Spin dynamics in the pseudogap state: phase fluctuation versus $d$-density wave

Hong-Min Jiang$^{1,2,3}$, Jian Zhou$^2$ and Jian-Xin Li$^{2,3}$

1 Department of Physics, Hangzhou Normal University, Hangzhou 310036, China
2 National Laboratory of Solid State of Microstructure and Department of Physics, Nanjing University, Nanjing 210093, China
E-mail: monsoonjhm@sina.com and jxli@nju.edu.cn

New Journal of Physics 13 (2011) 113016 (14pp)
Received 6 March 2011
Published 11 November 2011
Online at http://www.njp.org/
doi:10.1088/1367-2630/13/11/113016

Abstract. The dynamical spin susceptibility in the pseudogap phase of high-$T_c$ cuprates is examined for two different scenarios: the phase fluctuation (PF) of pairing and the $d$-density wave (DDW) order. In the PF scenario, while the resonant feature of the spin response at $Q = (\pi, \pi)$ is preserved at weak PF, the feature is lost as the fluctuation is increased. The dispersion of the spin response in the PF scenario is simply a broadened version of the spectrum in the $d$-wave superconducting (DSC) state at all the strengths of PFs being discussed. In the DDW scenario, there is no spin resonant mode found at the AFM wave vector in nature, and the spin response exhibits the almost dispersionless feature markedly different from that in the PF scenario. As far as the spin dynamics in the pseudogap state is concerned, our results support the scenario that the pseudogap phenomenon is derived from a distinct normal-state order.

$^3$ Authors to whom any correspondence should be addressed.
1. Introduction

One of the most unusual behaviors in the normal state of high-$T_c$ superconductors is the so-called 'pseudogap' phenomenon observed by various experimental techniques in the underdoped and optimal doped cuprates [1, 2]. The origin of the pseudogap and its relationship to superconductivity is one of the important open issues in the physics of high-$T_c$ superconductivity and represents the focal point of current theoretical debate. Among the proposals accounting for the pseudogap phenomenon, there are two distinctly different popular scenarios, depending on whether the pseudogap phase is independent of the Cooper pairing. One is the phase fluctuation (PF) scenario [3–13], where the pseudogap state is thought to be a 'phase-disordered superconductor' characterized by $|\Delta|\exp(i\varphi)$ with nonzero value of $|\Delta|$ but spatially fluctuating phase $\varphi$. In this scenario, the Cooper pair amplitude with $d$-wave symmetry is assumed to preform at temperature $T^*$ that is above the superconducting transition temperature $T_c$, while the coherence of the phase $\varphi$ develops at temperature $T_c$. In the intermediate temperature between $T^*$ and $T_c$, the PFs of the gap give rise to pseudogap phenomena. In an alternative scenario, the pseudogap phase is described as another distinct normal-state ordered phase [14–25], the $d$-density wave (DDW) order, which is a particle–hole condensate with $d$-wave symmetry in the internal momentum space. As a result, there are staggered fluxes originating from the orbital currents, which alter their direction from one plaquette to the neighboring one.

Although the proposals accounting for the pseudogap phenomenon generally fall into two categories, the physics outcome to distinguish them is fairly subtle [26, 27]. Recently, Hinkov et al [28] conducted an inelastic neutron scattering experiment on YBa$_2$Cu$_3$O$_{6.6}$ in the pseudogap state. There, they found that the singularity at resonant energy is no longer discernible in the pseudogap state, and the incommensurability $\delta$ is only weakly energy dependent over a wide energy range. This constitutes a distinct difference from the extensively studied spin resonant mode at the antiferromagnetic (AFM) wave vector $Q = (\pi, \pi)$ and the hourglass-shaped dispersion in the $d$-wave superconducting (DSC) state. Neutron scattering is
an ideal probe for characterizing the spin correlations that are present in the doped materials. Thus, it may overcome the embarrassment encountered by the measurements directly related to the gaps. This is because gaps at points on the Fermi surface connected by a density-wave ordering vector are particle–hole symmetric, just as in the case of a pairing gap [8, 26], rendering the standard analysis for distinguishing them inconclusive [13, 18, 20, 23, 27]. Hence, it is high time that the two scenarios mentioned above should be re-examined theoretically for the spin response to select the viable theory about the origin of the pseudogap phenomenon, a long-lasting puzzle in the field of high-$T_c$ superconductivity.

In this paper, we investigate the dynamical spin susceptibility in the pseudogap phase, which turns out to be markedly different for the two scenarios. In the PF scenario, the energy transfer (defined as frequency $\omega$) dependence of the spin response at the AFM wave vector $Q$ preserves the feature of the spin resonant peak at weak PF strength, whereas the peak intensity is suppressed and broadened by the increase of PFs and eventually loses the resonant feature at the strong PF strength. The dispersion of the spin response in the PF scenario is simply a broadened version of the spectrum in the DSC state at all the strengths of PFs being discussed. In the DDW scenario, on the other hand, there is no spin resonant mode at the AFM wave vector in nature as a result of the banned intraband excitation at the AFM wave vector, and the spin response exhibits the almost dispersionless feature markedly different from the PF scenario. Compared with experiments, our results support the scenario where the pseudogap phase is a distinct normal state order from the superconductivity.

This paper is organized as follows. In section 2, we introduce the model Hamiltonian and carry out the analytical calculations. In section 3, we present the numerical results and compare them with experiments. In section 4, we discuss other possibilities that have been proposed for the pseudogap phenomena. Finally, we give the conclusion of our results in section 5.

2. Theory and method

2.1. The phase fluctuation (PF) scenario

The effective mean field Hamiltonian for a $d$-wave superconductor in the PF scenario may be written as [29, 30]

$$H_{PF} = \sum_{ij}(\psi_i^\dagger h_{ij} \psi_j + \text{h.c.}) - \mu \sum_i \psi_i^\dagger \sigma_3 \psi_i,$$

where $\psi_i^\dagger = (f_i^\dagger, f_i)$ is the Nambu spinor, and

$$h_{ij} = -\tilde{t}_{ij} \delta_{i+\tau,j} \sigma_3 + \begin{bmatrix} 0 & \Delta_{ij}^* \\ \Delta_{ij} & 0 \end{bmatrix},$$

with $\tilde{t}_{ij} = \tilde{t}$ denoting the nearest-neighbor hopping if $\tau = \pm \hat{x}, \pm \hat{y}$, and $\tilde{t}_{ij} = \tilde{t}$ the next-nearest-neighbor hopping if $\tau = \pm \hat{x} \pm \hat{y}$. $\Delta_{ij} = \Delta_0 \eta_{ij} \delta_{i+\tau,j} \exp(i\phi_{ij})$, where $\Delta_0$ is the pairing amplitude, $\eta_{ij} = 1(-1)$ if $\tau = \pm \hat{x} (\pm \hat{y})$, and $\phi_{ij}$ is the phase. $\hat{x} (\hat{y})$ denotes the unit vector along the $x$ ($y$) direction. In the PF scenario, the phase $\phi_{ij}$ is disordered by thermal and/or quantum fluctuations of vortices at zero applied field.

We may adopt a singular gauge transform $\psi_i \rightarrow \exp(-i\phi_i \sigma_3/2) \psi_i$ such that the phase in $\Delta_{ij}$ is transferred to the hopping part in $h_{ij}$, leading to $\Delta_{ij} \rightarrow \Delta_0 \eta_{ij}$ and $-\tilde{t}_{ij} \sigma_3 \rightarrow -\tilde{t}_{ij} \sigma_3 \exp[i(\phi_i - \phi_j) \sigma_3/2]$. In the continuum limit, the phase difference between neighboring sites translates to the phase gradient $2\mathbf{q}_s = \exp(-i\phi) \frac{\hat{y}}{\sqrt{2}} \exp(i\phi)$, and corresponds to the
circulating supercurrent around the vortices. Using the semiclassical Doppler approximation, the Hamiltonian in the momentum space can be written as

$$H_{\text{PF}} = \sum_k \psi_k^\dagger \left[ \varepsilon_k \sigma_3 + (\mathbf{q} \cdot \mathbf{v}_k) \sigma_0 + \Delta_k \sigma_1 \right] \psi_k,$$

where \( \psi_k = (f_k^\dagger \cdot f_{k-1}) \), \( \mathbf{v}_k = \nabla_k \varepsilon_k \) and \( \Delta_k = 2J' \Delta (\cos k_x - \cos k_y) \). \( \varepsilon_k \) and \( J' \) will be given in the following. Appealing to the unitary transformations: \( f_k^\dagger = \sin \theta_k \alpha_k + \cos \theta_k \beta_k^\dagger \) and \( f_{k-1}^\dagger = -\cos \theta_k \alpha_k + \sin \theta_k \beta_k^\dagger \), where \( \sin 2\theta_k = -\Delta_k / g_k \), \( \cos 2\theta_k = -\varepsilon_k / g_k \) and \( g_k = \sqrt{\varepsilon_k^2 + \Delta_k^2} \), the Hamiltonian can be diagonalized in terms of \( \alpha_k \) and \( \beta_k \), with the two energy bands \( E_{k,\alpha} = E_{k} + \mathbf{q}_s \cdot \mathbf{v}_k \) and \( E_{k,\beta} = E_k - \mathbf{q}_s \cdot \mathbf{v}_k \).

Following previous studies, we choose a Gaussian distribution exp\((-\mathbf{q}_s^2 / 2n_v) / \sqrt{2\pi n_v}\) for \( \mathbf{q}_s \) [7], [30–32], with \( n_v \) scaling the density of the thermal vortices, i.e. the intervortice spacing \( d_t \sim \sqrt{1/n_v} \) [30, 32], and therefore characterizing the strength of PFs. The average spin susceptibility is thus

$$\chi(\mathbf{q}, \omega) = \langle \chi(\mathbf{q}, \omega; \mathbf{q}_s) \rangle_{\mathbf{q}_s},$$

where

$$\chi(\mathbf{q}, \omega; \mathbf{q}_s) = \frac{\chi_0(\mathbf{q}, \omega; \mathbf{q}_s)}{1 - U \chi_0(\mathbf{q}, \omega; \mathbf{q}_s)},$$

with

$$\chi_0(\mathbf{q}, \omega; \mathbf{q}_s) = \frac{1}{2N} \sum_k \left\{ \sin^2(\theta_{k+\mathbf{q}} - \theta_k) \left[ R(-E_{k+\mathbf{q},\alpha}, E_{k,\alpha}) + R(E_{k+\mathbf{q},\beta}, -E_{k,\beta}) \right] \\
+ \cos^2(\theta_{k+\mathbf{q}} - \theta_k) \left[ R(E_{k+\mathbf{q},\beta}, E_{k,\alpha}) + R(-E_{k+\mathbf{q},\alpha}, -E_{k,\beta}) \right] \right\},$$

and

$$R(E_{k+\mathbf{q},\alpha}, E_{k,\alpha}) = \frac{f(E_{k+\mathbf{q},\alpha}) - f(E_{k,\alpha})}{\omega + 2\mathbf{q}_s \cdot \mathbf{v}_k - E_{k+\mathbf{q},\alpha} - E_{k,\alpha} + i\Gamma},$$

where \( \Gamma = 0.02J \) is introduced to account for the energy resolution of the experiment.

### 2.2. The \( d \)-density wave (DDW) scenario

The effective Hamiltonian for the uniform DDW state is [15]

$$H_{\text{DDW}} = \sum_{k,\sigma} \left[ f_{k,\sigma}^\dagger f_{k+\mathbf{Q},\sigma} \left[ \varepsilon_k - \Phi_k \right] \left[ \varepsilon_{k+\mathbf{Q}} + \Phi_k \right] \right],$$

where the order parameter of the DDW is \( \Phi_k = 2iJ' \Phi(\cos k_x - \cos k_y) \). Diagonalization of the Hamiltonian by the unitary transformations \( f_{k,\sigma} = \sin \tilde{\theta}_k \tilde{\alpha}_{k,\sigma} - i \cos \tilde{\theta}_k \tilde{\beta}_{k,\sigma} \) and \( f_{k+\mathbf{Q},\sigma} = -i \cos \tilde{\theta}_k \tilde{\alpha}_{k,\sigma} + \sin \tilde{\theta}_k \tilde{\beta}_{k,\sigma} \), where \( \sin 2\tilde{\theta}_k = \Phi_k / \gamma_k \), \( \cos 2\tilde{\theta}_k = -\varepsilon_k / \gamma_k \) and \( \gamma_k = \sqrt{\varepsilon_k^2 + \Phi_k^2} \), we obtain two energy bands \( \tilde{E}_{k,\alpha} = \varepsilon_k + \gamma_k \) and \( \tilde{E}_{k,\beta} = \varepsilon_k - \gamma_k \) corresponding to \( \tilde{\alpha}_{k,\sigma} \) and \( \tilde{\beta}_{k,\sigma} \) quasiparticles.

In this case, due to the nonvanishing Umklapp susceptibility \( \chi_0(\mathbf{q}, \mathbf{q} + \mathbf{Q}, \omega) \), the bare dynamical spin susceptibility is expressed as a matrix,

$$\tilde{\chi}_0(\mathbf{q}, \mathbf{q}', \omega) = \left[ \begin{array}{cc} \chi_0(\mathbf{q}, \mathbf{q}, \omega) & \chi_0(\mathbf{q}, \mathbf{q} + \mathbf{Q}, \omega) \\
\chi_0(\mathbf{q} + \mathbf{Q}, \mathbf{q}, \omega) & \chi_0(\mathbf{q} + \mathbf{Q}, \mathbf{q} + \mathbf{Q}, \omega) \end{array} \right].$$

New Journal of Physics 13 (2011) 113016 (http://www.njp.org/)
where
\[
\chi_0(\mathbf{q}, \mathbf{q} + \mathbf{Q}, \omega) = \frac{1}{N} \sum_k \left[ \cos^2(\tilde{\theta}_{k+q} - \tilde{\theta}_k) [M(\tilde{E}_{k,\alpha}, \tilde{E}_{k+q,\alpha}) + M(\tilde{E}_{k,\beta}, \tilde{E}_{k+q,\beta})] \\
+ \sin^2(\tilde{\theta}_{k+q} - \tilde{\theta}_k) [M(\tilde{E}_{k,\alpha}, \tilde{E}_{k+q,\alpha}) + M(\tilde{E}_{k,\beta}, \tilde{E}_{k+q,\beta})] \right],
\]
and
\[
\chi_0(\mathbf{q}, \mathbf{q} + \mathbf{Q}, \omega) = \frac{i}{2N} \sum_k \left[ \sin(2\tilde{\theta}_{k+q} - 2\tilde{\theta}_k) [M(\tilde{E}_{k,\alpha}, \tilde{E}_{k+q,\alpha}) + M(\tilde{E}_{k,\beta}, \tilde{E}_{k+q,\beta})] \\
+ M(\tilde{E}_{k,\alpha}, \tilde{E}_{k+q,\alpha}) + M(\tilde{E}_{k,\beta}, \tilde{E}_{k+q,\beta}) \right],
\]
with
\[
M(\tilde{E}_{k,\nu}, \tilde{E}_{k+q,\nu}) = \frac{f(\tilde{E}_{k,\nu}) - f(\tilde{E}_{k+q,\nu})}{\omega - \tilde{E}_{k,\nu} + \tilde{E}_{k+q,\nu} + i\Gamma}.
\]

Then, the physical response is given by the diagonal elements of the following random-phase approximation (RPA) renormalized spin susceptibility:
\[
\hat{\chi}(\mathbf{q}, \mathbf{q}', \omega) = \hat{\chi}_0(\mathbf{q}, \mathbf{q}', \omega) [1 - U \hat{I} \hat{\chi}_0(\mathbf{q}, \mathbf{q}', \omega)]^{-1}.
\]

As for the tight-binding energy band, we will choose the following form in both scenarios:
\[
\varepsilon_k = -2t'(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu.
\]
Renormalized hopping parameters are \( t' = xt + J'\xi_0, \) \( t'' = xt' \) with doping level \( x \) and renormalized \( J' = \frac{5}{6}J \). This dispersion can be derived from the slave-boson mean-field calculation of the \( t-t'-J \) model; here we take it as a phenomenological form. In this way, the parameters \( \xi_0 \) and \( \mu \) are determined self-consistently [33, 34]. The parameters we used are \( J = 1.0, t = 2J, \xi_0 = 0.37, \Delta = \Phi = 0.26, \) and the chemical potential \( \mu \) is so chosen to set the doping \( x = 0.12 \).

3. Results and discussion

3.1. Spin response at the antiferromagnetic wave vector

The frequency dependence of the imaginary part of the dynamical spin susceptibility \( \chi(\mathbf{q}, \omega) \) at the AFM wave vector \( \mathbf{Q} = (\pi, \pi) \) for the DSC, PF and DDW states at temperature \( T = 0.05J \) is shown in figure 1(a). In the case of the DSC state, we see a well-known spin resonant mode peaked at about 2\( \Delta \), which is ascribed to a collective spin excitation mode. In the PF case, the PFs do not have a significant effect on the spin resonant peak when the fluctuation strength \( n_x \) is less than 0.005, corresponding to an inter-vortex spacing \( d_v \geq 14a_0 \) that is much larger than the coherent length \( \xi \), which is typically several \( a_0 \) in the cuprate superconductors (\( a_0 \) is the crystal lattice constant). When \( n_v \geq 0.05 \), the inter-vortex spacing \( d_v \leq 4.5a_0 \), which is comparable to \( \xi \). Then, the peak is suppressed, broadened and loses the resonant feature by the strong PFs in this case, as shown in figure 1(a). The same broadened nonresonant peak also occurs in the DDW case, as presented by the line with red circles in figure 1(a).

In figure 1(b), we give the frequency dependence of \( \text{Im} \chi_0(\mathbf{Q}, \omega) \) and \( \text{Re} \chi_0(\mathbf{Q}, \omega) \) for the DSC, PF and DDW states. In the DSC case, \( \text{Im} \chi_0(\mathbf{Q}, \omega) \) has a step and correspondingly
Reχ₀(Q, ω) has a logarithmic singularity (in realistic calculations, this divergence exhibits a maximum as shown in figure 1(b)), and causes a resonant peak due to the RPA renormalization, which satisfies the condition \( 1 - U/Re\chi_0 = 0 \) and vanishing Imχ₀ [35, 36]. A similar situation happens for low PFs in the PF state. However, for strong PFs and in the DDW state, Imχ₀(Q, ω) exhibits a continuous increase with ω, and Reχ₀(Q, ω) does not have a logarithmic singularity, so that the resonant condition is not satisfied anymore in the reasonable range of parameters.

To account for the notably different behaviors of Imχ₀(q, ω) and Reχ₀(q, ω) between the DSC state and the pseudogap phase, we note that Imχ₀(q, ω) at the AFM wave vector \( \mathbf{Q} \) in the DSC and PF states mainly comes from the term

\[
\chi_0(\mathbf{Q}, \omega) \approx \frac{1}{N} \sum_{\mathbf{k}} \left( 1 - \frac{\varepsilon_{\mathbf{k}} \varepsilon_{\mathbf{k}+\mathbf{Q}} + \Delta_{\mathbf{k}} \Delta_{\mathbf{k}+\mathbf{Q}}}{E_{\mathbf{k},\beta} E_{\mathbf{k}+\mathbf{Q},\beta}} \right) \frac{f(E_{\mathbf{k}+\mathbf{Q},\beta}) + f(E_{\mathbf{k},\beta}) - 1}{\omega + 2\mathbf{q}_s \cdot \mathbf{v}_k - g_{\mathbf{k}+\mathbf{Q}} - g_k + i\Gamma},
\]

where \( \mathbf{q}_s = 0 \) (≠0) corresponding to the DSC (PF) case. While in the DDW state, it comes exclusively from the interband term

\[
\chi_0(\mathbf{Q}, \omega) = \frac{1}{N} \sum_{\mathbf{k}} \left( 1 - \frac{\varepsilon_{\mathbf{k}+\mathbf{Q}} - \varepsilon_{\mathbf{k}} + \Phi_{\mathbf{k}+\mathbf{Q}} \Phi_{\mathbf{k}}}{\gamma_{\mathbf{k}+\mathbf{Q}} \gamma_{\mathbf{k}}} \right) \left[ \frac{f(\tilde{E}_{\mathbf{k},\alpha}) - f(\tilde{E}_{\mathbf{k}+\mathbf{Q},\beta})}{\omega - 2\gamma_k + i\Gamma} + \frac{f(\tilde{E}_{\mathbf{k},\beta}) - f(\tilde{E}_{\mathbf{k}+\mathbf{Q},\beta})}{\omega - 2\gamma_k + i\Gamma} \right].
\]

In this case, the spin response comes from the normal particle–hole excitations, so that the intraband excitations are forbidden at the wave vector \( \mathbf{Q} \) due to the relation \( \tilde{E}_{\mathbf{k}+\mathbf{Q},\alpha} = \tilde{E}_{\mathbf{k},\beta} \).

In the DSC state, the energy \( \Omega_\text{DSC} = g_{\mathbf{k}+\mathbf{Q}} + g_k \), which is the function of the 2D wave vector \( \mathbf{k} \), has a minimum \( \Omega_\text{DSC}^{\text{min}} = \min(g_{\mathbf{k}+\mathbf{Q}} + g_k) \approx 2\Delta \) near the hot spot regions shown as red areas in the \( \mathbf{k} \) distribution of H(\( \mathbf{k}, \omega \)). In figure 2(a), for \( \omega \leq \Omega_\text{DSC}^{\text{min}} \), the pattern of figure 2(a) is frequency independent, having small values for \( \omega < \Omega_\text{DSC}^{\text{min}} \). When \( \omega \) equals \( \Omega_\text{DSC}^{\text{min}}, H(\mathbf{k}, \omega) \) increases suddenly and becomes divergent in the hot spot regions. This effect is supported by a large magnitude in the same

*New Journal of Physics* 13 (2011) 113016 (http://www.njp.org/)
regions of the factor \(1 - \frac{\gamma_k Q + \Delta_k Q + \Delta_k}{E_{k,\beta} E_{k,\beta}}\) as shown in figure 2(b). The combined effect gives rise to the step of \(\text{Im} \chi_0(Q, \omega)\) and correspondingly the logarithmic singularity of \(\text{Re} \chi_0(Q, \omega)\). Thus, it causes a resonant peak due to the RPA renormalization.

To some extent, the above statement remains true for weak PFs in the PF scenario. But the situation changes a lot for the strong PFs. Specifically, the \(k\)-dependence of \(H(k, q_s, \omega) = \text{Im} \frac{-1}{\omega - \gamma_k q_s - \gamma_k + i\pi}\) exhibits different patterns, such that the regions with large values are smeared out by the fluctuations and become frequency dependent as presented in figures 2(c) and (d) for \(\omega = 0.2\) and \(\omega = 0.4\), respectively. As seen from figures 2(c) and (d), \(\max[H(k, q_s, \omega)]\) in \(k\) space varies little for different \(\omega\), but the regions with a large value spread out gradually as \(\omega\) is increased. Therefore, the combined effect of the \(\omega\)-dependent \(H(k, q_s, \omega)\) and the \(k\)-dependent coherent factor shown in figure 2(b) leads to a continuous increase of \(\text{Im} \chi_0(Q, \omega)\) with \(\omega\). In the DDW case, \(\Omega_{\text{DDW}} = \min(2\gamma_k) = 0\), so there are always some regions in the \(k\) space, where \(\text{Im} \frac{-1}{\omega - 2\gamma_k + i\pi}\) satisfy the divergent condition for arbitrary \(\omega \leq 2\Phi\) producing the ring-like area in \(k\) space as depicted in figures 3(b)–(d) with \(\omega = 0.2, 0.3\) and 0.42, respectively. The size of the ring increases with \(\omega\) and touches the region with a large magnitude in \(f(E_{k+Q,\beta}) - f(E_{k,\beta})\) shown in figure 3(a). This also causes a gradual increase of \(\text{Im} \chi_0(Q, \omega)\) with \(\omega\), just as in the PF case with strong PFs.

**Figure 2.** The \(k\)-space map of \(\text{Im} \frac{-1}{\omega - \gamma_k q_s - \gamma_k + i\pi}\) for \(\omega = 0.3\) (a) and the \(k\)-space map of the factor \(1 - \frac{\gamma_k Q + \Delta_k Q + \Delta_k}{E_{k,\beta} E_{k,\beta}}\) (b) in the DSC state. Im \(\frac{-1}{\omega + q_s v_k - \gamma_k + i\pi}\) in the PF state at a strong PF \(n_v = 0.05\) for \(\omega = 0.2\) (c) and \(\omega = 0.4\) (d), respectively. The Fermi surface is denoted by a dark line in panel (a) for reference.
3.2. The dispersion of the spin response

We now discuss the dispersion of the dynamical spin susceptibility in the two scenarios. Because the present model is appropriate for describing the well-defined low-energy spin excitations, only the dispersion in the low-energy regime ($\omega < 2\Delta(2\Phi)$) is calculated. Figures 4(a) and (b) show the results with $q_y = \pi$ in the PF and DDW scenarios, respectively. In the PF case, the feature of the dispersion is much like that in the DSC case, in which the distance between two branches, i.e. the incommensurability $2\delta$, decreases with an increase of $\omega$ and becomes zero at the AFM wave vector $Q$ when $\omega = \Omega_{\text{DSC}}^{\text{min}}$ forming the lower part of a hourglass dispersion,
Figure 5. (a) Contour plot shown in the first quadrant of the Brillouin zone for $g_k = \omega/2 = 0.15J$ and its image shifted by $(\pi, \pi)$ in the DSC case. The arrows denote the nesting wave vectors relative to $Q = (\pi, \pi)$. (b) Contour plot for $E_{k,\beta} = \omega/2 = 0.15J$ (red dotted curve) and $E_{k,\beta} = -\omega/2 = -0.15J$ (green dashed curve) in the DDW case. The yellow curve in figure 5(b) indicates the Fermi surface of the $\beta$ band in the DDW case.

except that a slight expansion of the spectra weight exists here due to the PFs. In the DDW case, on the other hand, the incommensurability $\delta$ is only weakly energy dependent over a wide frequency range including $\omega = 2\Phi_1$.

It is known that the hourglass dispersion in the DSC phase can be explained in terms of the nesting of the Fermi surface [37–39]. In the superconducting state, the nesting parts of the two contours $g_k \approx g_k + Q = \omega/2$ are connected by the incommensurate wave vector $\delta q$ as shown in figure 5(a). When $\omega$ increases, the two contours enlarge and approach each other. This gives rise to a decrease of the incommensurability $\delta q$. At the same time, the superconducting coherence factor $1 - \frac{\varepsilon_{k+q} - \varepsilon_k + \Phi_{k+q} \Phi_k}{\gamma_{k+q} \gamma_k}$ increases its value as $q \to Q$ and has the maximal value when $q = Q$. Therefore, the combined effect of these two factors leads to the lower part of hourglass dispersion in the DSC phase. In the PF case, the phase fluctuates about $q_s = 0$ with a Gaussian distribution; for a given $\omega$ the effect of $q_s$ in $H(k, q_s, \omega)$ leads to the expansion of the excitation channel, forming an excitation energy band, which centers about the contour $g_k \approx g_{k+q} = \omega/2$. Therefore, the dispersion in the PF case has a similar hourglass feature as in the DSC case, except that the excitation spectral weight is smeared.

While in the DDW state, without the restriction of $q = Q$, the main contribution to $\text{Im} \chi_0(q, \omega)$ at low energies now comes from the intraband excitations

$$
\chi_0(q, \omega) \approx \frac{1}{N} \sum_k \left( 1 + \frac{\varepsilon_{k+q} - \varepsilon_k + \Phi_{k+q} \Phi_k}{\gamma_{k+q} \gamma_k} \right) \frac{f(E_{k,\beta}) - f(E_{k+q,\beta})}{\omega + E_{k+q,\beta} - E_{k,\beta} + i\Gamma}.
$$

This indicates that $E_{k+q,\beta} < 0$ and $E_{k,\beta} > 0$ are required for appreciable spin excitations. In figure 5(b), we show the equal-energy contour with typically $E_{k,\beta} = \omega/2 = 0.15$ and $E_{k+q,\beta} = -\omega/2$, where the nesting parts of the two equal-energy contours are connected by the incommensurate wave vector $\delta q$. In contrast to the DSC case, the two contours move apart from each other when $\omega$ increases. It leads to an increase of the wave vector $\delta q$. On the other hand, the DDW coherence factor $1 - \frac{\varepsilon_{k+q} - \varepsilon_k + \Phi_{k+q} \Phi_k}{\gamma_{k+q} \gamma_k}$ decreases as $q \to Q$ and has the minimal value when $q = Q$. This opposite effect of the DDW coherent factor prevents decrease of
Figure 6. Effects of the order parameter amplitude fluctuations on $\text{Im}\chi(q,\omega)$. 
(a, c) Frequency dependence of $\text{Im}\chi(Q,\omega)$. (b, d) Peak position of $\text{Im}\chi$ for fixed $q_y=\pi$ as a function of $q_x$ and energy. Upper panels: the results with $n_a=0.005$ in the absence of PFs. Lower panels: the results with $n_a=0.005$ in the presence of PFs with $n_v=0.1$.

incommensurability as $\omega$ decrease, and results in weak energy dependence of the dispersion feature shown in figure 4(b).

4. Other possibilities

4.1. The amplitude fluctuation of the SC order parameter

We note that the amplitude of the superconducting order parameter is also expected to fluctuate significantly when the superconducting order is destroyed by the strong PF [9, 11]. The amplitude fluctuation can be taken into consideration by assuming $\Delta_0 = \Delta_0 + \hat{\Delta}$, where $\Delta_0$ is the average amplitude considered in the Hamiltonian equation (1) and $\hat{\Delta}$ describe the amplitude fluctuation around it. $\hat{\Delta}$ can also be approximated to have Gaussian distribution $\exp(-\hat{\Delta}^2/2n_a)/(\sqrt{2\pi n_a})$, which has been shown to give a good approximation within the pseudogap regime [9]. The results for $n_a=0.005$ both in the absence of PFs and in the presence of PFs with $n_v=0.1$ are displayed in the upper and lower panels of figure 6, respectively. One can see that the resonant feature in the $\omega$ dependence of the spin response at the AFM wave vector $Q$ is undiscernible in both cases, as shown by the dashed lines in figures 6(a) and (c). Meanwhile, the dispersion of spin excitations still exhibits a smeared hourglass feature as displayed in figures 6(b) and (d), just as in the pure PF scenario. Therefore, the results presented above remain qualitatively unchanged when the order parameter amplitude fluctuations are also included.
4.2. The coexistence of the d-wave superconducting and DDW

There has been evidence that the SC state and the pseudogap may coexist below $T_c$ [40]; thus it is interesting to examine the effects of this coexistence. In this case, the Hamiltonian is given by [41]

$$H_{DSC+DDW} = \sum_k \psi_k^\dagger H_k \psi_k,$$

where $\psi_k = (f_{k,\uparrow}^\dagger, f_{-k,\downarrow}^\dagger, f_{k+Q,\uparrow}^\dagger, f_{-k-Q,\downarrow})$ and

$$H_k = \begin{bmatrix}
\epsilon_k & \Delta_k & i\Phi_k & 0 \\
\Delta_k & -\epsilon_k & 0 & -i\Phi_{k-Q} \\
-i\Phi_k & 0 & \epsilon_{k+Q} & \Delta_{k+Q} \\
0 & i\Phi_{k+Q} & \Delta_{k+Q} & -\epsilon_{k+Q}
\end{bmatrix}.\quad(17)$$

The calculation detail of the spin susceptibility in the case of the coexistence can be found in [42]. In figure 7, we present the $\omega$ dependence of $\text{Im}\chi(\mathbf{Q}, \omega)$ and the $q$ dependence of $\text{Im}\chi(q, \omega)$ for several frequencies. As shown in figure 7(a), the resonant peak fades away gradually as the amplitude of the DDW order is increased, resulting in a broad peak when the DDW order amplitude is comparable to the DSC order. At the same time, the downward dispersion only remains at higher energies below the resonance energy, and it will shift to that with an almost dispersionless feature at low energies when the magnitude of the DDW order parameter is comparable to the DSC gap (figure 7(b)). Both of these features interpolate the results between the DSC and DDW states.

4.3. The stripe charge-density-wave order

The stripe charge-density wave (CDW) has also been proposed to account for the pseudogap phenomena. Here, we will consider the stripe CDW order with a period of $4a$ along the $x$-direction. The Hamiltonian for the period $4a$ CDW state is given by

$$H_{CDW} = \sum_{k,\sigma} \psi_{k,\sigma}^\dagger H_k \psi_{k,\sigma}.\quad(18)$$
Figure 8. Spin responses for the stripe CDW state (see text). (a, c) Frequency dependence of Im\(\chi(Q_c, \omega)\) (a) and Im\(\chi(Q, \omega)\) (c), respectively. Peak position of Im\(\chi(q, \omega)\) as a function of \(q_x\) and energy for fixed \(q_y = 0\) (b) and \(q_y = \pi\) (d), respectively.

where \(\psi_k^\dagger = (f_{k+Q_c,\sigma}^\dagger, f_{k+2Q_c,\sigma}^\dagger, f_{k+3Q_c,\sigma}^\dagger)\) and

\[
H_k = \begin{bmatrix}
\epsilon_k & \Phi_c & 0 & \Phi_c \\
\Phi_c & \epsilon_{k+Q_c} & \Phi_c & 0 \\
0 & \Phi_c & \epsilon_{k+2Q_c} & \Phi_c \\
\Phi_c & 0 & \Phi_c & \epsilon_{k+3Q_c}
\end{bmatrix},
\]

(19)

where \(Q_c = (\pi/2, 0)\) is the CDW order wave vector, and \(\Phi_c = 2J'\Phi\). The higher scattering term is weaker and will be neglected here. For the calculation of the spin susceptibility in the case of the stripe state, see [43] for details. In figure 8, we present the frequency dependence of the imaginary part of \(\chi(Q_c, \omega)\) and the dispersion of the dynamical spin susceptibility in the stripe CDW state. As shown in figure 8(a), although a peak appears at about \(\omega \approx 2\Phi_c\), it is not the resonant mode due to the small Re\(\chi_0(Q_c, \omega)\), so that the resonance condition is not satisfied. Above this energy, the over damping of the quasiparticles with the large Im\(\chi_0(Q_c, \omega)\) results in a long tail that persists to a very high energy, which exhibits a difference from that in both the DSC and DDW states. A broader peak structure and a more pronounced long tail feature can be seen at the AFM wave vector \(Q\) as a result of mismatch between the momentum transfer \(q = Q\) and the order wave vector \(Q_c\) (figure 8(c)). The dispersion shows a difference more clearly between \(q_y = 0\) and \(q_y = \pi\). For \(q_y = 0\), the wave vectors \(q = Q_c\) and \(q = 3Q_c\) connect the parts of the Fermi surface approaching the Van Hove singularity and thus result in the peak structures around \(\omega \approx 2\Phi_c\) at these wave vectors (figure 8(b)). In contrast, for \(q_y = \pi\), the broad peak structure appears around the wave vector \(q = Q\) with the energy range extending from \(\omega \sim 0.2\) to \(\omega \sim 0.8\) (figure 8(d)). In both cases, no obvious incommensurate spin excitations have been observed.
5. Remarks and conclusion

At present, there is no agreement as to which of these proposals is correct. The pseudogap in the PF scenario is thought to be directly related to the Cooper pair in the sense that it evolves smoothly into the superconducting gap and has the same $d$-wave symmetry \[5, 8, 12, 13, 44\]. In contrast, in the DDW scenario, the pseudogap phenomenon is described as another distinct normal-state order, which gives way to the SC order as temperature decreases below $T_c$. Thus, both scenarios are capable of describing the evolution from the pseudogap phase to the SC state, where a resonant peak emerges in the spin response at the AFM wave vector due to the collective spin excitation mode in the SC state, as discussed in section 3.1.

In the pseudogap state, our calculations presented above show that the dispersion relation of spin excitations for both scenarios exhibits a distinct difference; namely it has hourglass shape in the PF scenario and the almost dispersionless feature in the DDW scenario. The difference stems from their qualitatively different coherence factors and different topologies of the renormalized band structure, other than the association with the quantitative details such as the gap size, and therefore possesses a capability of distinguishing them unambiguously. By comparing with other possibilities, we find that both the $\omega$-dependent spin response at the AFM wave vector and the dispersion relation for spin excitations in the DDW scenario are consistent with experiments \[28\], lending support to the scenario of the normal-state order where the superconducting and pseudogap states are not directly related to each other.

We also found that the spin resonance and the downward dispersion in the spin responses remain for a small DDW order in the coexistence state of the DDW and the DSC order. In this case, the spin resonance disappears and the downward dispersion becomes dispersionless at low energies when the DDW order is comparable to the DSC order. In contrast, for the stripe CDW, no clear spin resonance and downward dispersion are observed. We note that there are other proposals for the origin of the pseudogap, such as the pair density wave, the AFM spin fluctuations and other types of orbital currents \[17\], \[45–47\], which remain to be investigated.

Acknowledgments

This work was supported by the National Natural Science Foundation of China (grant numbers 91021001 and 10904062), Hangzhou Normal University (HSKQ0043), the Ministry of Science and Technology of China (973 Project grant numbers 2011CB922101 and 2011CB605902) and the NSF of Zhejiang Province (No. Z6110033).

References

\[1\] Timusk T and Statt B 1999 Rep. Prog. Phys. 62 61
\[2\] Norman M R, Pines D and Kallin C 2005 Adv. Phys. 54 715
\[3\] Anderson P W 1987 Science 235 1196
\[4\] Emery V J and Kivelson S A 1995 Nature 374 434
\[5\] Loeser A G, Shen Z-X, Dessau D S, Marshall D S, Park C H, Fournier P and Kapitulnik A 1996 Science 273 325
\[6\] Geshkenbein V B, Ioffe L B and Larkin A I 1997 Phys. Rev. B 55 3173
\[7\] Franz M and Millis A J 1998 Phys. Rev. B 58 14572
\[8\] Renner Ch, Revaz B, Genoud J-Y, Kadowaki K and Fischer Ø 1998 Phys. Rev. Lett. 80 149
14

[9] Curty P and Beck H 2000 Phys. Rev. Lett. 85 796
[10] Eckl T, Scalapino D J, Arrigoni E and Hanke W 2002 Phys. Rev. B 66 140510
[11] Curty P and Beck H 2003 Phys. Rev. Lett. 91 257002
[12] Sutherland M et al 2003 Phys. Rev. B 67 174520
[13] Kanigel A, Chatterjee U, Randeria M, Norman M R, Koren G, Kadowaki K and Campuzano J C 2008 Phys. Rev. Lett. 101 137002
[14] Opel M et al 2000 Phys. Rev. B 61 9752
[15] Chakravarty S, Laughlin R B, Morr D K and Nayak C 2001 Phys. Rev. 63 094503
[16] McElroy K, Lee D-H, Hoffman J E, Lang K M, Lee J, Hudson E W, Eisaki H, Uchida S and Davis J C 2005 Phys. Rev. Lett. 94 197005
[17] Li J-X, Wu C-Q and Lee D-H 2006 Phys. Rev. B 74 184515
[18] Tanaka K et al 2006 Science 314 1910
[19] Ismer J-P, Eremin I and Morr D K 2006 Phys. Rev. B 73 104519
[20] Lee W S, Vishik I M, Tanaka K, Lu D H, Sasagawa T, Nagaosa N, Devereaux T P, Hussain Z and Shen Z-X 2007 Nature 450 81
[21] Kondo T, Takeuchi T, Kaminski A, Tsuda S and Shin S 2007 Phys. Rev. Lett. 98 267004
[22] Liu Y H, Takeyama K, Kurosawa T, Momono N, Oda M and Ido M 2007 Phys. Rev. B 75 212507
[23] Khasanov R, Kondo T, Strässle S, Heron D O G, Kaminski A, Keller H, Lee S L and Takeuchi T 2008 Phys. Rev. Lett. 101 227002
[24] Tewari S, Zhang C, Yakovenko V M and Das Sarma S 2008 Phys. Rev. Lett. 100 217004
[25] Kondo T, Khasanov R, Takeuchi T, Schmalian J and Kaminski A 2009 Nature 457 296
[26] Yang H-B, Rameau J D, Johnson P D, Valla T, Tsvelik A and Gu G D 2008 Nature 456 77
[27] Boyer M C, Wise W D, Chatterjee K, Yi M, Kondo T, Takeuchi T, Ikuta H and Hudson E W 2007 Nat. Phys. 3 802
[28] Hinkov V, Bourges P, Pailhès S, Sidis Y, Ivanov A, Frost C D, Perring T G, Lin C T, Chen D P and Keimer B 2007 Nat. Phys. 3 780
[29] Kwon H-J and Dorsey A T 1999 Phys. Rev. B 59 6438
[30] Wang Q-H 2002 Phys. Rev. Lett. 88 057002
[31] Choi H-Y, Bang Y and Campbell D K 2000 Phys. Rev. B 61 9748
[32] Sheehy D E, Adagideli I, Goldbart P M and Yazdani A 2001 Phys. Rev. B 64 224518
[33] Li J X, Mou C Y and Lee T K 2000 Phys. Rev. B 62 640
[34] Lee P A, Nagaosa N and Wen X G 2006 Rev. Mod. Phys. 78 17
[35] Liu D Z, Zha Y and Levin K 1995 Phys. Rev. Lett. 75 4130
[36] Bulut N and Scalapino D J 1996 Phys. Rev. B 53 5149
[37] Manske D, Eremin I and Bennemann K H 2001 Phys. Rev. B 63 054517
[38] Chubukov A V, Janko B and Thernshyov O 2001 Phys. Rev. B 63 180507
[39] Li J X, Yin W G and Gong C D 1998 Phys. Rev. B 58 2895
[40] Brinckmann J and Lee P A 1999 Phys. Rev. Lett. 82 2915
[41] Norman M R 2007 Phys. Rev. B 75 184514
[42] Li J X and Gong C D 2002 Phys. Rev. B 66 014506
[43] He R-H et al 2011 Science 331 1579
[44] Cappelluti E and Zeyher R 1999 Phys. Rev. B 59 6475
[45] Chen C-P, Jiang H-M and Li J-X 2010 J. Phys.: Condens. Matter 22 035701
[46] Zhou J, Guo J, Jiang H-M and Li J-X 2011 Eur. Phys. J. B 82 295
[47] Ding H, Norman M R, Yokoya T, Takeuchi T, Randeria M, Campuzano J C, Takahashi T, Mochiku T and Kadowaki K 1997 Phys. Rev. Lett. 78 2628
[48] Varma C M 1997 Phys. Rev. B 55 14554
[49] Chen H-D, Vafek O, Yazdani A and Zhang S-C 2004 Phys. Rev. Lett. 93 187002
[50] Daou R et al 2010 Nature 463 519

New Journal of Physics 13 (2011) 113016 (http://www.njp.org/)