Effects of Charge Density Modulation on Incommensurate Antiferromagnetism: Ginzburg-Landau Study

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In the vicinity of hole density, 1/8, La-based high-$T_c$ superconductors exhibit long-range order of incommensurate antiferromagnetism (IC-AF). Motivated by this observation, we explore the possible stabilization of IC-AF ordering due to the existence of static charge density modulation (CDM). We use Ginzburg-Landau free energy based on the mean field theory of the $t$-$J$ model. It is shown numerically that three kinds of CDM including a stripe pattern can stabilize static IC-AF ordering. We also argue that such CDMs can cause the saturation of the degree of incommensurability ($\eta$) as a function of hole density for IC-AF fluctuation. In our framework a principal effect of low-temperature tetragonal (LTT) structure is just to increase $\eta$ of IC-AF slightly larger only for the stripe pattern.

KEYWORDS: La-based high $T_c$-superconductors, GL free energy, $t$-$J$ model, Fermi surface, nesting, 1/8-phenomena, incommensurate antiferromagnetism, charge density modulation, stripe pattern

In the vicinity of hole density, 1/8, La-based high-$T_c$ superconductors show anomalous temperature dependence in various physical quantities such as in-plane electrical resistivity, Hall coefficient, static magnetic susceptibility and thermoelectric power, and the following characteristics are also observed: the suppression of d-wave superconductivity (dSC); the stabilization of static incommensurate antiferromagnetism (IC-AF) with higher onset temperature, $T_N$, than that for the other hole densities; and the appearance of static charge density modulation (CDM) accompanying with the structural phase transition from low-temperature orthorhombic (LTO1, space group Bmab) phase to low-temperature tetragonal (LTT, P$4_2/ncm$) phase in La$_{1.6-x}$Nd$_{0.4}$Sr$_x$CuO$_4$ (LNSCO) with $x = 0.13$. We will call these ‘1/8-phenomena’. This has been discussed so far in the context of the stripe model first suggested by Tranquada et al. However, the justification of the stripe model has not been established either experimentally or theoretically.

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Among many factors described above, we expect that static CDM plays a central role for the '1/8-phenomena'. In this paper we study the possibility that the presence of static CDM induces static IC-AF ordering at hole densities where the dSC is stabilized if static CDM is absent (the important role of the coupling between static CDM and static IC-AF is suggested in the study of antiferromagnetic vortex cores in the $t$-$J$ model\(^5\)). We will not restrict ourselves to the stripe model and examine all possible patterns of static CDM consistent with the spin pattern observed experimentally\(^3\),\(^4\),\(^7\),\(^8\),\(^12\). We will assume existence of those static CDMs a priori (in the following 'static CDM' will be abbreviated to 'CDM'). Explicit calculations will be done in the dSC state because it is implied experimentally\(^8\) that whether the system is in the dSC state or not is not essential to discuss the stabilization of static IC-AF ordering. Effects of LTT structure will also be studied.

To study effects of CDM on IC-AF in the Ginzburg-Landau (GL) free energy, we define two order parameters, static IC-AF, $M(q)$, and CDM, $N(q)$:

\[
\langle S^z_i \rangle = M(r_i) = \sum_q M(q)e^{i\mathbf{q}\cdot\mathbf{r}_i}, \quad (1)
\]

\[
\langle n_i \rangle - \delta = N(r_i) = \sum_q N(q)e^{i\mathbf{q}\cdot\mathbf{r}_i}, \quad (2)
\]

where $\langle S^z_i \rangle$ and $\langle n_i \rangle$ are average magnetization and average hole number at site $i$, respectively, and $\delta$ is average hole density (doping rate). Since the lowest order interaction allowed by symmetry is $\int d\mathbf{r}_1d\mathbf{r}_2d\mathbf{r}_3 g(\mathbf{r}_2 - \mathbf{r}_1, \mathbf{r}_3 - \mathbf{r}_1)N(\mathbf{r}_1)M(\mathbf{r}_2)M(\mathbf{r}_3)$, with $g$ being a coupling constant, we consider the following GL free energy in the wavevector space\(^9\):

\[
F = \sum_q \frac{1}{2\chi(q)} |M(q)|^2 + \sum_{q_a, q_b} g(q_a, q_b) N(q_a + q_b)M(-q_a)M(-q_b) + O(M^4). \quad (3)
\]

Careful treatment of the wavevector dependence of static susceptibility, $\chi(q)$, and the coupling constant, $g(q_a, q_b)$, is essential in this paper. For example, in the microscopic calculation explained below, $\chi(q)$ has a maximum at some incommensurate wavevectors, $(\pi, \pi \pm 2\pi\eta)$ and $(\pi \pm 2\pi\eta, \pi)$, owing to the nesting property of the Fermi surface. The parameter $\eta$ represents the degree of incommensurability. In eq. (3) we consider the hole density where $\chi(q)$ is positive, that is, there is no magnetic ordering in the absence of CDM; we then consider a situation that there exists some kind of CDM, $N(q_a + q_b)$, and examine the possibility that it induces static long-range order of IC-AF.

As the wavevector of $M(q)$, we consider $(\pi, \pi \pm 2\pi\eta)$ and $(\pi \pm 2\pi\eta, \pi)$, which are the same pattern as observed by neutron scattering\(^6\),\(^3\),\(^4\),\(^7\),\(^8\),\(^12\). In this case, CDMs which couple with this static IC-AF through the second term in eq. (3) are limited to only two types, type I (CDM(I)) and type II (CDM(II)), each having both 1-dimensional (1d) and 2-dimensional (2d) patterns. Their wavevectors are defined in Fig. 1. In particular, 1d-CDM(I) is the stripe pattern proposed by
Fig. 1. Four possible patterns of CDMs (●) which can couple with static IC-AF (×). They are represented by the spots in the Brillouin zone. There are two types, type I (CDM(I)) and type II (CDM(II)), which are characterized by the spots on $q_x$ and/or $q_y$ axes and by those on diagonal axes, respectively. Each type has both 1-dimensional (1d) and 2-dimensional (2d) patterns. (a) 1d-CDM(I) has $(\pm 4\pi \eta, 0)$ or $(0, \pm 4\pi \eta)$, and the case of $(0, \pm 4\pi \eta)$ is shown (b) 2d-CDM(I) (c) 1d-CDM(II) has $(\pm 2\pi \eta, \pm 2\pi \eta)$ or $(\pm 2\pi \eta, \mp 2\pi \eta)$, and the case of $(\pm 2\pi \eta, \mp 2\pi \eta)$ is shown (d) 2d-CDM(II). Note that spin pattern is 2-dimensional except for 1d-CDM(I).

Tranquada et al.\textsuperscript{3,4} We consider eq. (3) for each pattern whose existence is assumed a priori; for 2d-CDM(I) and 2d-CDM(II), two independent amplitudes are assumed to be the same.

In eq. (3) the coefficient of $M^2$ can change sign when $|N(q_a + q_b)|$ becomes large; this signals the onset of static long-range order of IC-AF. For convenience, we rescale Fourier component, $N(q)$, for each CDM so that the minimum of the real space hole number, $\langle n_i \rangle$, becomes simply $\delta - N(q)$. Using this redefined $N(q)$, the critical amplitude of each CDM for the onset of static IC-AF order
is given by

\[ N_{cr} = \frac{1}{g(q_1, q_1)\chi(q_1)} \] for 1d-CDM(I), \hspace{1cm} (4)

\[ N_{cr} = \frac{2}{g(q_1, q_1)\chi(q_1)} \] for 2d-CDM(I), \hspace{1cm} (5)

\[ N_{cr} = \frac{1}{g(q_1, q_2)\sqrt{\chi(q_1)\chi(q_2)}} \] for CDM(II), \hspace{1cm} (6)

where \( q_1 = (\pi, \pi + 2\pi\eta) \) and \( q_2 = (\pi + 2\pi\eta, \pi) \); CDM(II) represents both 1d-CDM(II) and 2d-CDM(II). We define

\[ a(\eta; \delta) \equiv \frac{N_{cr}}{\delta}, \hspace{1cm} (7) \]

which can be used as a measure of the strength of the coupling between CDM and IC-AF (see Fig. 2): smaller \( a(\eta; \delta) \) means stronger coupling. If \( a(\eta; \delta) \) is less than 1, CDM can stabilize static IC-AF ordering when its amplitude \( N(q) \) is larger than \( N_{cr} \). For \( a(\eta; \delta) > 1 \), CDM cannot stabilize static IC-AF order because \( N(q) \) cannot be larger than \( N_{cr} \), but will affect IC-AF fluctuation. For \( a(\eta; \delta) \gg 1 \), effects of CDM are negligible and IC-AF fluctuation is controlled only by \( \chi(q) \). Note that we expect that the GL free energy, eq. (3), can be used to discuss some properties of IC-AF fluctuation such as the value of \( \eta \), although it can only be used to study static ordering.

![Fig. 2](image-url)  
**Fig. 2.** Interpretation of \( a(\eta; \delta) \) as the strength of the coupling between CDM and IC-AF. Smaller value of \( a(\eta; \delta) \) means stronger coupling. If \( a(\eta; \delta) \) is less than 1, then static IC-AF can be stabilized. For \( a(\eta; \delta) \geq 1 \), CDM can not stabilize static IC-AF ordering but will affect IC-AF fluctuation, while in the case of \( a(\eta; \delta) \gg 1 \) effects of CDM are negligible and IC-AF fluctuation is controlled only by spin susceptibility, \( \chi(q) \).

To estimate \( a(\eta; \delta) \), we calculate \( g(q_a, q_b) \) and \( \chi(q) \) on the basis of the mean field theory of the \( t-J \) model with LSCO-type Fermi surface\(^{10} \). We assume the singlet-RVB state (d-wave paring) and work at temperature, \( T = 0.02J \), and in the doping range, \( 0.10 \leq \delta \leq 0.30 \). At this temperature, singlet-RVB state is developed for each \( \delta \). In RPA, \( \chi(q) = \chi_0(q)/(1 + 2J(q)\chi_0(q)) \) where \( \chi_0(q) \) is...
spin susceptibility without interactions and $J(\mathbf{q}) = \tilde{J}(\cos q_x + \cos q_y)$ with $\tilde{J} = J$. In this paper, however, we set $\tilde{J} = 0.2 J$ to simulate the possible effects of renormalization due to fluctuations or higher order contributions. This choice of $\tilde{J} = 0.2 J$ leads to positive value of $\chi(\mathbf{q})$ for all doping rate, $\delta > 0$. As will be discussed later, the precise value of $\tilde{J}$ is not essential for drawing main conclusions. First we show results calculated with isotropic parameters, $t_x = t_y$ and $J_x = J_y$, which will apply for LTO1 structure. Effects of LTT structure are also studied by introducing the spatial anisotropy ($t_x \neq t_y$ and $J_x \neq J_y$) and will be described later.

As reported earlier, $\chi(\mathbf{q})$ takes a maximum at the incommensurate wavevectors, schematically shown by ‘×’ in Fig. 1, whose $\eta$ is defined to be $\eta_\chi$. This is due to the nesting property of the Fermi surface. Fig. 3 shows $\eta$-dependence of $g(q_1, q_2)$ (a) and $a(\eta; \delta)$ (b) at various average hole density $\delta$ for CDM(II). It is seen that $g(q_1, q_2)$ is a step-like function, and we found that the value of $\eta$ at the step roughly coincides with $\eta_\chi$. The step-like behavior of $g(q_1, q_2)$ is clearly reflected in $a(\eta; \delta)$ for $\delta = 0.26, 0.30$, where $a(\eta; \delta)$ decreases with increasing $\eta$, takes a minimum at $\eta \equiv \eta_a$, and then suddenly increases. For $\delta \geq 0.26$, $a(\eta; \delta)$ becomes less than 1 around $\eta_a$ and thus CDM(II) can in principle stabilize static IC-AF.

Compared to the above results for CDM(II), $a(\eta; \delta)$ around $\eta_a$ is larger by $\sim 10 \%$ for 1d-CDM(I) and by about a factor of two for 2d-CDM(I). Except for these quantitative differences, the $\eta$-dependence of $a(\eta; \delta)$ is almost the same among four CDMs. Therefore CDM(II) can stabilize static IC-AF more easily than 1d-CDM(I), and 2d-CDM(I) has much more difficulty. In the following we will not consider 2d-CDM(I).

The above results are summarized in Fig. 4 as the $\delta$-dependence of $\eta_\chi$ and $\eta_a$, and the shaded region ($\eta_K$, an arrow and a dotted line will be explained later). The $\eta_\chi$ roughly represents $\eta$ where $g(q_1, q_2)$ drastically changes. The $\eta_a$ represents $\eta$ of IC-AF which couples with CDM most strongly for each $\delta$. In the shaded region, $a(\eta; \delta)$ becomes less than 1 and thus the coupling with CDM is so strong that static IC-AF can be stabilized. In this case, patterns of CDM are limited to three: 1d-CDM(II), 2d-CDM(II) or 1d-CDM(I) (stripe pattern), and the last one being less effective.

Now we can draw a following global picture. In the absence of the coupling between $M$ and $N$, IC-AF fluctuation has $\eta = \eta_K$ at which $\chi(\mathbf{q})$ takes a maximum and we assume that $\eta$ of CDM ($\eta_a$) is equal to $1/8 \eta_K$, which will be favored owing to some commensurability effects. In the presence of the coupling, if the coupling is strong, $M$ and $N$ will tend to have the same $\eta$ because $N$ couples with $M$ having the same $\eta$ (see Fig. 1). Thus the resulting $\eta$ will take some value between $\eta_K$ and $\eta_a$. From our results that $a(\eta; \delta)$ is as small as 1 for $\eta_a < \eta < \eta_K$ (for $\delta \geq 0.23$), and is much larger than 1 if $\eta$ exceeds $\eta_K$, we expect that $\eta$ of IC-AF fluctuation will deviate from $\eta_K$ as shown by a dotted line in Fig. 4. Therefore we suggest that the resulting $\eta$ tends to saturate at high hole density ($\delta \geq 0.23$) owing to the strong coupling with CDM and probably crosses the shaded region, where instability to static IC-AF order occurs if the amplitude of CDM exceeds $N_{cr}$. In this case

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Fig. 3. The $\eta$-dependence of $g(q_1, q_2)$ (a) and $a(\eta, \delta) \equiv N_{\text{cr}}/\delta$ (b) are shown at various hole density, $\delta$, for CDM(II) in LTO1 structure, where $q_1 = (\pi, \pi + 2\pi\eta)$ and $q_2 = (\pi + 2\pi\eta, \pi)$. In (b) the case of $\delta = 0.10$ is out of the frame and is not shown.

the static IC-AF can be stabilized in some doping range and has $\eta \approx 0.13$.

The saturation of $\eta$ as a function of $\delta$ for IC-AF fluctuation is qualitatively consistent with experiments\textsuperscript{6,12}. Static IC-AF can be stabilized in some doping range. We consider that the possible stabilization of static IC-AF represented by the arrow (intersection point between the dotted line and the curve of $\eta_a$) in Fig. 4 corresponds to the observed one in La$_{2-x}$Sr$_x$CuO$_4$ (LSCO)
Fig. 4. The $\eta$ as a function of $\delta$. The $\eta_\kappa$ roughly represents $\eta$ where $g(q_1, q_2)$ drastically changes. The $\eta_a$ is $\eta$ of IC-AF which couples with CDM most strongly for each $\delta$. These two lines are characteristic ones which determine the distribution of the strength of coupling between CDM and IC-AF on the plane of $\delta$ and $\eta$. The $\eta_\kappa$ and the $\eta_\chi$ are $\eta$ of CDM and IC-AF fluctuation in the absence of the coupling, respectively. In the presence of the coupling, the $\eta$ of IC-AF fluctuation will deviate from $\eta_\chi$ as shown by the dotted line, which probably crosses the shaded region where static IC-AF ordering can be stabilized. The arrow represents the intersection point between the dotted line and the curve of $\eta_a$.

with $x = 0.1234$ and LNSCO with $x = 0.1234$. This is because the IC-AF represented by the arrow couples with CDM stronger than that for the other hole densities and will have higher onset temperature, $T_N$. It is noteworthy that $\eta \approx 0.13$ is close to the observed one $0.13$. However, the average hole density in our calculation is much larger than that in experiments. This inconsistency may be resolved if we note the following. In the present theory the large amplitude is required for CDM to stabilize static IC-AF, because $a(\eta; \delta)$ is not so small compared to 1. The existence of such CDM will have some influence on the shape of the Fermi surface which is crucial to the value of $\eta$.
for given $\delta$. In this context, we note that the Fermi surface of LSCO determined by angle-resolved photoemission spectroscopy (ARPES) is centered at $(\pi, \pi)$ for $x = 0.10, 0.15$ and different from that used in this paper. We speculate that this discrepancy may be explained by the existence of CDM.

In LNSCO with $x = 0.12$, charge spots were observed at $q = (\pm 4\pi \epsilon, 0)$, $(0, \pm 4\pi \epsilon)$ with $\epsilon \approx 0.12$ by elastic neutron scattering and hard X-ray scattering, suggesting that there is a charge pattern of either 1d-CDM(I) or 2d-CDM(I). If the case of CDM(II) is excluded experimentally, the present theory suggests that 1d-CDM(I) is realized in LNSCO. In LSCO with $x = 0.12$, CDM has not been observed yet. But our theory implies either 1d-CDM(II), 2d-CDM(II) or 1d-CDM(I) exists. Further detail experiments will be required.

In LNSCO static ordering of IC-AF is realized in the wide region, $0.08 \leq x \leq 0.25$, $0.15$. The present theory predicts the possible stabilization of static IC-AF in some doping range (see Fig. 4 where the dotted line crosses the shaded region) and we have considered that static IC-AF represented by the arrow corresponds to the observed one at $x = 0.12$, $0.15$. It is not clear, however, whether the static IC-AF for $x = 0.15$, $0.20$, $0.25$ can be explained in our global picture because our theory involves the following ambiguities: the way to draw the dotted line in Fig. 4, the assumed value of $\eta_k$ and the value of $\tilde{J}$. Indeed, if $\tilde{J}$ is taken larger, $a(\eta; \delta)$ becomes smaller and the shaded region extends to both lower $\delta$ and lower $\eta$. On the other hand it seems difficult to explain static IC-AF for $x = 0.08, 0.10$. This implies that effects of disorders and perturbations of Nd$^{3+}$ will be important. In fact, disorders enhance static IC-AF as in the case of La$_{2-x}$Sr$_x$Cu$_{1-y}$Zn$_y$O$_{4-\delta}$ with $x = 0.14$, $y = 0.01$ and it is suggested that the magnetic moment of Cu$^{2+}$ couples with that of Nd$^{3+}$ antiferromagnetically. These problems will also be related to the recent observation of static IC-AF in LSCO with $x = 0.06$, $0.10$, $0.13$. These are future problems.

Finally we study the effects of LTT structure by introducing the spatial anisotropy into $t$ and $J$: $t_y = t_x(1 - 3.78 \tan^2 \theta)$, $J_y = J_x(1 - 2 \cdot 3.78 \tan^2 \theta)$. Here $\theta$ is the tilting angle around [100] axis (tetragonal notation) of a CuO$_6$ octahedron and we set $\theta = 5^\circ$. Since the renormalized transfer integral along $x$ direction becomes larger than that along $y$ direction, we take the charge pattern for 1d-CDM(I) as shown in Fig. 1(a). The following two results have been obtained: (i) effects of LTT structure are not essential to stabilize static IC-AF ordering, and (ii) its principal effect is to increase $\eta_k$ and $\eta_a$ by about 0.01 only for 1d-CDM(I). The first result (i) is consistent with experiments, in that static IC-AF has been observed in both LTO1 and LTT. If we assume that 1d-CDM(I) is realized in LNSCO, then the second result (ii) seems consistent with experimental results on LNSCO (LTT structure) and LSCO (LTO1 structure): the former shows static IC-AF with larger $\eta$ than IC-AF fluctuation of the latter, if the comparison is made at the same hole density.

We mention our preliminary calculations on YBCO-type Fermi surface. While we observe
similar structures of \( a(\eta; \delta) \) such as a minimum as a function of \( \eta \), its value is order of 10. This means that effects of CDM are negligible, and predicts commensurate AF fluctuation because \( \chi(q) \) takes a maximum at \( q = (\pi, \pi) \). Recent observation of IC-AF fluctuation in YBa\(_2\)Cu\(_3\)O\(_{6.7}\) is unlikely to be explained in the present framework.

To summarize, we have studied the possibility of static ordering of IC-AF due to the existence of CDM. We have assumed the lowest order interaction between them in GL free energy and made explicit calculations based on the mean field theory of the \( t-J \) model with LSCO-type Fermi surface in the singlet-RVB state. Effects of LTT have also been studied as spatial anisotropies in \( t \) and \( J \). We have found the following conclusions: (a) Owing to the strong coupling with CDM, static IC-AF order can be stabilized; the degree of incommensurability as a function of hole density for IC-AF fluctuation can tend to saturate. In this case the expected patterns of CDMs are 1d-CDM(II), 2d-CDM(II) or 1d-CDM(I) (stripe pattern) (b) Effects of LTT structure are not essential to stabilize static IC-AF ordering for each expected CDM but to increase the degree of incommensurability of IC-AF slightly larger only for 1d-CDM(I).

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