigma}\tilde{c}_{\ell\sigma} + J\sum_{\langle j,\ell\rangle}\mathbf{S}_j\cdot\mathbf{S}_\ell, \tag{1}$$

where the transfer integrals $t_{j\ell}$ are finite for the first- (t), second- (t'), and third-nearest-neighbor bonds (t''), or zero otherwise. J is the antiferromagnetic superexchange interaction, and $\langle j,\ell\rangle$ denotes nearest-neighbor bonds.[30] 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. $\tilde{c}_{j\sigma}$ is the electron operator in Fock space without double occupancy, and we treat this condition using the slave-boson method[30–32] by writing $\tilde{c}_{j\sigma} = b^{\dagger}_j f_{j\sigma}$ under the local constraint $\sum_\sigma f^{\dagger}_{j\sigma}f_{j\sigma} + b^{\dagger}_j b_j = 1$ at every j site. Here $f_{j\sigma}$ (b_j) is a fermion (boson) operator that carries spin σ (charge e); the fermions (bosons) are frequently referred to as spinons (holons). The spin operator is expressed as $\mathbf{S}_j = \frac{1}{2}\sum_{\alpha,\beta} f^{\dagger}_{j\alpha}\sigma_{\alpha\beta}f_{j\beta}$.

We decouple the Hamiltonian in the following manner.[33,34] The bond OPs $\sum_\sigma\langle f^{\dagger}_{j\sigma}f_{\ell\sigma}\rangle$ and

$\langle b_j^\dagger b_\ell \rangle$ are introduced, and we denote $\chi_{j,\ell} \equiv \sum_\sigma \langle f_{j\sigma}^\dagger f_{\ell\sigma} \rangle$ for nearest-neighbor bonds. Although the bosons are not condensed in purely two-dimensional systems at finite temperature (T), they are almost condensed at a low T and for finite carrier doping ($\delta \gtrsim 0.05$, δ being the doping rate). Since we are interested in the low temperature region ($T \lesssim 10^{-2} J \sim 10$K) and the doping rate $\delta \gtrsim 0.05$, we treat holons as Bose condensed. Hence, we approximate $\langle b_j \rangle \sim \sqrt{\delta}$ and $\langle b_j^\dagger b_\ell \rangle \sim \delta$, and replace the local constraint with a global one, $\frac{1}{N}\sum_{j,\sigma}\langle f_{j\sigma}^\dagger f_{j\sigma}\rangle = 1 - \delta$, where N is the total number of lattice sites. This procedure amounts to renormalizing the transfer integrals by multiplying δ, i.e., $t \to t\delta$, *etc.*, and rewriting $\tilde{c}_{j\sigma}$ as $f_{j\sigma}$. In a qualitative sense, this approach is equivalent to the renormalized mean-field theory of Zhang *et al.*[35] (Gutzwiller approximation). The spin-singlet resonating-valence-bond (RVB) OP on the bond $\langle j, \ell \rangle$ is given by $\Delta_{j,\ell} = \langle f_{j\uparrow} f_{\ell\downarrow} - f_{j\downarrow} f_{\ell\uparrow} \rangle / 2$. Under the assumption of the Bose condensation of holons, $\Delta_{j,\ell}$ is equivalent to the SCOP.

With the above definitions of the OPs, the mean-field Hamiltonian is written as

$$\begin{aligned} H_{MFA} = & -\sum_{j,\sigma}\Big[\sum_{\delta_1=\pm\hat{x},\pm\hat{y}}\Big(t\delta e^{i\phi_{j+\delta_1,j}} + \frac{3J}{8}\chi_{j,j+\delta_1}\Big) f_{j+\delta_1,\sigma}^\dagger f_{j\sigma} \\ & + t'\delta \sum_{\delta_2=\pm\hat{x}\pm\hat{y}} e^{i\phi_{j+\delta_2,j}} f_{j+\delta_2,\sigma}^\dagger f_{j\sigma} + t''\delta \sum_{\delta_3=\pm 2\hat{x},\pm 2\hat{y}} e^{i\phi_{j+\delta_3,j}} f_{j+\delta_3,\sigma}^\dagger f_{j\sigma} + \mu f_{j\sigma}^\dagger f_{j\sigma}\Big] \\ & + \frac{3J}{8}\sum_j \sum_{\delta_1=\pm\hat{x},\pm\hat{y}} \Big[\Delta_{j,j+\delta_1}\big(f_{j\uparrow}^\dagger f_{j+\delta_1\downarrow}^\dagger - f_{j\downarrow}^\dagger f_{j+\delta_1\uparrow}^\dagger\big) + h.c.\Big] + E_0, \end{aligned} \tag{2}$$

where

$$E_0 = \frac{3J}{2}\sum_j \sum_{\delta_1=\hat{x},\hat{y}} \Big(|\Delta_{j,j+\delta_1}|^2 + \frac{1}{4}|\chi_{j,j+\delta_1}|^2\Big), \tag{3}$$

and μ is the chemical potential. We divide $\chi_{j,\ell}$ into two parts

$$\chi_{j,\ell} = \chi_0 + Z_{j,\ell}, \tag{4}$$

where χ_0 is real and uniform in space, while $Z_{j,\ell}$ may be complex and describe the flux phase as we will see in the following.

Since the onset temperature of χ_0 is much higher than that for superconductivity (T_C) and the bare transition temperature of the flux phase, we treat only Δ and Z as the GL-expansion parameters, and determine χ_0 using the usual MFA. The self-consistency equations for χ_0 and μ in the absence of Δ, Z, and $\mathbf{A}$ are given as

$$\chi_0 = \frac{1}{N}\sum_p (\cos p_x + \cos p_y) f(\xi_p), \quad \delta = 1 - \frac{2}{N}\sum_p f(\xi_p), \tag{5}$$

where f is the Fermi distribution function, and

$$\xi_p = -\Big(2t\delta + \frac{3J}{4}\chi_0\Big)(\cos p_x + \cos p_y) - 4t'\delta\cos p_x\cos p_y - 2t''\delta(\cos 2p_x + \cos 2p_y) - \mu. \quad (6)$$

We set the lattice constant to be unity.

3. Ginzburg-Landau Equations and Free Energy

In this section we derive the GL equations and GL free energy. The Gor'kov equations for normal and anomalous Green's functions, respectively defined as, $G(j,\ell,\tau) \equiv -\langle T_\tau f_{j\uparrow}(\tau) f^\dagger_{\ell\uparrow}\rangle$ and $F^\dagger(j,\ell,\tau) \equiv -\langle T_\tau f^\dagger_{j\downarrow}(\tau) f^\dagger_{\ell\uparrow}\rangle$, can be derived by a standard procedure,[28,29,36)]

$$\begin{aligned}(i\epsilon_n+\mu)G(j,\ell,i\epsilon_n) &+ \sum_{\delta_1=\pm\hat{x},\pm\hat{y}}\Big(t\delta e^{i\phi_{j,j+\delta_1}} + \frac{3J}{8}\chi_{j+\delta_1,j}\Big)G(j+\delta_1,\ell,i\epsilon_n)\\
+\sum_{\delta_2=\pm\hat{x}\pm\hat{y}} t'\delta e^{i\phi_{j,j+\delta_2}}G(j+\delta_2,\ell,i\epsilon_n) &+ \sum_{\delta_3=\pm2\hat{x},\pm2\hat{y}} t''\delta e^{i\phi_{j,j+\delta_3}}G(j+\delta_3,\ell,i\epsilon_n)\\
&-\frac{3J}{4}\sum_{\delta_1=\pm\hat{x},\pm\hat{y}}\Delta_{j,j+\delta_1}F^\dagger(j+\delta_1.\ell,i\epsilon_n) = \delta_{jl},\end{aligned} \quad (7)$$

$$\begin{aligned}(i\epsilon_n-\mu)F^\dagger(j,\ell,i\epsilon_n) &- \sum_{\delta_1=\pm\hat{x},\pm\hat{y}}\Big(t\delta e^{i\phi_{j+\delta_1,j}} + \frac{3J}{8}\chi_{j,j+\delta_1}\Big)F^\dagger(j+\delta_1,\ell,i\epsilon_n)\\
-\sum_{\delta_2=\pm\hat{x}\pm\hat{y}} t'\delta e^{i\phi_{j+\delta_2,j}}F^\dagger(j+\delta_2,\ell,i\epsilon_n) &- \sum_{\delta_3=\pm2\hat{x},\pm2\hat{y}} t''\delta e^{i\phi_{j+\delta_3,j}}F^\dagger(j+\delta_3,\ell,i\epsilon_n)\\
&-\frac{3J}{4}\sum_{\delta_1=\pm\hat{x},\pm\hat{y}}\Delta^*_{j,j+\delta_1}G(j+\delta_1,\ell,i\epsilon_n) = 0,\end{aligned} \quad (8)$$

where ϵ_n is a fermionic Matsubara frequency. These equations can be combined as

$$\begin{aligned}G(j,\ell,i\epsilon_n) = \quad &\tilde{G}_0(j,\ell,i\epsilon_n) + \frac{3J}{4}\sum_k\sum_{\delta_1=\pm\hat{x},\pm\hat{y}}\tilde{G}_0(j,k,i\epsilon_n)\Big[\Delta_{k,k+\delta_1}F^\dagger(k+\delta_1,\ell,i\epsilon_n)\\
&-\frac{1}{2}Z_{k+\delta_1,k}G(k+\delta_1,\ell,i\epsilon_n)\Big],\end{aligned} \quad (9)$$

$$\begin{aligned}F^\dagger(j,\ell,i\epsilon_n) = \quad &-\frac{3J}{4}\sum_k\sum_{\delta_1=\pm\hat{x},\pm\hat{y}}\tilde{G}_0(k,j,-i\epsilon_n)\Big[\Delta^*_{k,k+\delta_1}G(k+\delta_1,\ell,i\epsilon_n)\\
&+\frac{1}{2}Z_{k,k+\delta_1}F^\dagger(k+\delta_1,\ell,i\epsilon_n)\Big],\end{aligned} \quad (10)$$

where the summation on k is taken over all sites, and $\tilde{G}_0(j,\ell,i\varepsilon_n)$ is the Green's function for the system without Δ and Z but with $\mathbf{A}$. $\tilde{G}_0(j,\ell,i\varepsilon_n)$ is related to Green's function for the system without $\mathbf{A}$, G_0, as $\tilde{G}_0(j,\ell,i\varepsilon_n) \sim G_0(j,\ell,i\varepsilon_n)e^{i\phi_{j,\ell}}$, with $G_0(j,\ell,i\varepsilon_n)$ being the Fourier transform of $G_0(\mathbf{p},i\varepsilon_n) = 1/(i\varepsilon_n - \xi_p)$. In the expression of ξ_p, χ_0 and μ determined by Eqs.(5) and (6) will be substituted.

$Z_{j,\ell}$ may have real ($X_{j,\ell}$) and imaginary ($Y_{j,\ell}$) parts;

$$Z_{j,\ell} = X_{j,\ell} + iY_{j,\ell}. \tag{11}$$

$X_{j,\ell}$ and $Y_{j,\ell}$ describe the bond-order phase and the flux phase, respectively, and we treat only the latter in this paper. The spin-singlet SCOP ($\Delta_{j\ell}$) and $Y_{j\ell}$ are expressed in terms of $F^\dagger$ and G, respectively,

$$(\Delta_{j,\ell})^* = -\frac{T}{2}\sum_{\varepsilon_n}\Big[F^\dagger(j,\ell,i\varepsilon_n) + F^\dagger(\ell,j,i\varepsilon_n)\Big], \tag{12}$$

$$Y_{j,\ell} = \frac{1}{2i}(\chi_{j,\ell} - \chi_{\ell,j}) = iT\sum_{\varepsilon_n}\Big[G(j,\ell,i\varepsilon_n) - G(\ell,j,i\varepsilon_n)\Big]. \tag{13}$$

We substitute Eqs.(9) and (10) into Eqs.(12) and (13) iteratively and keep terms up to the third order in the OPs. The s- (d-) wave SCOP Δ_s (Δ_d) and the OP for the flux phase Π can be constructed by making linear combinations of Eqs.(12) and (13),

$$\Delta_s(j) = \frac{1}{4}\sum_{\eta=\pm\hat{x},\pm\hat{y}} \Delta_{j,j+\eta}, \tag{14}$$

$$\Delta_d(j) = \frac{1}{4}\Big(\sum_{\eta=\pm\hat{x}} \Delta_{j,j+\eta} - \sum_{\eta=\pm\hat{y}} \Delta_{j,j+\eta}\Big), \tag{15}$$

$$\Pi(j) = \frac{1}{4}\Big(Y_{j+\hat{x},j} + Y_{j+\hat{x}+\hat{y},j+\hat{x}} + Y_{j+\hat{y},j+\hat{x}+\hat{y}} + Y_{j,j+\hat{y}}\Big)e^{i\mathbf{Q}\cdot\mathbf{r_j}}, \tag{16}$$

with $\mathbf{Q} \equiv (\pi,\pi)$. Here we define Δ_s and Δ_d at a lattice site $\mathbf{r}_j$, while Π is defined at the center of the plaquette, $\tilde{\mathbf{r}}_j = \mathbf{r}_j + \hat{x}/2 + \hat{y}/2$. The latter definition is necessary to get a gauge-invariant coupling between Π and the vector potential. (See Appendix A.) Assuming that the SCOPs and Π are slowly varying, we take a continuum limit. Terms linear in the OPs are expanded in powers of derivatives up to the second order, and the Peierls factor is also expanded in powers of $\mathbf{A}$. Then we get the following GL equations,

$$\alpha_s\Delta_s + 2\beta_s|\Delta_s|^2\Delta_s - K_s(D_x^2 + D_y^2)\Delta_s - K_{ds}(D_x^2 - D_y^2)\Delta_d$$
$$+\gamma_1|\Delta_d|^2\Delta_s + 2\gamma_2\Delta_d^2\Delta_s^* + \gamma_{s\Pi}\Delta_s\Pi^2 = 0, \tag{17}$$

$$\alpha_d\Delta_d + 2\beta_d|\Delta_d|^2\Delta_d - K_d(D_x^2 + D_y^2)\Delta_d - K_{ds}(D_x^2 - D_y^2)\Delta_s$$
$$+\gamma_1|\Delta_s|^2\Delta_d + 2\gamma_2\Delta_s^2\Delta_d^* + \gamma_{d\Pi}\Delta_d\Pi^2 = 0, \tag{18}$$

$$\alpha_\Pi\Pi + 2\beta_\Pi\Pi^3 - K_\Pi(\partial_x^2 + \partial_y^2)\Pi + \gamma_{s\Pi}|\Delta_s|^2\Pi + \gamma_{d\Pi}|\Delta_d|^2\Pi$$
$$+\frac{\alpha_0}{2}\cos(\mathbf{Q}\cdot\mathbf{r})(\partial_x A_y - \partial_y A_x) = 0, \tag{19}$$

where the coefficients appearing in Eqs.(17)-(19) are given in the Appendix B, and $\mathbf{D}$ is the gauge-invariant gradient defined as $\mathbf{D} = \nabla + \frac{2\pi i}{\phi_0}\mathbf{A}$.

The GL free energy F up to the fourth order in the OPs can be obtained from the above GL equations in such a way that the variation in F with respect to the OPs reproduce Eqs.(17)-(19). The result is,

$$F = F_\Delta + F_\Pi + F_{\Delta\Pi} + F_B, \tag{20}$$

$$\begin{aligned} F_\Delta = & \int d^2\mathbf{r}\Big[\alpha_d|\Delta_d|^2 + \beta_d|\Delta_d|^4 + K_d|\mathbf{D}\Delta_d|^2 + \alpha_s|\Delta_s|^2 + \beta_s|\Delta_s|^4 + K_s|\mathbf{D}\Delta_s|^2 \\ & +\gamma_1|\Delta_d|^2|\Delta_s|^2 + \gamma_2(\Delta_d^2(\Delta_s^*)^2 + c.c.) \\ & +K_{ds}\big((D_x\Delta_d)(D_x\Delta_s)^* - (D_y\Delta_d)(D_y\Delta_s)^* + c.c.\big)\Big], \end{aligned} \tag{21}$$

$$F_\Pi = \int d^2\mathbf{r}\Big[\alpha_\Pi\Pi^2 + \beta_\Pi\Pi^4 + K_\pi(\nabla\Pi)^2 + \alpha_0\cos(\mathbf{Q}\cdot\mathbf{r})(\partial_x A_y - \partial_y A_x)\Pi\Big], \tag{22}$$

$$F_{\Delta\Pi} = \int d^2\mathbf{r}(\gamma_{d\Pi}|\Delta_d|^2 + \gamma_{s\Pi}|\Delta_s|^2)\Pi^2, \tag{23}$$

$$F_B = \frac{1}{2\mu_0}\int d^3\mathbf{r}(\nabla\times\mathbf{A})^2. \tag{24}$$

Here, F_Δ and F_Π are the free energy for superconductivity and flux phase, respectively, and $F_{\Delta\Pi}$ represents the coupling between SCOPs and Π. F_B is the energy for the magnetic field.

The currents are obtained by varying F with respect to $\mathbf{A}$, namely, $J_\nu = -\frac{\partial}{\partial A_\nu}(F_\Delta + F_\Pi)$:

$$\begin{aligned} J_x = & -\alpha_0\cos(\mathbf{Q}\cdot\mathbf{r})\partial_y\Pi - \frac{2\pi i}{\phi_0}\Big[K_d(\Delta_d\partial_x\Delta_d^* - \Delta_d^s\partial_x\Delta_d) + K_s(\Delta_s\partial_x\Delta_s^* - \Delta_s^*\partial_x\Delta_s) \\ & +K_{ds}(\Delta_d\partial_x\Delta_s^* - \Delta_d^*\partial_x\Delta_s + \Delta_s\partial_x\Delta_d^* - \Delta_s^*\partial_x\Delta_d)\Big] \\ & -2\left(\frac{2\pi}{\phi_0}\right)^2 A_x\Big[K_d|\Delta_d|^2 + K_s|\Delta_s|^2 + K_{ds}(\Delta_d\Delta_s^* + \Delta_d^+\Delta_s)\Big], \end{aligned} \tag{25}$$

$$\begin{aligned} J_y = & \alpha_0\cos(\mathbf{Q}\cdot\mathbf{r})\partial_x\Pi - \frac{2\pi i}{\phi_0}\Big[K_d(\Delta_d\partial_y\Delta_d^* - \Delta_d^s\partial_y\Delta_d) + K_s(\Delta_s\partial_y\Delta_s^* - \Delta_s^*\partial_y\Delta_s) \\ & -K_{ds}(\Delta_d\partial_y\Delta_s^* - \Delta_d^*\partial_y\Delta_s + \Delta_s\partial_y\Delta_d^* - \Delta_s^*\partial_y\Delta_d)\Big] \\ & -2\left(\frac{2\pi}{\phi_0}\right)^2 A_y\Big[K_d|\Delta_d|^2 + K_s|\Delta_s|^2 - K_{ds}(\Delta_d\Delta_s^* + \Delta_d^+\Delta_s)\Big]. \end{aligned} \tag{26}$$

Equations (17)-(19), together with the Maxwell equation $\nabla\times\mathbf{B} = \mu_0\mathbf{J}$, determine Δ_d, Δ_s, Π, and $\mathbf{A}$ self-consistently.

Equations (25) and (26) show that when the flux phase OP, Π, has unidirectional spatial variation, a current would flow in a perpendicular direction. For example, near a (110) surface of a d-wave superconductor, SCOP is suppressed and then Π may become finite. Induced Π should be uniform along the surface and decays toward the bulk. In this case, staggered currents would flow along the surface, and their amplitudes vanish in the bulk. Near the surface, spontaneous magnetic fields would appear. Their spatial distribution can be determined by solving the GL equations numerically, and we expect that the amplitude of the magnetic field should be reduced, compared to the case where F_B is neglected and the magnetic field is not treated self-consistently (as in BdG calculations).

4. Summary

We have derived the GL equations and GL free energy for the flux phase and superconductivity microscopically from the two-dimensional $t-J$ model. The derived GL theory can be used to study various problems in high-T_c superconductivity, e.g., states near a surface or impurities, and the effect of an external magnetic field. The latter issue is important to distinguish theories proposed to explain surface-state properties of cuprates.[37,38] Since the GL theory derived microscopically directly reflects the electronic structure of the system, e.g., the shape of the Fermi surface that changes with doping, it can provide more useful information than that from phenomenological GL theories.[39,40] In order to discuss the above mentioned problems, numerical calculations that treat magnetic fields as well as the OPs self-consistently are necessary, and we will examine them in a separate study.

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Appendix A: Coupling between Flux Phase Order Parameter and Magnetic Field

In this appendix, we derive a term that couples the flux phase OP with the magnetic field, i.e., the last term in Eq.(19). This is the zeroth-order term in the GL equation for Π (first-order term in the GL free energy F_Π), which arises from the substitution of $\tilde{G}_0$ in Eq.(9) into Eq.(13). The contribution to $Y_{j+\hat{x},j}$ is calculated as

$$
\begin{aligned}
& iT\sum_{\varepsilon_n}[\tilde{G}_0(j+\hat{x},j,i\varepsilon_n)-\tilde{G}_0(j,j+\hat{x},i\varepsilon_n)] \\
= \quad & iT\sum_{\varepsilon_n}\frac{1}{N}\sum_{p}G_0(\mathbf{p},i\varepsilon_n)[e^{ip_x}e^{i\phi_{j+\hat{x},j}}-e^{-ip_x}e^{i\phi_{j,j+\hat{x}}}] \\
& \sim iT\sum_{\varepsilon_n}\frac{1}{N}\sum_{p}G_0(\mathbf{p},i\varepsilon_n)\Big[e^{ip_x}\Big(1-\frac{i\pi}{\phi_0}A_x(\mathbf{r}_j+\frac{\hat{x}}{2})\Big)-e^{-ip_x}\Big(1+\frac{i\pi}{\phi_0}A_x\Big(\mathbf{r}_j+\frac{\hat{x}}{2}\Big)\Big)\Big] \\
& =\frac{2\pi}{\phi_0}T\sum_{\varepsilon_n}\frac{1}{N}\sum_{p}\cos p_x G_0(\mathbf{p},i\varepsilon_n)A_x\Big(\mathbf{r}_j+\frac{\hat{x}}{2}\Big)
\end{aligned}
$$

$$= \frac{2\pi}{\phi_0}\frac{1}{N}\sum_p \cos p_x f(\xi_p) A_x\Big(\mathbf{r}_j + \frac{\hat{x}}{2}\Big)$$

$$= \frac{\pi\chi_0}{\phi_0} A_x\Big(\mathbf{r}_j + \frac{\hat{x}}{2}\Big) \tag{A·1}$$

Contributions to $Y_{j+\hat{x}+\hat{y},j+\hat{x}}$, $Y_{j+\hat{y},j+\hat{x}+\hat{y}}$, and $Y_{j,j+\hat{y}}$ can be calculated similarly. Substituting them into Eq.(16), the lowest-order term is given by

$$\frac{\pi\chi_0}{4\phi_0} e^{i\mathbf{Q}\cdot\mathbf{r}_j}\Big[A_x\Big(\mathbf{r}_j + \frac{\hat{x}}{2}\Big) - A_x\Big(\mathbf{r}_j + \frac{\hat{x}}{2} + \hat{y}\Big) + A_y\Big(\mathbf{r}_j + \hat{x} + \frac{\hat{y}}{2}\Big) - A_y\Big(\mathbf{r}_j + \frac{\hat{y}}{2}\Big)\Big]$$

$$\sim \frac{\pi\chi_0}{4\phi_0} e^{i\mathbf{Q}\cdot\mathbf{r}_j}\Big[\partial_x A_y(\tilde{\mathbf{r}}_j) - \partial_y A_x(\tilde{\mathbf{r}}_j)\Big]. \tag{A·2}$$

Here, we have expanded $\mathbf{A}$ around the center of a plaquette, $\tilde{\mathbf{r}}_j = \mathbf{r}_j + \hat{x}/2 + \hat{y}/2$. By multiplying an appropriate factor, this gives the last term in Eq. (19). Equation (A.2) shows that the flux phase OP, Π, which is defined at $\tilde{\mathbf{r}}_j$, couples to a magnetic field at the same point. In deriving the other terms of GL equations, we approximate $Y_{j+\hat{x}+\hat{y},j+\hat{x}} \sim -Y_{j-\hat{y},j}$ and $Y_{j+\hat{y},j+\hat{x}+\hat{y}} \sim Y_{j-\hat{x},j}$, assuming the slow variation of $|Y_{j,\ell}|$. Namely, in these terms, we approximate

$$\Pi(j) \sim \frac{1}{4}(Y_{j+\hat{x},j} + Y_{j-\hat{x},j} - Y_{j+\hat{y},j} - Y_{j-\hat{y},j}) e^{i\mathbf{Q}\cdot\mathbf{r}_j}. \tag{A·3}$$

This means that while the flux phase OP is defined at the center of a plaquette, $\tilde{\mathbf{r}}_j$, it couples to SCOPs defined at the neighboring site $\mathbf{r}_j$. If we use Eq. (A.3) to calculate the coupling between the flux phase OP and the vector potential, we would get a term of the form $\Pi(\partial_x A_x - \partial_y A_y)\cos(\mathbf{Q}\cdot\mathbf{r})$ in F_Π, which is not gauge invariant and thus inappropriate.

Appendix B: Coefficients in GL Equations and GL Free Energy

The coefficients appearing in the GL equations and GL free energy are given as follows:

$$\alpha_{d(s)} = 3J\Big(1 - \frac{3J}{4N}\sum_p I_1(p)\omega^2_{d(s)}(p)\Big), \tag{B·1}$$

$$\beta_{d(s)} = \frac{81J^4}{32N}\sum_p I_2(p)\omega^4_{d(s)}(p), \tag{B·2}$$

$$\gamma_1 = \frac{81J^4}{8N}\sum_p I_2(p)\omega_d^2(p)\omega_s^2(p), \quad \gamma_2 = \frac{1}{4}\gamma_1, \tag{B·3}$$

$$K_{d(s)} = \frac{9J^2}{8N}\sum_p I_2(p)\Big(\frac{\partial\xi_p}{\partial p_x}\Big)^2\omega^2_{d(s)}(p), \tag{B·4}$$

$$K_{ds} = \frac{9J^2}{8N}\sum_p I_2(p)\Big(\frac{\partial\xi_p}{\partial p_x}\Big)^2\omega_d(p)\omega_s(p), \tag{B·5}$$

$$\alpha_\Pi = \frac{3J}{4}\Big[1 + \frac{3J}{4N}\sum_p I_3(p)\omega_d^2(p)\Big], \tag{B·6}$$

$$\beta_\Pi = \frac{1}{2}\Big(\frac{3J}{4}\Big)^4 \frac{1}{N}\sum_p I_4(p)\omega_d^4(p), \tag{B·7}$$

$$K_\Pi = -\frac{1}{2}\Big(\frac{3J}{4}\Big)^2 \frac{1}{N}\sum_p \frac{\partial\xi_p}{\partial p_x}\frac{\partial\xi_{p+Q}}{\partial p_x} I_4(p)\omega_d^2(p), \tag{B·8}$$

$$\alpha_0 = -\frac{3\pi J}{8\phi_0}\chi_0, \tag{B·9}$$

$$\gamma_{d\Pi} = -4\Big(\frac{3J}{4}\Big)^4 \frac{1}{N}\sum_p \Big[I_5(p) + 2I_6(p)\Big]\omega_d^4(p), \tag{B·10}$$

$$\gamma_{s\Pi} = -4\Big(\frac{3J}{4}\Big)^4 \frac{1}{N}\sum_p \Big[I_5(p) + 2I_6(p)\Big]\omega_d^2(p)\omega_s^2(p), \tag{B·11}$$

where $\omega_d(p) = \cos p_x - \cos p_y$ and $\omega_s(p) = \cos p_x + \cos p_y$, and the summation on p is taken over the first Brillouin zone. The functions appearing in the integrals are defined as

$$I_1(p) = T\sum_{\varepsilon_n} G_0(p, i\varepsilon_n)G_0(p, -i\varepsilon_n), \tag{B·12}$$

$$I_2(p) = T\sum_{\varepsilon_n} G_0^2(p, i\varepsilon_n)G_0^2(p, -i\varepsilon_n), \tag{B·13}$$

$$I_3(p) = T\sum_{\epsilon_n} G_0(p, i\varepsilon_n)G_0(p+Q, i\varepsilon_n), \tag{B·14}$$

$$I_4(p) = T\sum_{\epsilon_n} G_0^2(p, i\varepsilon_n)G_0^2(p+Q, i\varepsilon_n), \tag{B·15}$$

$$I_5(p) = T\sum_{\epsilon_n} G_0(p, i\varepsilon_n)G_0(p, -i\varepsilon_n)G_0(p+Q, i\varepsilon_n)G_0(p+Q, -i\varepsilon_n), \tag{B·16}$$

$$I_6(p) = T\sum_{\epsilon_n} G_0^2(p, i\varepsilon_n)G_0(p, -i\varepsilon_n)G_0(p+Q, i\varepsilon_n). \tag{B·17}$$

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