The two-component spin–fermion model for high-$T_c$ cuprates: its applications in neutron scattering and ARPES experiments

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Abstract. Motivated by neutron scattering experiments in high-$T_c$ cuprates, we propose the two-component spin–fermion model as a minimal phenomenological model, which has both local spins and itinerant fermions as independent degrees of freedom (d.o.f.). Our calculations of the dynamic spin correlation function provide a successful description of the puzzling neutron experiment data and show that: (i) the upward dispersion branch of magnetic excitations is mostly due to local spin excitations; (ii) the downward dispersion branch is from collective particle–hole excitations of fermions; and (iii) the resonance mode is a mixture of both d.o.f. Using the same model with the same set of parameters, we calculated the renormalized quasiparticle (q.p.) dispersion and successfully reproduced one of the key features of the angle-resolved photoemission spectroscopy (ARPES) experiments, namely the high-energy kink structure in the fermion q.p. dispersion, thus supporting the two-component spin–fermion phenomenology.
Contents

1. Introduction .............................................. 2
2. The model ............................................. 3
   2.1. Formalism ........................................ 3
   2.2. How and why are one-component and two-component spin–fermion models different? ................................. 6
   2.3. Why do the $\Omega$-linear damping and $\Omega^2$ terms have comparable strength in our model? ...................... 6
3. Neutron scattering ...................................... 7
   3.1. $\chi_f(q, \Omega)$ along $(0,1/2) \rightarrow (1,1/2)$ ........................................... 7
   3.2. Origin of the resonance mode ........................................ 9
   3.3. Constant energy scans ................................... 11
   3.4. Parameters of our phenomenology ............................... 13
4. Angle-resolved photoemission spectroscopy and high-energy kink ................. 13
5. Conclusion ............................................. 16
6. Acknowledgments ....................................... 16
7. References ............................................. 16

1. Introduction

The study of spin dynamics has been of key interest since the discovery of the high-$T_c$ superconductor because it is expected that the spin correlation holds crucial information on the mechanism of high-$T_c$ superconductivity (HTS). For a long time the two main observations in neutron scattering experiments of high-$T_c$ cuprates (HTC) have been (i) the incommensurate (IC) peaks at low energy or at quasielastic excitations [1, 2] and (ii) the so-called resonance peak at commensurate wave vector at a relatively high energy (30–50 meV) [3–5]. In early experiments, the IC peaks were observed only in the deeply underdoped lanthanum cuprate and the resonance mode was the hallmark of the fully doped two-layer yttrium cuprate. However, later experiments reveal that both features appear in both groups of cuprate compounds, although they sensitively depend on doping level. More recently, with inelastic neutron scattering (INS) experiments [6–11] with high precision, a unifying form of the magnetic excitations in the cuprate superconductors has emerged as the ‘hourglass’ shape of excitations around the wave vector $(1/2,1/2)$ (hereafter in units of $2\pi/a$), in which the low-energy IC excitations form the downward dispersion branch and the high-energy IC excitations form the upward dispersion branch, and the two branches of excitations merge at the commensurate momentum $Q = (1/2, 1/2)$ and at the resonance frequency $\Omega_{\text{res}}$.

To understand the origin of these ‘hourglass’ shape excitations is a pressing problem. Theoretical proposals made up to now can be classified into two groups: (i) theories based on the spin dynamics in the presence of stripes [12–15] and (ii) Fermi liquid-type theories of itinerant fermions [16–20]. The key idea of the first group of theories is that the stripes formed by doping in the two-dimensional (2D) Cu–O plane split the commensurate spin wave excitations into two IC branches at the wave vectors $(1/2 \pm \delta, 1/2)$ or at their symmetry rotated positions by
x ↔ y depending on the directions of the stripes. The dispersions from each branch of the two IC modulations cross at the commensurate wave vector (1/2,1/2) at a higher energy, which is then identified as the resonance mode. This picture provides a qualitative explanation of the hourglass dispersion and the resonance mode. However, this type of theory is difficult to extend to the higher doping regime where the presence and nature of the stripes are questionable. The second group of proposals is itinerant fermion theories with interaction [16–20]. In this type of theory, the resonance mode and the downward dispersion can be obtained, but the upward dispersion branch is not satisfactorily reproduced.

In this paper, we propose a two-component spin–fermion model [21, 22] as a minimal phenomenological model to provide a natural and unifying explanation of the above-mentioned neutron experiments of HTC. In this phenomenological model, the minimal set of low-energy degrees of freedom (d.o.f.) are the spin wave excitations of local spins and the continuum particle–hole excitations of fermions. A similar phenomenological theory is known as the one-component spin–fermion model and has been intensively studied by Pines and coworkers (see [23] and references therein). The main difference between the two-component model and the one-component one is the introduction of spin wave excitations directly from the local spins in addition to the usual collective spin density excitations from fermions. In this paper, we show that the presence of the local spin fluctuations is essentially proven by the INS and angle-resolved photoemission spectroscopy (ARPES) experiments of HTC, thus supporting the two-component spin–fermion model as a minimal phenomenological model of HTS.

2. The model

2.1. Formalism

In a mixed momentum and real-space representation the two-component spin–fermion phenomenology Hamiltonian is written as

\[ H = \sum_{k,\alpha} c_{\alpha}^\dagger(k) \epsilon(k) c_{\alpha}(k) + \sum_{r,\alpha,\beta} \mathbf{g}\mathbf{S}(r) \cdot c_{\alpha}^\dagger(r) \mathbf{\sigma}_{\alpha\beta} c_{\beta}(r) + H_S(\mathbf{S}(r)), \]

where the first term is the fermionic kinetic energy and the second term describes the coupling between local spins \( \mathbf{S}(r) \) and the spin density of the conduction electrons \( \mathbf{s}(r) = c_{\alpha}^\dagger(r) \mathbf{\sigma}_{\alpha\beta} c_{\beta}(r) \). The last term \( H_S(\mathbf{S}(r)) \) represents an effective low-energy Hamiltonian for the local spins \( \mathbf{S}(r) \). Instead of specifying \( H_S \) and solving it, we assumed a phenomenological ansatz of the bare (before coupling to the fermions) local spin dynamics \( \langle \mathbf{S}_q \mathbf{S}_{-q} \rangle_0 = \chi_{0,S}(q, \Omega) \) with a short-range antiferromagnetic (AFM) correlation, which has the general form given below [24]:

\[ \chi_{0,S}^{-1}(q, \Omega) = \chi_{0,S}(Q, 0) \cdot [1 + \xi^2|q - Q|^2 - \Omega^2/\Delta_{SG}^2], \]

where \( Q \) is the 2D AFM ordering vector and the spin gap energy \( \Delta_{SG} \) and the magnetic correlation length \( \xi \) combine to give the spin wave velocity \( v_s = \Delta_{SG} \cdot \xi \) that can be determined by direct measurement [25].

The key difference of the Hamiltonian equation (1) from the one-component Hamiltonian [23] is in the definition and meaning of the spin fields \( \mathbf{S}(r) \). We assumed that \( \mathbf{S}(r) \)
is the local spin d.o.f. besides and independent of the fermions $c_a^\dagger (r)$ and the related itinerant spin density $\mathbf{s}(r) = c_a(r)\hat{\sigma}_{\alpha\beta}c_\beta(r)$. On the other hand, in the one-component spin–fermion model [23], the collective spin fields are defined as the itinerant spin density operators made up of fermions and hence fundamentally linked to the fermions, and there is no concept of local spins. Another important distinct feature of our two-component phenomenology is the local spin dynamics defined in equation (2). This form of the local spin correlation function with a short-range AFM order should be valid not only near $Q$ but also for the entire BZ of $\mathbf{q}$—if the precise form of the spin-wave dispersion is ignored—because at high energies the local spin dynamics becomes less sensitive to the long-range or short-range order. However, the similar form of the itinerant spin correlation function assumed in the one-component model [23] is valid only in a narrow region of $\mathbf{q}$ around $Q$ by definition.

Microscopic justification of the above two-component model, starting, for example, from the Hubbard or $t$–$J$ model, has been the heart of the problem of HTC for the last 20 years or so. We can only sketch here the underlying idea of our phenomenology. Starting from a Hubbard model, for example, dynamic mean field theory (DMFT) [26] demonstrated that the key consequence of the strong correlation of large $U$ Coulomb interaction is to split the electron spectral density into two parts: one near the Fermi level—the itinerant one, and the other at the lower and upper Hubbard bands far below and above the Fermi level—hence the localized one. Therefore this splitting of one bare electron spectral density into itinerant and localized parts is not a new observation but already has a solid theoretical justification.

A new step in our phenomenology is to propose that the localized spectral density far away from the Fermi level is not dormant for the low-energy physics. In the framework of the DMFT, once the coherent band is formed at the Fermi level in addition to the upper and lower Hubbard bands through the strong correlation effect, the low-energy physics is solely described by the coherent band near the Fermi level and the Hubbard bands appear only as high-energy charge fluctuations such as the incoherent absorption bands at high frequencies of order $O(U)$, for example, in optical conductivity. This picture is correct with respect to the charge degree of freedom because the DMFT is designed to capture the strong correlation of charge dynamics by being a single-site impurity model. However, it is physically rather obvious that the localized Hubbard bands can still contribute to low-energy physics through spin fluctuations. In order to capture this low-energy spin degree of freedom, it is, however, necessary to study the lattice model—not a small cluster but a thermodynamically large lattice. Then we have to give up all the merits of the DMFT. At the moment, there is no satisfactory microscopic theory for the lattice model which faithfully treats the strong correlation of large $U$.

To this end, we note that there exist two spin correlation functions in our two-component model: $\chi_S$ from the local spins $\mathbf{S}(r)$ and $\chi_f$ from the itinerant spin density $\mathbf{s}(r) = c_a^\dagger (r)\hat{\sigma}_{\alpha\beta}c_\beta(r)$. Counting the coupling term to one loop order (equivalent to the RPA), the dressed spin correlation functions of the Hamiltonian (1) are written as follows:

$$\chi_S^{-1}(\mathbf{q}, \Omega) = \chi_{0.S}^{-1}(\mathbf{q}, \Omega) - g^2 \cdot \chi_{0.f}(\mathbf{q}, \Omega),$$

$$\chi_f^{-1}(\mathbf{q}, \Omega) = \chi_{0.f}^{-1}(\mathbf{q}, \Omega) - g^2 \cdot \chi_{0.S}(\mathbf{q}, \Omega),$$

where $\chi_{0.S}$ is introduced in equation (2) and $\chi_{0.f}$ is the noninteracting spin susceptibility of the conduction band of the fermions. The diagrammatic illustration of the derivation of equations (3)
and (4) is shown in figure 1. The noninteracting spin susceptibility \( \chi_{0,f} \) is written as

\[
\chi_{0,f}(q, \Omega) = \sum_k \left[ \frac{1}{2} \left[ 1 + \frac{\epsilon(k + q)\epsilon(k) + \Delta(k + q)\Delta(k)}{E(k + q)E(k)} \right] \frac{f(E(k + q)) - f(E(k))}{\omega - [E(k + q) - E(k)] + i\Gamma} + \right. \\
+ \sum_k \frac{1}{4} \left[ 1 - \frac{\epsilon(k + q)\epsilon(k) + \Delta(k + q)\Delta(k)}{E(k + q)E(k)} \right] \frac{1 - f(E(k + q)) - f(E(k))}{\omega - [E(k + q) + E(k)] + i\Gamma} \\
+ \sum_k \frac{1}{4} \left[ 1 - \frac{\epsilon(k + q)\epsilon(k) + \Delta(k + q)\Delta(k)}{E(k + q)E(k)} \right] \frac{f(E(k + q)) + f(E(k)) - 1}{\omega + [E(k + q) + E(k)] + i\Gamma},
\]

where \( E(k) = \sqrt{\epsilon^2(k) + \Delta^2(k)} \) and the itinerant fermion dispersion \( \epsilon(k) \) is given by a tight binding model,

\[
\epsilon(k) = -2t \cos(k_x) - 2t' \cos(k_x) \cdot \cos(k_y) - \mu.
\]

For calculations in this paper, we chose \( t' = -0.4t \) and \( \mu = -0.81t \). The overall energy scale \( t \) and the choice of parameters \( t', \mu \) will be discussed later with the numerical results. For the superconducting state (SS), we assume a canonical d-wave gap function \( \Delta(k) = \Delta_0[\cos(k_x) - \cos(k_y)] \) and for the normal state (NS), we set \( \Delta_0 = 0 \) in equation (5).

Having two d.o.f. in the model, two spin susceptibilities \( \chi_S \) and \( \chi_I \) should be calculated on an equal footing. Previous studies of the local spin correlation embedded in the fermion bath [24] considered only the imaginary part of \( \chi_{0,I} \) (the so-called Landau damping) in equation (3) to damp the spin wave excitations of equation (2) and the real part of \( \chi_{0,I} \) is assumed to be either already included in the definition of the bare local spin dynamics described in equation (2) or having negligible effects. In fact, when the coupling \( g \) is weak, this approach is reasonable. But in the strong coupling limit when the dimensionless coupling constant \( \lambda \equiv g^2 \cdot \chi_{0,I}(Q, 0) \cdot \chi_{0,S}(Q, 0) \sim O(1) \), it is crucial to include both the real and imaginary parts as in equations (3) and (4). As we can see in the next section, in the strong coupling limit both dressed spin susceptibilities \( \chi_S(q, \Omega) \) and \( \chi_I(q, \Omega) \) become a mixture of the local spins and the itinerant fermions and assimilate to each other with increasing coupling strength \( \lambda \). In passing, equations (3) and (4) are loop expansions (one loop order) but not a coupling constant expansion. Therefore, the strong coupling limit of \( \lambda \sim O(1) \) is not a problem, but the higher loop diagrams—for example, vertex corrections in standard many-body terminology—need to be worried about. This problem is beyond the scope of this work.

Figure 1. (a) Interaction vertex of \( H_{\text{int}} \) and bare spin correlation functions \( \chi_{0,S} \) and \( \chi_{0,I} \). (b) Graphical illustration of the summations of the infinite series for the dressed spin correlation functions \( \chi_S \) and \( \chi_I \) as defined in equations (3) and (4).
2.2. How and why are one-component and two-component spin–fermion models different?

Here we summarize the difference between the two models and re-emphasize the necessity of the two-component phenomenology.

1. The standard one-component spin–fermion model [23] also starts with the same form of the bare spin propagator as equation (2) although it has conceptually different origin as it was argued that it can arise from fermions as a collective spin density mode by successively integrating out the high-energy fermions. Regardless of its origin, the bare spin propagator obtains the Landau damping, \( \Omega / \Omega_{sf} \), by coupling with fermions. However, the one-component model assumed \( \Omega^2 / \Delta^2_{SG} \gg \Omega_{sf}^2 / \Delta^2_{SG} \) and then dropped the term \( \Omega^2 / \Delta^2_{SG} \) in the model by arguing that this is justified when \( \xi_{AFM} \gg 1 \) (see below equation (38) of [23]). Neglecting the \( \Omega^2 / \Delta^2_{SG} \) term means that the spin d.o.f. has lost its active dynamics but becomes a passive relaxational mode, meaning that its frequency dependence is obtained only through the fermion damping process \( i\Omega / \Omega_{sf} \). The condition \( \xi_{AFM} \gg 1 \) also means that the one-component model is applicable near the AFM criticality and indeed in this case there is no need to consider the two-component model of this paper. However, our two-component model is designed to explain the hourglass dispersion of INS near the optimal doping region where \( \xi_{AFM} \sim 2–3 \) lattice constant. In this region, we argue that \( i\Omega / \Omega_{sf} \sim \Omega^2 / \Delta^2_{SG} \); hence the \( \Omega^2 \) term cannot be dropped and the independent spin dynamics is crucial for understanding the key features of the INS and ARPES experiments.

2. Therefore, the presence or absence of the \( \Omega^2 \) term in the spin dynamics is the technical criterion to distinguish the two-component model from the standard one-component spin fermion model. Depending on this choice, the two models are using two different effective Lagrangians and hence become two different phenomenologies. Also, at the level of phenomenology the \( \Omega^2 \) term cannot be self-consistently generated by the low-energy fermions; hence, it needs to be treated as independent d.o.f. Incidentally, a recent resonant x-ray scattering experiment [32] detected the persistence of spin wave excitations—similar to those of the undoped antiferromagnetically ordered parent compound—even in the over-doped YBa\(_2\)Cu\(_3\)O\(_7\) supporting the persistence of the independent spin dynamics and the concept of the local spin d.o.f. of our model.

2.3. Why do the \( \Omega \)-linear damping and \( \Omega^2 \) terms have comparable strength in our model?

1. In our model, the dimensionless coupling constant is defined as \( \lambda = g^2 \cdot \chi_{0,f} \cdot \chi_{0,s} \). As can be seen from equations (3) and (4) and also numerically demonstrated later in figure 4, \( \lambda \sim O(1) \) is the inevitable and necessary condition to produce the ‘resonance mode’ at \((\pi, \pi)\) in the SC state; this also implies that the observation of ‘the resonance mode’ itself is an indicator that the physical coupling strength ought to be \( \lambda \sim O(1) \) in that region. We use \( \lambda = 0.8 \) in our calculations and this value is independent of the separate normalizations of \( g, \chi_{0,f} \) and \( \chi_{0,s} \), respectively.

2. The coupled equations (3) and (4) automatically impose that the \( \Omega \)-linear damping and \( \Omega^2 \) terms should have comparable strengths near the resonance frequency when \( \lambda \sim O(1) \). Indeed, figures 2(c) and 3(c) show that the spectra of \( \text{Im}\chi_{f,s}(\omega) \) are smoothly connected from zero frequency to the resonance frequency \( \Omega_{res} \).
Figure 2. (a, b) (left column) The dressed itinerant spin susceptibility $\text{Im}\chi_f(q,\Omega)$ and the bare spin susceptibility $\text{Im}\chi_{0,f}(q,\Omega)$, respectively, in the SS. Parameters are $\Delta_{SG} = 1.1t$, $\Delta_0 = 0.2t$ and $\lambda = 0.8$. (c, d) (right column) $\text{Im}\chi_f(q,\Omega)$ and $\text{Im}\chi_{0,f}(q,\Omega)$, respectively, in the NS ($\Delta_0 = 0$).

3. Neutron scattering

In order to study the INS experiments, we calculated the fully dressed dynamic spin susceptibilities $\chi_S(q,\Omega)$ and $\chi_f(q,\Omega)$ of equations (3) and (4). As mentioned in the previous section, in the strong coupling limit of $\lambda \sim O(1)$, the behavior of $\chi_S(q,\Omega)$ and $\chi_f(q,\Omega)$ becomes qualitatively similar. Therefore, we conveniently discuss the numerical results of $\chi_f(q,\Omega)$ in this paper. But for completeness, we also show the numerical results of $\chi_S(q,\Omega)$ as well as the total spin susceptibility $\chi_{tot} = \chi_f + \chi_S$, too.

3.1. $\chi_f(q,\Omega)$ along $(0,1/2) \rightarrow (1,1/2)$

Figure 2(a) shows $\text{Im}\chi_f(q,\Omega)$ scanned along $q = (h, 1/2)$ in the SS. The superconducting gap $\Delta_0 = 0.2t$, the bare spin gap $\Delta_{SG} = 1.1t$ (it is not the physical spin gap), and the dimensionless coupling constant $\lambda = 0.8$ ($g^2 = 0.95\text{eV}^2$) were chosen. The main effect of the coupling is to renormalize down the bare spin gap energy $\Delta_{SG}$ below the particle–hole excitation gap of...
Figure 3. (a, b) (left column) The dressed local spin susceptibilities $\text{Im}\chi_S(q, \Omega) = (h, 1/2), \Omega)$ and the total spin susceptibilities $\text{Im}\chi_{\text{tot}}(q, \Omega) = \text{Im}\chi_S + \text{Im}\chi_f$, respectively, in the SS. (c, d) (right column) $\text{Im}\chi_S(q, \Omega)$ and $\text{Im}\chi_{\text{tot}}(q, \Omega)$, respectively, in the NS. Parameters are the same as in figure 2.

$\chi_0, f(q, \Omega) \sim 2\Delta_0$, which then forms a sharp resonance peak at $Q = (1/2, 1/2)$. Centering from this resonance mode, both the downward dispersion branch and the upward dispersion branch span out. The origin of the upward dispersion is apparently from the local spin wave mode (see equation (2)) and the origin of the downward dispersion is the itinerant spin excitations of $\chi_0, f$. The latter fact can be identified in figure 2(b) which shows the non-interacting fermion spin susceptibility $\text{Im}\chi_0, f(q, \Omega)$ scanned along $q = (h, 1/2)$ in the SS. The shape and strength of the downward whisker-like excitations in $\text{Im}\chi_0, f$ are sensitive to the Fermi surface (FS) curvature (controlled by $\mu$ and $t'$), and the size of the d-wave gap $\Delta(k) = \Delta_0[\cos(k_x) - \cos(k_y)]$.

With the coupling strength $\lambda = 0.8$, the dressed fermion spin susceptibility $\chi_f(q, \Omega)$ obtains features of both the local spin susceptibility $\chi_0, S$ and the itinerant spin susceptibility $\chi_0, f$. In particular, the high-energy parallel branches in $\chi_0, f$ (see figures 2(b) and (d)) are overwhelmed by the spin wave-like excitations of $\chi_0, S$ in the dressed susceptibility $\chi_f$ as seen in figures 2(a) and (c). With a smaller coupling strength ($\lambda < 0.5$) the two spin susceptibilities $\chi_S(q, \Omega)$ and $\chi_f(q, \Omega)$ are obtained.
and $\chi_t(\mathbf{q}, \Omega)$ retain more of the bare characteristics of the spin wave excitations and the itinerant fermion susceptibility, respectively, and the resonance peak at $\mathbf{Q} = (1/2, 1/2)$ is not formed.

Figures 2(c) and (d) are the same plots as in figures 2(a) and (b) but in the NS. Firstly, the resonance peak becomes severely overdamped having only a hump-like structure in $\text{Im}\chi_t(\mathbf{q}, \Omega)$. Secondly, the low-energy downward whisker-like dispersion disappears because the free fermion susceptibility $\chi_{0,f}(\mathbf{q}, \Omega)$ in the NS (see figure 2(d)) has no such structure. Lastly, the high-energy upward dispersion remains almost similar to the case of the SS. The results of figures 2(a) and (c) successfully reproduce the main features of recent neutron scattering experiments in HTC [6–11], i.e. the resonance mode in SS, the hourglass shape of the upward and downward dispersions and their drastic change between superconducting and NSs. In particular, these results strikingly resemble the INS data of YBCO$_{1.8}$ [8], which has a static stripe order and an extremely low $T_c = 2.5$ K [27]. In particular, the presence of the stripe ordering is likely to change the spin dynamics significantly [13–15] and introduce $a$–$b$ plane anisotropy.

For comparison, we also show in figure 3 the numerical results for the local spin susceptibility $\chi_S(\mathbf{q}, \Omega)$ as well as the total spin susceptibility $\chi_{tot}(\mathbf{q}, \Omega) = \chi_t(\mathbf{q}, \Omega) + \chi_S(\mathbf{q}, \Omega)$. As mentioned above, the overall behavior of $\chi_S(\mathbf{q}, \Omega)$ is indistinguishably similar to $\chi_t(\mathbf{q}, \Omega)$ and so is $\chi_{tot}(\mathbf{q}, \Omega)$. This is a typical feature of the strong coupling limit of $\lambda \sim O(1)$; remember that the value of $\lambda = 0.8$ used in our calculations was not an arbitrary choice, but was determined by the ($\pi, \pi$) resonance condition. As expected, however, a fine difference exists between $\chi_S$ and $\chi_f$ such that, in general, $\chi_S(\mathbf{q}, \Omega)$, in comparison to $\chi_t(\mathbf{q}, \Omega)$, has slightly more of a feature of the local spin dynamics at higher frequencies and slightly less of a feature of the itinerant fermion spin dynamics at low frequencies and vice versa. For example, we can see a slightly weaker downward dispersion branch in $\chi_S(\mathbf{q}, \Omega)$ in the SS (figure 3(a)) than in $\chi_t(\mathbf{q}, \Omega)$ in the SS (figure 2(a)).

Also although we plotted the total spin susceptibility as $\chi_{total} = \chi_t + \chi_S$, there is ambiguity as to whether the contributions from the local spin fluctuations $\chi_S$ and the itinerant spin fluctuations $\chi_t$ to the INS measurement should be equal as we have tentatively assumed here, because the form factors of the local and itinerant spins, in principle, should be different. However, our ignorance of the relative strength of the $\chi_t$ and $\chi_S$ fluctuations does not affect our phenomenology because the physical coupling strength between two spin fluctuations is determined by the effective dimensionless coupling $\tilde{\lambda}(q) \equiv g^2 \cdot \chi_{0,t}(q, 0) \cdot \chi_{0,S}(q, 0)$ and the value of $\lambda_t(\mathbf{Q})$ is determined once and for all by the ($\pi, \pi$) resonance condition, and all the other physical quantities are calculated without further ambiguity. Keeping in mind this point, the comparison of our numerical calculations with the INS experiments should be qualitatively the same whether we use the results of $\chi_t$, $\chi_S$ or $\chi_{tot}$.

3.2. Origin of the resonance mode

The mechanism of forming the resonance mode in our model is illustrated in figure 4. When the inverse of the dressed susceptibilities of equations (3) and (4) crosses zero (which occurs simultaneously in both susceptibilities), the dressed susceptibilities develop a resonance mode: a bound state or an overdamped mode depending on the presence and strength of the imaginary part at the position of the pole. In figure 4, we plot separately $\text{Re}\chi_{-1,0}(\mathbf{Q}, \Omega)$, $\text{Re}\chi_{0,t}(\mathbf{Q}, \Omega)$ and $\text{Im}\chi_{0,t}(\mathbf{Q}, \Omega)$ to make this point clear. Figure 4(a) is the case of an SS, where the pole of
Figure 4. (a) Plots of bare susceptibilities $\text{Re} \chi_{0,S}^{-1}(Q, \Omega)$, $g^2 \text{Re} \chi_{0,f}(Q, \Omega)$ and $g^2 \text{Im} \chi_{0,f}(Q, \Omega)$, respectively, in the SS. Parameters are $\Delta_{\text{SG}} = 1.1t$, $\Delta_0 = 0.2t$ and $\lambda = 0.8$. The vertical dashed line is a guide to the eyes indicating the position of the pole at $\Omega = 0.28t$. (b) The same as (a) in the NS (i.e. $\Delta_0 = 0$).

$\chi_{f,S}(q = Q, \Omega)$ occurs at $\Omega_{\text{res}} \sim 0.28t$. At this frequency the damping from $\text{Im} \chi_{0,f}$ is very weak below the p–h excitation gap, so that the pole becomes a sharp resonance peak. Figure 4(b) shows the case of the NS ($\Delta_0 = 0$) with the same parameters as in figure 2(c). The position of the pole occurs at a slightly higher frequency ($\Omega \sim 0.5t$) compared to the case of the SC phase (figure 4(a)). But this pole is strongly damped by $\text{Im} \chi_{0,f}$ (green line) that is linearly increasing with energy, and this linearly increasing damping shifts down the actual position of the peak to $\Omega_{\text{res}} \sim 0.35t$ (the maximum height position in figure 2(c)). We note that this overdamped resonance peak at NS is consistent with the data of [11] as shown in figure 2(c).

The resonance mode found in our model has physically different content than the resonance mode in the Fermi liquid-type theories [16–19]. The line of $\text{Re} \chi_{0,S}^{-1}(Q, \Omega)$ in figure 4 is not a simple inverse of a static potential (for example, $\frac{1}{U(q)}$ in a random phase approximation (RPA) calculation of the Hubbard model as in [17–19]), but carries its own dynamics and spectral density. Therefore, the resonance mode formed by the coupling of two dynamic susceptibilities $\chi_{0,f}$ and $\chi_{0,S}$ should carry the spectral densities from both the local spin wave and the fermion particle–hole continuum. In our coupled two-component spin–fermion model, the upward excitation branch and the resonance mode appear from a pole of equations (3) and (4) for a
given $\mathbf{q}$ but the downward excitation branch is made of particle–hole excitations of fermions in the d-wave SS and does not constitute a pole in equations (3) and (4). This is in contrast with the Fermi liquid-type theories [16–20] where both the downward branch and the resonance mode are constructed by the pole of an RPA-type spin susceptibility.

3.3. Constant energy scans

In the left column of figures 5(a)–(d), we show the constant energy scans of $\chi_t(\mathbf{q}, \Omega)$ in the SS for $\Omega = 0.2t$, $0.28t$, $0.6t$ and $0.8t$, respectively. Constant energy scans of neutron scattering data of YBCO [7] and LBCO [8] show peculiar patterns of IC peak positions in $(q_x, q_y)$ momentum space at different energy cuts. In particular, the $45^\circ$ rotation of the patterns from a low-energy scan (below the resonance energy $\Omega_{\text{res}}$) to a high-energy scan drew special attention and several theoretical explanations have been proposed [13–15, 17–19]. Results of figure 5 demonstrate that the two-component spin fermion model can consistently explain this phenomenon, too.

Figure 5(b) in the left column is the scan of $\chi_t(\mathbf{q}, \Omega)$ at the resonance energy, $\Omega_{\text{res}} = 0.28t$ with the same parameters as in figure 2(a). It shows a very intense peak at $(1/2, 1/2)$ indicating a very sharp resonance not only in energy but also in momentum space. Figures 5(c) and (d) are the scans at higher energies than the resonance energy and figure 5(a) is a scan of the lower-energy cut. We colored the highest intensity positions in black to emphasize the clear patterns. The lower-energy scan (figure 5(a)) shows the IC peaks at $(1/2 \pm \delta, 1/2)$ and $(1/2, 1/2 \pm \delta)$ forming a diamond-shaped pattern. The higher-energy scans (figures 5(c) and (d)) show that the IC peak positions at $(1/2 \pm \delta, 1/2 \pm \delta)$ and $(1/2 \pm \delta, 1/2 + \delta)$ form a square-shaped pattern which has the symmetry of $45^\circ$ rotated from the low-energy pattern. The results of figure 5 excellently reproduce the observed patterns of the constant-energy scan data of neutron experiments reported in YBCO [7] and LBCO [8]. This is rather surprising for LBCO since this compound is known to develop a static stripe ordering and our model has no ingredient for the stripes as mentioned before.

In our model we can trace the origins of the IC peak patterns. The low-energy IC peaks and diamond-shaped pattern are basically a reflection of the band structure and d-wave superconducting gap. The high-energy IC peaks and the square-shaped pattern have a more complicated origin. At and above the resonance energy the dressed spin susceptibility $\chi_t$ is the result of a strong interplay between the local spin correlation and the itinerant spin correlation. Therefore the high-energy scan pattern is the result of a subtle interplay/competition between $\chi_{0,5}(\mathbf{q}, \Omega)$ and $\chi_{0,t}(\mathbf{q}, \Omega)$. The presence of IC peaks at high energies itself is a manifestation of the high-energy spin wave dispersion spanning from the AFM wave vector $Q$; so the incommensurability increases with energy. However, whether the pattern will be a square or a diamond shape has no universal mechanism. We tested various combinations of parameters $t'$, $\mu$, $\Delta_{SG}$, $\Delta_0$ and $\lambda$. The low-energy diamond-shaped pattern is robust within our model. As to the patterns of higher energy scans, although the square shape is dominant, it is not absolutely robust; with different parameters the diamond pattern can appear, too. Therefore, we believe that the $45^\circ$ rotation of the IC peak patterns may not be a universal feature of HTC; it can change with doping and for different cuprate compounds. This non-universality is also seen in the scan of $\chi_S(\mathbf{q}, \Omega)$ at $\Omega_{\text{res}} = 0.6t$ in the central column of figure 5(c). However, as repeatedly emphasized, the patterns of the constant-energy scans for $\chi_S(\mathbf{q}, \Omega)$, $\chi_{0n}(\mathbf{q}, \Omega)$ and $\chi_t(\mathbf{q}, \Omega)$ are all basically the same in the strong coupling limit.
Figure 5. Constant-energy scans of $\text{Im} \chi_f(q, \Omega)$ (left column), $\text{Im} \chi_S(q, \Omega)$ (central column) and $\text{Im} \chi_{\text{tot}}(q, \Omega)$ (right column) at (a) $\Omega = 0.2t$, (b) $\Omega = 0.28t$, (c) $\Omega = 0.6t$ and (d) $\Omega = 0.8t$, respectively. In all cases, parameters are $\Delta_{SG} = 1.1t$, $\Delta_0 = 0.2t$ and $\lambda = 0.8$. 

New Journal of Physics 14 (2012) 043030 (http://www.njp.org/)
3.4. Parameters of our phenomenology

To make a comparison of our calculations with experiments, it is important to fix the energy scale of the model. The tight binding band of equation (6) is widely studied to fit the ARPES data and the estimate of $t$ varies from 150 to 400 meV depending on the doping and different cuprate compounds [28]. Our calculation results are in good agreement with neutron experiments in terms of energy scale if we choose $t \sim 150–180$ meV. This value of $t$ corresponds to the low end of the estimates from ARPES experiments. One possible reason for this is that the extraction of $t$ value from ARPES is carried out by fitting the whole Brillouin zone (BZ) of the quasiparticle (q.p.) dispersions. As a result, the high-energy dispersion sets the overall energy scale $t$. However, the low-energy spin susceptibility is determined by the low-energy particle–hole excitations near the Fermi level and irrelevant to the high-energy q.p. excitations. By this reasoning, it is quite possible that the effective $t$ particle–hole excitations near the Fermi level and irrelevant to the high-energy q.p. excitations.

The degree of incommensurability and the strength of the downward whisker-like dispersion in the fermion susceptibility $\chi_1$ (see figure 2(b)) are controlled by the FS curvature—which is tuned by $t'$ and the chemical potential $\mu$—and the SC gap size $\Delta_0$; this property is true even for Fermi liquid theories or one-component spin–fermion theories [16–19]. These parameters $t'$, $\mu$ and $\Delta_0$ should be independently determined by other experiments such as ARPES [28], tunneling [29], etc. Therefore, after fixing the overall energy scale of the model by $t$, the genuinely free fitting parameters of our phenomenological model are only two: the coupling strength $g$ (or equivalently $\lambda$) and the bare spin gap $\Delta_SG$. For all calculations in this paper we used $t' = -0.4t$, $\mu = -0.81t$, $\Delta_0 = 0.2t$, $\Delta_SG = 1.1t$ and $\lambda = 0.8$.

4. Angle-resolved photoemission spectroscopy and high-energy kink

As a consistency check of our phenomenological model, we calculate the renormalized band dispersion with the same parameter set that we used for neutron scattering in the previous section. In this calculation, the most important parameter is the coupling strength between fermions and spin fluctuations, for which there is neither a direct experimental measurement nor a reliable theoretical estimate from a microscopic Hamiltonian. In our phenomenology, this value $\lambda \equiv g^2 \cdot \chi_{1}(Q, 0) \cdot \chi_{2}(Q, 0) = 0.8$ was determined by the condition to produce ($\pi$, $\pi$) resonance mode in both the superconducting and the NS. So we can crosscheck the consistency of our phenomenology by comparing the outcomes of the q.p. renormalization from the spin–fermion interaction to the ARPES experiments.

The self-energy of the fermion q.p. is calculated in Born approximation with the fully dressed local spin fluctuations $\chi_S(q, \omega)$ as

$$\Sigma(k, \omega) = g^2 \sum_q \int \frac{d\omega'}{\pi} \frac{\text{Im} \chi_S(q, \omega')}{\omega - \omega' - \epsilon_{k+q} + i\Pi[n(\omega') + f(\epsilon_{k+q})]},$$

where $n(\omega)$ and $f(\omega)$ are the boson and fermion distribution functions, respectively. Note that this calculation of the fermion self-energy is the same one-loop approximation as the calculations of the spin susceptibility renormalization in equations (3) and (4), guaranteeing the consistency of our phenomenology. This is graphically demonstrated in figure 6. We then calculate the renormalized q.p. spectral density as $A(k, \omega) = \text{Im}G_R(k, \omega)$ with

$$G_R(k, \omega) = \frac{1}{\omega - \epsilon_k - \Sigma(k, \omega)}. $$
In figure 7, we show the contour plots showing the intensity of the q.p. spectral densities with and without the self-energy correction. Figures 7(a) and (b) show the dispersions along the nodal direction \((0, 0) \rightarrow (\pi, \pi)\) and figures 7(c) and (d) show the dispersions along the near antinodal direction \((0, 0.5\pi) \rightarrow (\pi, 0.5\pi)\). Two features are clearly seen as a result of the spin–fermion interaction: (i) the overall q.p. dispersion is renormalized by a factor of \(\sim O(2)\). This is consistent with the input \(\lambda = 0.8\) because the wave function renormalization factor is \(Z \approx (1 + \lambda)\); (ii) a very interesting point is that q.p.s with a certain energy below the Fermi level are so strongly renormalized that the bare dispersion is not continuously renormalized but is detached from the low-energy dispersion and forms a broad spectral puddle at further high-energy region (see figures 7(a) and (c)).

This second feature is commonly observed for both the nodal and the antinodal directions regardless of some differences in the fine details such as the breaking points of dispersion in energy and momentum space and the intensity of the broad spectral puddle at high energies. This behavior is remarkably similar to the so-called high-energy kinks (\(\sim 340\) meV) observed in the ARPES experiments with BSCCO and LBCO by Valla et al [27]. The breaking point of the dispersion occurs around \(\omega \sim 1.5\)–\(2\) in our model calculations. In fact, if we assume \(t \sim 150\)–\(180\) meV as discussed before, the kink energy we calculated corresponds to \(\sim 225\)–\(360\) meV, consistent with the experimental data. Our results even reproduce the overall differences in the dispersion and kink behavior between the nodal direction and the antinodal direction as observed in experiments [27].

We traced the origin of this jump or breaking of the q.p. dispersion and found that it is caused by the upper bound of the local spin wave excitations \(\chi_S(q, \Omega)\). The local spin wave excitations, defined in equations (2) and (3), disperse from the lowest energy \(\Delta_{SG}\) (renormalized one) at \(q = Q = (\pi, \pi)\) to the highest energy at the magnetic zone corners \(q = (2\pi, 2\pi)\) and its equivalent points. Even after being dressed by fermions as in equation (3) these damped spin wave excitations have a similar upper bound. With the parameters of our model, this high-energy upper bound of the local spin fluctuations is limited to around \(2t\). The physical meaning of it is that the local spin excitations exist only up to \(\sim 2t\) and the fermion q.p. cannot be scattered beyond this energy scale. Consequently, the real part of self-energy calculated with equation (7) develops a rapid variation at around \(2t\) in frequencies and the q.p. pole is not formed beyond.
Figure 7. Spectral densities of q.p. dispersions: (a, c) Renormalized band dispersions along (h, h) and (h, 0.5) cuts, respectively. (b, d) Bare band dispersions along (h, h) and (h, 0.5) cuts, respectively.

This energy scale in the dressed fermion Green’s function $G_R(\vec{k}, \omega) = \frac{1}{\omega - \epsilon_{\vec{k}} - \Sigma(\vec{k}, \omega)}$. Hence, we can understand the origin of the high-energy kink from the high-energy upper bound of the local spin excitations [30]. The consistency between our model calculations and experimental observation of the high energy kink strongly supports the existence and strength of local spin excitations which have a upper energy scale around 350 meV. In contrast, the itinerant spin fluctuations have a long tail of the particle–hole continuum excitations up to the band width ($\sim 8t$) which would be a couple of eV at least. Therefore, the one-component spin–fermion model with only the itinerant fermions would have difficulty in explaining the high-energy kink phenomena.

The reproduction of the high-energy kink feature in the renormalized q.p. dispersion also implies that not only the low-energy spin excitations near $(\pi, \pi)$ play an important role but also the high-energy spin excitations can play an important role. However, it does not necessarily mean that the coupling of the high-energy spin excitations to fermions has a strength comparable...
to the coupling of the low-energy spin excitations to fermions. In fact, the effective coupling between fermions and the local spins \( \lambda(q) \) becomes much weaker with \( q \) away from \( Q = (\pi, \pi) \). However, the phase space of the local spin excitations rapidly increases with increasing \( q \) from \( Q = (\pi, \pi) \), which compensates for the weakness of coupling.

Within our resolution, we did not find noticeable features in the low-energy q.p. dispersion, i.e. the low-energy kink, which might be related to the \( (\pi, \pi) \) resonance mode. Possibly it is because the spectral weight of the resonance mode in NS (see figure 3(c)) is not sufficiently dominant over the total spectral density of the spin fluctuations spread over the entire momentum space, and/or more possibly because the low-energy kink is in fact not an abrupt kink but rather a gentle variation of the dispersion slope as seen in the recent experiment [31].

5. Conclusion

In summary, we proposed a phenomenological two-component spin fermion model motivated by the neutron scattering experiments in HTC. With the two spin d.o.f. of the local spins and the itinerant spins, our calculations of the dynamic spin susceptibilities coherently reproduced the essential features of the neutron experiments in HTC: the hourglass dispersions, resonance mode, their changes in the normal and SS and the IC peak patterns of constant energy scans. Although our approach is phenomenological, considering that there are genuinely only two free fitting parameters, namely the coupling constant \( \lambda \) and the bare spin gap \( \Delta_{SG} \), the successful reproduction of several key features of neutron experiments with one set of parameters is quite encouraging. Then with the same model parameters, we calculated the renormalized fermion q.p. dispersion and reproduced both the nodal and the antinodal high-energy kinks with the correct energy scale in agreement with ARPES experiments [27]. It further strengthened the explanation for our phenomenology.

Finally, the main aim of this work on the two-component spin–fermion phenomenology was to demonstrate that there is compelling experimental evidence [32] for the presence and important role of local spin d.o.f. in addition to the fermionic q.p. in the cuprates. Interestingly, there is also accumulating experimental evidence for the coexistence of itinerant electrons and local moment of spins in the recently discovered iron-based superconducting compounds [33, 34]. The pressing question now is: what is the microscopic theory for the phenomenological two-component spin fermion model; in other words, how do the local spin d.o.f. survive doping from the parent insulating cuprate compounds, or more generally, how do the local moments and the itinerant fermions coexist in strongly correlated metallic systems such as cuprate and pnictide compounds.

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New Journal of Physics 14 (2012) 043030 (http://www.njp.org/)
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New Journal of Physics 14 (2012) 043030 (http://www.njp.org/)