Low-energy effective theory for spin dynamics of fluctuating stripes

Chi-Ho Cheng*
Institute of Physics, Academia Sinica, Taipei, Taiwan
and Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing, China

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We derive an effective Hamiltonian for spin dynamics of fluctuating smectic stripes from the *t*-*J* model in the weak coupling limit $t \gg J$. Besides the modulation of spin magnitude, the high energy hopping term would induce a low-energy antiferromagnetic interaction between two neighboring "blocks of spins." Based on the effective Hamiltonian, we applied the linear spin-wave theory and found that the spin-wave velocity is almost isotropic for $La_{2-x}Sr_xCuO_4$ unless the structural effect is considered. The intensity of the second harmonic mode is found to be about 10% to that of the fundamental mode.

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There is still a lot of interest on stripe physics.[1,2] The stripe modulation was found in a cuprate superconductor[3] of the sample $La_{2-x}Sr_xCuO_4$ (LSCO) in the low-temperature orthorhombic (LTO) structure. It is also consistent with the incommensurate magnetic peaks observed in the inelastic neutron scattering experiments,[4] in which the peak shift from (π,π) towards $(\pi,0)$ with the derivation very near to $2\pi\delta$ at doping concentration δ. By partial substitution of Nd for La, the LTO lattice structure is distorted to the low-temperature tetragonal (LTT) structure,[5] in which the horizontal stripe is enhanced and the fluctuating (dynamic) stripe becomes more ordered (static).

Theoretically, by the mean-field analysis of the single-band Hubbard model,[6] there is a possibility that the stripe phase is formed. On the other hand, by employing the Schwinger-boson mean-field theory[7] to the *t*-*J* model, it is found that the spiral spin state[8] can also give the deviation from (π,π) upon doping. However, it was studied by many approaches that the uniform phase is unstable towards phase separation in the range of interest ratio t/J.[9] One of the consequences of the phase separation is to form stripes in order to be consistent with the neutron scattering experiments. Because of the stripe fluctuation around the hole domain, the spins across the hole domain should be antiparallel. By considering just a small transverse fluctuation of the stripe, it was found that two neighboring spins across the hole domain feels an antiferromagnetic interaction of coupling J.[10]

Although there is still controversy about the stability of stripes,[11] in this paper the fact that the fluctuating smectic stripe phase is stable is our assumption. By including the Coulomb repulsion (which is neglected in the *t*-*J* model), the holes can only phase separate at microscopic scale instead of full phase separation. In order to balance the hole kinetic energy and the Coulomb repulsion, stripes is the simplest solution among those inhomogeneous states at microscopic scale.

In the following, we are going to derive the low-energy spin dynamics from the two dimensional (2D) *t*-*J* model of the site-centered stripe along the y direction. The period of hole domain is $2R$ where $R \gg 1$ in our model.

The hopping term H_t in the *t*-*J* model is written as

$$H_t = H_t^{\perp} + H_t^{\parallel} = \sum_{\alpha} (H_t^{\perp,\alpha} + H_t^{\parallel,\alpha}), \tag{1}$$

where $H_t^{\perp}$ is the transverse fluctuation of vertical stripes and $H_t^{\parallel}$ is the one-dimensional (1D) kinetic motion along the vertical stripes. Now

$$H_t^{\perp,\alpha} = -t\sum_{\sigma}\sum_{i}{}' (c_{i+\hat{x},\alpha,\sigma}^{\dagger}c_i + c_{i+2\hat{x},\alpha,\sigma}^{\dagger}c_{i+\hat{x},\alpha,\sigma} + \cdots + c_{i+R\hat{x},\alpha,\sigma}^{\dagger}c_{i+(R-1)\hat{x},\alpha,\sigma}) + \text{H.c.}, \tag{2}$$

where α label the smectic stripes and i_x is summed over the supercell of period $2R$. And also

$$H_t^{\parallel,\alpha} = -t\sum_{\sigma}\sum_{i}{}' c_{i+\hat{y},\alpha,\sigma}^{\dagger}c_{i,\alpha,\sigma} + \text{H.c.} \tag{3}$$

In the weak coupling limit, $t \gg J$, the fluctuating stripe induces a charge-density wave along the x direction. There are two almost degenerate ground states for $H_t^{\perp,\alpha}$, $|\psi_S\rangle$ and $|\psi_T\rangle$, which are expressed as

$$|\psi_S\rangle = \frac{1}{\sqrt{2}}(|\psi_1\rangle - |\psi_2\rangle), \tag{4}$$

$$|\psi_T\rangle = \frac{1}{\sqrt{2}}(|\psi_1\rangle + |\psi_2\rangle), \tag{5}$$

where

$$|\psi_1\rangle = a_0|\cdots\downarrow\uparrow\circ\downarrow\uparrow\cdots\rangle + a_1|\cdots\downarrow\uparrow\downarrow\circ\uparrow\cdots\rangle + a_{-1}|\cdots\downarrow\circ\uparrow\downarrow\uparrow\cdots\rangle + \cdots, \tag{6}$$

$$|\psi_2\rangle = a_0|\cdots\uparrow\downarrow\circ\uparrow\downarrow\cdots\rangle + a_1|\cdots\uparrow\downarrow\uparrow\circ\downarrow\cdots\rangle + a_{-1}|\cdots\uparrow\circ\downarrow\uparrow\downarrow\cdots\rangle + \cdots \tag{7}$$

The basis of $|\psi_1\rangle$ and $|\psi_2\rangle$ is different by the up and down spins. The corresponding coefficients are equal. Two subspaces $\{|\psi_1\rangle\}$ and $\{|\psi_2\rangle\}$ are orthogonal to each other. By Eq. (4), which is an orthogonal transformation from $|\psi_1\rangle$ and $|\psi_2\rangle$ to $|\psi_S\rangle$ and $|\psi_T\rangle$, two subspaces $\mathcal{H}_S$ and $\mathcal{H}_T$ spanned by

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$\{|\psi_S\rangle\}$ and $\{|\psi_T\rangle\}$, respectively, are also orthogonal to each other. Equation (2) can be written in the following matrix form under the above basis:

$$H_t^{\perp,\alpha} = (-t)\begin{pmatrix} 0 & 1 & 1 & 0 & \dots \\ 1 & 0 & 0 & 1 & \dots \\ 1 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \otimes (-t) \times \begin{pmatrix} 0 & 1 & 1 & 0 & \dots \\ 1 & 0 & 0 & 1 & \dots \\ 1 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{8}$$

where the two identical $(2R+1)$-dimensional matrices correspond to two orthogonal subspaces spanned by $\{|\psi_S\rangle\}$ and $\{|\psi_T\rangle\}$. Simultaneously, the Heisenberg term in the *t-J* model is written in the matrix form

$$H_J^{\perp,\alpha} = \left(-\frac{3J}{4}\right)\begin{pmatrix} 0 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & 1 & 0 & \dots \\ 0 & 0 & 0 & 1 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \otimes \left(\frac{J}{4}\right) \times \begin{pmatrix} 0 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & 1 & 0 & \dots \\ 0 & 0 & 0 & 1 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{9}$$

Now because two subspaces $\mathcal{H}_S$ and $\mathcal{H}_T$ are orthogonal to each other, the first-order correction to the ground-state energy due to perturbed term $H_J^{\perp,\alpha}$ is

$$E_S^{(1)} = \langle\psi_S|H_J^{\perp,\alpha}|\psi_S\rangle + O(J^2/t), \tag{10}$$

$$E_T^{(1)} = \langle\psi_T|H_J^{\perp,\alpha}|\psi_T\rangle + O(J^2/t), \tag{11}$$

and no correction to the wave function since two subspaces are orthogonal. Solving the eigenproblem for $H_t^{\perp,\alpha}$ gives the transverse density $\rho(x)$ in $(-R,R)$ to the leading order that can be obtained from

$$\rho(x) = |\langle x|\psi_S\rangle|^2 = |\langle x|\psi_T\rangle|^2 = \frac{\delta}{1+2/\pi}\left[1+\cos\left(\frac{\pi x}{2R}\right)\right] \tag{12}$$

and repeat for a period $2R$. It would be convenient to define $\vec{q}_0=(q_0,0)$, where $q_0=\pi/(2R)$. The charge-density wave induced by stripe fluctuation is

$$\rho(\vec{r}) = \delta + \rho_1\cos(2\vec{q}_0\cdot\vec{r}) + \rho_2\cos(4\vec{q}_0\cdot\vec{r}) + \cdots \tag{13}$$

where $\rho_1=4\delta/3(2+\pi)$ and $\rho_2=-4\delta/15(2+\pi)$.

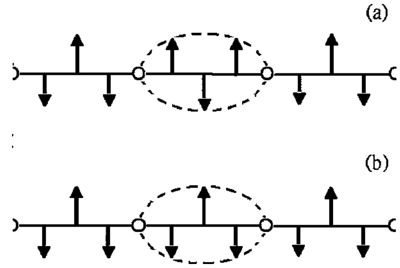

FIG. 1. Illustration of the flip of a "block of spins" from (a) to (b).

Equations (10) and (11) show that two almost degenerate states are split by an energy difference $E_T^{(1)}-E_S^{(1)}$, and hence the energy difference between two "block of spins" is

$$J' = 2R\delta(E_T^{(1)}-E_S^{(1)}) = \frac{2J\delta R^2}{R+1}. \tag{14}$$

Substitution of $q_0=2\pi\delta$ gives $J'=J/2(1+4\delta)$. Note also that the energy difference per site between the antiphase and inphase becomes $J'/(2R)=J\delta/(1+4\delta)$, which is almost linear in δ for $\delta\ll 1$. For $\delta=1/8$, the energy difference is $J/12$ $=130$ K (take $J=135$ meV), which is consistent with the observation of the incommensurate peak up to around 100 K.[4]

There is then an effective antiferrromagnetic coupling term between two neighboring blocks of spins. The antiphase described by $|\psi_S\rangle$ is of lower energy J' than the inphase by $|\psi_T\rangle$. Note that it is different from the case where two neighboring spins across the hole domain interact with an antiferromagnetic coupling.[10,12] The illustration of how to flip a block of spins is shown in Fig. 1. Several mean-field type studies neglecting this low-energy interaction[13] cannot distinguish antiphase and inphase.

Because of no-double occupancy at every site, the spin magnitude also forms a period of $2R$, in which

$$S(\vec{r}) = \frac{1}{2}[1-\rho(\vec{r})] = S_0 + S_1\cos(2\vec{q}_0\cdot\vec{r}) + S_2\cos(4\vec{q}_0\cdot\vec{r}) + \cdots \tag{15}$$

where $S_0=\frac{1}{2}(1-\delta)$, $S_1=-2\delta/3(2+\pi)$, and $S_2=2\delta/15(2+\pi)$.

Because of the antiferromagnetic interaction between two blocks of spins across the hole stripes, we can determine *classically* the z component of the spin $S^z(\vec{r})$ which gives

$$S^z(\vec{r})e^{i\vec{Q}\cdot\vec{r}} = S_1^z\sin(\vec{q}_0\cdot\vec{r}) + S_3^z\sin(3\vec{q}_0\cdot\vec{r}) + \cdots, \tag{16}$$

where $\vec{Q}=(\pi,\pi)$ $S_1^z=(2/\pi)-[3\delta/(2+\pi)]$, and $S_3^z=(2/3\pi)$ $-[5\delta/3(2+\pi)]$. Note that the components S_2^z, S_4^z etc., vanish because of the antiphase symmetry. The effect from lattice distortion gives the same result. The nonvanishing higher harmonic should have wave vector $3q_0$, $5q_0$, etc. The schematic diagram of the classical spin state is shown in Fig. 2.

Estimated up to the order of magnitude, the neutron scattering intensity is more or less proportional to

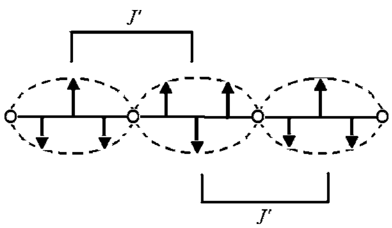

FIG. 2. Schematic diagram of spin state at doping concentration $\delta=1/8$ of LSCO ($q_0=2\pi\delta=\pi/4$). The circles represent the zero average of spin direction. The dashed line shows the envelope of the spin component in a z direction. Any two neighboring "blocks of spins" feel an antiferromagnetic interaction of coupling J'.

$$\int d\vec{r}e^{-\vec{k}\cdot\vec{r}}\langle S^z(\vec{r})S^z(0)\rangle \propto (S_1^z)^2[\delta(\vec{k}-\vec{Q}+\vec{q}_0)+\delta(\vec{k}-\vec{Q}-\vec{q}_0)] + (S_3^z)^2[\delta(\vec{k}-\vec{Q}+3\vec{q}_0) + \delta(\vec{k}-\vec{Q}-3\vec{q}_0)] + \cdots . \quad (17)$$

For $\delta \ll 1$, $(S_3^z/S_1^z)^2 \simeq 1/9$. Substituting $\delta=1/8$, the ratio is 0.093. In general, the ratio of the intensities of the second harmonic ($\vec{Q}\pm 3\vec{q}_0$) to that of the fundamental mode ($\vec{Q}\pm\vec{q}_0$) is about 10%. However, the signal-to-noise ratio in current neutron scattering experiments[3] is not high enough to observe the second harmonic peak. We expect further experiments on a larger pure single crystal measurement can verify our prediction. The first harmonic occuring at $\vec{Q}\pm 2\vec{q}_0$ vanishes. For LSCO, the structural effect at doping concentration $\delta=1/8$ enhances the fundamental mode so that the second harmonic is even harder to be observed.

In order to obtain the low-energy properties, we apply the linear spin-wave expansion,[14] i.e.,

$$\hat{S}^z(\vec{r}_i) = \pm[S(\vec{r}_i) - b_i^\dagger b_i], \quad (18)$$

$$\hat{S}^\pm(\vec{r}_i) = \sqrt{S(\vec{r}_i)}b_i, \quad (19)$$

$$\hat{S}^\mp(\vec{r}_i) = \sqrt{S(\vec{r}_i)}b_i^\dagger, \quad (20)$$

in which $b_i^\dagger$'s and b_i's describe the quantum fluctuation from the classical ground state. The effective Hamiltonian for spin dynamics is

$$H_J = E_0 + 4J\sum_i S(\vec{r}_i)b_i^\dagger b_i + 2J\sum_i (\sqrt{S(\vec{r}_i)S(\vec{r}_{i+1})}b_i b_{i+1} + \text{H.c.}). \quad (21)$$

In the long-wavelength limit, we replace the geometric mean $\sqrt{S(\vec{r}_i)S(\vec{r}_{i+1})}$ by the arithmetic mean $[S(\vec{r}_i)+S(\vec{r}_{i+1})]/2$, and then perform the Fourier transform to the variables $b_i^\dagger$ and b_i. Note that the sites of classical spin pointing up and down are merged together in their Fourier modes. Then

$$H_J = E_0 + 2S_0J\sum_{\vec{k}} (2b_{\vec{k}}^\dagger b_{\vec{k}} + \gamma_{\vec{k}} b_{\vec{k}} b_{-\vec{k}} + \gamma_{\vec{k}} b_{-\vec{k}}^\dagger b_{\vec{k}}^\dagger) + S_1J\sum_{\vec{k}} (2b_{\vec{k}+2\vec{q}_0}^\dagger b_{\vec{k}} + \gamma_{\vec{k}-2\vec{q}_0} b_{\vec{k}} b_{-\vec{k}+2\vec{q}_0} + \gamma_{\vec{k}+2\vec{q}_0} b_{\vec{k}} b_{-\vec{k}-2\vec{q}_0} + \text{H.c.}), \quad (22)$$

where $\gamma_{\vec{k}}=[\cos(k_x)+\cos(k_y)]/2$, and the terms involving higher harmonics are neglected. The Hamiltonian is quadratic and, in principle, can be straightforwardly diagonalized. Since we are only interested in the excitation spectrum around $\vec{k}=\pm 2\vec{q}_0$, write

$$H_J|_{\vec{k}\simeq\pm 2\vec{q}_0} = \sum_{\vec{k}\simeq 2\vec{q}_0} \eta_+^\dagger M_+ \eta_+ + \sum_{\vec{k}\simeq -2\vec{q}_0} \eta_-^\dagger M_- \eta_-, \quad (23)$$

where $\eta_\pm = (b_{\vec{k}} b_{\vec{k}\mp\vec{q}} b_{-\vec{k}}^\dagger b_{-\vec{k}\pm\vec{q}}^\dagger)^T$ and

$$M_\pm = J\begin{pmatrix} 4S_0 & 2S_1 & 4S_0\gamma_{\vec{k}} & 2S_1\gamma_{\vec{k}\mp 2\vec{q}} \\ 2S_1 & 4S_0 & 2S_1\gamma_{\vec{k}\mp 2\vec{q}} & 4S_0\gamma_{\vec{k}\mp 2\vec{q}} \\ 4S_0\gamma_{\vec{k}} & 2S_1\gamma_{\vec{k}\mp 2\vec{q}} & 4S_0 & 2S_1 \\ 2S_1\gamma_{\vec{k}\mp 2\vec{q}} & 4S_0\gamma_{\vec{k}\mp 2\vec{q}} & 2S_1 & 4S_0 \end{pmatrix}. \quad (24)$$

Note that it is the bosonic version of the spin-density wave induced by charge stripes instead of the fermionic one due to Fermi surface instability.[15]

Diagonalizing the Hamiltonian, we get the gapless excitation at $\vec{k}=\pm 2\vec{q}_0$, with the anisotropic spin-wave velocities, in which

$$\epsilon_{\vec{k}=(k_x,0)} = 4S_0J\left[1 - \frac{S_1^2}{4S_0^2}\sec^2(q_0)\right]^{1/2}|k_x \pm 2q_0| \quad (25)$$

and

$$\epsilon_{\vec{k}=(\pm 2q_0,k_y)} = 4S_0J|k_y|. \quad (26)$$

One can estimate the ratio of the anisotropic spin-wave velocities by the Eqs. (25) and (26),

$$\frac{v_x}{v_y} = \left[1 - \frac{S_1^2}{4S_0^2}\sec^2(q_0)\right]^{1/2}. \quad (27)$$

For LSCO, $q_0=2\pi\delta$. $v_x/v_y=1$ at $\delta=0$. At $\delta=1/8$, $v_x/v_y=0.9997$. Without the structural effect, one can safely ignore the anisotropy of spin-wave velocities. However, a perturbed structural effect can be straightforwardly considered by including the term

$$-V\sum_i \cos(2\vec{q}_0\cdot\vec{r}_i)b_i^\dagger b_i, \quad (28)$$

where $V>0$ enhances the spin ordering of magnitude of period $2R$. The term behaves as a perturbed term δM to enhance the first harmonic component S_1 of the spin magnitude.

$$\delta M = \frac{-V}{2}\begin{pmatrix} 0 & 1 & & \\ 1 & 0 & & 0 \\ & & 0 & 1 \\ 0 & & 1 & 0 \end{pmatrix} \quad (29)$$

For perturbed $V \ll t$ where the weak coupling limit is still valid, the density profile $\rho(x)$ in Eq. (12) does not vary. Equations (25) and (26) are just modified by replacing S_1 by $S_1 + V/(4J)$. At $\delta \ll 1$, we can estimate

$$\frac{v_x}{v_y} \simeq \sqrt{1 - \frac{V^2}{4J^2}}. \tag{30}$$

The anisotropy in the neutron scattering measurement is around 0.75.[16] Equation (30) gives an estimate of $V \simeq 1.3J$.

If the structural effect is strong enough $(V/t \gtrsim 1)$. For example, in the sample of the ordered stripe phase of $La_2NiO_{4+\delta}$, we should go beyond the weak coupling limit such that the density profile found in Eq. (12) should also depend on V. The case of the ordered stripe phase will be reported elsewhere.

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*Electronic address: phcch@phys.sinica.edu.tw

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