CHARGE SUSCEPTIBILITY IN STRONGLY CORRELATED ELECTRON SYSTEMS

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We investigate the charge susceptibility in strongly correlated electron systems by using a Bethe-Salpeter equation in a generalized cumulant expansion for the p-d model, at varying values of the doping and temperature. We find that for small values of the correlation U_d , the charge susceptibility decreases near the half-filling as hole-doping approaches zero, this behavior suggesting the precursor of the Mott-Hubbard gap formation. Particular attention is paid to the role played by the Van Hove singularity near the Fermi level in the density of states, in connection with the unusual normal state properties of the hole-doped cuprates.

Key words: p-d model, cumulant expansion, high- T_c superconductors.

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I. INTRODUCTION

Since the discovery of high temperature superconducting cuprates (HTSC), one of the central issues in the study of strongly correlated electron systems has been whether the two-dimensional systems behave as Fermi liquid or not [1]. Compared with the conventional superconductors, the HTSC seem to behave rather normally in the superconducting phase except for having high values of T_c but quite anomalously in the normal phase. Therefore, one may think that the key for clarifying origins of the high- T_c superconductivity must be in clarifying origins of the anomalous phenomena in the normal phase. On the other hand, studies done so far seem to suggest that those anomalous phenomena may be related intimately to the strong electronic correlations. Roughly speaking, one may classify effects of the electronic correlations into two different types, those due to spin density fluctuations and others due to charge density fluctuations. Up till now, the effects of spin density fluctuations have been studied extensively, while small attention has been devoted to those of charge density fluctuations. However, we believe that the mechanism of the high- T_c cannot be determined without clarifying the role of the charge fluctuations. Therefore, in the present work we intend to figure out thoroughly the properties of the charge fluctuations in the CuO_2-2D electronic systems by studying the charge susceptibility in the p-dmodel. In particular, we are interested in the dependence on the hole-doping x of the charge susceptibility. It is well known that when x approaches zero, the system exhibits a metal-insulator transition (MIT) becoming incompressible near the transition. So, it is generally expected that the charge susceptibility decreases and eventually vanishes when the MIT is approached. In fact, such a behavior has been obtained in some numerical studies on the basis of the quantum Monte Carlo (QMC) method [2] and in a perturbation study in the weak-coupling regime [3] of the two-dimensional Hubbard model. A completely different result, however, has

been reported in other QMC simulations [4]: The charge susceptibility diverges like $\sim 1/x$ as x approaches zero. The investigation of these controversial results provides a primary motivation for the present work. By using a generalized "cumulant" expansion around the atomic limit, we investigate the tendency of the change response near the MIT due to the correlation effects.

In order to evaluate the charge susceptibility properly in the vicinity of the half-filling, we utilize a Bethe-Salpeter equation for the vertex function taking into account the correlation effects through the inclusion of the cumulants of the first and second order. The calculations are performed in the framework of the well-known finite temperature Green function formalism.

II. MODEL HAMILTONIAN AND METHOD

Taking into account the characteristic feature of the 2D CuO₂ plane, we adopt the simplest p-d model, in which tight-binding holes are composed of $\text{Cu}-d_{x^2-y^2}$ orbitals which form a square lattice and $O-p_{\sigma}$ orbitals which connect the nearest-neighbor Cu sites (see Fig. 1).

The non-interacting part of the Hamiltonian consists of site energy terms of d- and p-orbitals and the Coulomb repulsion U_d on each d-orbital. As for the interaction, we consider the transfer term between nearestneighbor d- and p-orbitals. Thus we obtain the following Hamiltonian,

$$H = H_0 + H_1, (1)$$

where

$$H_{0} = (\varepsilon_{p} - \mu) \sum_{\mathbf{k},\sigma} p_{\mathbf{k}\sigma}^{\dagger} p_{\mathbf{k}\sigma} + (\varepsilon_{d} - \mu) \sum_{\mathbf{k},\sigma} d_{\mathbf{k}\sigma}^{\dagger} d_{\mathbf{k}\sigma} \qquad (2)$$
$$+ U_{d} \sum_{i} d_{i\uparrow}^{\dagger} d_{i\uparrow} d_{i\downarrow}^{\dagger} d_{i\downarrow},$$

$$H_1 = \sum_{\mathbf{k},\sigma} V_{\mathbf{k}} \left(d^{\dagger}_{\mathbf{k}\sigma} p_{\mathbf{k}\sigma} + h.c. \right), \tag{3}$$

where $d_{\mathbf{k}\sigma}^{\dagger}(d_{\mathbf{k}\sigma})$ and $p_{\mathbf{k}\sigma}^{\dagger}(p_{\mathbf{k}\sigma})$ are the creation (annihilation) operator for d- and p- holes of momentum \mathbf{k} and spin σ , respectively; $d_i = \frac{1}{N} \sum_{\mathbf{k}} d_{\mathbf{k}} e^{i\mathbf{k}\mathbf{R}_i}$. The site energy of d- and p-holes are given by $(\varepsilon_d - \mu)$ and $(\varepsilon_p - \mu)$, μ is the chemical potential. Finally, U_d represents the onsite Coulomb repulsion between Cu holes. The bonding orbital $p_{\mathbf{k}\sigma}$, hybridizing with the $d_{\mathbf{k}\sigma}$, orbital is given by the following combination of $p_{x\mathbf{k}\sigma}$ and $p_{y\mathbf{k}\sigma}$ orbitals:

$$p_{\mathbf{k}\sigma} = \left(-i\frac{\gamma_{k_x}}{\gamma_{\mathbf{k}}}p_{x\mathbf{k}\sigma} + i\frac{\gamma_{k_y}}{\gamma_{\mathbf{k}}}p_{y\mathbf{k}\sigma}\right),\tag{4}$$

where $\gamma_{k_{\alpha}} = \sin(k_{\alpha}/2)$, $(\alpha = x, y)$. The *p*-*d* mixing potential is given by

$$V_{\mathbf{k}}^{2} = 2V^{2}(2 - \cos k_{x} - \cos k_{y}) = -2V\gamma(\mathbf{k}), \qquad (5)$$

where V is the p-d hybridization. In the following calculation, we put V = 1.

By considering the atomic part of the Hamiltonian (1) as the unperturbed Hamiltonian and H_1 as the perturbation part, we determine the finite temperature Green functions for p and d operators through the standard S-matrix perturbative formula

$$G_{\alpha\beta}(i-j,\tau_1-\tau_2) = -\frac{\left\langle T_{\tau} \ c_{i\sigma}^{\alpha}(\tau_1)c_{i\sigma}^{\beta\dagger}(\tau_2)S(\beta)\right\rangle_0}{\langle S(\beta)\rangle_0}, \quad (6)$$

where the subscript (α, β) represents either p- or d-hole indices. The unperturbed atomic single-particle Green functions $G_{pp}^{(0)}$ and $G_{dd}^{(0)}$ are given by:

$$G_{pp}^{(0)}(i\omega_{\nu}) = \frac{1}{i\omega_{\nu} - (\varepsilon_p - \mu)}$$
(7)

and

$$G_{dd}^{(0)}(i\omega_{\nu}) = \frac{\langle 1 - n_{\bar{\sigma}}^d \rangle_0}{i\omega_{\nu} - (\varepsilon_d - \mu)} + \frac{\langle n_{\bar{\sigma}}^d \rangle_0}{i\omega_{\nu} - (\varepsilon_d + U - \mu)}, \quad (8)$$

where ω_{ν} are the fermion Matsubara frequencies at the temperature T and $\langle n \frac{d}{\sigma} \rangle_0$ is the average number of particles in the *d*-atomic orbital. In calculating the full Green functions (6), since H_0 does not mix different holes, the thermal averages appearing in the expansion can be expressed as products of p- and *d*-averages, separately. While the *p*-averages may be evaluated by using the conventional Wick decoupling procedure, the presence of the Coulomb interaction term (U_d) in H_0 prevents the application of it to the *d*-averages. For this reason, one can apply a nonstandard diagrammatic expansion, analogous to that developed by Metzner [5] for the one-band Hubbard model. Within this approach, the simplest approximation consists in decoupling the *d*-averages of four or more fermionic operators in products of local pair averages, or equivalently, in taking into account only the oneparticle cumulants. Diagrammatically, one obtains the chain-like diagrams which can be summed up by means of a Dyson-like equation leading for $G_{pp}^{(1)}$, $G_{dd}^{(1)}$, $G_{pd}^{(1)}$ to the following expressions at the first-order in the cumulant expansion [6]:

$$G_{pp}^{(1)}(\mathbf{k}, i\omega_{\nu}) = \frac{G_{pp}^{(0)}(i\omega_{\nu})}{1 - V_{\mathbf{k}}^2 G_{pp}^{(0)}(i\omega_{\nu}) G_{dd}^{(0)}(i\omega_{\nu})}, \qquad (9)$$

$$G_{dd}^{(1)}(\mathbf{k}, i\omega_{\nu}) = \frac{G_{dd}^{(0)}(i\omega_{\nu})}{1 - V_{\mathbf{k}}^2 G_{pp}^{(0)}(i\omega_{\nu}) G_{dd}^{(0)}(i\omega_{\nu})}.$$
 (10)

The average number of particles in both p- and d- orbitals is determined together with the chemical potential in a self-consistent way.

Next, we define the charge susceptibility $\chi_c^{\alpha\beta}(\mathbf{q}, i\omega_v)$, as

$$\chi_{c}^{\alpha\beta}(\mathbf{q},i\omega_{v}) = \frac{1}{N} \int_{0}^{\beta} d\tau \ e^{i\omega_{v}\tau} \langle T_{\tau}[\ \Delta n_{\mathbf{q}}^{\alpha}(\tau)\Delta n_{-\mathbf{q}}^{\beta}(0)] \rangle,$$
(11)

where N is the number of cells and $\Delta n_{\mathbf{q}}$ is given by

$$\Delta n_{\mathbf{q}} = n_{\mathbf{q}}(\tau) - \langle n_{\mathbf{q}} \rangle, \qquad (12)$$

with $n_{\mathbf{q}} = \sum_{\mathbf{k},\sigma} c^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma} c_{\mathbf{k}\sigma}$. The equation (11) can be recast into

$$\chi_{c}^{\alpha\beta}(\mathbf{q},i\omega_{\upsilon}) = 2\left[\chi_{\uparrow\uparrow}^{\alpha\beta}(\mathbf{q},i\omega_{\upsilon}) + \chi_{\uparrow\downarrow}^{\alpha\beta}(\mathbf{q},i\omega_{\upsilon})\right],\qquad(13)$$

where $\chi^{\alpha\beta}_{\sigma\sigma'}(\mathbf{q}, i\omega_v)$ is the generalized susceptibility in the "particle-hole" channel defined as

$$\chi_{\sigma\sigma'}^{\alpha\beta}(\mathbf{q}, i\omega_{\upsilon}) = \frac{1}{N} \int_{0}^{\beta} d\tau \ e^{i\omega_{\upsilon}\tau} \langle T_{\tau} \sum_{\mathbf{k}} c_{\mathbf{k}+\mathbf{q}\sigma}^{\alpha\dagger}(\tau) c_{\mathbf{k}\sigma}^{\beta}(\tau) \\ \times \sum_{\mathbf{p}} c_{\mathbf{p}+\mathbf{q}\sigma'}^{\alpha\dagger}(0) c_{\mathbf{p}\sigma'}^{\beta}(0) \rangle^{conn}, \tag{14}$$

where the superscript "conn" denotes the operation to take into account only the connected diagrams. The total susceptibility will be obtained by summing up the four contributions $\chi^{pp}_{\sigma\sigma'}, \chi^{dd}_{\sigma\sigma'}, \chi^{dp}_{\sigma\sigma'}$, and $\chi^{pd}_{\sigma\sigma'}$. The generalized susceptibility contains two terms: the Hartree– Fock's, expressed in terms of the single–particle propagators and the "irreducible" part containing the vertex correction. Taking into account expressions (9) and (10)

for the one–particle Green functions, the following analytic expression corresponds to the Hartree–Fock terms

$$\chi_{\uparrow\uparrow}^{(1)\alpha\beta}(\mathbf{q},i\omega_{\nu}) = -\beta^{-1} \sum_{\Omega_{\nu}} e^{i\Omega_{\nu}\varepsilon} \int \frac{d^2k}{(2\pi)^2} G_{\uparrow\alpha\beta}^{(1)}(\mathbf{k}+\mathbf{q},i\omega_{\nu}+i\Omega_{\nu}) \times G_{\uparrow\alpha\beta}^{(1)}(\mathbf{k},i\Omega_{\nu}).$$
(15)

In calculating the irreducible part of $\chi^{\alpha\beta}_{\sigma\sigma'}$, we first introduce the *d*-vertex function

$$\Gamma_{\sigma\sigma'}(\mathbf{q}, i\omega_{\upsilon}) = \sum_{\mathbf{k}} \int_{0}^{\beta} d\tau \ e^{i\omega_{\upsilon}\tau} \langle T_{\tau} \left(d^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma}(\tau) d_{\mathbf{k}\sigma}(\tau) d^{\dagger}_{\mathbf{k}+\mathbf{q}\sigma}(0) d_{\mathbf{k}\sigma}(0) \right) \rangle^{conn}$$
(16)

that can be determined approximately from the Bethe–Salpeter equation

$$\Gamma_{\sigma\sigma'}(\mathbf{q}, i\omega_{\upsilon}) = \Gamma^{(0)}_{\sigma\sigma'}(i\omega_{\upsilon}) + \sum_{\sigma''} \Gamma^{(0)}_{\sigma\sigma''}(i\omega_{\upsilon}) \Pi^{pp}_{\sigma''}(\mathbf{q}, i\omega_{\upsilon}) \Gamma_{\sigma''\sigma'}(\mathbf{q}, i\omega_{\upsilon}),$$
(17)

where $\Gamma_{\sigma\sigma'}^{(0)}(i\omega_v)$ is the atomic irreducible vertex function of four *d* operators (i.e. a two-particle cumulant for the *d*-holes) Π

$$\Gamma^{(0)}_{\sigma\sigma'}(i\omega_{\upsilon}) = \int_{0}^{\beta} d\tau \ e^{i\omega_{\upsilon}\tau} \langle T_{\tau}(d^{\dagger}_{i\sigma}(\tau)d_{i\sigma}(\tau)d^{\dagger}_{i\sigma'}(0)d_{i\sigma'}(0))\rangle_{0}^{irr},$$
(18)

in which the average is performed with respect to the atomic Hamiltonian and $\Pi^{pp}_{\sigma}(\mathbf{q}, i\omega_{\nu})$ is the polarization insertion

$$\Pi^{pp}_{\sigma}(\mathbf{q}, i\omega_{\nu}) = -\beta^{-1} \sum_{\Omega_{\nu}} e^{i\Omega_{\nu}\varepsilon} \int \frac{d^2k}{(2\pi)^2} V^2(\mathbf{k} + \mathbf{q}) G^{(1)}_{\sigma pp}(\mathbf{k} + \mathbf{q}, i\omega_{\nu} + i\Omega_{\nu}) \\ \times V^2(\mathbf{k}) G^{(1)}_{\sigma pp}(\mathbf{k}, i\Omega_{\nu}).$$
(19)

In terms of Eq. (16) we obtain for $\chi^{(2)\alpha\beta}_{\sigma\sigma'}(\mathbf{q},i\omega_v)$ the following expression

$$\chi_{\sigma\sigma'}^{(2)dd}(\mathbf{q}, i\omega_{\nu}) = \Gamma_{\sigma\sigma'}(\mathbf{q}, i\omega_{\nu}) \left[1 + \tilde{\Pi}_{\sigma'}^{pd}(\mathbf{q}, i\omega_{\nu})\right]^2,$$
(20)

$$\chi_{\sigma\sigma'}^{(2)pp}(\mathbf{q}, i\omega_{\nu}) = \Gamma_{\sigma\sigma'}(\mathbf{q}, i\omega_{\nu})\tilde{\Pi}_{\sigma'}^{pp2}(\mathbf{q}, i\omega_{\nu}), \qquad (21)$$

$$\chi_{\sigma\sigma'}^{(2)pd}(\mathbf{q},i\omega_{\nu}) = \chi_{\sigma\sigma'}^{(2)dp}(\mathbf{q},i\omega_{\nu}) = \Gamma_{\sigma\sigma'}(\mathbf{q},i\omega_{\nu})\tilde{\Pi}_{\sigma'}^{pp}(\mathbf{q},i\omega_{\nu}) \left[1 + \tilde{\Pi}_{\sigma'}^{pd}(\mathbf{q},i\omega_{\nu})\right],\tag{22}$$

where

$$\tilde{\Pi}^{\alpha\beta}_{\sigma}(\mathbf{q}, i\omega_{\nu}) = -\beta^{-1} \sum_{\Omega_{\nu}} e^{i\Omega_{\nu}\varepsilon} \int \frac{d^2k}{(2\pi)^2} V(\mathbf{k} + \mathbf{q}) G^{(1)\alpha\beta}_{\sigma}(\mathbf{k} + \mathbf{q}, i\omega_{\nu} + i\Omega_{\nu}) \times V(\mathbf{k}) G^{(1)\alpha\beta}_{\sigma}(\mathbf{k}, i\Omega_{\nu}).$$
(23)

The superscript ⁽²⁾ indicates that we are taking into account the two-particle cumulants contained in the irreducible part. Combining Eq. (13) with the explicit expressions of $\chi^{\alpha\beta}_{\sigma\sigma'}(\mathbf{q},i\omega_v) = \chi^{(1)\alpha\beta}_{\sigma\sigma'}(\mathbf{q},i\omega_v) + \chi^{(2)\alpha\beta}_{\sigma\sigma'}(\mathbf{q},i\omega_v)$, from Eqs. (15) and (20)-(22), we obtain $\chi_c(\mathbf{q},i\omega_v)$ in the form

$$\chi_{c}(\mathbf{q},i\omega_{\upsilon}) = -2\beta^{-1}\sum_{\alpha\beta}\sum_{\Omega_{\nu}}e^{i\Omega_{\nu}\varepsilon}\int\frac{d^{2}k}{(2\pi)^{2}}G_{\uparrow}^{(1)\alpha\beta}(\mathbf{k}+\mathbf{q},i\omega_{\upsilon}+i\Omega_{\nu})\times G_{\uparrow}^{(1)\alpha\beta}(\mathbf{k},i\Omega_{\nu})$$
$$+2(\Gamma_{\uparrow\uparrow}+\Gamma_{\uparrow\downarrow})(\mathbf{q},i\omega_{\upsilon})\left[1+\tilde{\Pi}_{\uparrow}^{pd}(\mathbf{q},i\omega_{\nu})+\tilde{\Pi}_{\uparrow}^{pp}(\mathbf{q},i\omega_{\nu})\right]^{2}.$$
(24)

III. RESULTS

In this section we investigate, first, the dependence on x of the charge susceptibility in the static and uniform limit, $\chi_c(\mathbf{0}, 0)$. The results are shown in Fig. 1 for T = 100K, $\varepsilon_d/V = -1$ and $\varepsilon_p/V = 0$ and $U_d/V = 5$. As the system is doped away from half-filling (x = 0)the susceptibility increases and reaches its maximum at $x_c \simeq 0.26$, then decreases. The dependence of the charge susceptibility on x can be explained according to a Van-Hove scenario.



Fig. 1. $\chi_c(\mathbf{0}, 0)$ as a function of x, for T = 100 K, $U_d/V = 5$, $\varepsilon_d/V = -1$ and $\varepsilon_p/V = 0$.

Since at low temperature χ_c reflects the thermal average of the density of states at the Fermi level $N(E_F)$, the presence of the maximum in χ_c for the critical doping of x_c can be related to the fact that, upon doping with holes, the Fermi level approaches the Van Hove singularity (VHS) arising from the nearest-neighbor hybridization term, and for the choice of the parameters that we have considered lies on it at $x = x_c$ [6]. Interpretation of many experimental results for LSCO and YBCO [7]–[8] in terms of a sharp feature in the density of states, consistent with photoemission spectroscopy data on cuprates [9], have been advanced in numerous works [10,12]. To have a better understanding of the change of χ_c with doping, in Fig. 2 (a), (b) we report $\chi_c(T)$ versus temperature for different values of the doping x. As shown,

upon doping with holes $\chi_c(T)$ increases with doping till the critical value $x_c \simeq 0.26$ and then behaves reversely for x > 0.26.



Fig. 2. (a)–(b): $\chi_c(0,0)$ as a function of T for (a) $x < x_c$ and (b) $x > x_c$ with the other parameters as in Fig. 1.

For $x \neq x_c = 0.26$ the VHS is not on the Fermi-level and then its contribution to the charge-susceptibility decreases as the temperature is lowered. As for the temperature dependence of χ_c , we find the maximum at a certain temperature T_m that moves to lower temperatures at the increasing value of the doping for $x < x_c$, while opposite behaviour is observed for $x > x_c$. We would like to stress that the same kind of behaviour is evinced for the spin susceptibility [6], we only find that the amplitude of the charge fluctuations is one order of magnitude smaller as compared with the spin-one. This means that in the range of the parameters considered, the system is more instable with respect to the spin fluctuations. A probe of the electronic correlations effects and the metallic or insulating character of the system is obtained by considering different values of U_d/V . In Fig. 3 the charge susceptibility is plotted as a function of the doping for the same values of the parameters as in Fig. 1, but $U_d/V = 0$ and $U_d/V = 5$. For $U_d/V = 0$ the VHS falls at the Fermi level at half-filling, consequently, $\chi_c(\mathbf{0}, 0)$ as x approaches zero. In the interacting case $(U_d/V = 5) \chi_c(0,0)$ shows a maximum at a critical value of the doping $x = x_c \simeq 0.26$ still due to a VHS in the density of states, and turns to decrease near half-filling.



Fig. 3. $\chi_c(\mathbf{0}, 0)$ as a function of x for $U_d/V = 0$ and 5 and the other parameters as in Fig. 1.

A large suppression of χ_c near half-filling is due to the vertex corrections which are not included in the Random Phase Approximation (RPA) and properly describes the MIT approaching. This behaviour can be considered as a precursor of the formation of the Mott-Hubbard gap at x = 0. Our results are consistent with those of the QMC simulations by A.Moreo *et al.* [2] and the perturbation study of the 2DHM by T. Hotta and S. Fujimoto, but not with the assertion by N. Furukawa and M. Imada [4] that the charge susceptibility diverges in the vicinity of halffilling. According to Ref. [4] this divergence reflects the realization of some non-Fermi liquid state in the metallic phase near the MIT. In conclusion, our results seem to support the possibility of a smooth transition from the Fermi liquid state to the Mott-insulating phase as x approaches zero. The same conclusion was reached in the study of the infinite-dimensional Hubbard model [11].

IV. CONCLUSIONS

We have investigated the doping and the temperature dependence of the charge susceptibility in the p-d model, by using a Bethe–Salpeter equation in a generalized cumulant expansion. Our results for the charge susceptibility as a function of the doping show that: a) it has the maximum at the critical value of the doping x_c ; b) as a function of the temperature it increases with the doping for $x < x_c$, and behaves reversely for $x > x_c$ due to the Fermi level lying very close to VHS; c) in the interacting case the charge susceptibility is much suppressed due to the correlations effect in the vicinity of half-filling. This suppression indicates a precursor of the formation of the Mott–Hubbard gap.

In conclusion, in the framework of the p-d model a VHS scenario well reproduces some of the "unusual" properties observed in the normal state of the HTSC. Besides, smooth behaviour of the charge susceptibility near the MIT is obtained as half-filling is approached.

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