



Collective spin and charge excitations in the t - J - U model of high- T_c cuprates

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ABSTRACT

The t - J - U model of high- T_c copper-oxide superconductors incorporates both the on-site Coulomb repulsion and kinetic exchange interaction and yields a semi-quantitative description of the static properties of those materials. We extend this analysis to dynamic quantities and address collective spin- and charge excitations in the correlated metallic state of the t - J - U model. We employ VWF+1/ \mathcal{N}_f approach that combines the variational wave function (VWF) approach with the expansion in the inverse number of fermionic flavors (1/ \mathcal{N}_f). It is shown that the resonant (paramagnon) contribution to the dynamic magnetic susceptibility remains robust as one interpolates between the Hubbard- and t - J -model limits, whereas the incoherent continuum undergoes substantial renormalization. Energy of the collective charge mode diminishes as the strong-coupling limit is approached. We also introduce the concept of effective kinetic exchange interaction that allows for a unified interpretation of magnetic dynamics in the Hubbard, t - J , and t - J - U models. The results are discussed in the context of recent resonant inelastic x-ray scattering experiments for the high- T_c cuprates.

1. Introduction

High-temperature (high- T_c) copper-oxide superconductors (SC) serve as paradigmatic strongly-correlated systems, evolving from the antiferromagnetic (AF) Mott insulating state, through high- T_c SC state, to normal metal phase as a function of chemical doping. The common theoretical frameworks, used to describe them, are based on (extended) Hubbard [1] and t - J [2] models, yet a unified quantitative description of static- and single-particle properties of high- T_c cuprates for a fixed set of microscopic parameters has not been achieved so far within those schemes. In effect, extended t - J - U Hamiltonian, encompassing both Hubbard and t - J models as special cases, has been proposed and demonstrated to yield a consistent description of principal experimental data for high- T_c cuprates within variational scheme [3–6]. However, the t - J - U -model studies have been hitherto restricted to static properties, whereas recent developments in spectroscopic techniques (in particular, resonant inelastic x-ray scattering (RIXS)) provide comprehensive evidence for the relevance of collective excitations across the phase diagram of high- T_c cuprates [7–28]. In this respect, the t - J - U model remains largely unexplored and is yet to be tested as a tool to study many-particle dynamics.

Here we analyze the structure of dynamical spin and charge susceptibilities in the paramagnetic metallic state of the two-dimensional t - J - U model and relate its predictions to those of the Hubbard and t - J

models that are used extensively [29–35] to study collective modes in correlated electron systems. We employ VWF+1/ \mathcal{N}_f scheme [30–32], combining Variational Wave Function (VWF) approach in its diagrammatic form with the field-theoretical 1/ \mathcal{N}_f expansion (\mathcal{N}_f denotes the number of fermionic flavors). The latter has been recently benchmarked [31] against determinant quantum Monte-Carlo for small systems. This allows us to incorporate both the effect of local correlations and long-range collective excitations, required to be able to analyze the strong-coupling (t - J -model) limit. We find that the resonant part of the magnetic response (paramagnon mode) remains comparable within Hubbard, t - J , and t - J - U models, provided that the parameters of those three Hamiltonians are appropriately mapped onto each other. On the other hand, the incoherent part of the spectrum is substantially affected by variation of the Hubbard U . We also find that the charge mode energy undergoes reduction as one moves from the Hubbard to the t - J -model regime, reflecting enhanced band renormalization effects near the t - J -model limit. This analysis supports the t - J - U model as a tool to study semi-quantitatively collective modes in high- T_c cuprates.

2. Model and method

We employ the t - J - U model on two-dimensional 200 × 200 square lattice, given by the Hamiltonian

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$$\widehat{\mathcal{H}} = \sum_{i \neq j, \sigma} t_{ij} \widehat{c}_{i\sigma}^\dagger \widehat{c}_{j\sigma} + U \sum_i \widehat{n}_{i\uparrow} \widehat{n}_{i\downarrow} + J \sum_{\langle i,j \rangle} \widehat{\mathbf{S}}_i \cdot \widehat{\mathbf{S}}_j, \quad (1)$$

where $\widehat{c}_{i\sigma}$ ($\widehat{c}_{i\sigma}^\dagger$) denote electron annihilation (creation) operators on site i with spin index $\sigma = \pm 1$, $\widehat{n}_{i\sigma} \equiv \widehat{c}_{i\sigma}^\dagger \widehat{c}_{i\sigma}$, and $\widehat{\mathbf{S}}_i \equiv (\widehat{S}_i^x, \widehat{S}_i^y, \widehat{S}_i^z)$ are spin operators. We retain only nearest- and next-nearest hopping integrals, $t \equiv -0.35$ eV and $t' \equiv 0.25|t|$, respectively. The on-site Coulomb repulsion, U , and exchange coupling, J , are treated as free parameters. To interpret the results on the U - J plane, we introduce *effective kinetic exchange interaction*, $J_{\text{eff}} \equiv J + \frac{4t^2}{U}$, combining J with the second-order kinetic exchange that results from the canonical perturbation expansion [36] for the Hubbard model. Unless stated otherwise, we restrict the parameter space by setting $J_{\text{eff}} \equiv 0.2$ eV so that the exchange coupling is determined by $U \geq 7|t|$ as $J = J_{\text{eff}} - \frac{4t^2}{U}$. In the Hubbard model limit ($J = 0$, $U = 7|t|$), this choice yields a semi-quantitative agreement with measured paramagnon spectra for the lanthanum cuprates [30]. Moreover, the selection of sizable J_{eff} favors AF correlations and thus places the system away from ferromagnetism [37–40] (cf. the phase stability analysis below). Hereafter we set the hole concentration to $\delta = 0.16$ and temperature $k_B T = 0.4|t|$ to ensure stability of the paramagnetic state against fluctuations.

The model is solved using VWF+1/ \mathcal{N}_f approach in the local-diagrammatic (LD) variant, LD_f+1/ \mathcal{N}_f [31]. First, the energy functional $E_{\text{var}} \equiv \langle \Psi_{\text{var}} | \widehat{\mathcal{H}} | \Psi_{\text{var}} \rangle$ is constructed based on the t - J - U Hamiltonian (1) and the trial state, $|\Psi_{\text{var}}\rangle \equiv C \prod_i \widehat{P}_i |\Psi_0\rangle$, where $|\Psi_0\rangle$ represents Slater determinant to be determined self-consistently,

$$\widehat{P}_i \equiv \lambda_0 |0\rangle_{ii}\langle 0| + \sum_{\sigma\sigma'} \lambda_{\sigma\sigma'} |\sigma\rangle_{ii}\langle \sigma'| + \lambda_d |\uparrow\downarrow\rangle_{ii}\langle \uparrow\downarrow| \quad (2)$$

introduces local correlations into $|\Psi_{\text{var}}\rangle$, and C is the normalization factor. The correlators, \widehat{P}_i , are expressed in terms of the local many-particle basis on site i , encompassing empty ($|0\rangle_i$), singly-occupied ($|\uparrow\rangle_i$, $|\downarrow\rangle_i$), and doubly occupied ($|\uparrow\downarrow\rangle_i$) configurations. The six coefficients, $\lambda_0, \lambda_{\sigma\sigma'} (\sigma, \sigma' = \uparrow, \downarrow)$, and λ_d , serve as variational parameters. By application Wick's theorem, energy is then expressed as $E_{\text{var}} = E_{\text{var}}(\mathbf{P}, \boldsymbol{\lambda})$, where \mathbf{P} is a vector composed of two-point correlation functions (lines) in the form $P_{i\sigma, j\sigma'} = \langle \Psi_0 | \widehat{c}_{i\sigma}^\dagger \widehat{c}_{j\sigma'} | \Psi_0 \rangle$, and $\boldsymbol{\lambda}$ denotes correlator parameters. We evaluate E_{var} within specialized diagrammatic scheme [41,2] and retain only local diagrams, which results in the so-called local

diagrammatic (LD) approximation [31]. The latter incorporates multiple-loop diagrams and goes beyond the renormalized mean-field theory already at the zeroth-order (saddle-point) level. Both \mathbf{P} and $\boldsymbol{\lambda}$ are then treated as (imaginary-time) dynamical fields, and their quantum and classical fluctuations around this correlated state are studied at the leading order in $1/\mathcal{N}_f$ expansion (note that the fields are subjected to additional constraints, cf. Ref. [31]). This allows us to calculate imaginary-time dynamical spin and charge susceptibilities (χ_s and χ_c , respectively), which are analytically continued to real frequencies as $i\omega_n \rightarrow \omega + i0.02|t|$.

3. Results

In Fig. 1, the calculated imaginary parts of spin (top) and charge (bottom) dynamical susceptibilities for the t - J - U model (1) with fixed $J_{\text{eff}} \equiv 0.2$ eV, are displayed. The left panels, (a) and (f), correspond to the Hubbard model ($U = 7|t|$ and $J = 0$), whereas (e) and (j) represent the t - J -model limit ($U = \infty, J = \frac{4}{7}|t|$). The middle panels show the results for intermediate values of the Hubbard U (parameters are detailed inside the figure). As is apparent from Fig. 1(a)–(e), the magnetic spectrum separates into intense and dispersive paramagnon contribution (ranging up to ~ 0.3 eV) and the incoherent part. The latter may be interpreted as particle-hole continuum, which has been verified explicitly in the Hubbard-model limit by comparison with correlated Lindhard susceptibility [32]. Remarkably, well-defined paramagnon persists along the anti-nodal (Γ - X) line and the magnetic Brillouin zone boundary (X - $M/2$) in the metallic state ($\delta = 0.16$), but it is absent in the nodal (Γ - M) direction. This shows that robust magnetic excitations may arise in strongly correlated systems and resist overdamping, even without long-range magnetic order. In the Hubbard-model limit, those highly anisotropic paramagnon characteristics have been recently shown to semi-quantitatively reproduce experimental inelastic neutron scattering and RIXS data for selected high- T_c superconductors [30,32]. As the main finding of the present study, we demonstrate *weak dependence of the peak paramagnon energy on U* for a fixed value of J_{eff} [cf. Fig. 1(a)–(e)]. This supports the proposed here interpretation of J_{eff} as the scale controlling paramagnons in the metallic state of the t - J - U model close to AF instability and should allow us to reconcile the Hubbard-model results for dynamic quantities with the t - J - U - (V) model analysis [3–6] of equilibrium properties. The particle-hole excitations exhibit qualitatively different behavior and are shifted to lower energies as the on-site

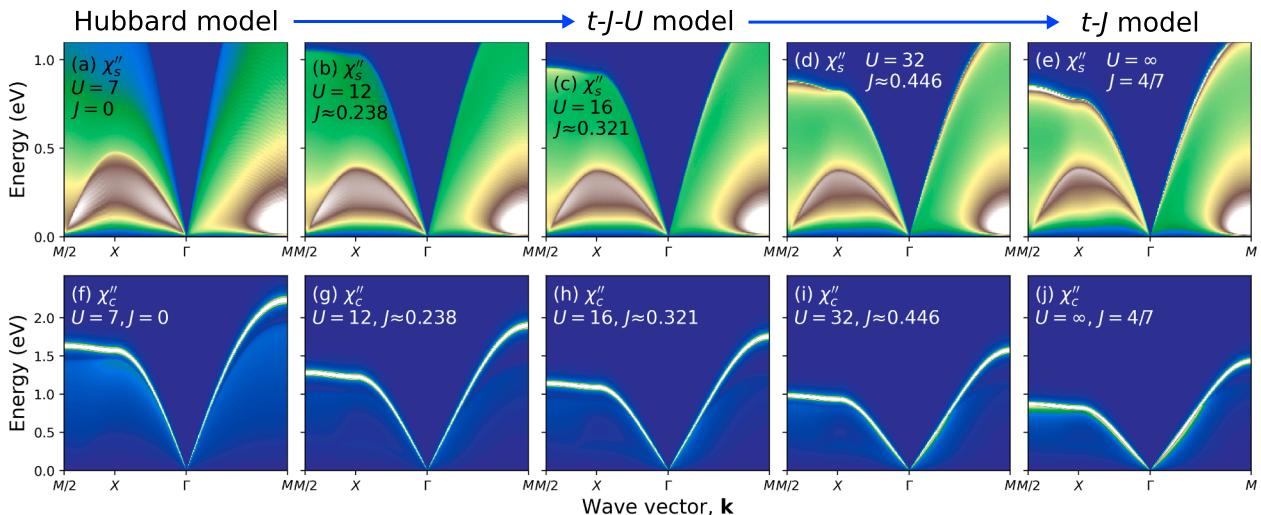


Fig. 1. Calculated imaginary parts of spin (top panels) and charge (bottom panels) dynamical susceptibilities for the t - J - U model along the $M/2$ - X - Γ - M contour. The common value of effective exchange interaction $J_{\text{eff}} = J + \frac{4t^2}{U} \equiv 0.2$ eV is adopted for all panels, whereas the on-site repulsion U varies from 7 on the left [(a) and (f)] to ∞ on the right [(e) and (j)]. The parameters are detailed inside the panels in units of $|t|$. Blue and white colors map to low- and high intensity, respectively. Note the model evolution marked on the top.

Coulomb interaction increases, which can be attributed to correlation-induced narrowing of single-particle bandwidth. The coherent- and incoherent magnetic excitations are thus, to large extent, decoupled and governed by distinct energy scales (J_{eff} and renormalized bandwidth, respectively).

Charge excitations may be decomposed in an analogous manner into coherent- and incoherent components, with a well-defined mode emerging above the continuum. From Fig. 1(f)–(j) it follows that the charge mode energy undergoes reduction as the system evolves from the Hubbard- to the t - J -model limits. Remarkably, the charge-mode energy approaches zero near the Γ point as a consequence of neglecting long-range three-dimensional Coulomb repulsion in the model (1), whose singular small- k behavior is known to open the Γ -point plasmon gap and induce dimensional crossovers in layered systems [42]. Both effects have been observed experimentally [24,26,28], so long-range interactions are necessary to reliably describe plasmons in the cuprates.

In Fig. 2 we display the energy dependence of the calculated imaginary parts of spin (left panels) and charge (right panels) dynamical susceptibilities for the Hubbard model ($U = 7$; red lines), t - J - U model ($U = 16$; blue lines), and the t - J model ($U = \infty$; green lines), all with $J_{\text{eff}} \equiv 0.2$ eV. The panels correspond to representative points in the Brillouin zone, detailed inside the plot (wave vectors are related to h and k as $\mathbf{k} = (\frac{2\pi}{a}h, \frac{2\pi}{a}k)$, with a being lattice constant). Several features of the spectra may be noted. First, a well-defined peak emerges from the continuum only along the anti-nodal (Γ - X) line, with maximum intensity corresponding to energy ~ 0.3 eV at the X point [panel (a)]. Its position weakly depends on U . For the nodal (Γ - M) direction, the spin response does not contain a clear paramagnon feature [(e) and (g)]. Second, the particle-hole continuum shifts towards lower energies for increasing U , with an intensity peak systematically building up at its boundary. Remarkably, this second peak appears only for U substantially exceeding the bare quasiparticle bandwidth [cf. red ($U = 16|t|$) and green ($U = \infty$) lines in Fig. 2]. The lack of a double-peak signature in RIXS experiments supports thus the t - J - U over the t - J model as an appropriate starting point for variational studies of collective dynamics in the cuprates.

For completeness, in Fig. 3 the stability of paramagnetic state against spin (a) and charge (b) fluctuations is verified for the parameter range encompassing that used in the analysis of collective excitations (cf. Figs. 1 and 2). The static susceptibilities are displayed along the high-symmetry $M/2$ - X - Γ - M contour (all curves correspond to $J_{\text{eff}} = 0.2$ eV and varying values of U and J , detailed inside the panels). Both magnetic and charge responses remain finite in the entire parameter range, implying local stability of the paramagnetic state against fluctuations. The spin susceptibility attains a maximum at the M point, reflecting the dominant role of AF correlations. The charge susceptibility is peaked at the Γ point, which is characteristic of the model with short-range interactions. The singular tail of the Coulomb repulsion tends to suppress the charge response around the Γ -point [43,32].

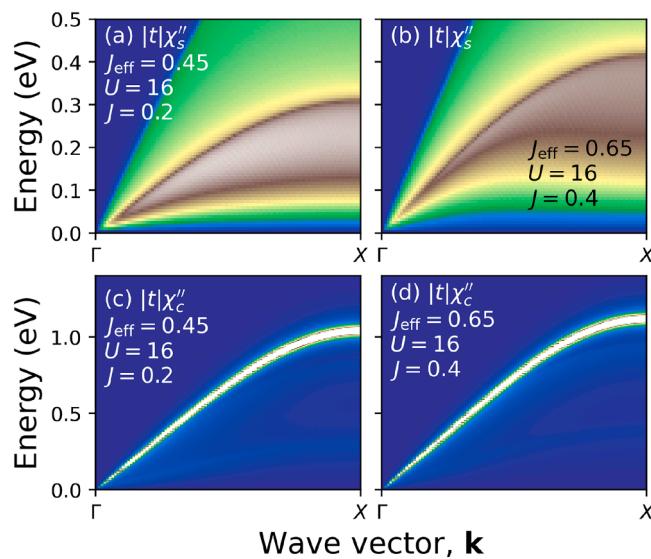


Fig. 4. Imaginary parts of spin (top panels) and charge (bottom panels) dynamical susceptibilities for the t - J - U model along the $M/2$ - X - Γ - M contour for $U = 16|t|$, and two selections of $J = 0.2|t|$ [(a), (c)] and $J = 0.4|t|$ [(b), (d)], resulting in $J_{\text{eff}} = 0.45|t|$ and $J_{\text{eff}} = 0.65|t|$, respectively. Model parameters inside the plot are given in units of $|t|$.

effective exchange interaction, $J_{\text{eff}} \equiv J + \frac{4t^2}{U}$, has been identified as the energy scale controlling the anti-nodal paramagnon energies close to AF ordering, which rationalizes experimentally reported similarity of Γ - X magnetic excitations in metallic and AF insulating state. It also means that the paramagnon dynamics is governed predominantly by short-range spin-flip correlations (either introduced through J or those originating from second-order exchange $\alpha t^2/U$), the same that provide pairing potential within the local-pairing scenario of high- T_c SC. Whereas generic occurrence of those magnetic excitations in the cuprates has revived the discussion about their role in high- T_c SC [20,44], our analysis supports the view that SC and persistent paramagnons may share a common microscopic origin, but need not to strictly couple to each other. The latter statement is consistent with the observation of high-energy paramagnons also in the overdoped regime, where SC is already suppressed [7,21].

We have also noted that the incoherent magnetic excitations are governed predominantly by renormalized single-quasiparticle bandwidth and thus remain sensitive to the magnitude of the on-site Coulomb repulsion. For U much larger than the bare bandwidth, a sharp feature builds up at the threshold of a particle-hole continuum, which is not unambiguously observed in experiments. This circumstance favors the t - J - U model with intermediate U over the t - J model as a starting point for the discussion of the paramagnons in hole-doped high- T_c cuprates. Similar conclusions follow from former studies of equilibrium and single-particle properties [3–6]. We have also demonstrated a substantial reduction of charge-mode energy with increasing U , which provides the flexibility required to interpret experimental data in real materials. In particular, the above characteristics of collective excitations in the t - J - U model may allow us to reconcile the observed persistent anti-nodal paramagnons with particularly low-energy acoustic plasmons [28] in lanthanum cuprates. Finally, the role of J_{eff} is expected to be diminished in the regime of extremely large U and small J , where ferromagnetic correlations may dominate [37–40]. Those aspects should be the subject of a separate study.

A separate future question concerns the influence of the collective excitations on the pairing induced by the correlations.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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