Systematic $1/S$ study of the two-dimensional Hubbard model at half-filling

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The two-dimensional Hubbard model is extended by placing $2S$ orbitals at each lattice site and studied in a systematic $1/S$ expansion. The $1/S$ results for the magnetic susceptibility and the spectra of spin-wave excitations at half-filling are consistent with the large-$S$ calculations for the Heisenberg antiferromagnet. The $1/S$ corrections to the fermionic spectrum lift the degeneracy along the edge of the magnetic Brillouin zone yielding minima at $(\pm \pi/2, \pm \pi/2)$. Relation to previous papers on the subject is discussed.

I. INTRODUCTION

The two-dimensional (2D) Hubbard model and the closely related $t$-$J$ model have been extensively used recently in the context of high-temperature superconductivity as the simplest models which capture at least some of the exciting physics of high-$T_c$ superconductors. At half-filling, the large-$U$ Hubbard model reduces to the nearest-neighbor Heisenberg antiferromagnet, which perfectly describes the properties of pure La$_2$CuO$_4$. While at sufficiently strong doping, it describes a strongly correlated metal and possibly a superconductor.

One of the crucial issues for lightly doped antiferromagnets is the role of quantum fluctuations. In La$_{2-x}$Sr$_x$CuO$_4$, they destroy long-range order in the ground state already at a very small doping. There is therefore a need for a systematic accounting of quantum fluctuations in the Hubbard model. For ordered Heisenberg antiferromagnets, a customary tool for this is the $1/S$ expansion. This expansion gives rather fast convergence and first-order $1/S$ results are quite accurate even for $S = 1/2$.

In this paper, we report the results of the large-$S$ studies of quantum fluctuations in the Hubbard model at half-filling. We view the results as a basis for future considerations of quantum fluctuations in doped antiferromagnets.

To perform $1/S$ studies, we need to extend the Hubbard model to higher spins. A straightforward way to do this is to place $2S$ equivalent orbitals at each lattice site. The hopping term remains the same as in the conventional Hubbard model; only the hopping integral $t$ now scales with $S$. At the same time, the $U_{\uparrow\uparrow}$ term is replaced by the Hund rule interaction term

$$H_{\text{int}} = \frac{U}{2} \sum_{\langle n,n',\alpha,i \rangle} \bar{\psi}_{n\alpha i} \bar{\psi}_{\bar{n}n'\bar{i}} \bar{\psi}_{\bar{n}'n'\bar{i}} \bar{\psi}_{n\alpha i} .$$

(1)

Here $\alpha = 1, 2$ is the spin index, and $i$ is the orbital index which runs over $i = 1, 2, ..., 2S$. For $S = 1/2$, the summation over spin index is absent and (1) reduces to the conventional on-site repulsion term. For $S > 1/2$, the coupling term ensures (at large $U$) a parallel alignment of the spins of electrons at all orbitals, i.e., total spin $S$ at each site, which forms a natural basis for $1/S$ expansion, and also ensures an equal number of electrons at each site. Fluctuations of this number cost energy of the order of $US \gg t$. The interaction term is simply related to the total spin per site as

$$H_{\text{int}} = -U \sum_n \left[ S_n^2 + (N_n - 2S)^2 \right] / 4 \text{ where } N_n = \psi_{\alpha n}^\dagger \psi_{\alpha n} \text{ is the fermion density, and } S_n = \sum_i \bar{S}_i = \frac{1}{2} \psi_{\alpha n}^\dagger \sigma_{\alpha \beta} \psi_{\bar{n} \beta n} \text{ is the total spin on a given site.}$$

The fluctuations of the square of the total density are irrelevant at large $U$, and we have checked explicitly that one can equally well use either Eq. (1) or $-U \sum_n S_n^2$ for the interaction term. The former choice is however advantageous for computational purposes.

In the momentum space, the extended Hubbard Hamiltonian takes the form

$$H = \sum_k \epsilon_k a_{j,k}^\dagger a_{j,k} + \frac{U}{2N} \sum_{k,k',q} a_{i,k,k'}^\dagger a_{j,k',-k+q} a_{i,k,-k+q} a_{j,k,k} .$$

(2)

Here $\epsilon_k = -2t(\cos k_x + \cos k_y)$, $N$ is the total number of lattice sites, and the momentum summations extend over the first Brillouin zone $-\pi < k_x, k_y < \pi$.

The large-$S$ expansion for magnetization and spin susceptibility of the Hubbard model has been previously studied in Ref. 10. Although a complete agreement with the similar expansion in the Heisenberg model was obtained, we believe that several relevant contributions were missed, and the agreement is thus a bit fortuitous. Below we will point out the discrepancies with Ref. 10 explicitly. The semiclassical expansion results for the magnetization were also reproduced in Ref. 11 by means of a $1/z$ expansion, where $z$ is the number of nearest neighbors.
II. MEAN-FIELD THEORY

We now briefly outline the results of mean-field \((S = \infty)\) studies of the Hubbard model.\(^{11-15}\) At the mean-field level, one introduces the condensate of \(S_z(q = Q)\) where \(Q = (\pi, \pi)\), and uses it to decouple the interaction term in (2). The resulting quadratic Hamiltonian then takes the form

\[
H_{\text{MF}} = \sum_k \epsilon_k a_{iak}^\dagger a_{iak} - \frac{U\langle S_z \rangle}{2} \sum_k a_{iak}^\dagger a_{iak} a_{iak+Q} a_{iak+Q}^\dagger \sigma_{\alpha \beta} a_{iak}^\dagger a_{iak+Q}^\dagger \sigma_{\alpha \beta} ,
\]

where the summations over momentum here and below are limited to the magnetic zone, i.e., half the Brilloin zone. Note that \(\langle S_z \rangle\) is the exact value of the condensate which includes all zero-point fluctuations. This quadratic Hamiltonian can be diagonalized by means of a Bogolubov transformation

\[
c_{iak} = u_k a_{iak} + v_k \sigma_{\alpha \beta} a_{iak+Q}^\dagger \sigma_{\alpha \beta}^\dagger , \quad d_{iak} = v_k a_{iak} - u_k \sigma_{\alpha \beta} a_{iak+Q}^\dagger \sigma_{\alpha \beta}^\dagger ,
\]

where \(c\) represents conduction, and \(d\) valence electrons. The transformation explicitly reads

\[
u_k = \left[ \frac{1}{2} \left( 1 + \frac{\epsilon_k}{E_k} \right) \right]^{1/2} , \quad \frac{1}{2} \left( 1 - \frac{\epsilon_k}{E_k} \right) \right]^{1/2} ,
\]

where \(E_k = (\epsilon_k^2 + \Delta^2)^{1/2}\) and \(\Delta = \frac{U\langle S_z \rangle}{2}\). The diagonalized Hamiltonian then takes the form

\[
H = \sum_k E_k (c_{iak}^\dagger c_{iak} - d_{iak}^\dagger d_{iak}) .
\]

The value of the gap \(\Delta\) is obtained from the self-consistency condition of the diagonalization procedure

\[
\frac{1}{U} = \sum_k \frac{2S}{E_k} .
\]

The bosonic spin-wave excitations appear in the theory as poles of the total transverse susceptibility

\[
\chi_{\alpha \beta}^+(q, q'; \omega) = i \int dt \langle \langle S_\alpha^+(t) S_\beta^-(0) \rangle \rangle e^{i\omega t} .
\]

To zeroth order in \(1/S\), the total static susceptibility is given by a sum of bubble diagrams in Fig. 1:

\[
\chi_{\alpha \beta}^+ = \frac{\chi_{\alpha \beta}^-(q, \omega = 0)}{1 - U \chi_{\alpha \beta}^- (q, \omega = 0)} .
\]

\[
\chi_{\alpha \beta}^-(q, \omega) = \frac{S}{N} \sum_k \left( 1 - \frac{\epsilon_k^2 + q_k + \Delta^2}{E_k E_{k+Q}} \right) \frac{2}{E_k + E_{k+Q}} .
\]

(10)

This simple form familiar from paramagnon theories exists, however, only for the static susceptibility. The total dynamical susceptibility is the solution of a \(2 \times 2\) problem because the antiferromagnetic ordering doubles the unit cell, and \(\chi_{\alpha \beta}^-(q, q'; \omega)\) is nonzero only when \(q = q'\) or when \(q = q' + Q\) (in the latter case \(\chi_{\alpha \beta}^-(q, q + Q, \omega) \sim \omega\)). Also notice the overall factor of \(S\) in \(\chi_{\alpha \beta}^-\). It comes from the summation over the orbital index in each bubble. Because of this factor, \(U\chi_{\alpha \beta}^+\) is \(O(1)\), and this makes the total transverse susceptibility very different from the bare one.

For large \(\Delta/t\), one can expand in (10) and simplify (9) to

\[
\chi_{\alpha \beta}^+ (q, \omega) = \frac{1}{2J (1 + \gamma_q)} ,
\]

(11)

where \(\gamma_q = (\cos k_x + \cos k_y)/2\) and \(J = 4t^2/(2S)^2 U\). As \(q\) approaches the ordering momentum \(Q\), \(\gamma_q \rightarrow -1\), and static susceptibility diverges as it, indeed, should because of the Goldstone theorem.

III. 1/S EXPANSION
FOR THE STATIC SUSCEPTIBILITY

We now proceed to the study of the fluctuation corrections to the static susceptibility. These corrections are related to the full residual interaction between fermions. In the longitudinal channel, we need to consider only the direct interaction between fermions with parallel spins as the renormalization due to scattering is small. In the transverse channel, however, the scattering between conduction and valence fermions produces low-energy spin-wave modes, and we therefore have to consider both the direct interaction of two fermions with opposite spins, and the interaction mediated by magnetic fluctuations (i.e., spin waves), (see Fig. 2). The latter interaction will in fact be responsible for all 1/S corrections to magnetic parameters. The effective Hamiltonian for fermion-magnon coupling was derived by Frenkel and one of us;\(^{11}\) here we quote only the result:

\[
\begin{align*}
\text{FIG. 1.} & \quad \text{The RPA series for the total transverse susceptibility for } S = \infty. \text{ The first term represents the simple bubble,} \\
& \quad \text{which is the building block of the ladder.}
\end{align*}
\]

\[
\begin{align*}
\text{FIG. 2.} & \quad \text{The vertex function for the exchange of magnetic fluctuations.} \text{ This interaction is obtained from the fermion-fermion coupling after a summation of ladder diagrams.}
\end{align*}
\]
\[
H_{tr} = \sum_{k,q} [c_{\alpha k}^\dagger c_{\alpha, k+q} c_{\beta k}^\dagger c_{\beta, k+q} + \Phi_{cc}(k, q) + d_{\alpha k}^\dagger d_{\alpha, k+q} + c_{\beta k}^\dagger c_{\beta, k+q} + \Phi_{cd}(k, q)] + \text{H.c.} \delta_{\alpha, -\beta} .
\]

Here \(c_{\alpha q}\) is the boson annihilation operator with polarization \(\alpha\), and the vertex functions are given by

\[
\Phi_{cc, dd}(k, q) = \left[ \pm (\epsilon_k + \epsilon_{k+q}) \eta_q + (\epsilon_k - \epsilon_{k+q}) \bar{\eta}_q \right] / \sqrt{2S} ,
\]

\[
\Phi_{cd, dc}(k, q) = \sqrt{\frac{2}{S}} \Delta \left[ \left( 1 - \frac{(\epsilon_k + \epsilon_{k+q})^2}{8\Delta^2} \right) \eta_q 
+ \left( 1 - \frac{(\epsilon_k - \epsilon_{k+q})^2}{8\Delta^2} \right) \bar{\eta}_q \right] ,
\]

and \(\eta_q\) and \(\bar{\eta}_q\) are given by

\[
\eta_q = \frac{1}{\sqrt{2}} \left( \frac{1 - \gamma_q}{1 + \gamma_q} \right)^{1/4} , \quad \bar{\eta}_q = \frac{1}{\sqrt{2}} \left( \frac{1 + \gamma_q}{1 - \gamma_q} \right)^{1/4} .
\]

In (13) we neglected all terms of the order \(J(t/U S)^m \ll J\) with \(m \geq 2\) which is consistent with our intention to calculate corrections on the scale of magnetic interaction \(J\). Observe that the vertex functions have the overall factor of \(1/\sqrt{S}\). The second-order self-energy corrections to the fermionic propagators then have \(1/S\) factor compared to the mean-field inverse propagators.

To calculate the spin susceptibility we will need the renormalized self-consistency condition, i.e., an expression for the order parameter \(S_z\) in terms of \(\Delta = U S_z\). It should ensure the cancellation of the leading \(O(1)\) term in the denominator of \(\chi^{zz}\). At \(S = \infty\), this condition was given by Eq. (7). For \(1/S\) corrections, however, we need the full expression for \(S_z\). Substituting (4) into the formula for the \(z\) component of the spin, we obtain after a simple algebra

\[
\langle S_z \rangle = \frac{1}{\Delta} \sum_{i, \alpha, k} \frac{\Delta}{E_k} (d_{i, \alpha k}^\dagger d_{i, \alpha k} - \langle c_{i, \alpha k}^\dagger c_{i, \alpha k} \rangle)
+ \frac{\epsilon_k}{\Delta} (\langle c_{i, \alpha k}^\dagger d_{i, \alpha k} \rangle + \langle d_{i, \alpha k}^\dagger c_{i, \alpha k} \rangle) .
\]

At \(S = \infty\), the only nonzero average is \(\langle d_{i, \alpha k}^\dagger d_{i, \alpha k} \rangle = 1\), and using \(\Delta = U \langle S_z \rangle\), we return to (7). However, at finite \(S\), one has to calculate pair averages with the self-energy corrections. These corrections include terms which transform a conduction fermion into a valence one and vice versa after emitting or absorbing a spin wave. Accordingly, all pair averages, including \(\langle c_{i, \alpha k}^\dagger d_{i, \alpha k} \rangle\), will have nonzero values at finite \(S\). The density diagrams are presented in Fig. 3. Note that we do not have to include the correction terms with direct interactions in both longitudinal and transverse channels, as these terms are already included in the mean-field diagonalization procedure. A straightforward calculation using (12) and (13) yields

\[
\langle S_z \rangle = \frac{2S}{N} \sum_k \frac{\Delta}{E_k} - \frac{1}{N^2} \sum_{k,p} \frac{4S^2 \Phi_{cd}^2}{(E_k + E_{k+p} + \Omega_p)^2}
+ \frac{4J}{U^2} (A - B) ,
\]

where \(\Omega_q = 4JS \sqrt{1 - \gamma_q^2}\) is the bare spin-wave frequency, and we defined

\[
A = \frac{1}{N} \sum_q \frac{1 - \sqrt{1 - \gamma_q^2}}{\sqrt{1 - \gamma_q^2}} , \quad B = \frac{1}{N} \sum_q \frac{\gamma_q^2}{\sqrt{1 - \gamma_q^2}} ,
\]

Retaining only terms of the order of \(U\) we arrive at a well-known result for the Heisenberg model,\(^7\)

\[
\langle S_z \rangle = S \left( 1 - \frac{1}{SN} \sum_q \frac{1 - \sqrt{1 - \gamma_q^2}}{\sqrt{1 - \gamma_q^2}} \right) .
\]

We are now in a position to compute \(1/S\) corrections to the static transverse susceptibility. Simple considerations show that to the first order in \(1/S\), the random phase approximation (RPA) approach is still exact, but one has to include all \(1/S\) corrections within a bubble and also take into account the renormalization of the relation between \(\Delta\) and \(U\). A special care should be given in selecting the diagrams as the valence-conduction bubble itself has the order of \(1/U\). However this leading contribution gets canceled in the denominator of (9), and the momentum dependence of \(\chi^{zz}\) is given by the subleading terms in \(\chi_0^{zz}\) which have the order of \(J/U^2\). The cancellation of the \(O(U)\) terms should clearly survive in \(1/S\) expansion, and we, therefore, have to keep all \(1/S\) diagrams to the order \(J/U^2 S\). Further, the inclusion of self-energy corrections due to interactions with spin waves flips the spins of intermediate fermions, and this makes fermionic spins on both sides of the bubble parallel to each other.
One then should also consider the effects of adding the direct longitudinal fermion-fermion interactions. Simple power counting arguments show that this does not give rise to an extra 1/S smallness because each time one includes an extra interaction, one also has to sum over the orbitals of intermediate fermions. We found however that in the large-U limit each inclusion of more than one triplet interaction does produce a smallness, not in 1/S but in (t/US)^2, because the frequency integration selects only those combinations of conduction and valence fermions for which the actual longitudinal interaction becomes small after being dressed by the Bogolubov coefficients. Altogether, we found 14 relevant diagrams. They are presented in Figs. 4–7. The diagrams in Fig. 4 contain no spin-wave propagator, but two direct fermion-fermion interactions. The diagrams in Fig. 5 contain self-energy corrections related to the exchange of spin waves and no direct fermion-fermion interactions. The diagrams in Fig. 6 contain one spin-wave propagator and one direct interaction between fermions with parallel spins. Finally, the diagrams in Fig. 7 contain one spin-wave propagator and two interactions in the triplet channel.

It is appropriate to comment at this point on the comparison of our results and those by Singh.\textsuperscript{10} The interaction potential used in Ref. 10 is somewhat different from ours because of different procedure of subtracting the total fermion density from the Hund rule coupling term. In particular, the interaction potential in Ref. 10 does not contain scattering with parallel spins. However, as we said above, fluctuations of the total density are irrelevant at large U, and therefore both approaches must yield the same results for susceptibility. We indeed explicitly checked that each diagram we consider has its analog for the form of the interaction term used in Ref. 10. In particular, we found analogous diagrams in Figs. 4 and 7 which were omitted in Ref. 10 together with several O(J/U^2S) terms in other diagrams. Altogether, the terms omitted in Ref. 10 cancel each other, but we do not believe that this could be anticipated in advance.

Calculation of the diagrams is tedious but straightforward. We list the expressions in the Appendix and quote here only the final result. We found that the modified self-consistency condition ensures an exact cancellation of the denominator in (9) at q = Q in accordance with the Goldstone theorem. The functional form of χ^{+-} is also unchanged compared to the mean-field result, but quantum fluctuations give rise to an overall renormalization factor Z_χ. We have

\begin{equation}
χ^{+-}(q, ω = 0) = \frac{Z_χ}{2J(1 + γ_q)},
\end{equation}

\begin{equation}
Z_χ = 1 - \frac{B}{S} = 1 - \frac{1}{NS} \sum_q \frac{γ_q^2}{\sqrt{1 - γ_q^2}}.
\end{equation}

As expected, this result coincides with the known 1/S expression for the static susceptibility of the Heisenberg antiferromagnet.\textsuperscript{7}

Finally, for completeness, we will also obtain the 1/S expansion result for the spin-wave velocity, c. From hydrodynamical considerations,\textsuperscript{16} we know that \(c^2 = \rho_σ/\chi_⊥\), where \(\chi_⊥\) is the static susceptibility.

\begin{equation}
χ_⊥ = \frac{1}{2} \chi^{+-}(q = 0, ω = 0) = \frac{Z_χ}{8J},
\end{equation}

FIG. 5. Diagrams for the irreducible susceptibility which do not contain a fermion-fermion interaction in the longitudinal channel. A half of the diagrams is presented. The rest are equivalent to those presented in Figs. 5–7 and can be obtained by replacing simultaneously all conduction electron propagators by valence ones and vice versa.

FIG. 6. Diagrams for the irreducible susceptibility which contain one direct fermion-fermion interaction line.

FIG. 4. The 1/S diagrams for the irreducible susceptibility which contain only direct fermion-fermion interactions. These diagrams should be irrelevant to magnetism, and we indeed found that they cancel each other.
and $\rho_s$ is the spin stiffness defined by
\[
\chi_{xx}^{zz}(q \approx Q) = \frac{S^2}{\rho_s(q - Q)^2}.
\]
(21)

Using the result for $S_z$ and expanding (19) near $q = Q$, we find
\[
\rho_s = JS^2 Z_{\rho},
\]
\[
Z_{\rho} = 1 - \frac{2A}{S} + \frac{B}{S} = 1 - \frac{2}{NS} \sum_q \frac{1 - \sqrt{1 - \gamma_q^2}}{1 - \gamma_q^2} + \frac{1}{NS} \sum_q \frac{\gamma_q^2}{\sqrt{1 - \gamma_q^2}}.
\]
(22)

Combining (20) and (22), we obtain
\[
e^2 = 2J^2 Z_c^2,\]
\[
Z_c^2 = \frac{Z_{\rho}}{Z_x} = 1 + \frac{2}{S} (B - A)
\]
\[
= 1 + \frac{2}{NS} \sum_q [1 - \sqrt{1 - \gamma_q^2}],
\]
(23)

which again coincides with the known spin-wave result.

**IV. SELF-ENERGY CORRECTIONS TO THE FERMIONIC SPECTRUM**

We now turn to the calculation of self-energy corrections to the single-particle excitation energy $E_k$. In the mean-field approximation we have $E_k = \sqrt{\Delta^2 + \epsilon_k^2}$. At large $U$, it can be simplified to $E_k = \Delta + 4JS(\cos k_x + \cos k_y)^2$. These forms for $E_k$ imply that the minimum of the fermion energy coincides with the whole edge of the magnetic Brillouin zone, $|k_x \pm k_y| = \pi$. This degeneracy in the position of the minima of $E_k$ was responsible for the singular behavior of the Hubbard model at infinitesimally small doping.\textsuperscript{12} We will show, however, that this degeneracy does not survive perturbative $1/S$ corrections, and the actual minima of the quasiparticle energy are located only at the particular points $(\pm \pi/2, \pm \pi/2)$ in the Brillouin zone. This is consistent with the results of other approaches.\textsuperscript{17-21}

Consider for definiteness the corrections to the energy of a valence fermion. As before, the dominant self-energy corrections at large $U$ are those which include the exchange of transverse magnetic fluctuations. To first order

\[
\Sigma = \ldots + \ldots
\]

FIG. 7. The same as in Fig. 6 but with two fermion-fermion interaction lines in the longitudinal channel.

in $1/S$, there are two such diagrams (Fig. 8). Performing the frequency integration in these diagrams, we obtain for the Green function of a valence fermion
\[
G^{-1}(k,\omega) = \omega + E_k
\]
\[
- \frac{2S}{N} \sum_q \left( \frac{\Phi_{cd}^2}{\omega - E_{k+q} - \Omega_q + i\delta} + \frac{\Phi_{dd}^2}{\omega + E_{k+q} + \Omega_2 - i\delta} \right).
\]
(24)

We now consider the two self-energy terms separately. The first term in (24) corresponds to a process when valence fermion transforms into a conduction one after emitting a spin wave. The matrix element for such a process and the energy denominator scale as $U$ and $US$, correspondingly. As a result, the first term yields the momentum-independent renormalizations of the gap, $\Delta \to \Delta(1 + A/S)$, and of the wave function residue, $Z = 1 - A/2S$. The latter is in fact related to the renormalization of the sublattice magnetization\textsuperscript{11} $\langle S_z \rangle = Z - 1/2$. This first self-energy term also has momentum-dependent contributions due to the $k$ dependence in $E_{k+q}$, but they scale as $J$ and, as we will see, are completely overshadowed by the momentum-dependent contributions from the second self-energy term.

The second self-energy term in (24) describes a process which includes only valence fermions. The vertex function for such a process scales as $t/S$, and so intuitively one may conclude that the second term is less relevant than the first one. However, at resonance, $\omega = -E_k$, and the leading $O(\Delta)$ terms in the denominator get canceled. The remaining terms scale as $JS$, so that the total self-energy correction behaves as $O(\Delta/S)$. More important, however, is that the $k$-dependent self-energy terms are not anymore suppressed by a factor $J/U$ and, therefore, may substantially modify the shape of the excitation spectrum.

The general structure of the $1/S$ self-energy correction is rather involved, and so below we will restrict calculations to the dispersion relation along the lines $|k_x \pm k_y| = \pi$ where the mean-field energy of valence fermions has a degenerate maximum. Simplifying Eq. (24) at $\gamma_k = 0$ and $US/t \gg 1$ we obtain for the pole of the Green function
\[
E_{k}^{1/S} = \Delta \left( 1 - \frac{1}{S} + \frac{\beta(k)}{2S} \right),
\]
(25)

where
\[
\beta(k) = \frac{2}{N} \sum_q \frac{1 + \sqrt{1 - \gamma_q^2}}{2\gamma_{k+q}^2 + \sqrt{1 - \gamma_q^2}}.
\]
(26)
TABLE I. Quasiparticle dispersion along $k_x + k_y = \pi$. Energies are in units of $\Delta$.

<table>
<thead>
<tr>
<th>$(\pi/2, \pi/2)$</th>
<th>$(5\pi/8, 3\pi/8)$</th>
<th>$(3\pi/4, \pi/4)$</th>
<th>$(7\pi/8, \pi/8)$</th>
<th>$(\pi, 0)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.739</td>
<td>0.751</td>
<td>0.784</td>
<td>0.824</td>
<td>0.842</td>
</tr>
</tbody>
</table>

It is not difficult to see that $\beta(k)$ does contain some momentum dependence, and, therefore, the excitation energy acquires dispersion along the edge of the magnetic Brillouin zone (see Table I). We evaluated the integral (26) numerically and found that $\beta(k)$ has four equivalent minima at $\pm(\pi/2, \pm\pi/2)$. Near each minimum, one can expand $k_{x,y} = \pm\pi/2 - k_{x,y}$ and obtain the dispersion relation typical for the anisotropic 2D Fermi gas:

$$E_{k}^{1/S} = \bar{\Delta} + \frac{p_{1}^{2}}{2m_{\perp}} + \frac{p_{||}^{2}}{2m_{||}}.$$ (27)

Here $\bar{\Delta}$ differs from $\Delta$ due to momentum-independent self-energy corrections, and we introduced $p_{1} = (k_{x} \pm \bar{k}_{y})/\sqrt{2}$, $p_{||} = (\bar{k}_{x} \pm \bar{k}_{y})/\sqrt{2}$ [the upper sign is for $(\pi/2, \pi/2)$ and $(-\pi/2, -\pi/2)$ and the lower sign is for the other two minima]. One of the effective masses is finite already at the mean-field level, and we easily obtain from $E_{k}^{S=\infty}$

$$m_{\perp} = \frac{1}{8JS} [1 + O(1/S)].$$ (28)

On the contrary, $m_{||}$ is infinite at the mean-field level, and acquires a finite value only due to $1/S$ corrections. The numerical evaluation of this mass yields

$$m_{||} \approx \frac{2S}{0.084\Delta}.$$ (29)

For the ratio of the effective masses we then obtain, to leading order in $1/S$, $m_{||}/m_{\perp} \approx 188(JS/U)$. Notice the surprisingly large numerical coefficient.

Care has to be taken in applying the $1/S$ results for the masses to the physical case of $S = 1/2$. We already mentioned that in resonance, the diagram with only valence fermions has a small energy denominator $O(JS)$ because the leading $\Delta$ term in $E_{k+q}$ gets cancelled by the external frequency. In this situation, vertex and self-energy corrections to the internal fermion line are important as they contain large factors of $U/J$. A simple analysis similar to that in Ref. 11 shows that self-energy and vertex corrections scale as $O(UJS)$ and $O(UJS)^2$ respectively. Neglecting these corrections is therefore legitimate only if $U/JS \ll 1$ and, in a rigorous sense, our $1/S$ expansion for the fermionic energy is valid only if $S \gg U/J$. It has, however, been argued several times that at large $U$, the actual (renormalized) interaction between fermions and spin waves (which includes the wave function renormalization factor of fermions) retains its functional form [at least near magnon momentum $q = (\pi, \pi)$], but has the same order of magnitude as the bandwidth. The argument here is that for $U_{\text{eff}} \sim JS$, self-energy and vertex corrections do not generate any new energy scales besides $JS$. In this situation, the actual expansion parameter for our studies is $O(1)$, and we can expect that the lowest-order approximation we are using still yields at least qualitatively correct results.

We conclude this section by a brief comparison with other approaches. Singh and Tesanovic, and Vignale and Hedayati considered the same perturbative corrections as we did, but resorted to self-consistent rather than perturbation analysis. They required that all corrections to the bare dispersion of quasiparticles be on the scale of $JS$, and solved self-consistently the Dyson equation for the quasiparticle energy. They found the band minimum at $(\pi/2, \pi/2)$, which agrees with our finding. We, however, did find the corrections of order $O(\Delta/S)$ in perturbative calculations. Boninsegni and Manousakis used a variational Monte Carlo simulation to compute the hole dispersion in the $t-J$ model. They also obtained band minima at $(\pm\pi/2, \pm\pi/2)$. The quantitative comparison with our results is, however, difficult because of the relatively small values of $t/J \leq 0.5$ considered in Ref. 18. The minima at $(\pm\pi/2, \pm\pi/2)$ in the $t-J$ model were also found in the perturbative calculations in the small $t/J$ limit. Trugman and Sachdev performed variational calculations for the Hubbard and $t$-$J$ models respectively and also found the minima at $(\pm\pi/2, \pm\pi/2)$ at large $t/J$. We compared the bandwidth along $k_{x} + k_{y} = \pi$ and found good agreement between Sachdev’s results and ours. Thus at $t/J = 2$, variational and our $1/S$ analysis yield $\Delta E = (E(\pi, 0) - E(\pi/2, \pi/2)) \approx 0.2t$ and 0.24$t$ correspondingly.

V. CONCLUSIONS

To summarize, in this paper we considered a large-$S$ extension of the Hubbard model and calculated in the $1/S$ expansion the leading quantum corrections to the static spin susceptibility, spin-wave velocity, and hole dispersion at half-filling. We found that the mean-field degeneracy of the quasiparticle spectrum does not survive in $1/S$ calculations, and the actual hole dispersion has minima at $(\pm\pi/2, \pm\pi/2)$. Our results for magnetic parameters agree (as they should) with the $1/S$ calculations in the Heisenberg model. Indeed, at half-filling, the use of the Hubbard model for magnetic calculations is not the easiest way to arrive at the final result. However, the method we presented here has a substantial advantage over other techniques in that it can be straightforwardly extended to doped antiferromagnets where quantum fluctuations are much more relevant than at half-filling. Work along these lines is now in progress.

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APPENDIX A

Here we give the expressions for the diagrams in Figs. 4–7. The two diagrams in Fig. 4 do not contain magnon propagators and therefore should be irrelevant to magnetism. They indeed cancel each other out giving contributions of $\pm J/2U^2S$. Two of the rest of the diagrams, namely, those of Figs. 5(a) and 6(a), contribute to order $1/US$, while the rest contribute to order $J/U^2S$. The explicit expressions for the first two diagrams are

$$\chi_{1a} = -\frac{1}{N^2} \sum_{k,p} \frac{1}{E_k} \left( 1 - \frac{(\epsilon_k + \epsilon_{k+p})^2}{4\Delta^2} \right) \times \left[ \frac{8S^2\Phi^2_{cd}}{(E_k + E_{k+p} + \Omega_p)^2} \right. + \left. \frac{4S^2\Phi^2_{cd}}{E_k(E_k + E_{k+p} + \Omega_p)} \right] \quad (A1)$$

for diagram 5(a), and

$$\chi_{2a} = -\frac{1}{N^2} \sum_{k,p} \frac{4S^2\Phi^2_{cd}}{E_k(E_k + E_{k+p} + \Omega_p)} - \frac{2J}{U^2S} (1 + \gamma_q) A - \frac{2J}{U^2S} B \quad (A2)$$

for diagram 6(a). Here all the sums are over a half of the Brillouin zone, and the constants $A$ and $B$ were defined in (17). Using the self-consistency condition (16), the total contribution from these diagrams can be immediately simplified to

$$\chi_{1a} + \chi_{2a} = \frac{1}{U} - \sum_k \frac{2S}{E_k} - \frac{2J}{U^2S} (2A - B) + \frac{2J}{U^2S} (1 + \gamma_q) A \quad (A3)$$

for $\chi_0^{+}$. The form for other diagrams are as follows:

$$\chi_{1b} = \frac{2J}{U^2S} \frac{1}{N} \sum_k \sqrt{1 - \gamma_k^2},$$

$$\chi_{1c} + \chi_{1d} = \frac{6J}{U^2S} (1 + \gamma_q) (A - B),$$

$$\chi_{1e} = \frac{2J}{U^2S} (1 + \gamma_q) A,$$

$$\chi_{2b} = -\frac{2J}{U^2S} \gamma_q (A - B),$$

$$\chi_{2c} = \frac{2J}{U^2S} \gamma_q B,$$

$$\chi_{2d} = -\frac{2J}{U^2S} (1 + \gamma_q) B,$$

$$\chi_{2e} = -\frac{2J}{U^2S} \frac{1}{N} \sum_k \sqrt{1 - \gamma_k^2},$$

$$\chi_{2f} = -\frac{2J}{U^2S} (1 + \gamma_q) A. \quad (A6)$$

Finally, the diagrams in Fig. 7 are

$$\chi_{3a} = \frac{2J}{U^2S} A, \quad \chi_{3b} = -\frac{2J}{U^2S} \gamma_q B \quad (A7)$$

Summing up all contributions and substituting them into Eq. (9), we obtain the result quoted in Eq. (19).

Broken Symmetry, and Correlation Functions (Benjamin/Cummings, Reading, MA, 1975).


22 For the calculations of the static susceptibility, vertex corrections of the type discussed in Sec. IV are irrelevant because the external frequency \( \omega_z \) is zero [or, more generally, it is \( O(JS) \) for all dynamical magnetic properties].