Spin-wave spectrum of a two-dimensional itinerant-electron antiferromagnet based on a CuO$_2$ layer: Approximate mapping onto an effective Heisenberg model

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We calculate the spin-wave spectrum of a CuO$_2$ antiferromagnetic layer with one hole per Cu site, as described by a three-band Hubbard model with a local repulsion $U$ at Cu sites, a hopping integral $t$ between Cu and O sites, and a charge-transfer energy $\Delta$ between Cu and O sites, by locating the poles of the transverse spin correlation function at given momentum and frequency within the random-phase approximation. We find that the calculated spin-wave spectrum can be fitted rather accurately over the whole Brillouin zone by the corresponding spectrum of a localized spin-$\frac{1}{2}$ Heisenberg model with a suitably chosen effective exchange coupling $J_{\text{eff}}$, the relative error $\Delta J_{\text{eff}}/J_{\text{eff}}$ introduced by the fitting being smaller than 15% when $\Delta/t + 2U/t \geq 5$. With the values for $U$, $t$, and $\Delta$ appropriate to La$_2$CuO$_4$, we find $J_{\text{eff}} \approx 0.12$ eV and $\Delta J_{\text{eff}}/J_{\text{eff}} \approx 4.5\%$, in good agreement with the estimated experimental values. Our results suggest that some caution is in order when embracing a localized-spin model to describe the magnetic properties of the parent compounds of oxide superconductors.

I. INTRODUCTION

The spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model with spins localized on a square lattice is often used to describe the dynamics of the spin degrees of freedom of undoped copper oxides and, in particular, of La$_2$CuO$_4$. The behavior of this model is controlled by the spin-wave excitations about a state characterized by long-range order. Upon further supplying this model with hole-hopping terms that lead to the $t$-$J$ model or its variations, it is also believed that one can get an appropriate description of the doped materials.

The only parameter of the Heisenberg model is the antiferromagnetic coupling $J_{\text{eff}}$, which can be determined from neutron- and Raman-scattering experiments [for the undoped La$_2$CuO$_4$, one gets typically $J_{\text{eff}} \approx 0.10-0.15$ eV (Ref. 1)]. In particular, Aeppli et al. were able to achieve good enough resolution to measure the spin-wave velocity accurately with about 5% error.

Already back from the work of Izuyama, Kim, and Kubo in ferromagnetic transition metals, however, the fact that neutron-diffraction phenomena could be successfully treated in terms of the localized-spin model had not been regarded as a proof of the unique validity of such a model. The itinerant (or band) -electron model was, in particular, shown to be capable of accounting equally well for the observed diffraction data on ferromagnetic transition metals. The itinerant-electron model of magnetism was shown, furthermore, to provide a good qualitative description of the one-electron properties of transition metals.

More recently, it has been pointed out that the single-band Hubbard model in the strong-coupling limit ($U \gg t$) yields the same behavior as obtained from the linear spin-wave analysis of the spin-$\frac{1}{2}$ Heisenberg model, when quantum spin fluctuations about the (band) Hartree-Fock state are properly included within the random-phase approximation (RPA). In this context the question naturally arises whether or not an itinerant model for antiferromagnets could, as far as the spin excitations are concerned, be mapped onto an effective Heisenberg model under more general circumstances, thereby providing one with a first-principles determination of the exchange integral $J_{\text{eff}}$ of the effective Heisenberg model.

The purpose of this paper is to set quantitative limits to the validity of this approximate mapping well outside the limited region of parameters where the mapping itself is expected to be exact. This will be achieved by comparing the spin-wave spectrum of a specific itinerant-electron model over the whole Brillouin zone with the characteristic spin-wave spectrum of the Heisenberg antiferromagnet as obtained from linear spin-wave theory. The comparison of the two spectra will provide us with an average effective exchange integral ($J_{\text{eff}}$) and with an associated root-mean-square deviation ($\Delta J_{\text{eff}}$). The latter gives an estimate of the overall error of the approximate mapping.

Specifically, we shall determine the spin-wave spectrum of a single CuO$_2$ layer whose one-electron properties are assumed to be described by three orbitals, namely, the $d_{x^2-y^2}$ orbital for copper and the $p_x$ and $p_y$ orbitals for oxygen. In the associated three-band Hubbard model, the relevant parameters are then the local repulsion $U$ at Cu sites, the hopping integral $t$ between Cu and O sites, and the charge-transfer energy $\Delta$ between O and Cu (hole) levels. The importance of introducing the charge-transfer energy $\Delta$ for the family of insulating oxides has been stressed by Zaanan, Sawatzky, and Allen (ZSA), $\Delta$ being directly related to the electronegativity of the anion and to the Madelung potential. Within the ZSA scheme, for $U < \Delta$, the band gap is proportional to $U$ (Mott-Hubbard regime), while for $U > \Delta$ the gap is proportional to $\Delta$ (charge-transfer region). The general consensus for the new superconductors based on CuO$_2$ layers is that
$U > \Delta$ and the first ionization state of the insulator is primarily O 2$p$ in character. Furthermore, with small doping a relatively low density of holes is introduced into the O 2$p$ states, and so it might be appropriate to neglect the local oxygen repulsion.

It turns out from our calculation that the effective exchange integral $J_{\text{eff}}$ (to be inserted into the spin-$\frac{1}{2}$ two-dimensional antiferromagnetic Heisenberg model) can be extracted with good accuracy from the spin-wave spectrum of the two-dimensional itinerant-electron antiferromagnet described above, essentially over the whole positive ($\Delta/t, U/t$) quadrant, with the sole exclusion of a limited region approximately bounded by $\Delta/t + 2U/t = 5$. On the outer boundary of this limited region, the ratio $\Delta J_{\text{eff}}/J_{\text{eff}}$ is at most 15%, and it rapidly decreases for larger values of $\Delta/t$ and $U/t$. Within this limited region the spin-wave spectrum of the itinerant-electron antiferromagnet acquires, in fact, an imaginary part owing to the “spin-wave disappearance phenomenon” that occurs when the spin-wave branch runs into the analog for an antiferromagnet of the Stoner continuum of spin-flip excitations. For the typical values $\Delta/t \approx 1.5$ and $U/t \approx 5.0$, which apply to La$_2$CuO$_4$, we obtain, in particular, $J_{\text{eff}}/t \approx 0.12$ and $\Delta J_{\text{eff}}/J_{\text{eff}} \approx 4.5\%$, in rather good agreement with the experimental value if we take the quoted value $t \approx 1.0$ eV.

Contrary to itinerant-electron ferromagnets, for which band-structure calculations suffice to reproduce the observed magnetic moments, for itinerant-electron antiferromagnets the inclusion of quantum fluctuations is essential for a comparison of the local (staggered) magnetic moment with the experimental value. This is especially true in two dimensions, where in the localized limit ($U/t \approx \infty$ and $\Delta/t \approx \infty$) quantum fluctuations are known to reduce the magnetic moment to about 60% of its nominal saturated value. Itineracy itself reduces the magnetic moment by spreading the wave function from a copper atom into the surrounding oxygens. The effects of quantum fluctuations on an itinerant-electron antiferromagnet need not, however, be as marked as one would naively expect by applying a uniform 60% rescaling over the whole ($\Delta/t, U/t$) quadrant. Rather, the effects of quantum fluctuations will be shown to decrease when itineracy effects get more pronounced, at least for $U/t \approx 10$, when some approximations we shall adopt specifically for the calculation of the magnetic moment hold. In particular, the value 0.35 of the local magnetic moment estimated by our calculation for $\Delta/t$ and $U/t$ corresponding to La$_2$CuO$_4$ is consistent with the experimental value 0.5±0.1 within the experimental error.

Quite generally, the spin-wave spectrum can be obtained for both the localized-spin and the itinerant-electron models by locating the poles of the transverse spin-correlation function at given wave vector and frequency. For the itinerant-electron model we consider, we restrict ourselves to the commonly adopted RPA to solve for the transverse spin-correlation function in a closed form. This approximation is related to the Hartree-Fock antiferromagnetic decoupling for the single-particle energy bands, in order for the approximation to be “conserving.” We shall assume consistently that antiferromagnetic long-range order exists in the ground state. (We expect on physical grounds that the bulk of our results and conclusions would be preserved qualitatively even beyond the RPA.) All calculations will be carried out at zero temperature since the RPA, by neglecting spin-wave interaction, is valid only in this limit. At any nonzero temperature the two-dimensional antiferromagnet is anyhow prohibited from developing long-range order.

The plan of the paper is the following. In Sec. II we derive the equation for the antiferromagnetic spin-wave spectrum of a two-dimensional three-band Hubbard model at zero temperature, by locating the poles of the frequency- and momentum-dependent transverse spin-correlation function. In Sec. III this equation is solved numerically essentially over the whole ($\Delta/t, U/t$) quadrant, and an approximate mapping is established with the spin-wave spectrum of the Heisenberg model. Section IV gives our conclusions. The exact mapping onto the spin-wave spectrum of the Heisenberg model in the limit $U/t \gg 1$ and $\Delta/t \approx 1$ is discussed in Appendix A. In Appendix B the conserving character of the RPA is exploited to show the absence of a gap in the spin-wave spectrum at zero wave vector for all values of $\Delta/t, U/t$ and doping, which sustain the antiferromagnetic Hartree-Fock solution.

II. TRANSVERSE SPIN-CORRELATION FUNCTION AND SPIN-WAVE SPECTRUM OF A TWO-DIMENSIONAL THREE-BAND HUBBARD MODEL WITHIN THE RPA

The spin dynamics of interest to us is embodied in the space and time dependence of the spin-correlation function. At zero temperature this function is defined by the tensor

$$
\chi_{\mu\nu}(rt, r't') = -\frac{i}{\hbar} \langle \mathcal{T}[S_{\mu}(rt)S_{\nu}(r't')] \rangle
$$

$$
+ \frac{i}{\hbar} \langle S_{\mu}(rt) \rangle \langle S_{\nu}(r't') \rangle,
$$

(2.1)

where $\mu$ and $\nu$ denote Cartesian components, the average $\langle \cdots \rangle$ is taken over the ground state of the system, and $\mathcal{T}$ stands for the time-ordering operator. The spin-$\frac{1}{2}$ density operator in Eq. (2.1) is given by

$$
S_{\mu}(rt) = \frac{\hbar}{2} \sum_{\alpha,\beta} \Psi_{\mu\alpha}(rt) \sigma_{\alpha\beta} \Psi_{\beta\nu}(rt)
$$

(2.2)

(\text{where $\sigma^{\alpha}$ are Pauli matrices and $\alpha,\beta = \pm 1$ are spin labels}) and evolves in time via the Heisenberg picture of the field operator, namely,

$$
\Psi_{\alpha}(rt) = e^{iHt/\hbar} \Psi_{\alpha}(r)e^{-iHt/\hbar},
$$

(2.3)

$H$ being the system Hamiltonian.

With the aid of expression (2.2), the spin-correlation function (2.1) can be conveniently expressed in terms of
the two-particle correlation function \( L \), in the form
\[
\chi_{\mu\nu}(r, r') = -\frac{i \hbar^2}{4} \sum_{\alpha, \beta, \beta'} \sum_{\lambda, \lambda'} \alpha_{\alpha \beta}^{\lambda \lambda'} \gamma_{\beta \beta' t'. t} \times \chi(r, r'; r, r') \times L(r, r', r', r''),
\]
(2.4)
where \( t = t + \eta \) with \( \eta = 0^+ \). Quite generally, the two-particle correlation function satisfies the following form of the Bethe-Salpeter integral equation:
\[
L(1, 2, 1', 2') = G(1, 2')G(2, 1') + \int d3d4d5d6 G(1, 3)G(4, 1') \times \Xi(3, 5; 4, 6)L(6, 2, 5, 2'),
\]
(2.5)
where 1, 2, \ldots signify the set of space, spin, and time variables.

\[
G(1, 2) = -\frac{i}{\hbar} \langle \mathcal{T}[\Psi(1)\Psi(2)] \rangle
\]
(2.6)
is the usual single-particle Green's function, and the kernel \( \Xi \) is an effective two-particle interaction. Any approximate functional form for \( \Xi \) must be related to the choice one makes for \( G \) in order for the approximation to be conserving.\(^{10}\) In particular, to the Hartree-Fock approximation for \( G \), there corresponds the RPA decoupling for \( \Xi \), namely,
\[
\Xi(3, 5; 4, 6) = -i\hbar \delta(3, 4) \delta(5, 6) \nu(3, 6)
+ i\hbar \delta(3, 6) \delta(4, 5) \nu(3, 4),
\]
(2.7)
where \( \nu \) is a static and spin-independent interparticle potential:
\[
\nu(1, 2) = \nu(r_1 - r_2) \delta(t_1 - t_2).
\]
(2.8)
As discussed in the Introduction, we shall restrict ourselves to these approximations in the following calculation.

The above expressions can be considerably simplified if we take the system Hamiltonian to be of the Hubbard form with on-site interparticle repulsion only. In particular, we are interested in a single CuO layer described by a Hubbard Hamiltonian with three orbitals per unit cell, namely, the \( d_{x^2-y^2} \) orbital for the copper atom and the \( p_x \) and \( p_y \) orbitals that point toward copper for the oxygen atoms (with suitable phase convention for the orbitals). We thus represent
\[
\Psi_{\alpha}(r) = \sum_{\tau} \left[ \phi_d(r - R) c_{\alpha \tau} + \sum_{\tau} \phi^*_\sigma(r - R) \sigma_{\alpha \tau} \right],
\]
(2.9)
where \( R \) is the lattice vector associated with cell \( i \) and the label \( \tau \) distinguishes the two \( p \) orbitals attached to a given cell. Introducing Bloch sums \( \phi \) for each type of local orbital \( \varphi \) and restricting the Bloch wave vector to the antiferromagnetic Brillouin zone, we can rewrite the field operator in the compact form
\[
\Psi_{\alpha}(r) = \sum_{k} \sum_{\lambda} \phi_{k\lambda}(r) c_{k\alpha}^\lambda,
\]
(2.10)
\[ n_{2d} = \frac{1}{2N} \sum_k \sum_{\alpha} \sum_n f_F(\epsilon_n(k\alpha)) \left[ W^*_{1\alpha}(k\alpha) W^*_{4\alpha}(k\alpha) + W^*_{4\alpha}(k\alpha) W^*_{1\alpha}(k\alpha) \right], \]
\[ \frac{1}{2N} \sum_k \sum_{\alpha} f_F(\epsilon_n(k\alpha)) = \frac{1 + \delta}{2}, \]
where \( f_F(\epsilon) \) is the (zero-temperature) Fermi function and \( \delta \) is the doping parameter introduced to eliminate the chemical potential [which is implicit in the diagonal elements of the matrix (2.14)].

The single-particle Green's function within the Hartree-Fock approximation, to be inserted into the integral equation (2.5), has then the structure
\[ G_{HF}(rt, r't', t') = \delta_{tt'} \left[ G_{HF}^I(r, r'; t) + \alpha G_{HF}^{II}(r, r'; t) \right], \]
with
\[ G_{HF}^I(rt, r't', t') = \frac{i}{\hbar} \sum_k \sum_{\lambda, \lambda'} \phi_{\lambda k}(r) W_{\lambda n}(k) \phi_{\lambda' k}(r') W^*_{\lambda' n}(k) \exp \left[ -\frac{i}{\hbar} \epsilon_n(k)(t - t') \right] \]
\[ \times \left[ \Theta(t - t') [1 - f_F(\epsilon_n(k))] - \Theta(t' - t) f_F(\epsilon_n(k)) \right] \]
\[ \times \left( \langle P_{\lambda} P_{\lambda'} + Q_{\lambda} Q_{\lambda'} \rangle \right), \]
and
\[ \epsilon_n(k\alpha) = \epsilon_n(k). \]

The approximations that lead to the Hubbard Hamiltonian with on-site interparticle repulsion only can be formally introduced into the integral equation (2.5) (or, equivalently, into the associated diagrammatic structure) by replacing the interparticle potential (2.8) with the expression
\[ v(1, 2) = v_0 \delta(r_1 - r_2) \delta(t_1 - t_2) \delta_{\alpha_1 - \alpha_2} \]
and by neglecting the overlap of local orbitals \( \varphi_d \) centered at different sites. The constant \( v_0 \) in Eq. (2.4) is thus related to the Hubbard repulsion \( U \) at Cu sites by
\[ U = v_0 \int d\tau |\varphi_d(\tau)|^4. \]

The replacement (2.24) makes it possible to solve for the spin-correlation function itself in a closed form. In particular, it can be shown that the transverse spin-\( \frac{1}{2} \) correlation function, defined by
\[ \chi_T^T(rt, r't') = \chi_T^{(0)}(rt, r't') - \frac{v_0}{\hbar^2} \int d\tau'' dt'' \chi_T^{(0)}(rt, r''t'') \chi_T^{T}(r''t', r't'') \]
(2.27)
In this expression the "bare" transverse spin-\( \frac{1}{2} \) correlation function can be obtained in terms of the single-particle Green's functions (2.21) as follows:
\[ \chi_T^{(0)}(rt, r't') = -i\hbar \left[ G_{HF}^I(rt, r't') G_{HF}^{II}(r't', rt) - G_{HF}^{II}(rt, r't') G_{HF}^I(r't', rt) \right] \]
\[ + \alpha i \hbar \left[ G_{HF}^I(rt, r't') G_{HF}^{II}(r't', rt) - G_{HF}^{II}(rt, r't') G_{HF}^I(r't', rt) \right]. \]
(2.28)

It is, in fact, enough to consider the function (2.26) since collective spin-wave modes develop as singularities of the Fourier transform of the spin correlators transverse to the broken-symmetry axis.\(^\text{11}\)

To solve Eq. (2.27), we take its space and time Fourier transform and introduce the notation
\[ \chi_T^T(q, q'; \omega) = \int d(t - t') e^{i\omega(t - t')} \frac{1}{V} \int dr dr' \int d\tau d\tau' e^{-iq\tau} \chi_T^T(rt, r't') e^{iq'\tau'} \]
\[ = \frac{1}{V_0} \sum_{\lambda, \lambda', \lambda''} A_{\lambda\lambda'}(q) \chi_T^T(\lambda\lambda', \lambda''; q, q'; \omega) A^*_{\lambda''\lambda}(-q'), \]
(2.29)
where $V$ and $V_0$ are the (two-dimensional) areas of the system and of the atomic unit cell, respectively, and
\[ A_{\lambda}(q) = \int d\tau \varphi_\lambda(\tau) e^{-iqr} \varphi_\lambda^*(\tau) \] (2.30)
are form factors. The integral equation (2.27) can now be reduced to a matrix equation for the elements $\chi^{(0)}_{\lambda}(\lambda',\lambda'';q,q';\omega)$ for given values of $q$, $q'$, and $\omega$. Among these elements, we shall consider in particular the subset with purely $d$ character, by neglecting the mixed form factors (2.30) between $d$ and $p$ orbitals and by recalling that $U_\sigma$ is not included in the present calculation. Let $f_{\alpha}(q,q';\omega)$ be the sum of all 16 elements $\chi^{(0)}_{\lambda}(\lambda',\lambda'';q,q';\omega)$ with purely $d$ character. Solution of the matrix equation then yields
\[ f_{\alpha}(q,q';\omega) = [f_{\alpha}^{(0)}(q,q';\omega) + \alpha f_{\alpha}^{(0)}(q-q,Q,q';\omega)] / D(q,q') \] (2.31)

Here
\[ a(q,q',\omega) = \frac{1}{N} \sum_{k} \sum_{n,n'} \left[ \frac{1 - f_{\alpha}(e_n(k))}{\hbar\omega - e_n(k) + e_n(k-q) + i\eta} - \frac{f_{\alpha}(e_n(k))}{\hbar\omega - e_n(k) + e_n(k-q) - i\eta} \right] \times \left[ W_{1n}(k) W_{1n}(k-q) - W_{4n}(k) W_{4n}(k-q) \right]^2, \] (2.32)
\[ b(q,q',\omega) = \frac{1}{N} \sum_{k} \sum_{n,n'} \left[ \frac{1 - f_{\alpha}(e_n(k))}{\hbar\omega - e_n(k) + e_n(k-q) + i\eta} - \frac{f_{\alpha}(e_n(k))}{\hbar\omega - e_n(k) + e_n(k-q) - i\eta} \right] \times \left[ W_{1n}(k) W_{1n}(k-q) - W_{4n}(k) W_{4n}(k-q) \right] \] (2.33)
and
\[ D(q,q',\omega) = [1 + Ua(q,q',\omega)][1 + Ua(q-q,Q,q',\omega)] - U^2b^2(q,q'), \] (2.34)

while
\[ \frac{1}{\hbar^2} f_{\alpha}^{(0)}(q,q';\omega) = \Delta(q,q') a(q,q') + \alpha \Delta(q,q'-Q) b(q,q') \] (2.35)
is the bare counterpart of $f_{\alpha}(q,q';\omega)$ [$\Delta(q,q')$ being the Kronecker delta function of the Bravais lattice]. The spin-wave spectrum $\Omega(q)$ results from the zeros of the denominator $D(q,q')$ in Eq. (2.31). Note that real solutions are obtained for given $q$ provided that the energy denominators in Eqs. (2.32) and (2.33) never vanish. Note also that $a(q,q',\omega)$ is even while $b(q,q',\omega)$ is odd in $\omega$.

The equation $D(q,q',\omega) = 0$ generalizes to the present context the known spin-wave equation for a single-band Hubbard model in the RPA, to which it readily reduces by properly identifying the notation. Inclusion of the charge-transfer gap $\Delta$, however, may affect considerably the spin-wave spectrum depending on the region of the ($\Delta/t, U/t$) quadrant. Detailed numerical calculations essentially over the whole quadrant will be presented in the next section, while in Appendix A we shall discuss the asymptotic region $U/t \gg 1$ and $\Delta/t \geq 1$ analytically.

We pass now to show how the reduction of the local (staggered) magnetic moment due to quantum fluctuations results for the itinerant-electron antiferromagnet we are considering. Quite generally, the local (staggered) magnetic moment at Cu sites can be related to the single-particle Green’s function by the expression
\[ m_S = \frac{1}{N} \sum_{\alpha} \sum_{\gamma} \alpha \langle d_{\gamma \alpha}^d d_{\gamma \alpha}^d \rangle e^{iQ \cdot R_\alpha} \] (2.36)
[with the convention (2.11)], where
\[ \langle G(k\alpha, \omega) \rangle_{\lambda,\lambda'}, \] (2.37)
\[ = \int d\tau d\tau' \phi_{\lambda,\lambda'}(\tau) G(\tau, \tau'; \omega) \phi_{\lambda,\lambda'}(\tau'). \]
At the level of the Hartree-Fock approximation, $\langle G(k\alpha, \omega) \rangle_{\lambda,\lambda'}$ is given by the inverse of the matrix $\hbar \omega \delta_{\lambda,\lambda'} - [M(k\alpha)]_{\lambda,\lambda'}$, where $M$ is the Hamiltonian matrix of Eq. (2.12) (with the understanding that the correct time-ordered boundary conditions have to be retained when taking the inverse). One recovers the well-known result
\[ m_S^{HF} = 2n_{2d}, \] (2.38)
where $n_{2d}$ is the Hartree-Fock self-consistent parameter given by Eq. (2.18). No quantum fluctuations are retained at this level, and consistently $m_S^{HF} \approx 1$ at zero doping in the localized limit $U/t \approx \infty$ and $\Delta/t \approx \infty$. The effect of quantum fluctuations appears when self-energy
corrections beyond the Hartree-Fock approximation are included. Consider, in particular, the effect of transverse spin fluctuations on the self-energy, as depicted in the diagrams of Fig. 1. This series can be readily summed, to yield

\[
\left[\Sigma_T^{\alpha}(k\alpha,\omega)\right]_{11} \Sigma_T^{\alpha}(k\alpha,\omega)\right]_{44} = U^2 i \Phi \sum_n \sum_{k'} \int \frac{d\omega'}{2\pi} \frac{F_n(k-k',\omega-\omega')}{D(k',\omega')} \left[\begin{array}{c}
W_{in}(k-k') \\
W_{4n}(k-k')
\end{array}\right]\left[\begin{array}{c}
W_{in}(k-k') \\
W_{4n}(k-k')
\end{array}\right],
\]

where \( b \) and \( D \) are given by Eqs. (2.33) and (2.34), respectively, and \( c \) is defined by

\[
c(k,\omega) = a(k,\omega)[1 + U a(k-Q,\omega)] - U b^2(k,\omega),
\]

with \( a \) given by Eq. (2.32) and with the notation

\[
F_n(k,\omega) = \frac{1 - f_n(\varepsilon_n(k))}{\hbar \omega - \varepsilon_n(k) + i\eta} + \frac{f_n(\varepsilon_n(k))}{\hbar \omega - \varepsilon_n(k) - i\eta}.
\]

Within the current approximation of retaining \( U \) only at the Cu sites, the matrix elements \( \left[\Sigma_T(k\alpha,\omega)\right]_{\lambda\lambda'} \) different from (2.40) vanish.

The matrix elements \( \left[G(k\alpha,\omega)\right]_{\lambda\lambda'} \) to be inserted in the expression (2.36) for the local magnetic moment at Cu sites are now obtained by inverting the matrix

\[
\hbar \omega \delta_{\lambda\lambda'} - \left[M(k\alpha)\right]_{\lambda\lambda'} - \left[\Sigma_T(k\alpha,\omega)\right]_{\lambda\lambda'}.
\]

To be consistent with the free-spin-wave approximation to the Heisenberg model in the localized limit,\(^14\) it is actually sufficient to invert this matrix to lowest significant order in \( \Sigma_T \). Thus we take

\[
\left[G(k\alpha,\omega)\right]_{\lambda\lambda'} = \left[G_{HF}(k\alpha,\omega)\right]_{\lambda\lambda'} + \sum_{\lambda'',\lambda'''} \left[G_{HF}(k\alpha,\omega)\right]_{\lambda\lambda''} \left[\Sigma_T(k\alpha,\omega)\right]_{\lambda\lambda''}.
\]

III. RESULTS AND DISCUSSION

In the previous section we have established a procedure to determine the spin-wave spectrum \( \Omega(q) \) over the whole Brillouin zone of a three-band Hubbard model within the RPA for all values of the parameters \( \Delta/t \) and \( U/t \) of that model and for arbitrary doping. It is further shown in Appendix A that, in the limit \( U/t \gg 1 \) and \( \Delta/t \gg 1 \) at zero doping, \( \Omega(q) \) acquires the simple form

\[
\hbar \Omega(q) = 2J_{eff}(t/\Delta) \left|1 - [\Gamma(q)]^2\right|^{1/2},
\]

where the prefactor \( J_{eff}(t/\Delta) \) is independent of \( q \) and \( \Gamma(q) \) given by Eq. (A.17) is the normalized structure factor characteristic of the two-dimensional Heisenberg model. The \( q \) dependence in Eq. (3.1), which coincides with the dispersion obtained by the spin-wave theory of the two-dimensional Heisenberg model, thus suggests the following procedure for arbitrary values of \( \Delta/t, U/t \) and of doping.

Without loss of generality, one can always cast (the real part of) the spin-wave spectrum \( \Omega(q) \) obtained by the procedure of Sec. II in the form\(^15\)

\[
\hbar \Omega(q) = 2J_{eff}(q)\left|1 - [\Gamma(q)]^2\right|^{1/2},
\]

where the function \( J_{eff}(q) \) is suitably chosen to reproduce the correct \( q \) dependence of \( \Omega(q) \) over the whole Brillouin zone, for given values of the parameters \( \Delta/t \) and \( U/t \) and of doping. In practice, not much would be gained by disentangling the characteristic \( q \) dependence of the Heisenberg model from the full spin-wave disper-
sion in Eq. (3.2), unless it turns out that the $q$ dependence of $J_{\text{eff}}(q)$ is rather weak. If this is the case, the values of $J_{\text{eff}}(q)$ lie close to the mean value,

$$J_{\text{eff}} = \frac{2}{N} \sum_q J_{\text{eff}}(q),$$  

(3.3)

with a small standard deviation

$$\Delta J_{\text{eff}} = \left[ \frac{2}{N} \sum_q [J_{\text{eff}}(q) - J_{\text{eff}}]^2 \right]^{1/2}. \quad (3.4)$$

$J_{\text{eff}}$ obtained from Eqs. (3.2) and (3.3) at zero doping is plotted in Fig. 2 versus $\Delta/t$ and $U/t$ over a wide range of values that extend to the region where the $q$ dependence of $J_{\text{eff}}(q)$ can be noticed, with the exclusion of a limited region bounded by $\Delta/t + 2U/t = 5$, where the spin-wave spectrum acquires an imaginary part near the boundary of the Brillouin zone. The corresponding relative standard deviation $\Delta J_{\text{eff}}/J_{\text{eff}}$ obtained from Eqs. (3.3) and (3.4) is plotted in Fig. 3. This figure shows, in particular, that $\Delta J_{\text{eff}}/J_{\text{eff}}$ is at most of the order 15% and thus that the details of the $q$ dependence of $J_{\text{eff}}(q)$ in Eq. (3.2) can be disregarded within this overall accuracy for the reported range of $\Delta/t$ and $U/t$. A more detailed look at the goodness of the fit of the spin-wave spectrum $\Omega(q)$ by the simplified expression $2J_{\text{eff}}[1-(\Gamma(q))^2]^{1/2}$ is shown in Fig. 4 along the symmetry lines of the Brillouin zone for two characteristic sets of values ($\Delta/t, U/t$) corresponding (a) to the estimated parameters for $\text{La}_x\text{CuO}_4$ (Ref. 16) and (b) to the boundary of the region where the fit can be applied. In both cases we see that the fit approximates rather well the original spin-wave spectrum on the average, although sizable differences begin to appear on the boundary of the Brillouin zone when $\Delta/t$ and $U/t$ approach the line $\Delta/t + 2U/t = 5$.

These results show that, as far as the spin excitations are concerned, the itinerant antiferromagnetic system we are considering can be properly mapped onto an effective localized Heisenberg model with a suitable identification of the effective exchange integral $J_{\text{eff}}$. This conclusion does not necessarily mean, however, that the system itself bears magnetic moments localized at the copper sites with negligible spread over the surrounding oxygen atoms. Rather, it turns out that the $q$ independence of $J_{\text{eff}}(q)$ discussed above is compatible with a substantial $p$

FIG. 2. Effective mean exchange integral $J_{\text{eff}}/t$ vs $\Delta/t$ and $U/t$ at zero doping.

FIG. 3. Relative standard deviation $\Delta J_{\text{eff}}/J_{\text{eff}}$ vs $\Delta/t$ and $U/t$ at zero doping.

FIG. 4. Spin-wave energy $\Omega(q)/t$ (solid line) compared with the Heisenberg-type expression $2J_{\text{eff}}[1-(\Gamma(q))^2]^{1/2}/t$ (dashed line) along the symmetry lines of the Brillouin zone for (a) $\Delta/t = 1.5$ and $U/t = 5.0$ and (b) $\Delta/t = 1.0$ and $U/t = 2.0$ at zero doping.
FIG. 5. d percentage at the Fermi level of the Hartree-Fock bands vs Δ/t and U/t at zero doping.

component in the electronic wave function. This feature is shown in Fig. 5, where the d percentage at the Fermi level is seen to decrease to about 58% near the region Δ/t ≈ 1 and U/t ≈ 2 where the maximum ΔJₐeff/Jₐeff occurs and to 66% for the La₂CuO₄ parameters, consistently with cluster calculations on the same material.¹⁷ Note also that the d percentage depends only weakly on U/t.

Several additional features can be noted from the above figures. From Fig. 2 one sees that the dependence of Jₐeff on Δ/t is considerably more pronounced than the dependence on U/t, suggesting that the crossover from “weak” to “strong-coupling” regimes is driven more quickly by Δ/t than by U/t. One notes also from Fig. 2 that near the boundary Δ/t + 2U/t = 5 of the excluded region the values of Jₐeff/t are quite substantial (if we take t ∼ 1.0 eV) on the scale of conventional magnetic couplings. This finding is consistent with experimental data on cuprates. In particular, for the parameters corresponding to La₂CuO₄, we obtain Jₐeff/t ≈ 0.12, in good agreement with the value obtained by neutron and Raman scattering.¹² For the same parameters we also obtain from Fig. 3 the value ΔJₐeff/Jₐeff = 4.5%, which agrees with the bound set on the experimental determination of the spin-wave velocity in that material.²

The calculation of the reduction of the local (staggered) magnetic moment due to transverse spin fluctuations according to Eqs. (2.36)–(2.43) can be considerably simplified if we exploit the results obtained above and in Appendix A for the mapping onto an effective Heisenberg model. We thus replace the quantities a(1k, ω) and b(1k, ω) entering expression (2.40) for the self-energy by their expressions that hold in the limit U/t >> 1 and Δ/t ≥ 1 (cf. Appendix A) with Jₐeff appropriate to the chosen values of Δ/t and U/t. In this way the frequency integrations in Eqs. (2.40) and (2.36) can be performed analytically and the numerical effort reduces to evaluating sums over wave vectors. The effect of itineracy on mₛ is then contained in the k dependence of the eigenvalues and eigenvectors of the Hartree-Fock matrix of Eq. (2.12) in the factor 1b of Eq. (A14) and in the appropriate value of Jₐeff.¹⁸ Owing to these approximations, our calculation for mₛ is expected to provide reliable estimates only when U/t is large enough, say, U/t ≥ 10.

The ratio (mₐHF − mₛ)/mₐHF at zero doping is shown in Fig. 6(a) versus Δ/t and U/t, while in Fig. 6(b) the reference Hartree-Fock value mₐHF is reported. Note that the ratio (mₐHF − mₛ)/mₐHF decreases from the value 0.39 in the localized-spin limit (U/t ∼ ∞ and Δ/t ∼ ∞) to 0.25 when Δ/t ≈ 1 and U/t ≈ 10, with mₐHF decreasing from 1.0 to 0.6 correspondingly. Transverse spin fluctuations have thus a less marked effect on mₛ when itineracy is more pronounced, resulting in a nonuniform rescaling of mₛ by decreasing Δ/t (at least when U/t is sufficiently large) and in values of mₛ which are not too sensitive to Δ/t. For the parameters corresponding to La₂CuO₄, we obtain mₐHF ≈ 0.59 and the estimate mₛ ≈ 0.35, which is consistent with the experimental value 0.5 ± 0.1,¹ although a more refined calculation might reduce the difference.¹⁸

FIG. 6. (a) (mₐHF − mₛ)/mₐHF and (b) mₐHF vs Δ/t and U/t at zero doping, showing the combined effects of itineracy and of transverse spin fluctuations on the local (staggered) moment.
IV. CONCLUDING REMARKS

In this paper we have examined to what extent one can use an effective Heisenberg model (with a suitably chosen exchange coupling) to reproduce the spin-wave spectrum of a two-dimensional itinerant antiferromagnet described by a three-band Hubbard model. We have shown that the overall accuracy achieved by the fit (in the case of zero doping) can be good enough whenever \( \Delta / t + 2U / t \gtrsim 5 \), so that it would be admittedly difficult to detect band-structure (itinerary) effects by measuring the spin-wave spectrum or related physical quantities for many transition-metal compounds characterized via the Zaanen-Sawatzky-Allen scheme. This conclusion actually holds in spite of the strong chemical mixing between the metal ion and its surroundings, which does not allow the magnetic moments to be completely localized at the metal sites.

Nonetheless, we have also shown that differences between the spin-wave spectra obtained by the localized-spin and itinerant-electron approaches may be revealed near the boundary of the Brillouin zone, where the spectra obtained by the two approaches differ most markedly and where the “spin-wave disappearance phenomenon” is bound to occur. This remark implies that, while short-wavelength magnons can be affected by band-structure effects, long-wavelength magnons are not.

We have based our calculation on the random-phase approximation for the spin-correlation function, which does not obviously exhaust all effects of the electron correlation (especially for large values of \( U / t \)). By analogy with recent results\(^{19}\) for the one-band Hubbard model, however, we expect that most of our conclusions might be preserved beyond the RPA by properly renormalizing the parameters of the three-band Hubbard model, although an explicit renormalization procedure is not yet known.

We comment, finally, that the value 0.61, which we have quoted for the zero-temperature magnetic moment \( m_s \) of the two-dimensional Heisenberg antiferromagnet, is obtained by linear-spin-wave theory\(^{14}\) and thus does not necessarily represent an absolute upper bound on \( m_s \). Improved approximations for the Heisenberg model give, in fact, a larger value (= 0.72) for \( m_s \).\(^{20}\) It would, therefore, not be surprising that even experimental values for \( m_s \) larger than 0.5 are compatible with a description of the spin dynamics in terms of an itinerant-electron model.

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APPENDIX A: ANALYTIC RESULTS IN THE LIMIT \( U / t \gg 1 \) AND \( \Delta / t \gtrsim 1 \)

The zeros of the function \( D(q, \omega) \) given by Eq. (2.34), which yield the spin-wave spectrum \( \Omega(q) \), can be determined analytically in the limit \( U / t \gg 1 \) and \( \Delta / t \gtrsim 1 \) as follows.

In this limit the calculation of the quantities \( a(q, \omega) \) and \( b(q, \omega) \) that enter the expression of \( D(q, \omega) \) proceeds over a frequency range where the energy denominators of Eqs. (2.32) and (2.33) never vanish. We can then ignore the infinitesimal imaginary part therein and reduce the expression within square brackets to

\[
\left[ \cdots \right] \to \frac{f_F(e_n(k-q)) - f_F(e_n(k))}{\hbar \omega - e_n(k) + e_n(k-q)}.
\]

(A1)

To find the eigenvalues and eigenvectors of the Hartree-Fock Hamiltonian matrix (2.13)–(2.15), which are needed in Eqs. (2.32) and (2.33), in the limit of interest, it is convenient to perform at the outset the following transformations on that matrix.

A bonding-nonbonding decoupling within the \( p \) sub-space can be achieved by transforming each diagonal block of Eq. (2.13) via the matrix

\[
V_b(q) = \begin{pmatrix}
2\gamma(q) & 0 & 0 \\
0 & \tau_\uparrow(q) & -\tau_\downarrow(q) \\
0 & \tau_\downarrow(q) & \tau_\uparrow(q)
\end{pmatrix},
\]

(A2)

where \( q \) equals \( k \) for the upper and \( k-Q \) for the lower diagonal block, respectively, and where we have set

\[
\gamma(q) = \left( \sin^2(k_x a) + \sin^2(k_y a) \right)^{1/2}.
\]

(A3)

In this way the matrix \( A(q) \) given by Eq. (2.14) is replaced by the real matrix

\[
A'(q) = \begin{pmatrix}
\epsilon_d + Un_{1d} & 2\gamma(q) & 0 \\
2\gamma(q) & \epsilon_p & 0 \\
0 & 0 & \epsilon_p
\end{pmatrix},
\]

(A4)

while the eigenvector components \( W_{1n} \) and \( W_{4n} \) needed in Eqs. (2.32) and (2.33) are left untouched by the transformation. (For the same reason, these components can be taken to be real.) Note that the nonbonding combination of \( p \) orbitals does not couple with the \( d \) orbitals and can be dismissed from further consideration.

It is also convenient to eliminate the off-diagonal \( U \) terms from the Hamiltonian matrix by making even and odd combinations of the \( d \) components. With a suitable rearrangement of the indices, the matrix to be diagonalized eventually reduces to

\[
K(k) = \begin{pmatrix}
\epsilon_d + Un_{1d} - n_{2d} & u(k) & v(k) & 0 \\
u(k) & \epsilon_p & 0 & u(k) \\
v(k) & 0 & \epsilon_p & -v(k) \\
0 & u(k) & -v(k) & \epsilon_d + Un_{1d} + n_{2d}
\end{pmatrix}.
\]

(A5)
with the notation $u(k) = \sqrt{2}\gamma(k)$ and $v(k) = \sqrt{2}\gamma(k-Q)$. Let $Z(k)$ be the orthogonal matrix which diagonalizes $K(k)$. The matrix elements needed in the expressions (2.32) and (2.33) are then given by

$$W_{1n}(k) = \frac{1}{\sqrt{2}}[Z_{1n}(k) + Z_{4n}(k)] , \quad (A6a)$$

$$W_{4n}(k) = \frac{1}{\sqrt{2}}[Z_{1n}(k) - Z_{4n}(k)] . \quad (A6b)$$

The self-consistent parameters $n_{1d}$ and $n_{2d}$ of Eq. (A5) can also be expressed in terms of the matrix $Z$, in the form [cf. Eqs. (2.17) and (2.18)]

$$n_{1d} + n_{2d} = \frac{2}{N} \sum_{k} \sum_{n} f_{f}(e_{n}(k))Z_{1n}^{2}(k) , \quad (A7)$$

$$n_{1d} - n_{2d} = \frac{2}{N} \sum_{k} \sum_{n} f_{f}(e_{n}(k))Z_{4n}^{2}(k) . \quad (A8)$$

The transformations performed thus far are still exact. We now consider the limit $U/t \gg 1$ explicitly at zero doping. In this limit the dominant ($\sim U$) matrix element in (A5) is $K_{44}$ since it turns out that $n_{1d} + n_{2d} \sim \text{const}$ while $n_{1d} - n_{2d} \sim 1/U^2$. For this reason perturbation theory in $t/U$ can be conveniently organized by prediagonalizing the upper $3 \times 3$ diagonal block of $K$, which is degenerate at the leading order in $U$. Let $K^{0}$ be the $4 \times 4$ matrix obtained from the matrix $K$ by neglecting the elements $K_{4j}$ with $j = 1, 2, 3$, which mix the threfold-degenerate level with the level split off by $U$. Corrections to all eigenvalues of this matrix due to the remnant $K-K^{0}$ are of order $1/U$, while the only eigenvector components with $1/U$ corrections are $Z_{4n}$, with $n=1, 2, 3$, and $Z_{44}$, with $j=1, 2, 3$ (all other components having $1/U^2$ corrections). To the leading order we obtain, for the matrix that diagonalizes $K^{0}$,

$$Z^{0}(k) = \begin{pmatrix}
S_{-} & 0 & 0 & 0 \\
(4t^2 + S_{-}^2)^{1/2} & 0 & 0 & 0 \\
0 & -v(k) & u(k) & 0 \\
(4t^2 + S_{+}^2)^{1/2} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
\end{pmatrix} , \quad (A9)$$

with $S_{\pm} = \left[-\Delta \Delta^2 + 16t^2 \right]^{1/2}$, while we obtain

$$\delta Z_{4n} = \frac{1}{U(n_{1d} + n_{2d})} \times \begin{pmatrix}
\frac{u^{2}(k) - v^{2}(k)}{(4t^2 + S_{-}^2)^{1/2}} , & n = 1 \\
-\frac{u(k)v(k)}{t} , & n = 2 \\
\frac{u^{2}(k) - v^{2}(k)}{(4t^2 + S_{+}^2)^{1/2}} , & n = 3 \\
\end{pmatrix} \quad (A10)$$

for its $1/U$ corrections.

It is clear that, in the limit $U/t \gg 1$, the expression (2.34) for $D(q, \omega)$ will have meaningful zeros provided $1 + Ua \sim 1/U$ and $b \sim 1/U^2$. It can be, in fact, verified that

$$a(q, \omega) = -\frac{1}{U} - \frac{\epsilon_{e}^{0} - \epsilon_{d}}{U^2(n_{1d} + n_{2d})} + \frac{2}{N} \sum_{k} \sum_{n=2, 3} \frac{\epsilon_{e}^{0} - \epsilon_{d}^{0}}{\left(\epsilon_{e}^{0} - \epsilon_{d}^{0}\right)^2 - \left(\epsilon_{e}^{0} - \epsilon_{d}^{0}\right)^2} \left[Z_{11}^{0}(k)\delta Z_{4n}(k-q) + Z_{1n}^{0}(k-q)\delta Z_{41}(k)\right] \quad (A11)$$

and

$$b(q, \omega) = -\frac{\hbar \omega}{U^2(n_{1d} + n_{2d})} + \frac{2}{N} \sum_{k} \sum_{n=2, 3} \frac{\hbar \omega}{\left(\epsilon_{e}^{0} - \epsilon_{d}^{0}\right)^2 - \left(\epsilon_{e}^{0} - \epsilon_{d}^{0}\right)^2} \left[Z_{11}^{0}(k)\delta Z_{4n}(k-q) - Z_{1n}^{0}(k-q)\delta Z_{41}(k)\right] \quad , \quad (A12)$$

to the leading significant order, where $\epsilon_{e}^{0}$ are the $k$-independent eigenvalues of the matrix $K^{0}$.

Further progress is achieved by neglecting the term $\left(\hbar \omega\right)^2$ in the energy denominators of Eqs. (A11) and (A12). Since this approximation introduces only errors of order $(t/\Delta)^{3}$, for the following results to hold, it is enough that $\Delta/t \gg 1$. In this way we obtain

$$1 + Ua(q, \omega) \approx \frac{1}{2U} \frac{S_{+}^2}{S_{+} - S_{-}} \gamma^2(q-Q) \quad (A13)$$

and

$$b(q, \omega) \approx \frac{\hbar \omega}{U^2} \left[ \frac{S_{+} - S_{-}}{S_{-}} \frac{1}{S_{+} - S_{-}} \left[ \frac{3}{4} S_{+} \Delta^2 + t^2(\Delta + 12S_{+}) \right] \right] \equiv \frac{\hbar \omega}{U^2} \tilde{b} , \quad (A14)$$

where the coefficient $\tilde{b}$ depends on $t/\Delta$. The spin-wave equation $D(q, \omega) = 0$ thus becomes
\[
\frac{1}{4} \left( \frac{S_+^2}{S_+ - S_-} \right) ^2 \gamma^2(q-Q)\gamma^2(q) = (\mathbf{q})^2 \text{b}^2,
\]  
\tag{A15}

where \(\text{cf. Eq. (A3)}\)

\[
\gamma^2(q-Q)\gamma^2(q) = [\cos^2(q_x a) + \cos^2(q_y a)] [\sin^2(q_x a) + \sin^2(q_y a)]
\]

\[
= [1 + \frac{1}{2}\cos(2q_x a) + \frac{1}{2}\cos(2q_y a)] [1 - \frac{1}{2}\cos(2q_x a) - \frac{1}{2}\cos(2q_y a)]
\]

\[
= 1 - [\Gamma(q)]^2.
\]  
\tag{A16}

In this expression the quantity

\[
\Gamma(q) = \frac{1}{2}[\cos(2q_x a) + \cos(2q_y a)]
\]  
\tag{A17}

refers to the network of the (magnetic) Cu sites at a distance 2\(a\) apart and yields the characteristic \(q\) dependence of the spin-wave spectrum of the two-dimensional Heisenberg model. From Eq. (A15) we, in fact obtain

\[
\mathbf{q}\Omega(q) = 2\mathbf{q}\text{eff}(t/\Delta)\sqrt{1 - [\Gamma(q)]^2},
\]  
\tag{A18}

where the prefactor

\[
\text{eff}(t/\Delta) = \frac{1}{4|b|} \left( \frac{S_+^2}{S_+ - S_-} \right)
\]  
\tag{A19}

is \(q\) independent and plays the role of the exchange integral of an effective Heisenberg model. In particular, to leading order in \(\Delta/t\), we recover from Eq. (A19) the well-known perturbative expression for the three-band Hubbard model when \(U/t \approx \infty\) and \(\Delta/t\) is large, namely,

\[
\text{eff}(t/\Delta) \approx \frac{4t^5}{\Delta^3}.
\]  
\tag{A20}

The limit \(U/t \gg 1\) and \(\Delta/t \gtrsim 1\) discussed here is relevant to the charge-transfer region of the ZSA scheme. In the complementary limit \(\Delta/t \gg 1\) and \(U/t\) arbitrary (which is relevant instead to the Mott-Hubbard region of the ZSA scheme), the three-band Hubbard model that we have considered throughout this paper reduces to the one-band Hubbard model with effective hopping integral \(t_{\text{eff}} = t^2/\Delta\) between two copper atoms at a distance 2\(a\) apart. We have verified numerically that the effective exchange coupling obtained by our calculation in the limit \(\Delta/t \gg 1\) coincides with the results reported in Refs. 6 and 7 with the appropriate rescaling \(U/t \rightarrow U/t_{\text{eff}}\) for the parameter of the one-band Hubbard model. We then refer to the above papers for the analytic results in this limit.

**APPENDIX B: PROOF OF THE ABSENCE OF A GAP IN THE SPIN-WAVE SPECTRUM**

Direct inspection of the denominator \(D(q, \omega)\) in the transverse spin-correlation function suffices to establish that \(\Omega(q=0)=0\) at the RPA level of the one-band Hubbard model for which a closed-form solution is available.\(^6,7\) In this case, in fact, one can readily verify that \(D(q, \omega)=0\) in the limit \(q=0\) and \(\omega=0\) for all values of \(U/t\) and doping \(\delta\), provided that the one-electron energies and wave functions entering the definition of \(D(q, \omega)\) are taken consistently within the antiferromagnetic Hartree-Fock approximation.

Extension of this argument to the three-band Hubbard model considered in this paper proceeds along the following lines. To prove that \(D(q, \omega)\) given by Eq. (2.34) vanishes for \(q=0\) and \(\omega=0\), it is sufficient to show that either one of the two factors \(1 + \text{Ua}(0, 0)\) or \(1 + \text{Ua}(Q, 0)\) vanishes since \(b(q, \omega)\) is an odd function of \(\omega\). The results of Appendix A, and in particular Eq. (A13) that holds at zero doping, show that only the factor \(1 + \text{Ua}(Q, 0)\) vanishes in the limit \(U/t \gg 1\) and \(\Delta/t \gtrsim 1\). To establish that \(1 + \text{Ua}(Q, 0)=0\) for all values of \(\Delta/t\), \(U/t\), and \(\delta\) which sustain the antiferromagnetic Hartree-Fock solution, we manipulate the self-consistent antiferromagnetic condition (2.18) by expressing it in terms of the eigenvectors \(\overline{W}(k)\) of the matrix

\[
\bar{\mathbf{M}}(k) = \begin{pmatrix} A(k) & e^{-i\varphi}B \\ e^{i\varphi}B & A(k-Q) \end{pmatrix},
\]  
\tag{B1}

where the \(3 \times 3\) blocks \(A(k)\) and \(B\) are given by Eqs. (2.14) and (2.15), respectively, and \(\varphi\) is an arbitrary real constant. Condition (2.18) can thus be rewritten in the form

\[
e^{i\varphi}i_{\text{2d}} = \frac{2}{N} \sum_k \sum_n f_p (\epsilon_n(k)) \overline{W}^*_{1n}(k) \overline{W}_{4n}(k),
\]  
\tag{B2}

with the same eigenvalues \(\epsilon_n(k)\) of the matrix (2.13) (with \(\alpha=+1\)). Equation (B2) holds, in particular, for **infinitesimal** values of \(\varphi\). Comparing linear terms in \(\varphi\) on both sides then yields

\[
i\varphi n_{\text{2d}} = \frac{2}{N} \sum_k \sum_n f_p (\epsilon_n(k)) [\delta \overline{W}^*_{1n}(k) W_{4n}(k) + W_{1n}(k) \delta \overline{W}_{4n}(k)],
\]  
\tag{B3}
where the corrections $\delta \bar{W}_{\lambda n}(k)$ can be calculated from first-order perturbation theory. One obtains eventually the expression

$$1 + U \frac{2}{N} \sum_k \sum_n f_k(e_n(k)) \sum_{n' \neq n} \frac{1}{e_n(k) - e_{n'}(k)} \times [W'_{1n}(k) W'_{4n}(k) - W'_{1n}(k) W_{4n}(k)]^2 = 0,$$

whenever $n_{2d}$ is nonvanishing. Upon symmetrizing Eq. (B4) with respect to the band labels and recalling that $W_{4n}(k) = W'_{1n}(k - Q)$ as well as the definition (2.32), Eq. (B4) provides the desired result $1 + Ua(Q,0) = 0$. Note, finally, that this result coincides with the antiferromagnetic instability condition when merging from the paramagnetic phase.

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1. For a recent review, see E. Manousakis, Rev. Mod. Phys. 63, 1 (1991), and references therein.
12. Time-ordered boundary conditions can be replaced with retarded ones in Eqs. (2.32) and (2.33) by letting $\omega \to \omega + i\eta$ in both denominators.
13. In what follows all single-particle Green's functions will be approximated by their Hartree-Fock expressions (2.20) and (2.21).
15. We always find numerically that $\Omega(q=0) = 0$, in agreement with the general argument of Appendix B.
16. Within the Hartree-Fock approximation, the antiferromagnetic single-particle gap differs only slightly from the input parameter $\Delta$ when $U/t = 5$.
18. Expressions (A13) and (A14) for $a(k,\omega)$ and $b(k,\omega)$, respectively, hold in the limit $U/t \gg 1$ and $\Delta/t \gtrsim 1$, where the functional form of the transverse spin-correlation function is rescaled by the factor $|\tilde{b}|^{-1}$ with respect to its Heisenberg form. (Recall, in particular, that $|\tilde{b}| \approx 2.4$ for $\Delta/t \approx 1$ and $|\tilde{b}| \approx 1.0$ for $\Delta/t = \infty$.) The difference $m_{S}^{\text{HF}} - m_{S}$ is similarly rescaled. Additional itinerancy effects, which arise when the full expressions of $a(k,\omega)$ and $b(k,\omega)$ are retained in Eqs. (2.40) and the frequency integrations in Eqs. (2.40) and (2.36) are performed exactly, are expected on physical grounds to reduce further the difference $m_{S}^{\text{HF}} - m_{S}$. We then regard the values reported in Fig. 6(a) to be upper bounds for the ratio $(m_{S}^{\text{HF}} - m_{S})/m_{S}^{\text{HF}}$.
FIG. 2. Effective mean exchange integral $J_{\text{eff}}/t$ vs $\Delta/t$ and $U/t$ at zero doping.
FIG. 3. Relative standard deviation $\Delta J_{\text{eff}}/J_{\text{eff}}$ vs $\Delta/t$ and $U/t$ at zero doping.
FIG. 5. $d$ percentage at the Fermi level of the Hartree-Fock bands vs $\Delta/t$ and $U/t$ at zero doping.
FIG. 6. (a) $(m_s^{HF} - m_s)/m_s^{HF}$ and (b) $m_s^{HF}$ vs $\Delta/t$ and $U/t$ at zero doping, showing the combined effects of itineracy and of transverse spin fluctuations on the local (staggered) moment.