Magnetic susceptibility and the Landau Fermi-liquid parameter of the Hubbard model and the three-band CuO_2 model

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Magnetic susceptibilities of interacting (d) electrons in the Hubbard model and the three-band CuO_2 model are worked out within the Gaussian fluctuations of the functional integral in the slave boson representation. The normalized Landau Fermi-liquid parameter $|F_0^a|/\alpha$ ($\alpha \equiv W_0 N_F^0$, N_F^0 the density of states at the Fermi level, and W_0 the bare bandwidth) defined from the susceptibility expression is investigated for the two models as functions of Coulomb repulsion U, charge-transfer energy Δ, and doping concentration δ. It is shown that the Landau parameter for the three-band model is larger and exhibits different renormalization behaviors than that for the Hubbard model in both the weak- and strong-coupling regimes except in the Mott-Hubbard weak-coupling regime, where it takes the same random-phase approximation form U/W_0 as the latter. The reasons for these results are analyzed. The slave-boson Landau parameter for the Hubbard model exactly reproduces the T-matrix expression $|F_0^a|/\alpha = U/W_0/(1+U/W_0)$ in the low-density limit, whose renormalization has the different origin from that in the dilutely doped regime. [S0163-1829(96)01426-9]

I. INTRODUCTION

Considerable interest is drawn on the unique magnetic excitations observed in some cuprate superconductors with the view that such excitations may be related to the nature of the high-temperature superconductivity in these compounds. The particularly unique magnetic properties among others are the unusual temperature dependence and enhancement of the NMR relaxation rate $1/T_1$ at Cu sites,[1] the spin gap in the neutron inelastic-scattering intensity,[2] etc. These unusual phenomena are now well documented with firm experimental evidences, for which several theoretical interpretations have been proposed: phenomenological antiferromagnetic spin-fluctuation theories,[3] a weak-coupling random-phase approximation (RPA) treatment of the Hubbard model,[4] a Fermi-liquid formalism of quasiparticles with the phenomenological exchange-coupling constant for the three-band CuO_2 model,[5] and a quantum Monte Carlo simulation of the attractive-U Hubbard model.[6] These theories have indeed revealed some new aspects of the strong correlation models. For example, the first three showed that unusual temperature dependences of the Cu NMR relaxation rate $(T_1T)^{-1}$ and the neutron inelastic-scattering intensity can arise at low temperatures by taking into account simple RPA spin fluctuations using the phenomenological coupling constant. The last pointed out that the same attractive interaction that causes the high-temperature superconductivity pairing can lead to these unique magnetic properties.

However, these theories are all rather phenomenological in that they are not based on a microscopic derivation of the expression for the magnetic susceptibility which is used to calculate the magnetic properties in the Hubbard model or the three-band model. For example, the effective magnetic coupling which enters into the magnetic susceptibility expression is so strongly renormalized under a strong Coulomb repulsion that the susceptibility expression can be totally different from a simple RPA type formula. It is not clear that the attractive pairing interaction is so dominant that one can ignore other residual magnetic interactions in the renormalized quasiparticle states. It is naturally difficult to extract from these theories the microscopic understandings of the important physical processes taking place behind the anomalous magnetic excitations.

For a correct description of the magnetic properties, therefore, one first needs to obtain a microscopic expression for the magnetic susceptibility with the renormalized effective coupling constants. In this paper we will do this within the Kotliar-Ruckenstein (KR) slave-boson scheme.[7] The main advantages of employing the slave-boson approach under strong correlation, in comparison to other methods, lie in that it allows to incorporate coupling constant renormalization as well as band renormalization in a simplest possible way of the saddle-point approximation and further permits to take into account fluctuations beyond this $O(1/N)$ Gaussian level. One difficult point of this functional approach is that to incorporate fluctuations beyond the Gaussian level in a sensible manner is in fact not so simple because residual interactions generally become nonlocal strong-coupling interactions. However, the magnetic properties of the Hubbard model as well as the three-band model have not been studied in any detail along this line even within the Gaussian approximation.

In this paper we derive the expression for the renormalized magnetic susceptibility for the Hubbard model[7–10] and the three-band CuO_2 model[11] in two dimensions (2D) within the Gaussian level of the KR slave-boson approach.[7] From this result we define the magnetic coupling constants, i.e., the asymmetric Landau Fermi-Liquid parameter F_0^a. We investigate the renormalization behaviors of this Landau parameter as the system goes from the weak coupling to the strong coupling regime (i.e., from the itinerant metallic regime to the localized insulator regime) or from the low carrier-density limit to the dilute doping limit. We will show how closely the magnetic susceptibility of the three-band model is related to that of the Hubbard model and compare the Landau parameters of the two models. We will then examine the reason why the Landau parameter of the three-band model is larger than that of the Hubbard model. The Landau parameters both at the half-filling and in the low-density limit can be analytically expressed using the bare physical parameters of the Coulomb repulsion U, the bare bandwidth W_0, doping concentration δ, etc. In particular, it is shown that the present slave-boson scheme can exactly reproduce the T-matrix result for the effective interaction[12] in the low-density limit of $\delta \sim 1$. We will defer to a later publication our studies on the anomalous magnetic properties which are obtained from our magnetic susceptibility expression.

Earlier studies on the magnetic susceptibility and the Landau parameter F_0^a have been performed mostly for the Hubbard model by Lavagna,[8] Li *et al.*,[9] Li and P. Bénard[10] using the slave-boson scheme and by Vollhardt *et al.*[13] with the Gutzwiller method. Lavagna[8] showed[14] the renormalization behaviors of the Landau parameter and the formal equivalence between the magnetic saddle-point approach and the Gaussian-fluctuation RPA approximation in deriving the magnetic susceptibility for the Hubbard model. So far only very little work has been done on the three-band model except for the brief study of the coupling constants by Schmalian *et al.*[11]

II. MAGNETIC PART OF THE FREE ENERGY

Using the slave-boson formulations of Kotliar and Ruckenstein,[7] the Lagrangian for the two dimensional (2D) Hubbard model is written as

$$\mathcal{L}^{(\mathcal{H})}(\tau)=\sum_{i\sigma} f_{i\sigma}^{*}(\partial_\tau+\lambda_{i\sigma}^{(2)}-\mu)f_{i\sigma}-\sum_{\langle ij\rangle\sigma} t z_{i\sigma}^{*}z_{j\sigma}f_{i\sigma}^{*}f_{j\sigma}+\sum_i e_i^{*}(\partial_\tau+\lambda_i^{(1)})e_i+\sum_{i\sigma} s_{i\sigma}^{*}(\partial_\tau+\lambda_i^{(1)}-\lambda_{i\sigma}^{(2)})s_{i\sigma}$$
$$+\sum_i w_i^{*}\left(\partial_\tau+U+\lambda_i^{(1)}-\sum_\sigma \lambda_{i\sigma}^{(2)}\right)w_i-\sum_i \lambda_i^{(1)}, \quad (1)$$

and that for the 2D three-band model[15] is

$$\mathcal{L}^{(3\mathrm{B})}(\tau)=\sum_{i\sigma} f_{i\sigma}^{*}(\partial_\tau+\lambda_{i\sigma}^{(2)}-\mu)f_{i\sigma}+\sum_{j_\alpha\sigma} p_{j_\alpha\sigma}^{*}(\partial_\tau+\varepsilon_p-\mu)p_{j_\alpha\sigma}-\sum_{\langle ij_\alpha\rangle\sigma} t_{pd}(z_{i\sigma}^{*}f_{i\sigma}^{*}p_{j_\alpha\sigma}+\mathrm{H.c.})+\sum_{\langle j_x j_y'\rangle\sigma} t_{pp}(p_{j_x\sigma}^{*}p_{j_y'\sigma}+\mathrm{H.c.})$$
$$+\sum_i e_i^{*}(\partial_\tau+\lambda_i^{(1)})e_i+\sum_{i\sigma} s_{i\sigma}^{*}(\partial_\tau+\lambda_i^{(1)}-\lambda_{i\sigma}^{(2)})s_{i\sigma}+\sum_i w_i^{*}\left(\partial_\tau+U+\lambda_i^{(1)}-\sum_\sigma \lambda_{i\sigma}^{(2)}\right)w_i-\sum_i \lambda_i^{(1)}. \quad (2)$$

In the expressions (1) and (2) the interacting d-electron Grassman field $d_{i\sigma}$ has been projected onto the composite fields, $d_{i\sigma}\equiv z_{i\sigma}f_{i\sigma}$, of quasiparticle-fermion Grassman number $f_{i\sigma}$ and boson variables

$$z_{i\sigma}\equiv(1-w_i^{*}w_i-s_{i\sigma}^{*}s_{i\sigma})^{-1/2}(e_i^{*}s_{i\sigma}+s_{i-\sigma}^{*}w_i)$$
$$\times(1-e_i^{*}e_i-s_{i-\sigma}^{*}s_{i-\sigma})^{-1/2},$$

where e_i, $s_{i\uparrow}$, $s_{i\downarrow}$, and w_i are the slave-boson variables representing the empty, single-occupied with up or down spin, and doubly-occupied interacting electron sites, respectively.[15] μ is the chemical potential and energy is measured from the bare d-electron level ($\varepsilon_d^0=0$). In the three-band model (2), i sites are the Cu sites of interacting d electrons and j_α sites ($\alpha=x,y$) the oxygen sites of noninteracting p electrons, and the external field h is applied only at Cu sites to calculate the magnetic susceptibilities of Cu d electron. Using the radial gauge, we split out the complex boson variables into the saddle-point values $(e_0,s_{0\sigma},w_0,\lambda_0^{(1)},\lambda_{0\sigma}^{(2)})$ and the fluctuating real variables such as $e_i\rightarrow(e_0+\delta e_i)\times\exp[i\theta_i^e]$, $s_{i\sigma}\rightarrow(s_{0\sigma}+\delta s_{i\sigma})\exp[i\theta_i^{s\sigma}]$, $w_i\rightarrow(w_0+\delta w_i)\times\exp[i\theta_i^w]$, $\lambda_i^{(1)}\rightarrow\lambda_0^{(1)}+\delta\lambda_i^{(1)}$, and $\lambda_{i\sigma}^{(2)}\rightarrow\lambda_{0\sigma}^{(2)}+\delta\lambda_{i\sigma}^{(2)}$. (Accordingly, $z_{i\sigma}\rightarrow z_0+\delta z_{i\sigma}$ and $q_{ij\sigma}\equiv z_{i\sigma}^{*}z_{j\sigma}\rightarrow q_0+\delta q_{ij\sigma}$.) Here we denote again the fluctuating variables $\delta s_{i\sigma}$, $\delta\lambda_{i\sigma}^{(2)}$, $\delta z_{i\sigma}$, etc., by $s_{i\sigma}$, $\lambda_{i\sigma}^{(2)}$, $z_{i\sigma}$, etc., unless they are confusing. The initially time-independent constraint Bose fields $\lambda_i^{(1)}$ and $\lambda_{i\sigma}^{(2)}$ become time-dependent incorporating the derivatives of other local gauge fields $\theta_i^e(\tau)$, etc.[16,8,15] Furthermore, we define the new spin-dependent fluctuating boson variables by $s_{i\pm}\equiv(s_{i\uparrow}\pm s_{i\downarrow})/\sqrt{2}$ and $\lambda_{i\pm}^{(2)}\equiv(\lambda_{i\uparrow}^{(2)}\pm\lambda_{i\downarrow}^{(2)})/\sqrt{2}$, resulting in the following replacements in Eqs. (1) and (2): $\Sigma_{i\sigma}s_{i\sigma}^{*}(\partial_\tau+\lambda_i^{(1)}-\lambda_{i\sigma}^{(2)})s_{i\sigma}\rightarrow\Sigma_{i\pm}s_{i\pm}^{*}[\partial_\tau+\lambda_i^{(1)}-(1/\sqrt{2})\lambda_{i+}^{(2)}]s_{i\pm}-(1/\sqrt{2})\lambda_{i-}^{(2)}(s_{i+}^{*}s_{i-}+s_{i-}^{*}s_{i+})$ and $\Sigma_i w_i^{*}(\partial_\tau+U+\lambda_i^{(1)}-\Sigma_\sigma\lambda_{i\sigma}^{(2)})w_i\rightarrow\Sigma_i w_i^{*}(\partial_\tau+U+\lambda_i^{(1)}-\sqrt{2}\lambda_{i+}^{(2)})w_i$, and the $s_{i\sigma}$ in the terms with $z_{i\sigma}$ by $s_{i\pm}$, etc. As we shall see later, the new boson variables allow the boson-propagator matrix to be block diagonal of the charge-charge correlation sector and the spin-spin correlation sector, being maintained in the expansion up to second order fluctuations in boson-fermion interaction [the same order as $O(1/N)$ in the $1/N$ expansion]. Notice here that boson-fermion interactions arise in the hopping term of the interacting fermion and in the terms with the constraint fields in the projected Lagrangians (1) and (2).

Let us perform a functional-integral expansion for the Lagrangian $\mathcal{L}(\tau)$ in the partition function

$$Z=\int [Df][Dp][D\phi_\alpha]\exp\left[-\int_0^\beta \mathcal{L}(\tau)d\tau\right], \quad (3)$$

where $\{\phi_\alpha\}$ is a set of the real Bose fields defined above $\{\phi_\alpha\}\equiv\{e,s_+,w,\lambda^{(1)},\lambda_+^{(2)};s_-,\lambda_-^{(2)}\}$. Here we illustrate this expansion for the single-band Hubbard model and make a brief remark on the expansion for the three-band model. We first represent the fermion part $\mathcal{L}_F^{(\mathcal{H})}(\tau)$ of the Lagrangian $\mathcal{L}^{(\mathcal{H})}(\tau)$ [the first two terms in Eq. (1)] using the above splittings of the boson variables. Integrating out the fermion variables from $\mathcal{L}_F^{(\mathcal{H})}(\tau)$ and then Fourier transforming we obtain

$$\mathcal{L}_F^{*(\mathcal{H})}(\tau)=-\sum_{ij}\ \mathrm{Tr}\ \ln[\{(\partial_\tau+\lambda_{0\sigma}^{(2)}-\mu)\delta_{ij}-q_{0\sigma}t\,\delta_{\langle ij\rangle}\}-\{z_{0\sigma}t(\delta z_{i\sigma}+\delta z_{j\sigma})+t\,\delta z_{i\sigma}\delta z_{j\sigma}\}\delta_{\langle ij\rangle}+\delta\lambda_{i\sigma}^{(2)}\delta_{ij}]$$

$$=-\sum_{\mathbf{kq}\sigma}\ \mathrm{Tr}\ \ln\left[(\mu_\tau+q_{0\sigma}\varepsilon_{\mathbf{k}}+\lambda_{0\sigma}^{(2)}-\mu)\delta_{\mathbf{q}}+z_{0\sigma}(\varepsilon_{\mathbf{k+q}}+\varepsilon_{\mathbf{k}})\delta z_{\mathbf{q}\sigma}+\sum_{\mathbf{p}}\ \varepsilon_{\mathbf{k+p+q}}\delta z_{-\mathbf{p}\sigma}\delta z_{\mathbf{p+q}\sigma}+\delta\lambda_{\mathbf{q}\sigma}^{(2)}\right],\qquad(4)$$

using the unrenormalized saddle-point fermion band $\varepsilon_{\mathbf{k}}\equiv-2t\gamma_{\mathbf{k}}^{(H)}$ with $\gamma_{\mathbf{k}}^{(H)}\equiv\cos k_xa+\cos k_ya$. In Eq. (4) we separate out the Tr ln form of the inverse saddle-point fermion propagator, $\mathcal{G}^{(0)}(\mathbf{k},\tau)^{-1}\equiv-(\partial_\tau+\xi_{\mathbf{k}\sigma}^{(H)}-\mu)$, and expand the rest in fluctuating boson variables $\delta z_{\mathbf{q}\sigma}$, etc., where $\xi_{\mathbf{k}\sigma}^{(H)}$ is the renormalized band $\xi_{\mathbf{k}\sigma}^{(H)}\equiv q_{0\sigma}\varepsilon_{\mathbf{k}}+\lambda_{0\sigma}^{(2)}$ with $q_{0\sigma}\equiv z_{0\sigma}^2$. In the latter boson terms we keep the self-energy corrections of single fermion line and two fermion lines to boson propagators. Consequently $\mathcal{L}_F^{*(\mathcal{H})}(\tau)$ is written as

$$\mathcal{L}_F^{*(\mathcal{H})}(\tau)=-\sum_{\mathbf{k}\sigma}\ \mathrm{Tr}\ \ln[-\mathcal{G}^{(0)}(\mathbf{k},\tau)^{-1}]+\sum_q\ \mathrm{Tr}\left\{\sum_{\mathbf{k}\sigma}\ (\delta A_{\mathbf{kq}\sigma}^{(H)}+\delta B_{\mathbf{kq}\sigma}^{(H)})\mathcal{G}^{(0)}(\mathbf{k},\tau)\right.$$

$$\left.+\frac{1}{2}\sum_{\mathbf{k}\sigma}\ (\delta A_{\mathbf{kq}\sigma}^{(H)}+\delta\lambda_{\mathbf{q}\sigma}^{(2)})\mathcal{G}^{(0)}(\mathbf{k},\tau)(\delta A_{\mathbf{k+qq}\sigma}^{(H)}+\delta\lambda_{\mathbf{q}\sigma}^{(2)})\mathcal{G}^{(0)}(\mathbf{k+q},\tau)\right\},\qquad(5)$$

where we have used the definitions $\delta A_{\mathbf{kq}\sigma}^{(H)}\equiv z_{0\sigma}(\varepsilon_{\mathbf{k+q}}+\varepsilon_{\mathbf{k}})\delta z_{\mathbf{q}\sigma}$ and $\delta B_{\mathbf{kq}\sigma}^{(H)}\equiv\Sigma_{\mathbf{p}}\varepsilon_{\mathbf{k+p+q}}\delta z_{-\mathbf{p}\sigma}\delta z_{\mathbf{p+q}\sigma}$. Fluctuations $\delta z_{\mathbf{q}\sigma}$, etc., in $\delta A_{\mathbf{kq}\sigma}^{(H)}$, etc., are further expanded into the terms with boson variables $\{\phi_\alpha\}$ in bilinear form.

A similar functional-integral expansion is made for the three-band model using the fermion part $\mathcal{L}_F^{(3\mathrm{B})}(\tau)$ (the first four terms) of the Lagrangian (2). The standard method to deal with mixing bands in a functional integral is to first form hybridized fields out of $f_{i\sigma}$ and $p_{j_\alpha\sigma}$ fermion variables using the saddle-point separation of the Lagrangian $\mathcal{L}_F^{(3\mathrm{B})}(\tau)$, and then integrate out these hybridized fields. One obtains a Lagrangian $\mathcal{L}_F^{*(3\mathrm{B})}(\tau)$ similar to the expression (5) but with the sum over the three hybridized bands $\xi_{n\mathbf{k}\sigma}^{(3\mathrm{B})}$ ($n=1,2,3$) in this case. In the case with $t_{pp}=0$, the fermion bands are simply given by $\xi_{n\mathbf{k}\sigma}^{(3\mathrm{B})}(n=3,1)=(1/2)\{\varepsilon_p+\lambda_{0\sigma}^{(2)}\pm[(\varepsilon_p-\lambda_{0\sigma}^{(2)})^2+4q_\sigma\tau_{\mathbf{k}}^2]^{1/2}\}$ and $\xi_{2\mathbf{k}\sigma}^{(3\mathrm{B})}=\varepsilon_p$, where $\tau_{\mathbf{k}}\equiv-2t_{pd}\gamma_{\mathbf{k}}^{(3\mathrm{B})}$, $(\gamma_{\mathbf{k}}^{(3\mathrm{B})})^2\equiv(\gamma_{k_x}^{(3\mathrm{B})})^2+(\gamma_{k_y}^{(3\mathrm{B})})^2$ and $\gamma_{k_\alpha}^{(3\mathrm{B})}=\sin(k_\alpha/2)$, $(\alpha=x,y)$.

As to the boson part (the last four terms) of the Lagrangians in Eqs. (1) and (2), one obtains only the saddle-point boson free energy $\mathcal{F}_B^{(0)}$ and the noninteracting boson-propagator $[\mathcal{D}(q)^{(0)^{-1}}]$ terms. Collecting these fermion and boson terms together and taking the trace, one obtains the partition function $\mathcal{Z}$ (common for the two models):

$$\mathcal{Z}=\mathcal{Z}^{(0)}\delta\mathcal{Z}_B,\qquad(6)$$

where

$$\mathcal{Z}^{(0)}=\exp[-\beta(\mathcal{F}_F^{(0)}+\mathcal{F}_B^{(0)})],\qquad(7)$$

$$\delta Z_B=\int\ [D\boldsymbol{\phi}(-\mathbf{q})][D\boldsymbol{\phi}(\mathbf{q})]\exp[-\delta\mathcal{S}_B],\qquad(8)$$

$$\mathcal{F}_F^{(0)}=-\frac{1}{\beta}\sum_{n\mathbf{k}\sigma}\sum_{\omega_n}\ \ln[-i\omega_n+\xi_{n\mathbf{k}\sigma}-\mu],\qquad(9)$$

$$\mathcal{F}_B^{(0)}=Uw_0^2+\lambda_0^{(1)}\left(e_0^2+\sum_\sigma\ s_{0\sigma}^2+w_0^2\right)-\sum_\sigma\ \lambda_{0\sigma}^{(2)}(s_{0\sigma}^2+w_0^2),\qquad(10)$$

$$\delta\mathcal{S}_B=\sum_q\ \boldsymbol{\phi}(-\mathbf{q})\mathcal{D}(q)^{-1}\boldsymbol{\phi}(\mathbf{q})$$

$$=\sum_q\sum_{\alpha\beta}\ \sigma_\alpha(-\mathbf{q})[\mathcal{D}(q)^{-1}]_{\alpha\beta}\phi_\beta(\mathbf{q}),\qquad(11)$$

and the action $\mathcal{S}=\int_0^\beta\mathcal{L}(\tau)d\tau=\mathcal{S}_F^{(0)}+\mathcal{S}_B$ is written as the sum of the saddle-point fermionic part $\mathcal{S}_F^{(0)}\equiv\beta\mathcal{F}_F^{(0)}$ and the bosonic part $\mathcal{S}_B$, the latter being further divided, $\mathcal{S}_B=\mathcal{S}_B^{(0)}+\delta\mathcal{S}_B$, into the c-number free energy $\mathcal{S}_B^{(0)}\equiv\beta\mathcal{F}_B^{(0)}$ and the fluctuating bosonic-field part $\delta\mathcal{S}_B$. Here q, etc., denote the four-vector components $[q\equiv(\mathbf{q},i\omega_n)]$ and $\boldsymbol{\phi}(\mathbf{q})\equiv\{\phi_\alpha(\mathbf{q})_s;\phi_\alpha(\mathbf{q})_a\}\equiv\{e_{\mathbf{q}},s_{\mathbf{q}+},w_{\mathbf{q}},\lambda_{\mathbf{q}}^{(1)},\ \lambda_{\mathbf{q}+}^{(2)};s_{\mathbf{q}-},\ \lambda_{\mathbf{q}-}^{(2)}\}$. The inverse boson propagators for the Hubbard model are written as the sum

$$\mathcal{D}_{\alpha\beta}(q)^{-1}=\mathcal{D}_{\alpha\beta}^{(0)^{-1}}+\Sigma_{\alpha\beta}(\mathbf{q})+\Pi_{\alpha\beta}(q),\qquad(12)$$

of the noninteracting term $\mathcal{D}_{\alpha\beta}^{(0)^{-1}}$, the single-fermion-line (first order) self-energy term given by

$$\Sigma_{\alpha\beta}(\mathbf{q})=\sum_{k\sigma} \mathcal{G}^{(0)}(k)\partial^2(A^{(H)}_{\mathbf{kq}\sigma}+B^{(H)}_{\mathbf{kq}\sigma})/\partial\phi_\alpha(-\mathbf{q})\partial\phi_\beta(\mathbf{q}), \tag{13}$$

and the two-fermion-line (second order) correlation-bubble term defined by

$$\Pi_{\alpha\beta}(q)=\frac{1}{2}\sum_{k\sigma} \{\partial(A^{(H)}_{\mathbf{k-q}\sigma}+\lambda^{(2)}_{-q\sigma})/\partial\phi_\alpha(-\mathbf{q})\}\{\partial(A^{(H)}_{\mathbf{k+qq}\sigma} +\lambda^{(2)}_{\mathbf{q}\sigma})/\partial\phi_\beta(\mathbf{q})\}\mathcal{G}^{(0)}(k)\mathcal{G}^{(0)}(k+q). \tag{14}$$

[This expansion is equivalent to the order $O(1/N)$ in the $1/N$ expansion.] It is easy to see that the resulting boson-propagator matrix $\mathcal{D}(q)^{-1}$ under the present expansion scheme is maintained to be block diagonal of the 5×5 charge-sector matrix $\mathcal{D}(q)_s^{-1}$ and the 2×2 spin-sector matrix $\mathcal{D}(q)_a^{-1}$:

$$\mathcal{D}(q)^{-1}=\begin{pmatrix}\mathcal{D}(q)_s^{-1} & 0\\ 0 & \mathcal{D}(q)_a^{-1}\end{pmatrix}. \tag{15}$$

Let us now write down explicitly the elements of the spin-sector boson matrix $\mathcal{D}(q)_a^{-1}=\mathcal{D}_a^{(0)^{-1}}+\Sigma(\mathbf{q})_a+\Pi(q)_a$ for the vector $\{\phi_\alpha(\mathbf{q})_\alpha\}=\{s_{\mathbf{q}-},\lambda^{(2)}_{\mathbf{q}-}\}$ since the charge-sector boson propagator $\mathcal{D}(q)_s^{-1}$ makes no contribution to the magnetic susceptibility. The noninteracting matrix $\mathcal{D}_a^{(0)^{-1}}$ is the same for the two models:

$$\mathcal{D}_a^{(0)^{-1}}=\begin{pmatrix}\lambda_0^{(1)}-\lambda_0^{(2)} & -s_0\\ -s_0 & 0\end{pmatrix}. \tag{16}$$

The one-fermion-loop self-energy matrix $\Sigma(q)_a$

$$\Sigma(\mathbf{q})_a=\begin{pmatrix}\Sigma_{s_-s_-}(\mathbf{q}) & 0\\ 0 & 0\end{pmatrix}, \tag{17}$$

has only $\Sigma_{s_-s_-}(\mathbf{q})$ element, which is given for the two models by

$$\Sigma^{(H)}_{s_-s_-}(\mathbf{q})=\left(\frac{\partial z_\uparrow}{\partial s_-}\right)^2\omega^{(H)}_{\mathbf{q}}+z_0\left(\frac{\partial^2 z_\uparrow}{\partial s_-^2}\right)\omega_0^{(H)}, \tag{18}$$

$$\Sigma^{(3B)}_{s_-s_-}=z_0\left(\frac{\partial^2 z_\uparrow}{\partial s_-^2}\right)\omega_0^{(3B)}, \tag{19}$$

where

$$\frac{\partial z_\uparrow}{\partial s_-}=\frac{1}{\sqrt{2}}\left(\frac{\partial z_\uparrow}{\partial s_\uparrow}-\frac{\partial z_\uparrow}{\partial s_\downarrow}\right),$$

$$\frac{\partial^2 z_\uparrow}{\partial s_-^2}=\frac{1}{2}\left(\frac{\partial^2 z_\uparrow}{\partial s_\uparrow^2}-2\frac{\partial^2 z_\uparrow}{\partial s_\uparrow\partial s_\downarrow}+\frac{\partial^2 z_\uparrow}{\partial s_\downarrow^2}\right), \tag{20}$$

$\omega^{(H)}_{\mathbf{q}}\equiv\Sigma^{\mathbf{k}_F}_{\mathbf{k}\sigma}\varepsilon_{\mathbf{k+q}}$ and $\omega_0^{(3B)}\equiv\Sigma^{\mathbf{k}_F}_{\mathbf{k}\sigma}\{-\tau^2_{\mathbf{k}}/[(\varepsilon_p-\lambda_0^{(2)})^2+4q_0\tau^2_{\mathbf{k}}]^{1/2}\}$. There exists an explicit $\mathbf{q}$ dependence in the one-fermion-loop self-energy $\Sigma^{(H)}_{s_-s_-}(\mathbf{q})$ for the Hubbard model, however, no such $\mathbf{q}$ dependence arises in the $\Sigma^{(3B)}_{s_-s_-}$ for the three-band model due to its nature of the on-site hybridization term. The latter $\mathbf{q}$-dependent dispersion of the s-slave-boson energy is brought by inclusion of the correlation-bubble $\Pi^{(3B)}_{s_-s_-}(q)$, which enables a Cu-to-Cu intersite hopping through oxygen sites. We will see later that due to this term the d-electron magnetic susceptibility of the three-band model becomes very similar to that of the Hubbard model. The correlation-bubble self-energy matrix $\Pi(q)_a$

$$\Pi(q)_a=\begin{pmatrix}\Pi_{s_-s_-}(q) & \Pi_{s_-\lambda_-^{(2)}}(q)\\ \Pi_{\lambda_-^{(2)}s_-}(q) & \Pi_{\lambda_-^{(2)}\lambda_-^{(2)}}(q)\end{pmatrix}, \tag{21}$$

has the elements $\Pi_{\alpha\beta}(q)$ given by

$$\Pi_{s_-s_-}(q)=-8z_0^2\left(\frac{\partial z_\uparrow}{\partial s_-}\right)^2\chi_2(q), \tag{22}$$

$$\Pi_{s_-\lambda_-^{(2)}}(q)=2\sqrt{2}z_0\left(\frac{\partial z_\uparrow}{\partial s_-}\right)\chi_1(q), \tag{23}$$

$$\Pi_{\lambda_-^{(2)}\lambda_-^{(2)}}(q)=-\frac{1}{2}\chi_0(q). \tag{24}$$

Here $\chi_n(q)$ $(n=0,1,2)$ are given for the Hubbard model by

$$\chi_0^{(H)}(q)=-\frac{1}{\beta}\sum_k \mathcal{G}^{(0)}(k+q)\mathcal{G}^{(0)}(k), \tag{25}$$

$$\chi_1^{(H)}(q)=-\frac{1}{\beta}\sum_k (-\varepsilon_{\mathbf{k}})\mathcal{G}^{(0)}(k+q)\mathcal{G}^{(0)}(k), \tag{26}$$

$$\chi_2^{(H)}(q)=-\frac{1}{\beta}\sum_k \left(\frac{\varepsilon_{\mathbf{k}}+\varepsilon_{\mathbf{k+q}}}{2}\right)^2\mathcal{G}^{(0)}(k+q)\mathcal{G}^{(0)}(k), \tag{27}$$

using $\mathcal{G}^{(0)}(k)\equiv1/(i\omega_n-\xi^{(H)}_{\mathbf{k}\sigma}+\mu)$, where $k\equiv(\mathbf{k},i\omega_n)$. For the three-band model they are written as

$$\chi_0^{(3B)}(q)=-\frac{1}{\beta}\sum_k \mathcal{G}^{(0)}_{ff}(k+q)\mathcal{G}^{(0)}_{ff}(k), \tag{28}$$

$$\chi_1^{(3B)}(q)=-\frac{1}{\beta}\sum_k \frac{1}{z_0}\tau_{\mathbf{k}}\mathcal{G}^{(0)}_{ff}(k+q)\mathcal{G}^{(0)}_{pf}(k), \tag{29}$$

$$\chi_2^{(3B)}(q)=-\frac{1}{\beta}\sum_k \frac{1}{2z_0^2}\{\tau^2_{\mathbf{k}}\mathcal{G}^{(0)}_{ff}(k+q)\mathcal{G}^{(0)}_{pp}(k)+\tau_{\mathbf{k}}\tau_{\mathbf{k+q}}\mathcal{G}^{(0)}_{fp} \times(k+q)\mathcal{G}^{(0)}_{fp}(k)\}. \tag{30}$$

Here we have used the propagators of f fermion and p electron, $\mathcal{G}^{(0)}_{\alpha\beta}(k)\equiv\Sigma^3_{n=1}u_{n\alpha}(\mathbf{k})u_{n\beta}(\mathbf{k})/(i\omega_n-\xi^{(3B)}_{n\mathbf{k}\sigma}+\mu)$ $(\alpha,\beta=f,p)$, which are also given more explicitly in Ref. 17, and for the $t_{pp}=0$ model, $u_{nf}(\mathbf{k})=\{\partial\xi^{(3B)}_{n\mathbf{k}\sigma}/\partial\varepsilon_{d\sigma}\}^{1/2}$ and $u_{np}(\mathbf{k})=\{\partial\xi^{(3B)}_{n\mathbf{k}\sigma}/\partial\varepsilon_p\}^{1/2}$.

Now that the boson propagator $\mathcal{D}(q)^{-1}$ is set up, we can integrate out the remaining boson variables $\boldsymbol{\phi}(\mathbf{q})\equiv\{\phi_\alpha(\mathbf{q})_s;\phi_\alpha(\mathbf{q})_a\}$ from the bosonic action $\delta\mathcal{S}_B$, Eq. (11). We obtain the partition function $\mathcal{Z}$ represented in terms of the total free energy, $\mathcal{F}\equiv\mathcal{F}_F^{(0)}+\mathcal{F}_B^{(0)}+\delta\mathcal{F}_B$:

$$\mathcal{Z}=\exp[-\beta(\mathcal{F}_F^{(0)}+\mathcal{F}_B^{(0)}+\delta\mathcal{F}_B)], \tag{31}$$

$$\delta\mathcal{F}_B=\frac{1}{\beta}\sum_q \ln[\det(\mathcal{D}(q)^{-1})]. \quad (32)$$

These treatments naturally lead to the same expressions for the magnetic susceptibilities.

III. DERIVATIONS OF MAGNETIC SUSCEPTIBILITY

In this section we derive the frequency and momentum dependent magnetic susceptibility, $\chi(\mathbf{q},\omega)$, of interacting d electron in several different approaches, which, as we shall see later, help us understand the complicated contributions to the susceptibility expressions in the slave-boson treatments. In subsections A and B, the magnetic susceptibilities for the two models $[\chi^{(H)}(\mathbf{q},\omega),\chi^{(3B)}(\mathbf{q},\omega)]$ are obtained by applying the RPA approximation to boson propagators which is equivalent to the $O(1/N)$ Gaussian fluctuation treatment for fermions in the $1/N$ expansion. In subsection C, the static uniform susceptibility $\chi^{(3B)}(0,0)$ for the three-band model is calculated in the spin-dependent saddle-point treatment.

A. Standard derivation of $\chi^{zz}(q)$ with magnetic field applied to fermion fields

We calculate the generalized magnetic susceptibility at Cu sites by applying spatially and time-varying magnetic field $h_{\mathbf{q}}e^{-i\omega_n\tau}$ with frequency ω_n only to interacting d electrons. This adds the effects of time-varying magnetic field interaction with fermions, $H_h=\Sigma_{\mathbf{qk}}h_{\mathbf{q}}(f^\dagger_{\mathbf{k+q}\uparrow}f_{\mathbf{k}\uparrow}-f^\dagger_{\mathbf{k+q}\downarrow}f_{\mathbf{k}\downarrow})e^{-i\omega_n\tau}$, to the free energy terms $\mathcal{F}_F^{(0)}$ and $\delta\mathcal{F}_B$ which contain fermion lines. We expand the total free energy $\mathcal{F}$ in terms of magnetic field $h_{\mathbf{q}}$ to second order $O(h_{\mathbf{q}}^2)$. Then taking the second derivatives with respect to $h_{\mathbf{q}}$, one obtains the frequency-dependent longitudinal susceptibility $\chi^{zz}(q)$ $[q\equiv(\mathbf{q},\omega)]$, of d electrons for the two models:

$$\chi^{zz}(q)=-\frac{1}{2}\frac{\partial^2}{\partial h_{\mathbf{q}}^2}\{\mathcal{F}_F^{(0)}(h_{\mathbf{q}})+\delta\mathcal{F}_B(h_{\mathbf{q}})\}=\chi_0^{zz}(q)+\frac{1}{\det\mathcal{D}(q)^{-1}}\left\{-\frac{1}{2}\frac{\partial^2[\det\mathcal{D}(q,h_{\mathbf{q}})^{-1}]}{\partial h_{\mathbf{q}}^2}\right\}$$
$$=\frac{\chi_0^{zz}(q)}{1-g_0(\mathbf{q})\chi_0(q)-g_1\chi_1(q)+\left(\frac{g_1}{2}\right)^2\{\chi_1(q)^2-\chi_0(q)\chi_2(q)\}}, \quad (33)$$

where we have used the relations

$$-\frac{1}{2}\frac{\partial^2[\det\mathcal{D}(q,h_{\mathbf{q}})^{-1}]}{(-s_0^2)\partial h_{\mathbf{q}}^2}=\chi_0^{zz}(q)\bigg[g_0(\mathbf{q})\chi_0(q)+g_1\chi_1(q)-\left(\frac{g_1}{2}\right)^2\{\chi_1(q)^2-\chi_0(q)\chi_2(q)\}\bigg], \quad (34)$$

$$\frac{\det\mathcal{D}(q)^{-1}}{(-s_0^2)}=1-g_0(\mathbf{q})\chi_0(q)-g_1\chi_1(q)+\left(\frac{g_1}{2}\right)^2\times\{\chi_1(q)^2-\chi_0(q)\chi_2(q)\}, \quad (35)$$

$$g_0(\mathbf{q})=-\frac{1}{2s_0^2}\{\lambda_0^{(1)}-\lambda_0^{(2)}+\Sigma_{s_-s_-}(\mathbf{q})\}, \quad (36)$$

$$g_1=2\sqrt{2}\left(\frac{z^0}{s_0}\right)\left(\frac{\partial z_\uparrow}{\partial s_-}\right), \quad (37)$$

and the saddle-point contribution $\chi_0^{zz}(q)$ in the numerator given by $\chi_0^{zz}(q)=\chi_{00}^{zz}(q)/q_0$ with the noninteracting susceptibility $\chi_{00}^{zz}(q)$ and the renormalization factor q_0. The multiplicative factors $g_0(\mathbf{q})$ and g_1 for the correlation functions $\chi_0(q)$ and $\chi_1(q)$ are the effective coupling constants for the magnetic interactions and are explicitly given with the saddle-point parameters by

$$g_0^{(H)}(\mathbf{q})=\frac{16x^2s_0^2}{1-\delta_d^2}\Bigg[|\omega_0^{(H)}|\left\{\frac{1+2\delta_d^2}{(1-\delta_d^2)^2}-\frac{1}{16s_0^4}-\frac{\delta_d^2}{2x^2s_0^2(1-\delta_d^2)}\right\}-\omega_{\mathbf{q}}^{(H)}\left\{\frac{\delta_d^2}{(1-\delta_d^2)^2}+\frac{x^2-4e_0w_0}{16x^2s_0^4}-\frac{\delta_d^2}{2x^2s_0^2(1-\delta_d^2)}\right\}\Bigg], \quad (38)$$

$$g_0^{(3B)}=\frac{16x^2s_0^2}{1-\delta_d^2}|\omega_0^{(3B)}|\left\{\frac{1+2\delta_d^2}{(1-\delta_d^2)^2}-\frac{1}{16s_0^4}-\frac{\delta_d^2}{2x^2s_0^2(1-\delta_d^2)}\right\}, \quad (39)$$

$$g_1^{(H)}=g_1^{(3B)}=\frac{8\delta_d}{1-\delta_d^2}\{1-z_0^2\}. \quad (40)$$

Here, δ_d is the d-electron doping $\delta_d>0$ (or the d-hole doping $\delta_d<0$) which, in the present hole-representation, is defined by $\delta_d=1-n^f$ $(n^f=n^d)$ for the Hubbard model and by $\delta_d=1-n^f=\delta+n^p$ for the three-band model using the total doping concentration $\delta=1-(n^f+n^p)$ measured from the half-filling, $n^f+n^p=1$. Therefore, $\delta_d=0$ in the undoped $(\delta=0)$ three-band model which corresponds no hybridization hopping indicates the one d-hole $(n^d=1)$ insulating state.

One can also derive the magnetic susceptibility expression $\chi^{zz}(q)$ by converting the fermion coupling with magnetic field, $H_h=\Sigma_{\mathbf{qk}}h_{\mathbf{q}}(f^\dagger_{\mathbf{k+q}\uparrow}f_{\mathbf{k}\uparrow}-f^\dagger_{\mathbf{k+q}\downarrow}f_{\mathbf{k}\downarrow})e^{-i\omega_n\tau}$, to the magnetic slave-boson coupling with magnetic field, $H_h^B=\Sigma_{\mathbf{q}}\sqrt{2}s_0h_{\mathbf{q}}s_{-\mathbf{q}-}e^{-i\omega_n\tau}$, where one uses the constraint with a partial saddle-point substitution, $m_i\equiv f^\dagger_{i\uparrow}f_{i\uparrow}-f^\dagger_{i\downarrow}f_{i\downarrow}$

$=s_{i\uparrow}^{\dagger}s_{i\uparrow}-s_{i\downarrow}^{\dagger}s_{i\downarrow}\rightarrow\sqrt{2}s_0 s_{i-}$. This approach has been employed by Wang *et al.* for the t-J model,[18] by Li *et al.* for the Hubbard model,[9,10] and by Schmalian *et al.* for the three-band model.[11] The slave-boson coupling with magnetic field introduces an additional term for the energy of the $[\mathcal{D}(q)^{-1}]_{s_-s_-}$ element as $[\mathcal{D}(q)^{-1}]_{s_-s_-}=\lambda_0^{(1)}-\lambda_0^{(2)}+\Sigma_{s_-s_-}(\mathbf{q})+\Pi_{s_-s_-}(q)-2s_0^2h_{\mathbf{q}}^2$. Now that the coupling of magnetic field has been switched onto magnetic slave bosons $s_{\mathbf{q}-}$, the magnetic-field dependence of the free energy $\mathcal{F}$ enters the boson propagator $\mathcal{D}(q,h_{\mathbf{q}})^{-1}$ only through $[\mathcal{D}(q,h_{\mathbf{q}})^{-1}]_{s_-s_-}$ in Eq. (32). Then we take the second derivatives of $\delta\mathcal{F}_B(h_{\mathbf{q}})$ with respect to $h_{\mathbf{q}}$:

$$\chi^{zz}(q)=-\frac{1}{2}\frac{\partial^2}{\partial h_{\mathbf{q}}^2}\,\delta\mathcal{F}_B(h_{\mathbf{q}})$$
$$=\frac{1}{\det\,\mathcal{D}(q)^{-1}}\left\{-\frac{1}{2}\frac{\partial^2[\det\,\mathcal{D}(q,h_{\mathbf{q}})^{-1}]}{\partial h_{\mathbf{q}}^2}\right\}$$
$$=4s_0^2\mathcal{D}(q)_{s_-s_-}=4s_0^2\frac{\Pi_{\lambda_-^{(2)}\lambda_-^{(2)}}(q)}{\det\,\mathcal{D}(q)^{-1}}, \tag{41}$$

which leads to the result obtained in Eq. (33) because $-4\Pi_{\lambda_-^{(2)}\lambda_-^{(2)}}(q)=2\chi_0(q)=\chi_0^{zz}(q)$.

B. Diagrammatic derivation of $\chi^{zz}(q)$

Suppose we represent the Hamiltonians of the two models as the sum of the saddle-point fermion term, the noninteracting boson term, and the fermion-boson interaction term. Then the interacting Hamiltonians are written as

$$H_{\rm int}^{(H)}=2z_0\frac{\partial z_\uparrow}{\partial s_\pm}\sum_{\mathbf{kq}\pm}\left(\frac{\varepsilon_{\mathbf{k}}+\varepsilon_{\mathbf{k+q}}}{2}\right)s_{\mathbf{q}\pm}(f_{\mathbf{k+q}\uparrow}^{\dagger}f_{\mathbf{k}\uparrow}\pm f_{\mathbf{k+q}\downarrow}^{\dagger}f_{\mathbf{k}\downarrow})$$
$$+\frac{1}{\sqrt{2}}\sum_{\mathbf{kq}\pm}\lambda_{\mathbf{q}\pm}^{(2)}(f_{\mathbf{k+q}\uparrow}^{\dagger}f_{\mathbf{k}\sigma\uparrow}\pm f_{\mathbf{k+q}\downarrow}^{\dagger}f_{\mathbf{k}\downarrow}), \tag{42}$$

$$H_{\rm int}^{(3B)}=2z_0\frac{\partial z_\uparrow}{\partial s_\pm}\sum_{\mathbf{kq}\pm}\left(\frac{\tau_{\mathbf{k}}+\tau_{\mathbf{k+q}}}{2z_0}\right)\left\{s_{\mathbf{q}\pm}\left(\frac{1}{2}\right)(f_{\mathbf{k+q}\uparrow}^{\dagger}p_{\mathbf{k}\uparrow}\right.$$
$$\left.\pm f_{\mathbf{k+q}\downarrow}^{\dagger}p_{\mathbf{k}\downarrow})+\text{H.c.}\right\}+\frac{1}{\sqrt{2}}\sum_{\mathbf{kq}\pm}\lambda_{\mathbf{q}\pm}^{(2)}(f_{\mathbf{k+q}\uparrow}^{\dagger}f_{\mathbf{k}\uparrow}$$
$$\pm f_{\mathbf{k+q}\downarrow}^{\dagger}f_{\mathbf{k}\downarrow}). \tag{43}$$

The saddle-point $(\mathbf{q},\tau)$-dependent longitudinal magnetic susceptibility of d electron is defined by

$$\chi_0^{zz}(\mathbf{q},\tau)=\langle T_\tau[m_{-\mathbf{q}}(\tau)m_{\mathbf{q}}(0)]\rangle_0$$
$$=\Sigma_{\mathbf{k}}\langle T_\tau\{[f_{\mathbf{k+q}\uparrow}^{\dagger}(\tau)f_{\mathbf{k}\uparrow}(\tau)-f_{\mathbf{k+q}\downarrow}^{\dagger}(\tau)f_{\mathbf{k}\downarrow}(\tau)]$$
$$\times[f_{\mathbf{k}\uparrow}^{\dagger}(0)f_{\mathbf{k+q}\uparrow}(0)-f_{\mathbf{k}\downarrow}^{\dagger}(0)f_{\mathbf{k+q}\downarrow}(0)]\}\rangle_0,$$

whose Fourier transform $\chi_0^{zz}(\mathbf{q},\omega)\equiv\chi_0^{zz}(q)$ is represented by the diagram of Fig. 1(a). Starting with this unperturbed susceptibility diagram of the f-fermion bubble, the diagrammatic expansion including second order corrections in the fermion-boson interactions $H_{\rm int}^{(H)}$ (or $H_{\rm int}^{(3B)}$) then introduces the series of the correction terms whose diagrams are shown in Fig. 1(b) for the three-band model. These diagram series exactly corresponds to the Hubbard model if the fp-propagator (half-solid and half-dashed) lines are replaced by the ff-propagator (solid) lines. Except this, all the following discussions and expressions including the vertex factors can be applied to the two models.

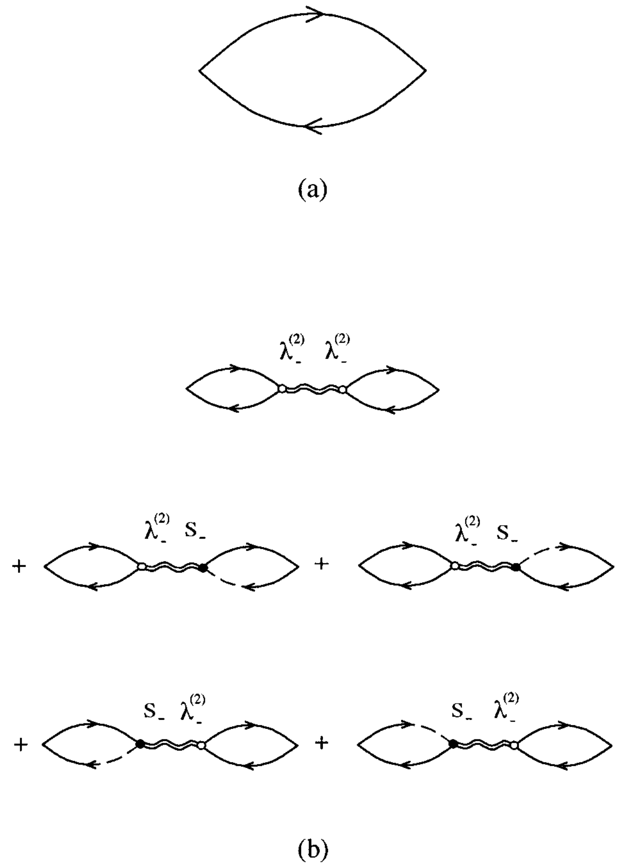

FIG. 1. The diagrammatic perturbation expansion for the momentum-dependent dynamical longitudinal magnetic susceptibility $\chi^{zz}(q)$ $[q\equiv(\mathbf{q},\omega)]$ of d electron for the Hubbard and the three-band models in the Gaussian-fluctuation approximation, i.e., the RPA self-energy corrections to the boson propagators. (a) The unperturbed saddle-point contribution $\chi_0^{zz}(q)$ of $O(1)$, and (b) the perturbation series diagrams of $O(1/N)$ obtained from the diagram in (a) due to fermion fluctuations by bosons. In the three-band model the solid and solid-dashed lines are the saddle-point propagators of f-fermion $\mathcal{G}_{ff}^{(0)}$ and fp-mixed fermion $\mathcal{G}_{fp}^{(0)}$, respectively, while in the Hubbard model the solid-dashed lines should be replaced by the f-fermion solid lines $\mathcal{G}^{(0)}$. The double wavy lines are the RPA renormalized boson propagators $[\mathcal{D}(q)_a]_{\lambda_-^{(2)}\lambda_-^{(2)}}$, $[D(q)_a]_{\lambda_-^{(2)}s_-}$, etc., and the open and solid circles are the vetices $1/\sqrt{2}$ and $2z_0(\partial z_\uparrow/\partial s_-)$, respectively, of the fermion-boson interactions given in Eqs. (42) and (43).

Now notice that these correction diagrams are made up of the two kinds of diagrams involving either the boson propagator $[\mathcal{D}(q)_a]_{\lambda_-^{(2)}\lambda_-^{(2)}}$ or $[\mathcal{D}(q)_a]_{\lambda_-^{(2)}s_-}$ which accompanies the magnetic correlation bubble $\chi_0(q)$ or $\chi_1(q)$. Here we emphasize that the diagram involving the s_--boson propagator $[\mathcal{D}(q)_a]_{s_-s_-}$ does not appear in this perturbation expansion because the unperturbed susceptibility bubble of $\chi_0^{zz}(q)$ which must exist on one end of each diagram cannot be connected to this boson line. The absence of the s_--boson propagator in the perturbation series is quite natural since the propagator $[\mathcal{D}(q)_a]_{s_-s_-}$ itself is directly related to the renormalized susceptibility $\chi^{zz}(q)$ as we have seen in (41). The vertices connecting the bubbles and the $\lambda_-^{(2)}$ and s_- boson lines are $1/\sqrt{2}$ and $2z_0(\partial z_\uparrow/\partial s_-)$, respectively. The total of the diagrams shown in Figs. 1(a) and 1(b) then leads to the sum

$$\chi^{zz}(q)=\chi_0^{zz}(q)\left\{1+\frac{1}{2}\left(\frac{1}{\sqrt{2}}\right)([\mathcal{D}(q)_a]_{\lambda_-^{(2)}\lambda_-^{(2)}})\left(\frac{1}{\sqrt{2}}\right)2\chi_0(q)-\frac{1}{2}\left(\frac{1}{\sqrt{2}}\right)([\mathcal{D}(q)_a]_{s_-\lambda_-^{(2)}}+[\mathcal{D}(q)_a]_{\lambda_-^{(2)}s_-})\left(2z_0\frac{\partial z_\uparrow}{\partial s_-}\right)2\chi_1(q)\right\}. \tag{44}$$

For the boson propagators $\mathcal{D}(q)_a$ in (44) we substitute the RPA propagators obtained by inverting $\mathcal{D}(q)^{-1}$ in Eq. (15). The boson propagators are found from Eqs. (16), (17), and (21), and are rewritten as

$$[\mathcal{D}(q)_a]_{\lambda_-^{(2)}\lambda_-^{(2)}}=\frac{\lambda_0^{(1)}-\lambda_0^{(2)}+\Sigma_{s_-s_-}(\mathbf{q})+\Pi_{s_-s_-}(q)}{\det\mathcal{D}(q)^{-1}}=\frac{2g_0(\mathbf{q})+2(g_1/2)^2\chi_2(q)}{\det\mathcal{D}(q)^{-1}/(-s_0^2)}, \tag{45}$$

$$\frac{1}{\sqrt{2}}\left(4z_0\frac{\partial z_\uparrow}{\partial s_-}\right)[\mathcal{D}(q)_a]_{s_-\lambda_-^{(2)}}=\left(2\sqrt{2}z_0\frac{\partial z_\uparrow}{\partial s_-}\right)\frac{s_0-\Pi_{s_-\lambda_-^{(2)}}(q)}{\det\mathcal{D}(q)^{-1}}=\frac{-g_1+(g_1/2)^2\chi_1(q)}{\det\mathcal{D}(q)^{-1}/(-s_0^2)}. \tag{46}$$

Substituting these expressions into Eq. (44), one finds the result for $\chi^{zz}(q)$ given in Eq. (33).

C. Derivation of $\chi^{zz}(0)$ from magnetic saddle-point solutions

As Kotliar and Ruckenstein[7] and Lavagna[8] showed previously for the Hubbard model, one can also derive the uniform susceptibility $\chi^{zz}(0)$ directly from the saddle-point free energy of fermions under applied magnetic field h_0. This is obtained by taking into account the effects of the spin-dependent band renormalization q_σ and the effective internal field $\lambda_{\mathbf{q}-}^{(2)}$ for $\mathbf{q}=0$. Since the result for the Hubbard model is available,[8] we will obtain here the saddle-point susceptibility expression for the three-band model. Using the fermion free energy $\mathcal{F}_F^{(0)}(m_d)$ with magnetic field h_0 applied to Cu sites only, the d-electron magnetic moment is $m_d=-\partial\mathcal{F}_F^{(0)}(m_d)/\partial h_0=\Sigma_{\mathbf{k}\sigma}u_{1f}(\mathbf{k},h_0)^2\sigma f(\xi_{1\mathbf{k}\sigma}^{(3B)})$ and the magnetic susceptibility $\chi^{zz}(0)=\partial m_d/\partial h_0$ is given by

$$\chi^{zz}(0)=\sum_{\mathbf{k}\sigma}\left(\frac{\partial u_{1f}(\mathbf{k},h_0)^2}{\partial h_0}\right)\sigma f(\xi_{1\mathbf{k}\sigma}^{(3B)})+\sum_{\mathbf{k}\sigma}u_{1f}(\mathbf{k},h_0)^2\sigma\times\left(-\frac{\partial f(\xi_{1\mathbf{k}\sigma}^{(3B)})}{\partial\xi_{1\mathbf{k}\sigma}^{(3B)}}\right)\left(-\frac{\partial\xi_{1\mathbf{k}\sigma}^{(3B)}}{\partial h_0}\right), \tag{47}$$

where $\xi_{1\mathbf{k}\sigma}^{(3B)}=\frac{1}{2}\{\varepsilon_p+\lambda_{0\sigma}^{(2)}-[(\varepsilon_p-\lambda_{0\sigma}^{(2)})^2+4q_\sigma\tau_{\mathbf{k}}^2]^{1/2}\}$ and $u_{1f}(\mathbf{k},h_0)^2=\frac{1}{2}\{1+(\varepsilon_p-\lambda_{0\sigma}^{(2)})/[(\varepsilon_p-\lambda_{0\sigma}^{(2)})^2+4q_\sigma\tau_{\mathbf{k}}^2]^{1/2}\}$ with the d level given by $\lambda_{0\sigma}^{(2)}\equiv\lambda_{0+}^{(2)}-\sigma(h_0-\lambda_{0-}^{(2)})$ under applied magnetic field h_0 together with the internal field $-\lambda_{0-}^{(2)}$. The internal field is calculated as $-\lambda_{0-}^{(2)}=-\partial\mathcal{F}_F^{(0)}(m_d)/\partial m_d=\Sigma_\sigma(-\partial q_\sigma/\partial m_d)\omega_\sigma^{(3B)}$, where $\omega_\sigma^{(3B)}$ is given by $\omega_\sigma^{(3B)}\equiv\Sigma_{\mathbf{k}}(-\tau_{\mathbf{k}}^2)f(\xi_{1\mathbf{k}\sigma}^{(3B)})/[(\varepsilon_p-\varepsilon_{d\sigma})^2+4q_\sigma\tau_{\mathbf{k}}^2]^{1/2}$ and is related to the energy $\omega_0^{(3B)}$, $\Sigma_\sigma\omega_\sigma^{(3B)}=\omega_0^{(3B)}$, which was defined earlier [see below Eq. (20)]. Now to obtain the expression for $\chi^{zz}(0)$ we need to calculate $-\partial\xi_{1\mathbf{k}\sigma}^{(3B)}/\partial h_0$ and $\partial u_{1f}(\mathbf{k},h_0)^2/\partial h_0$, and furthermore $-\partial\lambda_{0-}^{(2)}/\partial h_0$. Substituting these results into the expression (47) and rearranging the terms, we obtain the saddle-point uniform susceptibility of d electron as

$$\chi^{zz}=\frac{\chi_0^{zz}}{1-\{2q_2-(q_1/z_0)^2\}|\omega_0^{(3B)}|\chi_0-4q_1\chi_1+(2q_1)^2\{(x_1)^2-\chi_2\chi_0\}}, \tag{48}$$

where $\chi^{zz}\equiv\chi^{zz(3B)}(0)$, $\chi_0\equiv\chi_0^{(3B)}(0)$, etc., and we have used the relation $\chi_0^{zz}=2\chi_0$ and the definitions $q_1\equiv(1/2)\Sigma_\sigma\sigma\partial q_\sigma/\partial m_d$ and $q_2\equiv\partial^2q_\sigma/\partial m_d^2$. As regards the relationship with the coupling constants $g_0^{(3B)}$ and $g_1^{(3B)}$ obtained in Eqs. (38)–(40), it can be shown using the explicit quantities of q_1 and q_2 that $\{2q_2-(q_1/z_0)^2\}|\omega_0^{(3B)}|=g_0^{(3B)}$ and $4q_1=g_1^{(3B)}$. Therefore, the expression (48) exactly coincides with that in (33). In relation to the Hubbard model susceptibility, where only the term $2q_2|\omega_0^{(H)}|$ alone becomes equal to $g_0^{(H)}$ with the term $(q_1/z_0)^2|\omega_0^{(H)}|$ missing, the difference between $g_0^{(3B)}$ and $g_0^{(H)}$ in Eqs. (38) and (39) comes from the term $(q_1/z_0)^2|\omega_0^{(3B)}|$ by cancelling out the second term of $g_0^{(H)}$ in (38). In the three-band model a nonvanishing contribution equal to $(q_1/z_0)^2|\omega_0^{(3B)}|\chi_0$ further arises from the d-p interband term $-(2q_1)^2\chi_2\chi_0$, which cancels out the above $-(q_1/z_0)^2|\omega_0^{(3B)}|$ term in the $g_0^{(3B)}$, thus reducing the effective coupling constant of the three-band model multiplied by χ_0 to $2q_2|\omega_0^{(3B)}|$, which is very similar to the Hubbard $g_0^{(H)}=2q_2|\omega_0^{(H)}|$. For the nonuniform susceptibility $\chi^{zz}(\mathbf{q})$ of the three-band model, a similar contribution arises from the last $(g_1^{(3B)})^2$ term in (33) which has a $\mathbf{q}$ dependence from $\chi_0(\mathbf{q})$, $\chi_1(\mathbf{q})$, $\chi_2(\mathbf{q})$, and this leads the originally missing $\mathbf{q}$ dependence of $g_0^{(3B)}$ to the $\mathbf{q}$-dependent coupling constant as the $g_0^{(H)}(\mathbf{q})$.

It is a common observation in the linear response theory that the response function of the system under an external field which is derived by treating fluctuations in the RPA approximation is identically reproduced by expanding the saddle-point free energy, which implements the internal field, with respect to that external field. For example, it is well known that in the Hubbard model the self-consistent mean-field free energy under magnetic field which incorporates the internal field $-Um(m\equiv n_\uparrow - n_\downarrow)$ leads to the uniform susceptibility $\chi(0)=\chi_0(0)/(1-U\chi_0(0))$ with the same enhancement Stoner factor as that of the RPA susceptibility $\chi(0)$. Lavagna has pointed out that this feature remains also in the slave-boson treatment of the Hubbard model.[8]

IV. EFFECTIVE INTERACTIONS AND LANDAU FERMI-LIQUID PARAMETERS

In this section we examine the renormalizations of the magnetic interaction or the Landau Fermi-liquid parameter F_0^a as functions of doping concentration δ as well as Coulomb repulsion U and charge-transfer (CT) energy $\Delta\equiv\varepsilon_p$, $(\varepsilon_d^0=0)$. We define the magnetic Landau parameter F_0^a by the Wilson ratio R of the static uniform magnetic susceptibility to the linear specific-heat coefficient $\gamma\equiv C/T$ as follows:

$$R\equiv\frac{\chi^{zz}(0)/\gamma}{\chi_{00}^{zz}(0)/\gamma_0}=\frac{\chi^{zz}(0)}{\chi_0^{zz}(0)}\equiv\frac{1}{1+F_0^a}, \tag{49}$$

where $\chi_{00}^{zz}(0)$ and γ_0 are the bare susceptibility and specific-heat coefficient of noninteracting d electrons, respectively, and the relations $\chi_0^{zz}(0)=\chi_{00}^{zz}(0)\gamma/\gamma_0=\chi_{00}^{zz}(0)/q_0$ have been used. Combining this definition (49) with the expression (33) for $\chi^{zz}(0)$ with $q\equiv(\mathbf{q},\omega)=(0,0)$ leads to

$$F_0^a\equiv-g_0(0)\chi_0(0)-g_1\chi_1(0)+\left(\frac{g_1}{2}\right)^2\{\chi_1(0)^2-\chi_0(0)\chi_2(0)\}. \tag{50}$$

We now analyze the renormalization behaviors of the Landau parameter F_0^a of the two models, changing from the weak coupling to strong coupling regimes.

A. The Hubbard model

In the case of the single-band Hubbard model, the susceptibility functions $\chi_1^{(H)}(0)$ and $\chi_2^{(H)}(0)$ for $q=0$ involving one and two slave-boson interaction vertices, respectively, can be represented in terms of the transverse susceptibility $\chi_0^{(H)}(0)$ with energy factors $\varepsilon_{\mathbf{k}}$ and $\varepsilon_{\mathbf{k+q}}$ being evaluated on the Fermi surface $\varepsilon_F(=\mu)$. This leads to the vanishing of the last term with $(g_1)^2$ in Eq. (50). In the resulting expression of F_0^a we replace $\chi_0^{(H)}(0)$ by the density of states per spin at the Fermi energy, N_F, and obtain

$$\frac{F_0^{a(H)}}{\alpha}=-\frac{g_0^{(H)}(0)}{W}+\varepsilon_F\frac{g_1^{(H)}}{W}, \tag{51}$$

where we have introduced the normalization factor $\alpha\equiv WN_F$ and the renormalized bandwidth $W\equiv 8q_0t$. Here α represents the the structural parameter of the model reflecting on the density of states, which equals unity if we employ a constant density of states and takes a large value for the ε_F close to the van Hove singularity of the two-dimensional lattice.

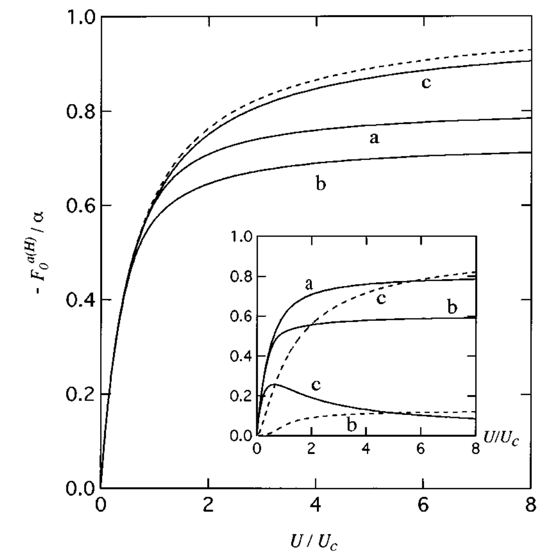

FIG. 2. The normalized Landau Fermi-liquid parameter $-F_0^{a(H)}/\alpha$ as a function of U/U_c for the Hubbard model. The solid curves a, b, c correspond to the doping concentrations of δ=0, δ=0.15, δ=0.95, respectively. The dashed curve is the T-matrix result, $-U_{\rm eff}/W_0=-(U/W_0)/(1+U/W_0)$, valid for the low carrier density limit, being exact for the two-particle system. The inset shows the separate contributions of the $g_0^{(H)}(0)/W$ (solid) and $\varepsilon_F g_1^{(H)}/W$ (dashed) terms in (51) for these dopings.

Using the expressions (38) and (40) of $g_0^{(H)}(0)$ and $g_1^{(H)}$ given by the saddle-point slave-boson parameters, one can easily evaluate the Landau parameter $F_0^{a(H)}/\alpha$ in the limiting cases. In the half-filled metallic regime defined by δ=0 and $u\equiv U/E_c<1$ (E_c is given by $E_c\equiv 8|\omega_0^{(H)}|\sim 1.6W_0$ in terms of the average kinetic energy per site $|\omega_0^{(H)}|\sim 1.6t$ for the half-filling or the unrenormalized bandwidth $W_0\equiv 8t$ and equals the critical Coulomb repulsion U_c for the metal-insulator transition), we obtain

$$\frac{F_0^{a(H)}}{\alpha}=-\frac{4|\omega_0^{(H)}|}{W_0}\left\{1-\frac{1}{(1+u)^2}\right\}=-0.8\left\{1-\frac{1}{(1+u)^2}\right\}. \tag{52}$$

So the metallic Landau parameter $F_0^{a(H)}/\alpha$ goes down to -0.6. In particular, in the weak-coupling limit $U\ll W_0$ we have $F_0^{a(H)}/\alpha\sim-1.6u\sim-U/W_0$, reproducing the known weak-coupling result of the RPA approximation. On the other hand, in the dilutely doped insulator regime of $\delta\ll1$ and $u>1$, we obtain

$$\frac{F_0^{a(H)}}{\alpha}=-0.8\left\{1-\frac{1+\delta\zeta}{4u}\right\}, \tag{53}$$

where $\zeta\equiv(1-1/u)^{1/2}$. In the strong-coupling regime $U\to\infty$, therefore, $F_0^{a(H)}/\alpha$ tends to -0.8 from above, which is different, due to the lattice structure, from the result $(F_0^{a(H)}/\alpha\to-1.0)$ obtained with a constant density of states. These results (52) and (53) are essentially the same except for the factor $4|\omega_0^{(H)}|/W_0=0.8$ as those obtained earlier[8–13] for the structureless Hubbard model where $4|\omega_0^{(H)}|/W_0=1$. In the intermediate-coupling regime, the behavior of the Landau parameter $F_0^{a(H)}/\alpha$ as a function of U/U_c is calculated numerically and is plotted in Fig. 2 for various dopings, which shows a typical crossover renormalization from the weak-coupling to the strong coupling parameter. The inset indicates the individual contributions of the $g_0^{(H)}$ and $g_1^{(H)}$ terms. As doping δ increases, the $g_1^{(H)}$ term (dashed lines) starts from 0 for $\delta=0$ and becomes larger than the $g_0^{(H)}$ term. In the weak coupling regime, however, the $g_0^{(H)}$ term always dominates over the $g_1^{(H)}$ term.

In Fig. 2 we have also plotted the Landau parameter (the dashed curve) corresponding to the effective interaction $U_{\rm eff}$, i.e., $-U_{\rm eff}/W_0=-(U/W_0)/(1+U/W_0)$. This is the exact result for the two-particle system and is identical to that of the T-matrix approximation valid for low carrier density. As it is expected, this T-matrix curve is quite well fitted by our result for the high-doping case (curve c for $\delta=0.95$). Not only this but we can also show that the expression (51) for $F_0^{a(H)}/\alpha$ exactly reduces to the above T-matrix expression in the low carrier-density limit with $\delta\sim1$; $g_0^{(H)}(0)/W=(U/W_0)/(1+U/W_0)^2$, $\varepsilon_F g_1^{(H)}/W=-(U/W_0)^2/(1+U/W_0)^2$, and $F_0^{a(H)}/\alpha=-(U/W_0)/(1+U/W_0)$. These two expressions were obtained by evaluating the slave-boson expressions (38) and (40) for the high-doping limit $\delta\sim1$, using the saddle-point self-consistent equation to determine the slave-boson parameters. In the weak-coupling regime the Landau parameter reduces to $-U_{\rm eff}/W_0\to-U/W_0$, coming from the first $g_0^{(H)}$ term, and in the strong-coupling regime it leads to $-U_{\rm eff}/W_0\to-1$, arising from the second $g_1^{(H)}$ term. The inset shows that the relative contributions of these two terms depend on the carrier concentration. It is important to notice that the mechanism of the strong-coupling renormalization of $F_0^{a(H)}$ is quite different in the two cases of the low carrier-density limit and the low-doping limit; in the latter case the strong-coupling renormalization $F_0^{a(H)}/\alpha\sim-1$ arises from the $g_0^{(H)}$ term and corresponds to the coupling constant $U_{\rm eff}\sim W(\ll W_0)$ contrary to $U_{\rm eff}\sim W_0$ in the former case. However, the weak-coupling parameter, which is $-U_{\rm eff}/W_0\sim-U/W_0$ for both the limits, always results from the $g_0^{(H)}$ term. In Sec. V we analyze in a more physically transparent way the processes which take place in the slave-boson representation to lead to the coupling constants $g_0^{(H)}$ and $g_1^{(H)}$.

B. The three-band model

Having studied the behaviors of the Landau parameter for the Hubbard model, it is now interesting to investigate the renormalizations of this parameter as the system of the three-band model goes from a metallic regime to an insulator regime. In this case we treat the $t_{pp}=0$ model and calculate F_0^a as functions of U and Δ for half-filling in the metallic regime and for infinitesimal electron and hole doping in the insulator regime. When a system of this model goes into an insulator, there are two types of insulator regimes; the Mott-Hubbard (MH) insulator and the charge-transfer (CT) insulator. We have recently found[15] that these insulators respond quite differently to a dilute electron and hole doping. Therefore, it would be interesting to examine how the Landau-parameter renormalizations differ in the two insulator regimes for electron and hole dopings.

We rewrite the Landau parameter of the three-band model, Eq. (50), as

$$F_0^{a(3B)}=-\left\{g_0^{(3B)}+\left(\frac{g_1^{(3B)}}{2}\right)^2\chi_2^{(3B)}(0)\right\}\chi_0^{(3B)}(0)-g_1^{(3B)}\chi_1^{(3B)}(0)+\left(\frac{g_1^{(3B)}}{2}\right)^2[\chi_1^{(3B)}(0)]^2, \quad (54)$$

where the susceptibility expressions for $q=0$ of the three-band model can be written down, considering the contributions from the lower $\xi_{1\mathbf{k}\sigma}^{(3B)}$ and the upper $\xi_{3\mathbf{k}\sigma}^{(3B)}$ bands, as

$$\chi_0^{(3B)}(0)=[\mu_{1f}(\mathbf{k}_F)]^4N_F+2\sum_{\mathbf{k}}^{\mathbf{k}_F}\frac{[u_{1f}(\mathbf{k})u_{1p}(\mathbf{k})/z_0]^2}{\xi_{3\mathbf{k}\sigma}^{(3B)}-\xi_{1\mathbf{k}\sigma}^{(3B)}}, \quad (55)$$

$$\chi_1^{(3B)}(0)=\tau_{\mathbf{k}_F}[u_{1f}(\mathbf{k}_F)]^2\frac{1}{z_0}u_{1f}(\mathbf{k}_F)u_{1p}(\mathbf{k}_F)N_F-\sum_{\mathbf{k}}^{\mathbf{k}_F}\frac{u_{1f}(\mathbf{k})^2u_{1p}(\mathbf{k})^2}{z_0^2}, \quad (56)$$

$$\chi_2^{(3B)}(0)=\tau_{\mathbf{k}_F}^2\frac{u_{1f}(\mathbf{k}_F)^2u_{1p}(\mathbf{k}_F)^2}{z_0^2}N_F+\frac{1}{2}(\varepsilon_p-\lambda_0^{(2)})^2\sum_{\mathbf{k}}^{\mathbf{k}_F}\frac{[u_{1f}(\mathbf{k})u_{1p}(\mathbf{k})/z_0]^2}{\xi_{3\mathbf{k}\sigma}^{(3B)}-\xi_{1\mathbf{k}\sigma}^{(3B)}}, \quad (57)$$

with the renormalized Fermi-level density of states $N_F\equiv N_F^0/z_0^2$ defined by the unrenormalized one N_F^0 and

$$[u_{1f}(\mathbf{k})]^2=\frac{\xi_{1\mathbf{k}\sigma}^{(3B)}-\lambda_0^{(2)}}{\xi_{3\mathbf{k}\sigma}^{(3B)}-\xi_{1\mathbf{k}\sigma}^{(3B)}}, \quad (58)$$

$$[u_{1p}(\mathbf{k})]^2=\frac{\xi_{1\mathbf{k}\sigma}^{(3B)}-\varepsilon_p}{\xi_{3\mathbf{k}\sigma}^{(3B)}-\xi_{1\mathbf{k}\sigma}^{(3B)}}, \quad (59)$$

$$u_{1f}(\mathbf{k})u_{1p}(\mathbf{k})=\frac{z_0\tau_{\mathbf{k}}}{\xi_{3\mathbf{k}\sigma}^{(3B)}-\xi_{1\mathbf{k}\sigma}^{(3B)}}. \quad (60)$$

We notice here that when z_0 tends to a small value such as near a metal-insulator transition, the susceptibility functions are all of order $O(1/z_0^2)$ while the coupling constants $g_0^{(3B)}$ and $g_1^{(3B)}$ are of order $O(z_0^2)$ because $[u_{1f}(\mathbf{k})]^2\to O(1)$, $[u_{1p}(\mathbf{k})]^2\to O(z_0^2)$, and $u_{1f}(\mathbf{k})u_{1p}(\mathbf{k})\to O(z_0)$. Therefore, each term of $F_0^{a(3B)}$ in the expression (54) equally contributes a quantity of order $O(1)$. Furthermore the terms with the factor $(N_F)^2$ which come from the interband terms of

$\chi_2^{(3B)}(0)\chi_0^{(3B)}(0)$ and $[\chi_1^{(3B)}(0)]^2$ exactly cancel out each other, which corresponds to the cancellation of the $(g_1)^2$ term in the Hubbard model for $q=0$.

We first evaluate $F_0^{a(3B)}$ for the half-filled metallic states ($u\equiv U/E_c<1$, $E_c\equiv 8|\omega_0^{(3B)}|$) of the Mott-Hubbard regime defined by $\Delta\equiv\varepsilon_p\gg U$ and $\Delta\gg t_{pd}$, where $\delta=0$, $\delta_d\sim 0$, and $z_0^2\sim O(1)$. In this case we find $\chi_0^{(3B)}(0)\sim O(1)$ but $\chi_1^{(3B)}(0)\ll 1$ and $\chi_2^{(3B)}(0)\ll 1$, $g_0^{(3B)}\sim O(1)$ but $g_1^{(3B)}\ll 1$, $[u_{1f}(\mathbf{k})]^2\sim 1$ but $[u_{1p}(\mathbf{k})]^2\ll 1$ and $u_{1f}(\mathbf{k})u_{1p}(\mathbf{k})\ll 1$. Therefore, $F_0^{a(3B)}$ can be written simply as

$$\frac{F_0^{a(3B)}}{\alpha}=-\frac{g_0^{(3B)}}{W}, \tag{61}$$

using the normalization factor $\alpha\equiv WN_F\equiv W_0N_F^0$ defined earlier for the Hubbard model. Evaluating $g_0^{(3B)}$ from Eq. (39) in the half-filled metallic case, one obtains

$$\frac{F_0^{a(3B)}}{\alpha}=-\frac{4|\omega_0^{(3B)}|}{W_0}\left\{1-\frac{1}{(1+u)^2}\right\}=-2.8\left\{1-\frac{1}{(1+u)^2}\right\}, \tag{62}$$

where we have used the expressions $|\omega_0^{(3B)}|=5.6t_{\rm eff}$ and $W_0=8t_{\rm eff}$ with $t_{\rm eff}\equiv t_{pd}^2/(\Delta-\lambda_0^{(2)})$ which are valid in the present limit. Therefore, although F_0^a/α in the Mott-Hubbard regime of the three-band model takes the same form as that for the Hubbard model, the magnitude $|F_0^a/\alpha|$ of the former is larger than the latter, becoming as large as 2.1 as opposed to the latter's maximum value 0.6 close to the metal-insulator transition.

We next evaluate the $F_0^{a(3B)}$ of Eq. (54) in the infinitesimal-doping limits in the insulator regimes where $\delta=0^{\pm}$, $\delta_d=0^{\pm}$, and $z_0^2\to 0$. In these limits $[u_{1f}(\mathbf{k})]^2\to 1$, $[u_{1p}(\mathbf{k})]^2\to 0$, and $u_{1f}(\mathbf{k})u_{1p}(\mathbf{k})\to 0$, and $\xi_{1\mathbf{k}\sigma}^{(3B)}-\xi_{1\mathbf{k}\sigma}^{(3B)}\to\Delta-\lambda_0^{(2)}$, and then F_0^a/α can be written as

$$\frac{F_0^{a(3B)}}{\alpha}=-\frac{g_0^{(3B)}}{W}-\left(\frac{g_1^{(3B)}}{2z_0^2}\right)^2\frac{|\omega_0^{(3B)}|}{4W_0}+\frac{g_1^{(3B)}}{2z_0^2}. \tag{63}$$

Here the second term is the contribution from the interband term of $\chi_2^{(3B)}(0)$ in (57) and becomes $(0.7/4)(g_1^{(3B)}/2z_0^2)^2$ performing the sum $\Sigma_{\mathbf{k}}^{\mathbf{k}_F}(\gamma_{\mathbf{k}}^{(3B)})^2=\frac{1}{2}+2/\pi^2\sim 0.7$. Using the expression (37) for $g_1^{(3B)}$, this term can be rewritten as $-(1/2s_0^2)(\partial_{z_\uparrow}/\partial_{s_-})^2|\omega_0^{(3B)}|$. This indicates the recovery of the originally missing $\mathbf{q}$-dependent term in $g_0^{(3B)}$, corresponding to the $\omega_{\mathbf{q}}^{(H)}$ term of the Hubbard $g_0^{(H)}(\mathbf{q})$ for $\mathbf{q}=0$, if we use Eqs. (36) and (19). As we already noticed in Sec. III C, the $\omega_{\mathbf{q}}^{(H)}$ term of the Hubbard $g_0^{(H)}(\mathbf{q})$ for the general nonzero $\mathbf{q}$, however, corresponds not only to the $\chi_2^{(3B)}(\mathbf{q})$ term but to the $\chi_0^{(3B)}(\mathbf{q})$ and $\chi_1^{(3B)}(\mathbf{q})$ terms as well. Furthermore, if the last term of (63) is written as $[\tau_{\mathbf{k}_F}^2/(\Delta-\lambda_0^{(2)})]g_1^{(3B)}/W$ in the present limits where $\tau_{\mathbf{k}_F}^2/(\Delta-\lambda_0^{(2)})=4t_{pd}^2/(\Delta-\lambda_0^{(2)})$ with $(\gamma_{\mathbf{k}_F}^{(3B)})^2=1$ is the effective band energy and $W=8z_0^2t_{pd}^2/(\Delta-\lambda_0^{(2)})$, then it is easy to notice that this term corresponds to the Hubbard term, $-\varepsilon_F g_1^{(H)}/W$ (which vanishes though at half-filling), and the first two terms of (63) to the Hubbard $-g_0^{(H)}(0)/W$ term of the $F_0^{a(H)}$ in (51). Now let us evaluate each term of (63) in the infinitesimal doping limits; we find $g_0^{(3B)}/W=2.1$ and $g_1^{(3B)}$ is given by $g_1^{(3B)}/2z_0^2=2\zeta(0^{\pm})\mathrm{sgn}\,\delta_d$ with $\zeta(0^{\pm})\equiv[1-E(0^{\pm})/U]^{1/2}=[1-1/u^{\pm}]^{1/2}$, $(1\geq\zeta(0^{\pm})\geq 0)$, where $E(\delta)\equiv 8|\omega_0^{(3B)}(\delta)|$, $u^{\pm}\equiv U/E(0^{\pm})$, and sgn δ_d is the sign of δ_d which is $\delta_d>0$ for electron doping $\delta>0$ but can be $\delta_d>0$ or $\delta_d<0$ for hole doping $\delta<0$ which depends on the regime in the insulator phase, as we clarified earlier.[8] Thus the Landau parameter in the insulator regimes for the infinitesimal dopings $\delta=0^{\pm}$ takes the form

$$\frac{F_0^{a(3B)}}{\alpha}=-\left\{2.1+0.7\left(1-\frac{1}{u^{\pm}}\right)-2\,(\mathrm{sgn}\ \delta_d)\left(1-\frac{1}{u^{\pm}}\right)^{1/2}\right\}. \tag{64}$$

From this we can extract the asymptotic values of $F_0^{a(3B)}/\alpha$ in the typical parameter regions; (i) near the boundary but inside the insulator phase of a metal-insulator transition in the Mott-Hubbard (MH) regime where $u^{\pm}\to 1+0,[\zeta(0^{\pm})\to 0]$, this $F_0^{a(3B)}/\alpha$ again takes the same value -2.1 as that from (62) in the metallic side, and (ii) in the charge-transfer (CT) insulator limit of $u^{\pm}\to\infty$ where both infinitesimal electron $\delta=0^+$ and hole $\delta=0^-$ dopings give $\delta_d=0^+$, we obtain $F_0^{a(3B)}/\alpha=-0.8$. This hole-doping value, however, changes very quickly to the value $F_0^{a(3B)}/\alpha=-4.8$ as $|\delta|$ increases to a finite hole doping ($\delta<0$) because δ_d changes its sign to the negative ($\delta_d<0$).[15] This CT value $F_0^{a(3B)}/\alpha=-0.8$ corresponds to the asymptotic value of the Hubbard $F_0^{a(H)}/\alpha$ for $U\to\infty$ at the half-filling. [Note that $\zeta(0^{\pm})\sim 1$ is not approached in the MH insulator regime.] Therefore, the structure of the Landau parameter (64) in the insulator phase of the three-band model is different from that (53) of the Hubbard model.

Other than the extreme MH and CT limits, next we investigate the behaviors of the Landau parameter for infinitesimal dopings through the parameter set of the high-temperature superconductors, which is assumed here as $U/t_{pd}\sim 10$ and $\Delta/t_{pd}\sim 9$ and exists just inside the insulator phase of CT character, as we showed before.[15] In Fig. 3(a) we plot $-F_0^{a(3B)}/\alpha$ as a function of U/U_c for $\Delta/t_{pd}=9$ and in Fig. 3(b) as a function of Δ/Δ_c for $U/t_{pd}=10$. In these figures we show separately (i) the contribution of the sum of the first and second terms of Eq. (64) and (ii) the contribution of the third term, which are plotted by the dashed and dash-dotted lines, respectively (the critical values for the metal-insulator transitions are, respectively, $U_c/t_{pd}=7.89$ and $\Delta_c/t_{pd}=8.33$). Contrary to the half-filled region in the metallic regime ($U/U_c<1$ and $\Delta/\Delta_c<1$) where the Landau parameter $-F_0^{a(3B)}/\alpha$ is continuous across the half-filling for $\delta=0^+$ and $\delta=0^-$, it is seen that in the insulator regimes $-F_0^{a(3B)}/\alpha$ jumps from $\delta=0^+$ doping to $\delta=0^-$ doping. The larger hole-doping value of $-F_0^{a(3B)}/\alpha$ than the electron-doping value is explained by the contribution (ii) with this trend while the contribution (i) has the opposite but smaller trend. The behavior of the contribution (i) is similar to the Hubbard $F_0^{a(H)}/\alpha$ at half-filling where the second term $-\varepsilon_F g_1^{(H)}/W$ corresponding to the contribution (ii) of the three-band model vanishes.

Figures 3(a) and 3(b) show that, contrary to the Hubbard model, the Landau parameter of the three-band model for dilute doping can increase beyond the critical value of unity corresponding to a ferromagnetic phase transition, especially even for the value of Coulomb repulsion U or charge-

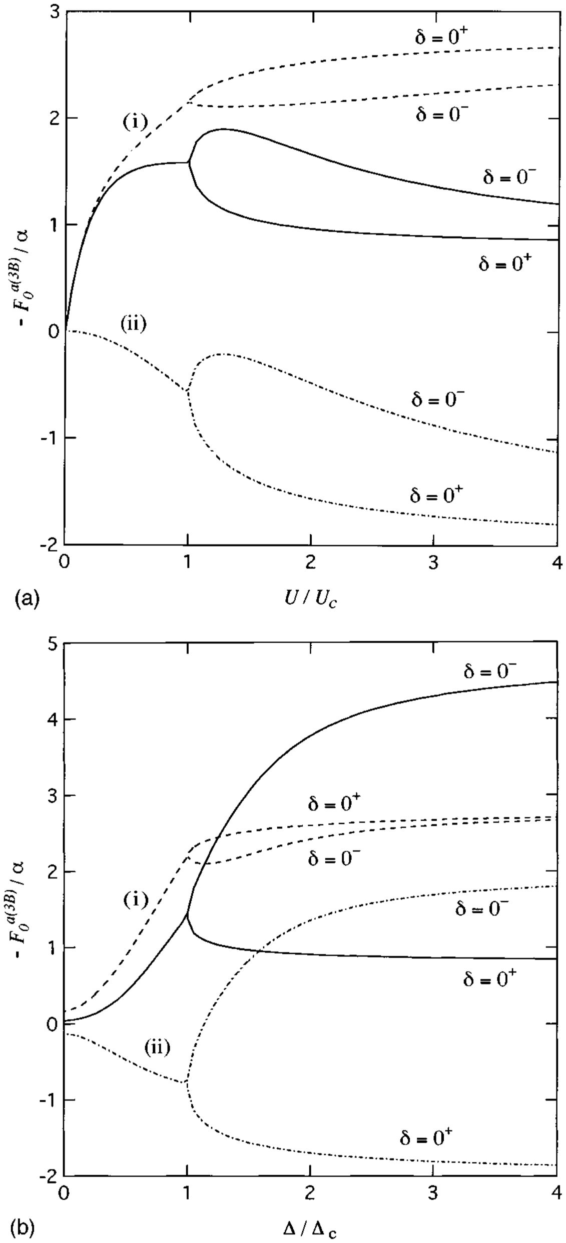

FIG. 3. The normalized Landau Fermi-liquid parameter $-F_0^{a(3B)}/\alpha$ (solid curves) for the three-band model. (a) $-F_0^{a(3B)}/\alpha$ as a function of U/U_c for $\Delta/t_{pd}=9$ in the Mott-Hubbard regime ($U_c/t_{pd}=7.89$), and (b) $-F_0^{a(3B)}/\alpha$ as a function of Δ/Δ_c for $U/t_{pd}=10$ in the charge-transfer regime ($\Delta_c/t_{pd}=8.33$). The dashed and dot-dashed curves are the contributions (i) [the first two terms of (64)] and (ii) [the last term of (64)], respectively. In (a) and (b) the parameter set $U/t_{pd}\sim10$ and $\Delta/t_{pd}\sim9$ roughly corresponds to that of the high-T_c cuprates. $\delta=0^+$ and $\delta=0^-$ on the curves for $U/U_c>1$ in (a) and $\Delta/\Delta_c>1$ in (b) correspond to infinitesimal electron and hole dopings, respectively, in the MH (a) and in the CT (b) insulator regimes.

transfer energy Δ less than the critical value U_c or Δ_c. Here the value of $-F_0^{a(3B)}/\alpha$ beyond unity is not itself physically meaningful, but our analyses beyond this value help understand the origins of this Landau parameter in the more realistic cases also because these infinitesimal doping behaviors persist even in finite doping concentrations. The fact that $-F_0^{a(3B)}/\alpha$ is larger than $-F_0^{a(H)}/\alpha$ in the same MH regime indicates that the three-band model is a more magnetic model than the Hubbard model.

V. DISCUSSION

We showed in subsection IV A that the weak-coupling Landau parameter $F_0^{a(H)}/\alpha\sim-U/W_0$ of the Hubbard model is always dominated by the $g_0^{(H)}$ term in both the low density limit and the dilute doping limit, whereas the strong-coupling parameter arises from the $g_1^{(H)}$ term in the low density case and from the $g_0^{(H)}$ term in the dilute doping case. In order to understand these origins we analyze here the physical processes leading to the coupling constants $g_0^{(H)}$ and $g_1^{(H)}$. If we look at the diagrammatic derivation of the susceptibility $\chi^{zz}(q)$ given in (44), it is easy to find that the $g_0^{(H)}$ and $g_1^{(H)}$ terms in the denominator of $\chi^{zz}(q)$ are derived by scatterings of fermions with $\lambda_-^{(2)}$ bosons and mixed $\lambda_-^{(2)}s_-$ bosons, being represented by $[\mathcal{D}(q)_a]_{\lambda_-^{(2)}\lambda_-^{(2)}}$ and $[\mathcal{D}(q)_a]_{s_-\lambda_-^{(2)}}$ boson propagating terms, respectively. These terms give the RPA contributions of $g_0^{(H)}\chi_0(q)$ and $g_1^{(H)}\chi_1(q)$ in $\chi^{zz}(q)$ as obtained by substituting the expressions (45) and (46) into (44). $\lambda_-^{(2)}$ boson and $\lambda_-^{(2)}s_-$-boson excitations represent the phase part and the mixed phase-amplitude part of spin fluctuations from their original definitions, which correspond, respectively, to the spin fluctuation of itinerant *quasiparticles* and to the spin fluctuation of *local moments* of d electrons. Excitations of the latter spin fluctuation with s_- bosons are suppressed in the strong-coupling dilute-doping regime where the local moments are strongly renormalized with the small factor z_0 which enters the vertex in (42). Let us briefly look at our result for $g_0^{(H)}$ and $g_1^{(H)}$ in the low-density limit in the light of the T-matrix derivation of the Landau parameter $-U_{\text{eff}}/W_0$. In the T-matrix approximation the effective interaction U_{eff} is formally given as the sum of the single scattering term U and the multiple scattering term UGU (G is the dressed Green's function), $U_{\text{eff}}=U+UGU$. The Landau parameter $-U_{\text{eff}}/W_0=-(U+UGU)/W_0$ is calculated as $-U_{\text{eff}}/W_0=-U/W_0+(U/W_0)^2/(1+U/W_0)=-(U/W_0)/(1+U/W_0)$. These individual terms have opposite signs tending to cancel each other when they grow, which is quite different from the division into the weak-coupling parameter $g_0^{(H)}$ and the strong coupling parameter $g_1^{(H)}$ obtained in the low-density limit. It is natural that our slave-boson terms do not correspond to the T-matrix perturbation expansion terms.

Another way to understand the two coupling constants $g_0^{(H)}$ and $g_1^{(H)}$ is to examine the derivations of these terms in the saddle-point derivation of $\chi^{zz}(0)$ in Sec. III C. As we have seen there, the coupling constants are given by $g_0^{(H)}=2q_2|\omega_0^{(H)}|$, $g_1^{(H)}=4q_1$, and the internal field by $-\lambda_{0-}^{(2)}=\Sigma_\sigma(-\partial q_\sigma/\partial m_d)\omega_\sigma$ where $q_1\equiv(1/2)\Sigma_\sigma\sigma\partial q_\sigma/\partial m_d$ and $q_2\equiv\partial^2 q_\sigma/\partial m_d^2$. Therefore, the $g_0^{(H)}$ and $g_1^{(H)}$ terms in the Fermi-liquid parameter are related to the internal-field effects through the second and first derivatives of the spin-dependent band renormalization q_σ, respectively, while the spin-independent renormalization q_0 yields the mass enhancement of the numerator $\chi_0^{zz}=\chi_{00}^{zz}(0)/q_0$.

Figure 2 shows that the Landau parameter $-F_0^{a(H)}/\alpha$ of the Hubbard model first decreases (curve b) and then increases (curve c) with increase in doping from the half-filling $\delta=0$ (curve a). This nonmonotonous variation is the result from the two competing terms of $g_0^{(H)}$ and $g_1^{(H)}$, the former decreasing and the latter increasing with doping δ. The strong correlation regime ($U \gg U_c$) near half-filling ($\delta \sim 0$) does not necessarily lead to the largest Landau parameter.

We have noticed in Sec. IV B that the contribution (i) of the first two terms of the expression (63) (and (64) for $-F_0^{a(3B)}/\alpha$ in the Mott-Hubbard insulator is very similar to $-F_0^{a(H)}/\alpha$ of the Hubbard model. In fact, the sum of these two terms exactly reproduces the $g_0^H(0)/W$ expression of the Hubbard model. However, there is some difference from the Hubbard model; in the insulator regime ($U \gg U_c$) the contribution (i) shows a jump on going from $\delta=0^+$ to $\delta=0^-$ doping. This is due to the existence of the two different values of $\zeta(0^\pm)$ for $\delta=0^+$ and $\delta=0^-$. The different $\zeta(0^\pm)$ values in turn result from the different average kinetic energies $E(0^\pm) \equiv 8|\omega_0^{(3B)}(0^\pm)|$ because the quasiparticle fermion level $\lambda_0^{(2)}$ which enters $\omega_0^{(3B)}$ jumps across $\delta=0$ corresponding to the jump in the chemical potential.

We have seen in Sec. IV that while the Landau parameter defined by $-F_0^{a(H)}/\alpha$ of the Hubbard model does not exceed the value of unity for arbitrary value of U and doping (Fig. 2), $-F_0^{a(3B)}/\alpha$ of the three-band model can exceed this value [Figs. 3(a) and 3(b)]. Particularly, this is true even for the expression (61) for the half-filled metallic region and the first two terms of (63) for the insulating region in the Mott-Hubbard regime which precisely correspond to the Hubbard model expression $-F_0^{a(H)}/\alpha$. To understand this large Landau parameter of the three-band model it will suffice basically to show why the metallic half-filling of the Mott-Hubbard regime leads to the larger prefactor 2.8 in (62) as compared to the corresponding prefactor 0.8 for the Hubbard model. The average kinetic energy $|\omega_0^{(3B)}|$ of the three-band model is the value calculated taking the nonhopping level $\lambda_0^{(2)}$ (the top of the lowest band) as the energy zero, as opposed to the value $|\omega_0^{(H)}|$ of the Hubbard model calculated with the center of the band as the nonhopping energy zero. This difference leads to the kinetic energy $|\omega_0^{(3B)}|=5.6t_{\rm eff}=(5.6/8)W_0$ for the three-band model and $|\omega_0^{(H)}|=(1.6/8)W_0$ for the Hubbard model. This also means that the critical Coulomb repulsion for metal-insulator transition is larger for the former, $U_c \sim E_c = 8|\omega_0^{(3B)}| \sim 5.6W_0$, than for the latter, $U_c = E_c = 8|\omega_0^{(H)}| \sim 1.6W_0$. For the weak coupling limit $U \ll U_c$, however, both the three-band model and the Hubbard model give the same Landau parameter value, $F_0^{a(3B)}\alpha \sim -5.6u = -U/W_0$ and $F_0^{a(H)}/\alpha \sim -1.6u \sim -U/W_0$.

We have noticed that our results (52) and (53) for the Landau parameter of the structureless Hubbard model reproduce those obtained by Lavanga[10] and Li *et al.*[11] within the same Kotliar-Ruckenstein slave-boson scheme and by Vollhardt *et al.*[13] in the Gutzwiller approximation. This indicates that our results for the three-band model are also valid at the same approximation level. The Landau parameters for the lattice Hubbard and three-band models can be evaluated from these expressions by simply multiplying the normalization factor $\alpha \equiv W_0 N_F^0$ using the unrenormalized bandwidth W_0 and density of states N_F^0 at the Fermi level N_F^0. Recently, Li and Bernard[10] have performed an extensive numerical study of several Landau parameters including $F_0^{a(H)}$ for the structureless Hubbard model, from which they deduced the pressure dependences of the effective-mass enhancement m^*/m, the compressibility k, the magnetic susceptibility χ, etc., of normal liquid ^{3}He, being in reasonable agreement with the experimental results.[19,20] We therefore expect that our results obtained for the three-band model can also explain the similar physical quantities of the normal states of the high-T_c compounds to the same extent.

As we have seen above, in contrast to other theoretical approaches the slave-boson Gaussian-fluctuation scheme can easily take into account coupling-constant renormalizations as well as bandwidth renormalization in the magnetic susceptibility expression as functions of Coulomb repulsion and doping concentration. Studies on the magnetic properties including these renormalization effects have just been started and we would therefore expect in near future to obtain further new information on the magnetic properties of the Hubbard and the three-band models. Our slave-boson approach fot the three-band CuO_2 model has revealed the different renormalization behaviors for the Fermi-liquid parameter (also for other magnetic properties described below) than for the 2D Hubbard model, which seems to be quite reasonable in view of the presence of the intervening oxygen ions.

Here we have only discussed the uniform Landau parameters F_0^a/α for $\mathbf{q}\neq 0$ and defined them by introducing the normalization factor $\alpha \equiv WN_F = W_0 N_F^0$ in order to avoid the particular model-dependent density-of-states effect. It would be interesting to examine the $\mathbf{q}$-dependent Landau parameters for the study of the magnetic instabilities and magnetic properties of these models, for which we have to consider explicitly the band-structure effect of α. We have recently derived the phase diagrams for the paramagnetic-to-antiferromagnetic and the paramagnetic-to-ferromagnetic instabilities in the 2D three-band model, which are compared with those in the 2D Hubbard model. The results will be published in a separate forthcoming paper.

In summary, we have derived the magnetic susceptibilities of the Hubbard model and the three-band CuO_2 model in several different methods within the Gaussian fluctuations of the functional integral in the slave-boson approach. We have analyzed the relationships between the two magnetic susceptibilities and the uniform Landau Fermi-liquid parameters $|F_0^a|/\alpha$ ($\alpha \equiv W_0 N_F^0$, N_F^0 the density of states at the Fermi level and W_0 the bare bandwidth) defined from the susceptibility expressions. It has been found that the Landau parameter for the three-band model becomes larger than that for the Hubbard model, indicating a more magnetic model. The reason for this is due to the fact that a larger kinetic energy is stabilized for quasiparticles in the three-band model, which leads to the larger effective magnetic-coupling constants. The Landau parameters in the doped strong-coupling insulator regime of the three-band model are found such that it is always larger for a hole doping than for an electron doping. We have given the explanation for this result using the infinitesimal doping cases. Furthermore, we have found that our Landau parameter expression for the Hubbard model reproduces the T-matrix expression of $|F_0^a|/\alpha = U/W_0/(1+U/W_0)$ for the highly doped low-density limit where the renormalization mechanism is different from that in the dilutely doped high-density regime.

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