INCOMMENSURATE ANTIFERROMAGNETISM INDUCED BY CHARGE DENSITY MODULATION: GINZBURG-LANDAU STUDY

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In the vicinity of hole density, 1/8, of La-based high-T_c superconductors, static incommensurate antiferromagnetism (IC-AF) is observed. We explore the possible stability of static IC-AF due to the existence of static charge density modulation (CDM) using Ginzburg-Landau free energy based on the mean field theory of the t-J model. We show numerically that on the plane of hole density and incommensurability of IC-AF fluctuation, there exists a region where instability to static IC-AF is possible. In this case CDM is not necessarily a stripe pattern.

KEYWORDS: A. superconductors, D. spin density wave, D. charge-density waves, D. Fermi surface, D. magnetic properties.

1. INTRODUCTION

In the vicinity of hole density,[1] 1/8, La-based high-T_c superconductors show anomalous temperature dependence in various physical quantities such as in-plane 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 onset temperature, T_N, higher than those of other hole densities; the appearance of static charge density modulation (CDM); and the structural phase transition. We call these phenomena '1/8-phenomena'. This '1/8-phenomena' has been discussed so far in the context of the stripe model first suggested by Tranquada *et al.*.[2,3] But its justification has not been established either experimentally or theoretically.

In this paper we will investigate '1/8-phenomena' searching for possible interrelationship between the stabilization of static IC-AF and the existence of static CDM. In the following 'static CDM' will be abbreviated to 'CDM'.

2. GL FREE ENERGY

To explore the possible interrelationship between static IC-AF and CDM, we take the following Ginzburg-Landau (GL) free energy:

$$\begin{aligned} F = \quad & \sum_{\boldsymbol{q}} \frac{1}{2\chi(\boldsymbol{q})} |M(\boldsymbol{q})|^2 + \sum_{\boldsymbol{q}_a, \boldsymbol{q}_b} g(\boldsymbol{q}_a, \boldsymbol{q}_b) N(\boldsymbol{q}_a + \boldsymbol{q}_b) M(-\boldsymbol{q}_a) M(-\boldsymbol{q}_b) \\ + \quad & \frac{b}{4} \sum_{\boldsymbol{q}_a, \boldsymbol{q}_b, \boldsymbol{q}_c} M(-\boldsymbol{q}_a) M(\boldsymbol{q}_b) M(-\boldsymbol{q}_b - \boldsymbol{q}_c) M(\boldsymbol{q}_a + \boldsymbol{q}_c) \end{aligned} \tag{1}$$

where $N(\boldsymbol{q}_a + \boldsymbol{q}_b)$ is an order parameter of CDM whose existence is assumed a priori; $M(\boldsymbol{q})$ is an order parameter of static IC-AF; $\chi(\boldsymbol{q}) > 0$ is spin susceptibility; and the second term is the lowest order interaction between static IC-AF and CDM, and $g(\boldsymbol{q}_a,\ \boldsymbol{q}_b)$ is the coupling constant. We consider only the static IC-AF having the same pattern as observed by neutron scattering:[2–6] $(\pi,\ \pi \pm 2\pi\eta)$ and $(\pi \pm 2\pi\eta,\ \pi)$. η is the degree of incommensurability. In this case, CDMs which couple with this static IC-AF through the second term in eq. (1) are limited to only four patterns: 1d-CDM(I) (Fig. 1 (a)), 2d-CDM(I) (Fig. 1 (b)), 1d-CDM(II) (Fig. 1 (c)) and 2d-CDM(II) (Fig. 1 (d)). Each figure shows spin and charge patterns in the wavevector space, and η of CDM is taken as the same as that of static IC-AF. Here 1d-CDM(I) is the stripe pattern proposed by Tranquada *et al.*[2,3]

In eq. (1) the coefficient of the second order of $M(\boldsymbol{q})$ can change its sign when $|N(\boldsymbol{q}_a + \boldsymbol{q}_b)|$ becomes large. A critical amplitude of CDM, above which the sign of this coefficient becomes negative, is given by: $N_{\rm cr} = 1/(g(\boldsymbol{q}_1,\ \boldsymbol{q}_1)\chi(\boldsymbol{q}_1))$ for 1d-CDM(I); $N_{\rm cr} = 2/(g(\boldsymbol{q}_1,\ \boldsymbol{q}_1)\chi(\boldsymbol{q}_1))$ for 2d-CDM(I); and $N_{\rm cr} = 1/\left(g(\boldsymbol{q}_1,\ \boldsymbol{q}_2)\sqrt{\chi(\boldsymbol{q}_1)\chi(\boldsymbol{q}_2)}\right)$ for both 1d-CDM(II) and 2d-CDM(II), where $\boldsymbol{q}_1 = (\pi,\ \pi + 2\pi\eta)$ and $\boldsymbol{q}_2 = (\pi + 2\pi\eta,\ \pi)$. Since the charge density must be positive, $N_{\rm cr}$ should be less than average hole density (doping rate), δ, if instability to static IC-AF occurs. Depending on the value of $a(\eta\,;\ \delta) \equiv N_{\rm cr}/\delta$, we classify three regions: (1) $a(\eta\,;\ \delta) < 1$. Static IC-AF can be stabilized by CDM (2) $a(\eta\,;\ \delta) \gtrsim 1$. CDM can not stabilize static IC-AF, but effects of CDM is still strong and will affect IC-AF fluctuations (3) $a(\eta\,;\ \delta) \gg 1$. Effects of CDM are negligible and IC-AF fluctuation is controlled only by $\chi(\boldsymbol{q})$.

3. RESULTS OF NUMERICAL CALCULATIONS BASED ON THE *t-J* MODEL

To estimate $a(\eta; \delta)$ we calculate[7] $g(\boldsymbol{q}_a,\ \boldsymbol{q}_b)$ and $\chi(\boldsymbol{q})$ based on the mean field theory of the *t-J* model with LSCO-type Fermi surface[8] in the singlet-RVB state at temperature, $T = 0.02J$, in the doping region, $0.10 \leq \delta \leq 0.30$. In the mean field theory $\chi(\boldsymbol{q}) = \chi_0(\boldsymbol{q})/(1 + 2J(\boldsymbol{q})\chi_0(\boldsymbol{q}))$ where $\chi_0(\boldsymbol{q})$ is spin susceptibility without interactions and $J(\boldsymbol{q}) = \tilde{J}(\cos q_x + \cos q_y)$ with $\tilde{J} =$

J. For explicit calculations we set $\tilde{J} = 0.2\,J$ to simulate the possible effects of renormalization due to fluctuations or higher order contributions. This choice of $\tilde{J} = 0.2\,J$, however, is rather arbitrary (see end of § 4).

The condition that $\chi(\boldsymbol{q}) > 0$ in eq. (1) is confirmed numerically. As reported earlier,[8] $\chi(\boldsymbol{q})$ takes a maximum at $(\pi,\, \pi \pm 2\pi\eta)$ and $(\pi \pm 2\pi\eta,\, \pi)$; we defined this η as η_χ. The η-dependences of $a(\eta;\delta)$ for both 1d-CDM(II) and 2d-CDM(II) are shown in Fig. 2. As a function of η, $a(\eta;\delta)$ decreases monotonically and takes a minimum at $\eta \equiv \eta_a$ then suddenly increases for $\delta \geq 0.22$, while it monotonically increases for $\delta \leq 0.20$. δ-dependence of η_χ and $\eta_{\rm a}$ is shown in Fig. 3, where $\eta_{\rm a}$ grows rapidly around $\delta \approx 0.20$ and gets close to η_χ. Around the thick line in Fig. 3, $a(\eta;\delta)$ becomes less than 1. Thus both 1d-CDM(II) and 2d-CDM(II) can in principle stabilize static IC-AF.

For 1d-CDM(I), $a(\eta\,;\,\delta)$ becomes larger than that for both 1d-CDM(II) and 2d-CDM(II) about a few % $\sim$ 10 % depending on η at each δ. For 2d-CDM(I), $a(\eta\,;\,\delta)$ is twice as large as that for 1d-CDM(I). Except for these quantitative differences, the η-dependence of $a(\eta\,;\,\delta)$ does not change among four CDMs.

4. CONCLUSION AND DISCUSSION

We have seen that both 1d-CDM(II) and 2d-CDM(II) can in principle stabilize static IC-AF more easily than 1d-CDM(I) around the thick line in Fig. 3 ($\delta \gtrsim 0.26,\ \eta \approx 0.13 \sim 0.15$). The possibility of 2d-CDM(I) is much smaller than the other CDM patterns. CDM is not necessarily a stripe pattern (1d-CDM(I)) in the present framework.

To get a global picture of how instability to static IC-AF occurs, we discuss δ-dependence of η for IC-AF fluctuation. In the absence of the coupling between N and M, η of IC-AF fluctuation is η_χ giving a maximum of $\chi(\boldsymbol{q})$ while we assume that η of CDM, η_κ, is equal to $1/8$ resulting from some commensurability effects. In the presence of the coupling, if η_χ is not equal to η_κ and effects of coupling are strong, N and M will tend to have the same η because N couples with M having the same η. Since we have found numerically that $a(\eta\,;\,\delta) \gg 1$ for $\eta_\chi < \eta < \eta_\kappa$ while $a(\eta\,;\,\delta) \sim 1$ for $\eta_\kappa < \eta < \eta_\chi$, we expect that the resulting η of IC-AF fluctuation deviates from η_χ as shown by the dotted line in Fig. 3. That is, η tends to saturate at high hole density and probably crosses the thick line at $(\eta,\ \delta) \approx (0.13,\ 0.26)$, where instability to static IC-AF can occur.

This global picture is consistent with experiments[2–6,9] qualitatively. It is noteworthy that the value of $\eta \approx 0.13$ for static IC-AF is close to the observed one, $\eta \approx 0.12$.[2,3,5,6] But the absolute value of hole density is much larger than that of experiments. To improve this problem, the following theoretical consideration may be required: (1) effects of gauge fluctuation on the mean field solutions (2) effects of disorders (3) and ambiguity of Fermi surface.

Finally we mention the value of $\tilde{J} = 0.2J$. If $\tilde{J}$ is taken larger, $a(\eta\,;\,\delta)$ becomes smaller and the region of the thick line in Fig. 3 extends to lower hole density.

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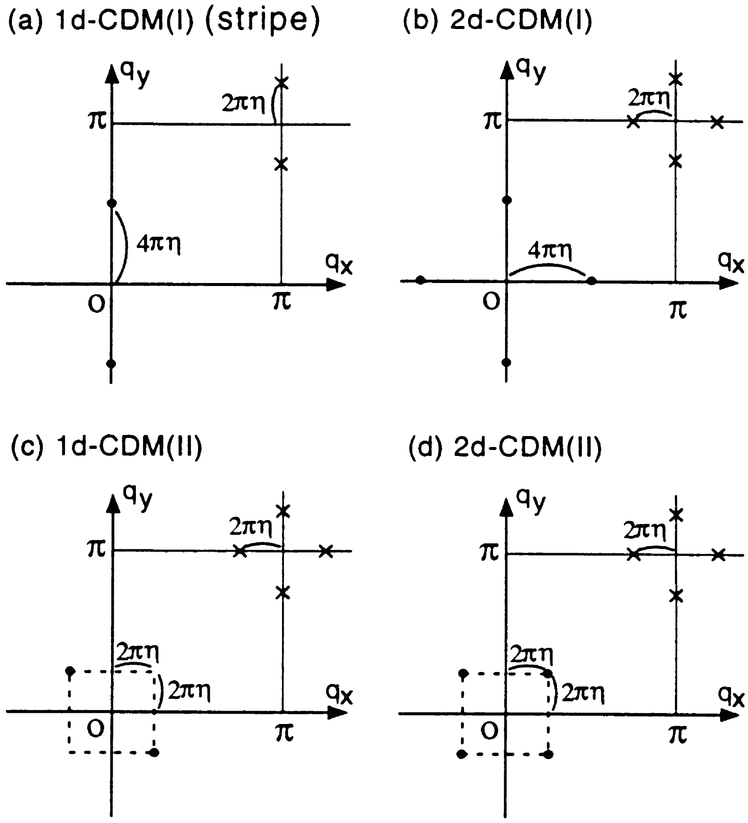

Fig. 1. Four possible patterns of static CDMs are represented by '•' when static IC-AF has wavevectors as shown by '×' in each figure: (a) 1d-CDM(I) has ($\pm 4\pi\eta$, 0) or (0, $\pm 4\pi\eta$), and the case of (0, $\pm 4\pi\eta$) is shown (b) 2d-CDM(I) (c) 1d-CDM(II) has ($\pm 2\pi\eta$, $\pm 2\pi\eta$) 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).

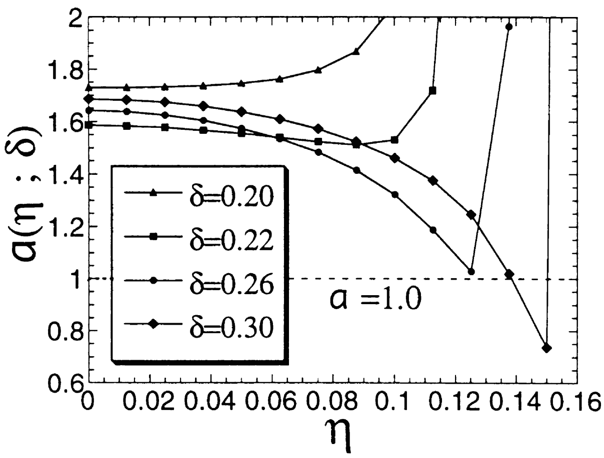

Fig. 2. The η-dependence of $a(\eta; \delta)$ for both 1d-CDM(II) and 2d-CDM(II). The case of $\delta = 0.10, 0.15$ is out of the frame and is not shown.

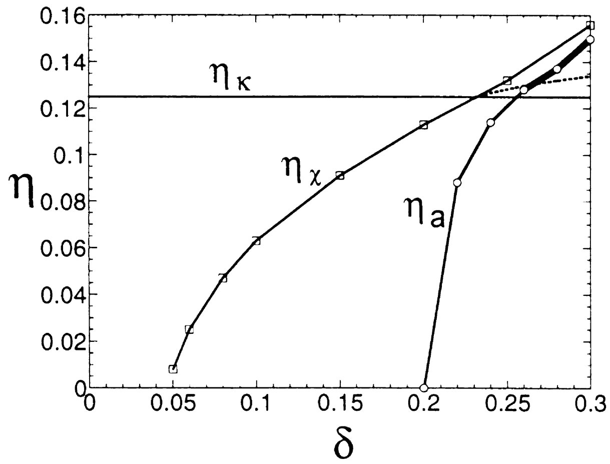

Fig. 3. The δ-dependence of η_χ and $\eta_{\rm a}$ is shown for both 1d-CDM(II) and 2d-CDM(II). Around the thick line $a(\eta\,;\,\delta)$ becomes less than 1, thus CDM can induce static IC-AF. In the absence of the coupling, IC-AF fluctuation has $\eta = \eta_\chi$ and we assume that η of CDM, η_κ, is equal to 1/8. We expect that owing to the strong coupling with CDM, η of IC-AF fluctuation deviates from η_χ as shown by the dotted line and crosses the thick line, where static IC-AF can be stabilized.

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