Collective excitations in a doped antiferromagnet

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We develop a systematic procedure for studying a doped antiferromagnet in the intermediate-coupling regime. Starting with the Hartree-Fock (HF) solution to the Hubbard model in the half-filled-band case, we obtain the spin-wave spectrum and find that in the strong-coupling limit the spin-wave mode is identical to that obtained from the corresponding spin-$\frac{1}{2}$ Heisenberg model. We self-consistently evaluate the one-loop correction to the sublattice magnetization due to spin-wave excitations and in the $U/t \to \infty$ limit find that the sublattice magnetization is reduced to 0.6, i.e., to 60% of its HF or saturation value. As a first step toward applying this systematic procedure to a doped antiferromagnetic, we numerically study in detail the HF ground state with few holes, which become self-consistently trapped by the self-induced spin polarization, resulting in the spin-bag ground state. We find that for $U/t < 20$ the transverse terms in the HF Hamiltonian iterate toward zero. We examine the nature of collective excitations in the spin-bag ground state in a 10×10 lattice system for $U/t = 5$, which is representative of the intermediate-coupling regime. We explicitly show that the spin-bag state admits to a stable Goldstone mode, confirming the local stability of this HF state. We analytically examine the self-consistent HF state, obtained in the rigid-band approximation, of a system with finite hole density. We find that, although self-consistent, this HF state is unstable with respect to collective excitations toward the formation of a two-dimensional incommensurate structure with a wave vector proportional to the linear hole density.

I. INTRODUCTION

The classical problem of holes doped into an antiferromagnetic system, discussed first in some detail by Brinkman and Rice,[1] has recently attracted renewed interest in an effort to understand the physical properties of the superconducting copper oxides. The parent copper oxides exhibit, in most cases, antiferromagnetic ground states, and the onset of the superconducting ground state upon doping seems to be related to the destruction of antiferromagnetic long-range order. While it was this association that initially motivated a search for possible mechanisms of superconductivity involving some bosonic excitation of magnetic origin, the problem of holes doped in an antiferromagnet has since proven to be of sufficient richness in itself as evidenced by the variety of unconventional ground states that have been proposed.[2–6]

Recent progress in the theoretical understanding of low-dimensional antiferromagnetism, specifically on the issue of long-range order in two dimensions, has provided a good starting point to study the consequences of doping by holes (or electrons). The destruction of antiferromagnetic long-range order by doping, observed in the layer copper oxides with just a few percent concentration of holes, is therefore the next important issue that has to be resolved in developing a progressive understanding towards the metallic phase and eventually the superconducting phase itself. While frustration of the copper-copper antiferromagnetic bonds through the direct exchange interaction of copper spins with spin of the hole residing on the intervening oxygen atoms has been proposed as a possible mechanism, there has been extensive effort to explore whether there is any instability within the single-band model itself, originating from an inherent frustration induced by the doped holes, that might play an important role in the destruction of long-range order of the antiferromagnetic ground state.

As has been the case quite generally with the history of magnetism, both localized spin as well as itinerant-electron models have been taken as starting points for the study of holes doped in an antiferromagnet. In the t-J and t-t'-J models,[7–11] the interaction between copper spins is taken to be of the Heisenberg exchange form. In the itinerant model studied first by Schrieffer *et al.*,[12] the spin correlation arise from the Hubbard interaction term which is treated within the Hartree-Fock approximation. In this case the added hole is self-consistently trapped by the spin polarization it induces, and this results in the formation of the spin bag. We shall refer to the self-consistent HF state containing the spin bag as the spin-bag ground state.

The Heisenberg model can be canonically obtained from the Hubbard model when U/t is large, so that it provides an accurate description of the electronic correlation effects in the "strong-coupling" limit. On the other hand, the Hartree-Fock approximation is a good one for small U/t when fluctuation effects are small, and therefore does well in the "weak-coupling" limit. Experimentally, as well as from the band-structure calculations, the electronic correlation energy is found to be of the same order as the band width in two dimensions, and therefore one is really in an "intermediate-coupling" limit. One therefore needs a systematic method to approach and study the behavior of the system in this intermediate-coupling regime, and to develop this is precisely the intent of this paper.

Here we have developed a formulation to incorporate, in a systematic and self-consistent fashion, the effects of quantum fluctuation (represented by the low-lying collective modes) about the self-consistent Hartree-Fock state of the Hubbard Hamiltonian. Within the random phase approximation (RPA), for example, in a half-filled-band system the lowest-lying excitations, represented by poles in the transverse spin susceptibility, are the collective spin-wave modes that significantly renormalize the sublattice magnetization and the ground-state energy. In fact, thermally excited spin waves destroy long-range order completely in a two-dimensional ferromagnetic system. Even at zero temperature there exist quantum zero-point fluctuations in an antiferromagnet, so much so that in one dimension such fluctuations completely destroy long-range order.[13]

In Sec. III we develop the formalism in the sublattice-basis representation and present our results regarding the nature and spectrum of the spin-wave modes in a half-filled-band system. In Sec. IV we self-consistently incorporate the quantum fluctuations about the HF state of the half-filled-band system. We find that, to one-loop order, the self-energy corrections due to spin-wave excitations lead to a reduction in the sublattice magnetization from its Hartree-Fock value of 1 in the large U/t limit to 0.6, i.e., to about 60% of its saturation value. This value, being in excellent agreement with the exact result recently obtained by Monte Carlo studies[14] and the linear spin-wave analysis of the Heisenberg model, suggests that the one-loop correction, done self-consistently, provides surprisingly good results just as the first-order term in a $\frac{1}{2}S$ expansion.[15,16]

The self-consistent treatment of quantum fluctuations evidently works well for the half-filled-band system. As a first step toward applying it to the doped system, we study, in Sec. V the nature of the low-lying bosonic collective modes in the self-consistent spin-bag ground state with precisely one hole. We explicitly show that the spin-bag ground state admits to a stable Goldstone mode. We also numerically obtain the wave functions of the low-lying collective modes and compare with the spin-wave modes of the half-filled-band system.

Section VI deals with a particular self-consistent state—the commensurate spin-density-wave state obtained in the rigid-band approximation—of a system with a finite fraction of holes. We show that the Goldstone mode is unstable in this case and that, due to fluctuations, the system develops an instability toward an incommensurate structure. We present this state as an example of a perfectly self-consistent state, which nonetheless does not represent a local minimum in the free energy.

The nature of the spin-bag ground state itself is discussed in detail in Sec. II for a wide range of the interaction strength. In the following we introduce the concept of the spin-bag ground state. This concept has been originally introduced in Ref. 12.

Consider that an $\uparrow$-spin hole in a localized state is introduced in a certain region of the Fermi sea of a half-filled-band antiferromagnetic system. The resulting local depletion in the $\uparrow$-spin electronic density results in a lower Hartree-Fock potential term locally for the $\downarrow$-spin electrons which, therefore, pile up in this region. An $\uparrow$-spin hole thus effectively attracts $\downarrow$-spin electrons. The bump in the $\downarrow$-spin density profile leads to a potential hill for $\uparrow$-spin electrons but a potential *valley* for the $\uparrow$ *hole.* The hole is, therefore, self-consistently trapped in the region with a localized wave function. In terms of the macroscopic gap parameter Δ, the hole reduces the sublattice magnetization and hence Δ around itself. This leads to a reduction in the energy gap around the hole, which, in turn, traps the hole. This self-consistent, localized state for a hole in an antiferromagnetic background is referred to as the spin-bag or the spin-polaron state. It should be stressed, however, that the particle that is trapped is not distinct from the particles providing the potential for it, and in this respect this problem is different from the classical problem of polarons in a lattice.

The formation of a localized spin-polaron state is closely tied in with the presence of the spin-density-wave (SDW) structure in the antiferromagnet. In a paramagnetic system, the local spin-density polarization formed by the introduction of a hole in a localized state amounts to a local spin-density fluctuation which decays rapidly (unless the system is very close to a magnetic instability). In the antiferromagnetic state, however, the SDW structure, which is responsible for lowering the ground-state energy, resists being reduced globally and forces a local reduction in the gap parameter. Another way of putting this is that the electrons in an itinerant antiferromagnet are tried up in forming the SDW structure, and the localized hole state that lies in the energy gap cannot couple strongly to the superposed plane-wave states and thereby decay.

In the weak-coupling limit an estimate for the size ξ of the spin bag can be made by minimizing, with respect to ξ, the total energy of the system, which is considered to consist of the occupied lower band and the hole. As already discussed, the localized $\uparrow$-spin hole introduces perturbations in the local electronic densities around the spin-bag site. These perturbations, denoted by $\delta n^{\uparrow,\downarrow}(\mathbf{r})$, also decay exponentially with the characteristic length scale ξ, and affect the band energy and the energy of the hole. Treating $U\delta n^{\uparrow,\downarrow}(\mathbf{r})$ as a perturbation, we evaluate the first-order energy correction to each quasiparticle state, and thus to the lower band. For the $\uparrow$-spin band, for example, the energy correction to the occupied band is $\Delta\delta n^{\downarrow}(0)\xi$, where we have made use of the fact that $\delta n^{\uparrow,\downarrow}(\mathbf{r})$ have opposite sign on the two sublattices. Using a localized wave function for the $\uparrow$-spin hole, with nonzero amplitudes only on the $\uparrow$-spin sublattice, the increase in the hole energy is similarly given by $U\delta n^{\downarrow}(0)$. Now, we consider $\delta n_{\downarrow}$ as arising from a response to a "field," $Un_h^{\uparrow}$, over a length scale ξ, due to a depletion in $\uparrow$-spin density equal to the hole density $n_h^{\uparrow}$. The susceptibility over a length scale ξ is $\approx(1/t)\ln\xi$. Therefore, using $n_h^{\uparrow}=1/\xi$, required by normalization, we have

$$\delta n^{\downarrow}(0)=(U/t)(1/\xi)\ln\xi \ .$$

The total change in the energy of the band plus hole system is therefore given by

$$\delta E_{\rm tot} = U\frac{\Delta}{t}\ln\xi + U\frac{1}{\xi} , \tag{1}$$

where in the second term, we have retained only the leading-order term in $\delta n^{\downarrow}(0)$. Minimizing this energy with respect to ξ, we see that the spin-bag size ξ is given by $\xi \approx t/\Delta$, which is essentially the spin-correlation length.

II. SELF-CONSISTENT STUDY OF THE SPIN-BAG GROUND STATE

In this section we describe the numerical self-consistent calculations with the Hubbard Hamiltonian in the Hartree-Fock (HF) approximation for a system that has one electron less (or one hole more) than required for half-filling. The added hole goes into a self-consistently localized state which lies within the band gap leading to the formation of the spin bag. We discuss the nature of the resulting spin-bag ground state in several regimes of the interaction strength. We start with a Hartree-Fock approximation in which all possible linearizations of the Hubbard term are considered, as shown below:

$$H_I = U\sum_i a_{i\uparrow}^\dagger a_{i\uparrow} a_{i\downarrow}^\dagger a_{i\downarrow}$$

$$\approx U\sum_i (\langle a_{i\uparrow}^\dagger a_{i\uparrow}\rangle a_{i\downarrow}^\dagger a_{i\downarrow} + \langle a_{i\downarrow}^\dagger a_{i\downarrow}\rangle a_{i\uparrow}^\dagger a_{i\uparrow} \tag{2}$$

$$- a_{i\uparrow}^\dagger \langle a_{i\downarrow}^\dagger a_{i\uparrow}\rangle a_{i\downarrow} - a_{i\downarrow}^\dagger \langle a_{i\uparrow}^\dagger a_{i\downarrow}\rangle a_{i\uparrow}) . \tag{3}$$

In terms of the expectation values of the spin-density operators and the spin-lowering and spin-raising operators, we obtain

$$H_I^{\rm HF} = -\sum_i (a_{i\uparrow}^\dagger a_{i\downarrow}^\dagger) \begin{bmatrix} \Delta_i^z - n_i U & \Delta_i^- \\ \Delta_i^+ & -\Delta_i^z - n_i U \end{bmatrix} \begin{bmatrix} a_{i\uparrow} \\ a_{i\downarrow} \end{bmatrix} , \tag{4}$$

where $n_i = (n_i^{\uparrow} + n_i^{\downarrow})/2$ is the local spin-averaged density, $2\Delta_i^z \equiv (n_i^{\uparrow} - n_i^{\downarrow})U$, and

$$(\Delta_i^+)^* = \Delta_i^- = U\langle a_{i\downarrow}^\dagger a_{i\uparrow}\rangle .$$

Separating the spin and charge operators, we can write this as

$$H_I^{\rm HF} = -\sum_i \hat{\sigma}_i \cdot \mathbf{B}_i + U\sum_i n_i \hat{n}_i , \tag{5}$$

where

$$\hat{\sigma}_i = (a_{i\uparrow}^\dagger a_{i\downarrow}^\dagger)\boldsymbol{\sigma} \begin{bmatrix} a_{i\uparrow} \\ a_{i\downarrow} \end{bmatrix}$$

is the local electronic spin operator in terms of the Pauli spin matrix;

$$\hat{n}_i = (a_{i\uparrow}^\dagger a_{i\downarrow}^\dagger)\underline{\mathbb{1}} \begin{bmatrix} a_{i\uparrow} \\ a_{i\downarrow} \end{bmatrix}$$

is the local charge operator and $\mathbf{B}_i$ is given in terms of the longitudinal and transverse components Δ_i^z and Δ_i^-.

The full Hamiltonian that we consider for the self-consistent calculation is

$$H^{\rm HF} = -t\sum_{\langle ij\rangle\sigma} (a_{i\sigma}^\dagger a_{j\sigma} + a_{j\sigma}^\dagger a_{i\sigma}) + H_I^{\rm HF} , \tag{6}$$

which represents the motion of particles in a spin-dependent potential, determined self-consistently and representing an effective field due to all the particles. The self-consistent procedure consists of (i) diagonalizing H (which is constructed initially from the spin densities and a "seed' for the transverse terms around the spin-bag site) to obtain the eigenfunctions $\{|\phi_l\rangle\}$, (ii) evaluating the spin densities and the transverse terms, Δ_i^-, using the eigenfunctions and (iii) reiterating to obtain self-consistency. The spin densities and the transverse (spin-flip) terms are evaluated using

$$n_{i\sigma} = \sum_{E_l < E_F} (\phi_l^\sigma)_i^* (\phi_l^\sigma)_i ,$$

$$(\Delta_i^+)^* = \Delta_i^- = \sum_{E_l < E_F} (\phi_l^{\downarrow})_i^* (\phi_l^{\uparrow})_i . \tag{7}$$

We use the unrestricted Hartree-Fock method in which both spins are treated simultaneously. This doubles the size of the Hamiltonian matrix and our study is limited to lattice system sizes of up to 10×10. We use periodic boundary conditions in both directions. At zero temperature the sum is to be done over all states with energies less than the Fermi energy. Since the diagonalization routine arranges the eigensolutions in increasing order of eigenvalues, the sum contains the lower $l_F = N^{\uparrow} + N^{\downarrow} = N - 1$ states, N being the total number of lattice sites.

In the absence of any transverse component the field term that couples to the spin operator is due to the sublattice magnetization and is only in the z direction. The presence of a transverse field term in the effective Hamiltonian is significant in that it allows the spin vector to tilt out of the z direction. This is important in the large U/t limit because the stiffness against such angular distortions decreases inversely with the interaction strength. In this situation it becomes energetically favorable to obtain the magnetization profile in the spin bag by tilting the spin vector rather than by decreasing its magnitude. In the strong-coupling limit, we do see evidence of this tendency of the local spin vector to tilt in the vicinity of the spin bag. However, for $U/t < 20$ zero spin-flip terms is the fixed point. All this is discussed in more detail later. We first discuss the results of the self-consistent calculation in the $U/t < 20$ range, without the spin-flip terms. The Hamiltonian in this case is diagonal in spin, nonetheless the diagonalizations were done in the expanded basis involving both spins simultaneously.

The results for the self-consistent $\uparrow$-spin densities on the sites of the 10×10 lattice system for $U/t = 5$ are shown in Table I. For this case we have 49 $\uparrow$-spin and 50 $\downarrow$-spin electrons. The spin bag is seen to have the C_4 symmetry around the spin-bag site. For much smaller values of the interaction strength, we find self-consistent solutions with two distinct symmetries, both with nearly equal energies. The cigar shaped spin bag lies along one of the diagonals of the lattice and this solution has been

TABLE I. ↑-spin densities on lattice sites in the HF spin-bag ground state for $U/t=5$ with an ↑-spin hole localized near the lattice center. The nearly equal ↑-spin densities near the spin-bag site allow delocalization of ↓-spin electrons leading to the formation of the ferromagnetic core.

Sites	1	2	3	4	5	6	7	8	9	10
1	0.114	0.886	0.114	0.886	0.114	0.886	0.114	0.886	0.114	0.886
2	0.886	0.114	0.885	0.114	0.885	0.114	0.885	0.114	0.885	0.114
3	0.114	0.886	0.114	0.881	0.113	0.881	0.113	0.881	0.114	0.886
4	0.886	0.114	0.885	0.113	0.843	0.122	0.843	0.113	0.885	0.114
5	0.114	0.886	0.114	0.881	0.122	0.093	0.122	0.881	0.114	0.886
6	0.886	0.114	0.885	0.113	0.843	0.122	0.843	0.113	0.885	0.114
7	0.114	0.886	0.114	0.881	0.113	0.881	0.113	0.881	0.114	0.886
8	0.886	0.114	0.885	0.114	0.885	0.114	0.885	0.114	0.885	0.114
9	0.114	0.886	0.114	0.886	0.114	0.886	0.114	0.886	0.114	0.886
10	0.886	0.114	0.886	0.114	0.886	0.114	0.886	0.114	0.886	0.114

discussed earlier by Su.[17,18] There is, however, another solution that energetically does better than the cigar shaped one. Though marginal at $U/t=2$, the difference in energy becomes increasingly pronounced with increasing U/t.

At $U/t=2$, this other solution actually shows two identical centers (with the maximum depression in $n^{\uparrow}$) situated on the diagonal, one in the center of the lattice (by choice) and a secondary one at the corner, and each having a local C_4 symmetry around itself. With increasing interaction strength, the secondary spin bag at the corner becomes less distinct and eventually loses identity. Also the size of the spin bag shrinks with increasing interaction strength and as shown in Table I, already for $U/t=5$, the hole is almost completely site localized. Spin bags with the C_4 symmetry has been discussed by Choi and Mele.[19]

A study of the spectrum of eigenvalues for the case $U/t=5$ shows two sites inside the gap (at energies $1.5t$ and $2t$), corresponding respectively to the localized ↑-spin and ↓-spin hole states, which appear due to the formation of the spin bag. The reason for the ↓-spin state at $2t$ (and another one at $-2t$, slightly below the bottom edge of the lower band), has to do with the formation of a ferromagnetic core near the spin-bag site, and is discussed in detail below. The ↑-spin hole state is precisely the one created by the removal of one ↑-spin electron from the half-filled band. This ↑-spin hole is, as discussed before, self-consistently localized (trapped) due to its binding with the excess ↓-spin electron density at the spin-bag site which is, in turn, induced by its presence. The energy separation between the top of the valence band and the energy of this ↑ hole, thus corresponds to its binding energy.

We now discuss the nature of the ↓-spin electron states in the spin-bag ground state in the strong-coupling limit. As we shall show, the energy states seen in the spectrum at $-2t$ and $2t$ arise from a delocalization of ↓-spin electrons in a ferromagnetic core around the spin bag. Since in the large U/t limit the ↑-spin hole is almost site localized, the ↑-spin density on the spin-bag site is vanishingly small. Also the ↑-spin densities are similarly small on the four nearest-neighboring sites belong to the ↓-spin sublattice. Therefore, a ↓-spin electron feels the same Hartree-Fock potential (≈ 0), due to the ↑-spin densities, on every one of the five sites in the core, consisting of the spin-bag site and the four nearest-neighbor sites that are connected to it via the hopping terms. (That this is indeed the case even when $U/t=5$ can be seen from Table I which shows that the ↑-spin densities on the five sites of the core are small and all roughly equal.) Furthermore, the ↑-spin density on the sites surrounding the core is almost 1. Therefore, the ↓-spin electrons in the core feel a huge barrier surrounding the core but can move freely among the five core sites.

The Hamiltonian for the ↓-spin electrons within the core can be represented as a 5×5 matrix in which the central site is connected to all four surrounding sites with matrix elements $-t$ and all other matrix elements are zero.

$$H_{\text{core}}=\begin{bmatrix} 0 & 0 & -t & 0 & 0 \\ 0 & 0 & -t & 0 & 0 \\ -t & -t & 0 & -t & -t \\ 0 & 0 & -t & 0 & 0 \\ 0 & 0 & -t & 0 & 0 \end{bmatrix}. \tag{8}$$

The five eigenvalues, in units of t, are -2, 2, and three zeroes. These two isolated states with energies 2 and -2 are precisely the ones seen outstanding in the spectrum. The other three states merge in the lower band centered around zero. The corresponding wave functions are

$$\frac{1}{2\sqrt{2}}\begin{bmatrix}1\\1\\2\\1\\1\end{bmatrix},\ \frac{1}{2\sqrt{2}}\begin{bmatrix}1\\1\\-2\\1\\1\end{bmatrix},\ \frac{1}{2}\begin{bmatrix}1\\1\\0\\-1\\-1\end{bmatrix},\ \frac{1}{2}\begin{bmatrix}1\\-1\\0\\-1\\1\end{bmatrix},\ \frac{1}{2}\begin{bmatrix}1\\-1\\0\\1\\-1\end{bmatrix}. \tag{9}$$

Since the four ↓-spin electrons in the core fill up the lower four of thees five states, the total ↓-spin density on the central spin-bag site is $\frac{1}{2}$. This explains why a ↓-spin density close to a half is seen on the central site in the large U/t limit within the self-consistent calculation. Also, it is the ↓-spin density of $\approx\frac{1}{2}$ which completes the ferromagnetic core together with the neighboring four sites, each having a ↓-spin density of $\approx\frac{7}{8}$.

We make two observations at this point. The first is concerned with the charge-density depression present in the HF state around the spin-bag site. This charge-density depression, arising from the delocalization already discussed, is an important feature of the HF ground state, considering that the energy gained from delocalization happens to be *the total HF ground-state energy* in the strong-coupling limit. The second is that the situation can be consistently viewed as well in terms of holes. The two holes of opposite spin on the spin-bag site, resulting from the removal of the ↑-spin electron, repel each other. The ↓-spin hole can delocalize to the nearest-neighboring sites (resulting in the ↓-spin electron density at the spin-bag site), however, the ↑-spin hole cannot do so because there are ↑-spin holes already present on these four sites.

Study of the total HF ground-state energy for the system with one hole shows that it approaches $-2t$ as U/t increases. Considering the narrowing of the bands with increasing U/t and that the lower, occupied band is centered at zero, this suggests that all of the ground-state energy is coming from the delocalization of the ↓-spin electrons in the core. The core itself is distinctly ferromagnetic in nature and, in fact, represents the seed for a ferromagnetic phase which is the true ground state in the limit $U/t\rightarrow\infty$.[20] The delocalization energy increases from $-2t$ for the five-site core eventually to $-4t$ as the size of the ferromagnetic core becomes infinite. In a Hartree-Fock study where the number of ↑- and ↓-spin electrons is conserved individually (that is no spin-flip terms are present) the antiferromagnetic and the ferromagnetic phase lie in disjoint subspaces and one can never go from one to the other. If the spin-flip terms are present, however, a relentless growth in the spin-flip terms is a possible indication of an instability of the antiferromagnetic state toward the ferromagnetic one.

This analysis of delocalization of ↓-spin electrons in the strong-coupling limit can be carried further to study the interaction between holes. Consider first the interaction between parallel-spin holes that are trapped on two sites belonging to the same sublattice. If the two holes are not next-nearest neighbors, then the ferromagnetic cores due to each do not overlap. The delocalization energy gained in this case is $-2t$ per hole. If, however, the two holes are next-nearest neighbors then the individual cores due to each hole overlap resulting in an enlarged ferromagnetic core containing nine sites or eight sites depending on whether the two holes are separated by $2a$ or $\sqrt{2}a$, respectively. The electrons of opposite spin are therefore delocalized to a greater extent, and the lowest eigenvalue in this case is indeed lower than $-2t$. But when the total energy is evaluated by summing over the occupied states, the result is slightly higher than $-4t$. Parallel-spin holes therefore marginally repeal each other in the strong-coupling limit.

Consider now the interaction between two holes of opposite spins. If a ↓-spin hole is to be placed in the vicinity of the ↑-spin hole, it has to go in the highest occupied of the ↓-spin states formed due to delocalization among the five sites in the ferromagnetic core. Placing it in one of three degenerate states with energy 0 leaves the total system energy unchanged at $-2t$. On the other hand, if the ↓-spin hole is introduced locally on any site that is not a nearest neighboring of the ↑-spin hole, then an additional energy of $-2t$ is gained by the delocalization of the surrounding ↑-spin electrons. Hence in the strong-coupling limit holes with opposite spin repel strongly when they are in the vicinity of each other. By numerically studying the total energies in the self-consistent states with two holes, we find that even for the case of $U/t=5$ the repulsion is present between holes with parallel or antiparallel spins.

We now discuss the results of the self-consistent calculation with the spin-flip terms present in the Hartree-Fock Hamiltonian. The presence of the spin-flip term Δ_i^- on a site merely reflects, as mentioned before, that the local magnetization vector is not pointing in the z direction; rather it is tilted with respect to it. As we shall show in the following, the results indicate that for large U/t, the self-consistent ground state in which only the diagonal spin-density terms are present develops an instability. This instability is towards a state in which the local magnetization vectors in the vicinity of the spin bag develop a tilt with respect to the z direction. The natural question that arises is why this tilting of spins in the vicinity of the spin bag should energetically favor the ground state. A simplified argument in terms of a Landau free energy functional-type picture is given in the following.

The presence of a spin bag locally induces a dip in the magnetization (or the S_z profile). This, one may expect, is associated with a $|\Delta S_z|^2$ type gradient term in the free energy. Now there two ways in which the given S_z profile across the system may be achieved. One is to simply have the magnitude of the spin vectors follow the profile, while keeping them all aligned in the z direction, as turns out to be case for $U/t<20$. The other possibility is to have the spin vectors in the vicinity of the spin-bag tilt with respect to the z direction, yielding the required profile in the projection on the z axis. In this situation the characteristic energy scale would be associated with angular distortion (rather than amplitude distortion as in the first case). But this energy scale associated with angular distortion is just the spin-wave stiffness, which goes as $\approx 4t^2/U$ in the strong-coupling limit. For large U/t, it is therefore energetically favorable for the system to accommodate the spin bag by having angular distortion in the local spin vectors.

In order to find the onset of this instability towards angular distortion, we start with a set of small seed values for the off-diagonal, spin-flip terms $\Delta_i^{-,+}$ around the spin-bag site in the Hartree-Fock Hamiltonian. As described earlier, we then iterate the procedure of diagonalization and evaluation of the spin-diagonal and off-

diagonal densities seeking self-consistency. We find two distinct behaviors as we iterate (up to 50 times) depending on the interaction strength. For $U/t<20$, with iterations the spin-flip terms slowly decrease towards zero, the rate itself slowing down as U/t approaches 20. This is accompanied with the total system energy, obtained by adding up the quasiparticle energies of the occupied states, approaching, from below, the energy of the self-consistent HF state with no spin-flip terms. However, for $U/t>20$, the spin-flip terms keep on increasing relentlessly, while the total energy goes on decreasing with iterations. This behavior of the total energy as a function of iteration is shown in Fig. 1.

The interaction strength $U/t\approx 20$, therefore, is a critical value at which the self-consistent spin-diagonal HF state of the 8×8 lattice system with one hole develops an instability toward a state in which the spin vectors in the vicinity of the spin bag are tilted with respect to the z axis.

The half-filled-band antiferromagnetic state. We first briefly review the characteristics of the antiferromagnetic state for a half-filled-band system obtained within the Hartree-Fock approximation. The Hartree-Fock Hamiltonian can be represented in the basis formed by the two sublattices as

$$H=\begin{bmatrix} -\Delta & \varepsilon_{\mathbf{k}} \\ \varepsilon_{\mathbf{k}} & \Delta \end{bmatrix} . \tag{10}$$

The eigenvalues yield the quasiparticle energies

$$E_k^{\uparrow,\downarrow}=\pm(\Delta^2+\varepsilon_{\mathbf{k}}^2)^{1/2} \tag{11}$$

in terms of the free-particle band energies

$$\varepsilon_{\mathbf{k}}=-2t[\cos(k_x a)+\cos(k_y a)]$$

and the gap parameter, Δ. The $-/+$ spin is associated with $\mathbf{k}$ states lying inside/outside the magnetic Brillouin zone (MBZ). The gap parameter is related to the sublattice magnetization m by $2\Delta=mU$. The sublattice magnetization is defined as the average over one sublattice of the expectation value of the z component of the spin operator, $S_z^i=a_i^\dagger\sigma_z a_i$. The quasiparticle wave functions are linear superposition of plane waves on the two sublattices A and B; the superposition amplitudes, $a_{\mathbf{k}}$, $b_{\mathbf{k}}$ on the two sublattices are given by the eigenvectors of H:

$$\phi_{\mathbf{k}}^{\uparrow}=\left[\frac{2}{N}\right]^{1/2}\sum_{\mathbf{r}}(a_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}\delta_{rA}+b_{\mathbf{k}}e^{i\mathbf{k}\cdot\mathbf{r}}\delta_{rB}) \tag{12}$$

$a_{\mathbf{k}}$ and $b_{\mathbf{k}}$ are interchanged in the $\downarrow$-spin wave function. The components $a_{\mathbf{k}}$ and $b_{\mathbf{k}}$ are given by

$$\begin{aligned} a_{\mathbf{k}}^2&=\frac{\varepsilon_{\mathbf{k}}^2}{\varepsilon_{\mathbf{k}}^2+(E_{\mathbf{k}}+\Delta)^2}\ , \\ b_{\mathbf{k}}^2&=1-a_{\mathbf{k}}^2\ . \end{aligned} \tag{13}$$

The sublattice magnetization m can be obtained from the difference in the spin densities on a site:

$$m=\frac{2}{N}\sum_{E_{\mathbf{k}}<E_F}(a_{\mathbf{k}}^2-b_{\mathbf{k}}^2)=\frac{2}{N}\sum_{E_{\mathbf{k}}<E_F}\frac{\Delta}{(\Delta^2+\varepsilon_{\mathbf{k}}^2)^{1/2}}\ . \tag{14}$$

This leads to the self-consistency condition

$$\frac{1}{U}=\frac{1}{N}\sum_{E_{\mathbf{k}}<E_F}\frac{1}{(\Delta^2+\varepsilon_{\mathbf{k}}^2)^{1/2}}\ . \tag{15}$$

The gap parameter can be obtained by inverting this relationship of U on Δ, from which the sublattice magnetization can be determined as a function of U. Figure 2 shows a plot of the sublattice magnetization obtained in this manner.

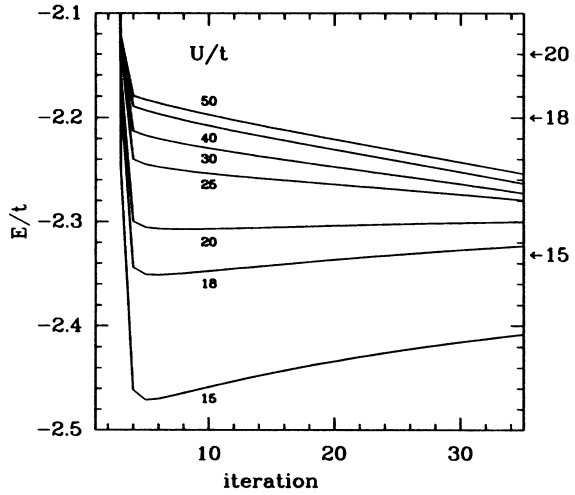

FIG. 1. Total system energy with iteration steps in the HF procedure when the spin flip are terms are present. When $U/t<20$ the spin-flip terms iterate to zero and the total energy approaches the HF ground-state energy with no spin-flip terms (indicated by arrows on the right margin). When $U/t>20$ the spin-flip terms grow slowly with iterations accompanied with a decreasing total energy.

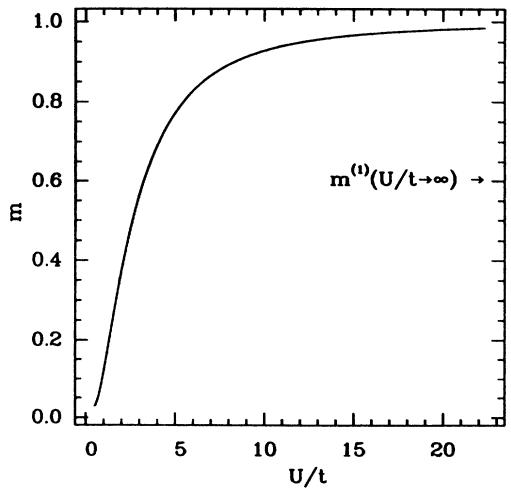

FIG. 2. Sublattice magnetization as a function of the interaction strength for a half-filled-band system in the HF approximation. The arrow indicates the value of the sublattice magnetization in the $U/t\rightarrow\infty$ limit when quantum fluctuations are self-consistently treated at the one-loop level.

The relationship between particle and hole amplitudes, used in the following sections, are given here:

$$(a_{\mathbf{k}}^{+})^2=(b_{\mathbf{k}}^{-})^2 ,$$

$$(b_{\mathbf{k}}^{+})^2=(a_{\mathbf{k}}^{-})^2 ,$$

where the superscripts $-$ and $+$ refer to particle (lower band) and hole (upper band) states, respectively.

III. SPIN WAVES IN A HALF-FILLED-BAND SYSTEM

Spin waves are the lowest-lying collective excitations that represent transverse spin fluctuations about the antiferromagnetic ground state. The spin-wave mode shows up in the form of a pole in the dynamical transverse spin susceptibility evaluated in the antiferromagnetic ground state. The transverse spin susceptibility is defined in terms of the spin raising and lowering operators as given in the following. The retarded two-particle Green's function of interest can be obtained from the corresponding time-ordered one,

$$\chi^{-+}(\mathbf{r},t;\mathbf{r}',t') =i\Theta(t-t')\langle\Psi_{\mathrm{AF}}|[\sigma^{-}(\mathbf{r},t),\sigma^{+}(\mathbf{r}',t')]|\Psi_{\mathrm{AF}}\rangle . \quad (16)$$

Within the RPA or the ladder approximation for the transverse susceptibility, we formally have

$$\chi^{-+}=\frac{\chi_0^{-+}}{1-U\chi_0^{-+}} \quad (17)$$

and the spin-wave modes are obtained from

$$1-U\chi_0^{-+}=0 . \quad (18)$$

The zeroth-order term in the susceptibility, χ_0^{-+}, is evaluated with respect to the antiferromagnetic ground state and is given, in terms of one-particle Green's functions, by

$$\chi_0^{-+}(\mathbf{r},\mathbf{r}';\omega)=i\int_{-\infty}^{+\infty}\frac{d\omega'}{2\pi}G^{\uparrow}_{\mathbf{r},\mathbf{r}'}(\omega')G^{\downarrow}_{\mathbf{r}',\mathbf{r}}(\omega'-\omega) . \quad (19)$$

Because translational symmetry is reduced by the sublattice magnetization, $(\chi_0^{-+})_{\mathbf{r},\mathbf{r}'}$ in the antiferromagnetic state depends on the sublattices that $\mathbf{r}$ and $\mathbf{r}'$ belong to. $(\chi_0^{-+})_{\mathbf{r},\mathbf{r}'}$ can hence be represented as a 2×2 matrix, each component of which still depends only on $\mathbf{r}-\mathbf{r}'$. Fourier transformation of each component can therefore be done keeping $\mathbf{r}$ and $\mathbf{r}'$ belonging to a fixed pair of sublattices yielding the 2×2 matrix $[\chi_0^{-+}](\mathbf{Q},\omega)$ in the sublattice basis. As we shall show in the following, the full RPA susceptibility of Eq. (17) can be inverse Fourier transformed:

$$[\chi^{-+}](\mathbf{r},\mathbf{r}';\omega) =\frac{1}{N}\sum_{\mathbf{Q}}\left[\frac{\chi_0^{-+}(\mathbf{Q},\omega)}{1-U\chi_0^{-+}(\mathbf{Q},\omega)}\right]_{\mathbf{r},\mathbf{r}'}e^{-i\mathbf{Q}\cdot(\mathbf{r}-\mathbf{r}')} . \quad (20)$$

Indicated by the subscripts, the appropriate matrix element to be taken in the right-hand side of the preceding equation is determined from the sublattices that $\mathbf{r}$ and $\mathbf{r}'$ belong to. The RPA form is thus clearly retained in the sublattice basis, and this is a distinct advantage of our matrix formulation in which the spin susceptibility, Green's function, self-energy, etc., are 2×2 matrices.

Equation (18) for the spin-wave mode is, therefore, really an eigenvalue equation. If $\lambda_{\max}(\mathbf{Q},\omega)$ denotes the bigger of the two eigenvalues, then the spin-wave mode is obtained from

$$1-U\lambda_{\max}(\mathbf{Q},\omega)=0 . \quad (21)$$

We now discuss in detail the evaluation of the susceptibility matrix, $[\chi_0^{-+}(\mathbf{Q},\omega)]$, and also the inverse Fourier transform. If we write the Green's functions in Eq. (19) in terms of the quasiparticle wave functions and energies, we obtain the sublattice basis

$$[\chi_0^{-+}(\mathbf{r}-\mathbf{r}';\omega)]=\left[\frac{2}{N}\right]^2\sum_{\mathbf{k},\mathbf{k}'}\begin{bmatrix}a_{\mathbf{k}}^2b_{\mathbf{k}'}^2 & a_{\mathbf{k}}b_{\mathbf{k}}a_{\mathbf{k}'}b_{\mathbf{k}'}\\ a_{\mathbf{k}}b_{\mathbf{k}}a_{\mathbf{k}'}b_{\mathbf{k}'} & b_{\mathbf{k}}^2a_{\mathbf{k}'}^2\end{bmatrix}D(\mathbf{k},\mathbf{k}',\omega)e^{i(\mathbf{k}'-\mathbf{k})\cdot(\mathbf{r}-\mathbf{r}')} , \quad (22)$$

where

$$D(\mathbf{k},\mathbf{k}',\omega)=\left[\frac{\Theta(E_F-E_{\mathbf{k}}^{\uparrow})\Theta(E_{\mathbf{k}'}^{\downarrow}-E_F)}{(E_{\mathbf{k}'}^{\downarrow}-E_{\mathbf{k}}^{\uparrow}+\omega)}+\frac{\Theta(E_F-E_{\mathbf{k}'}^{\downarrow})\Theta(E_{\mathbf{k}}^{\uparrow}-E_F)}{(E_{\mathbf{k}}^{\uparrow}-E_{\mathbf{k}'}^{\downarrow}-\omega)}\right] . \quad (23)$$

Using the following property of Fourier transform on sublattices,

$$(2/N)\sum_{\mathbf{r}-\mathbf{r}'}e^{i\mathbf{K}\cdot(\mathbf{r}-\mathbf{r}')}=\begin{cases}\delta_{\mathbf{K},0}+\delta_{\mathbf{K},\pi}, & \mathbf{r}\in A/B,\ \ \mathbf{r}'\in A/B\\ \delta_{\mathbf{K},0}-\delta_{\mathbf{K},\pi}, & \mathbf{r}\in A/B,\ \ \mathbf{r}'\in B/A ,\end{cases} \quad (24)$$

we obtain

$$[\chi_0^{-+}(\mathbf{Q},\omega)]\equiv\sum_{\mathbf{r}-\mathbf{r}'}[\chi_0^{-+}(\mathbf{r}-\mathbf{r}')]\exp[i\mathbf{Q}\cdot(\mathbf{r}-\mathbf{r}')] \tag{25}$$

$$=\frac{2}{N}\sum_{E_{\mathbf{k}}<E_F}\begin{bmatrix} a_{\mathbf{k}}^2 b_{\mathbf{k}-\mathbf{Q}}^2 & a_{\mathbf{k}}b_{\mathbf{k}}a_{\mathbf{k}-\mathbf{Q}}b_{\mathbf{k}-\mathbf{Q}} \\ a_{\mathbf{k}}b_{\mathbf{k}}a_{\mathbf{k}-\mathbf{Q}}b_{\mathbf{k}-\mathbf{Q}} & b_{\mathbf{k}}^2 a_{\mathbf{k}-\mathbf{Q}}^2 \end{bmatrix}\frac{1}{E_{\mathbf{k}-\mathbf{Q}}^{+}-E_{\mathbf{k}}^{-}+\omega}$$

$$+\frac{2}{N}\sum_{E_{\mathbf{k}}<E_F}\begin{bmatrix} b_{\mathbf{k}}^2 a_{\mathbf{k}-\mathbf{Q}}^2 & a_{\mathbf{k}}b_{\mathbf{k}}a_{\mathbf{k}-\mathbf{Q}}b_{\mathbf{k}-\mathbf{Q}} \\ a_{\mathbf{k}}b_{\mathbf{k}}a_{\mathbf{k}-\mathbf{Q}}b_{\mathbf{k}-\mathbf{Q}} & a_{\mathbf{k}}^2 b_{\mathbf{k}-\mathbf{Q}}^2 \end{bmatrix}\frac{1}{E_{\mathbf{k}-\mathbf{Q}}^{+}-E_{\mathbf{k}}^{-}-\omega}\ . \tag{26}$$

Here the sign to be taken for the quasiparticle energies with momenta $\mathbf{k}$ and $\mathbf{k}-\mathbf{Q}$ are explicitly shown as superscripts. The two δ-function terms in Eq. (24) effectively render the condition in Eq. (23) redundant that one of the momenta lie outside the magnetic Brillouin zone. This is because if $\mathbf{k}$ lies inside the MBZ then one and only one of $\mathbf{k}-\mathbf{Q}$ or $\mathbf{k}-\mathbf{Q}+\pi$ always lies outside. Therefore the sum over $\mathbf{k}$ inside the MBZ can be done without any further restriction. In obtaining Eq. (26) we have also taken $a_{\mathbf{k}}$ to carry the sign of $\varepsilon_{\mathbf{k}}$ [Eq. (13)] so that $a_{\mathbf{k}-\mathbf{Q}+\pi}=-a_{\mathbf{k}-\mathbf{Q}}$. This cancels the sign coming from the second δ-function term in the Fourier transform for the off-diagonal elements.

These same properties are used, perhaps a little more obviously, in obtaining the inverse Fourier transformation. One obtains

$$[\chi_0^{-+}(\mathbf{r}-\mathbf{r}';\omega)]=\frac{1}{N}\sum_{\mathbf{Q}}[\chi_0^{-+}(\mathbf{Q},\omega)]e^{-i\mathbf{Q}\cdot(\mathbf{r}-\mathbf{r}')}\ , \tag{27}$$

where $[\chi_0^{-+}(\mathbf{Q},\omega)]$ is as defined in Eq. (26). This can be checked explicitly by Fourier transforming both sides of Eq. (27) and using the following property of the susceptibility matrix:

$$[\chi_0^{-+}(\mathbf{Q}+\pi,\omega)]=\sigma_3[\chi_0^{-+}(\mathbf{Q},\omega)]\sigma_3\ . \tag{28}$$

At this stage we also note the following property of the inverse Fourier transform of product of two matrices, $\sum_{\mathbf{r}_1}A(\mathbf{r},\mathbf{r}_1)B(\mathbf{r}_1,\mathbf{r}')$, the elements of which exhibit translational symmetry within the 2×2 sublattice basis:

$$\sum_{\mathbf{r}_1}A(\mathbf{r},\mathbf{r}_1)B(\mathbf{r}_1,\mathbf{r}')=\left[\frac{1}{N}\right]^2\sum_{\mathbf{Q},\mathbf{Q}',\mathbf{r}_1}[A(\mathbf{Q})]_{\mathbf{r},\mathbf{r}_1}[B(\mathbf{Q}')]_{\mathbf{r}_1,\mathbf{r}'}e^{-i\mathbf{Q}\cdot(\mathbf{r}-\mathbf{r}_1)}e^{-i\mathbf{Q}'\cdot(\mathbf{r}_1-\mathbf{r}')} \tag{29}$$

$$=\left[\frac{1}{N}\right]^2\frac{N}{2}\sum_{\mathbf{Q}}\{[A(\mathbf{Q})B(\mathbf{Q})]_{\mathbf{r},\mathbf{r}'}+[A(\mathbf{Q})\sigma_3B(\mathbf{Q})\sigma_3]_{\mathbf{r},\mathbf{r}'}\}e^{-i\mathbf{Q}\cdot(\mathbf{r}-\mathbf{r}')}\ . \tag{30}$$

In view of the way in which $[\chi_0^{-+}(\mathbf{Q},\omega)]$ transforms under momentum translation by π, and using the property just derived, we can now easily inverse Fourier transform the full RPA susceptibility

$$[\chi^{-+}](\mathbf{r},\mathbf{r}';\omega)=\frac{1}{N}\sum_{\mathbf{Q}}\left[\frac{\chi_0^{-+}(\mathbf{Q},\omega)}{1-U\chi_0^{-+}(\mathbf{Q},\omega)}\right]_{\mathbf{r},\mathbf{r}'}e^{-i\mathbf{Q}\cdot(\mathbf{r}-\mathbf{r}')}\ . \tag{31}$$

We now proceed with the evaluation of $\chi_0^{-+}(\mathbf{Q},\omega)$. Since $E_{\mathbf{k}-\mathbf{Q}}^{+}-E_{\mathbf{k}}^{-}$ in Eq. (26) is $(\Delta^2+\varepsilon_{\mathbf{k}-\mathbf{Q}}^2)^{1/2}+(\Delta^2+\varepsilon_{\mathbf{k}}^2)^{1/2}$, which is at least 2Δ, we can expand the energy denominators in powers of $\omega/(E_{\mathbf{k}-\mathbf{Q}}-E_{\mathbf{k}})$ when the frequency is small compared to the energy gap. Since the off-diagonal terms in the two matrices in Eq. (26) are identical, they cancel when taken with odd powers of ω. This cancellation of the linear in ω terms in the off-diagonal elements is significant as it ensures that the eigenvalues depend only quadratically on ω. Keeping terms up to second order in ω, we see that $[\chi_0^{-+}(\mathbf{Q},\omega)]$ can be written in the following form:

$$[\chi_0^{-+}(\mathbf{Q},\omega)]=\begin{bmatrix}\mathcal{A}-\alpha\omega & \mathcal{B} \\ \mathcal{B} & \mathcal{A}+\alpha\omega\end{bmatrix}\ , \tag{32}$$

where $\mathcal{A}$ and $\mathcal{B}$ contain the $O(\omega^2)$ terms. To $O(\omega^2)$,

$$\lambda_{\max}=\mathcal{A}+(\mathcal{B}^2+\alpha^2\omega^2)^{1/2}\ ,$$

the larger one of the two eigenvalues of this matrix can be written as

$$\lambda_{\max}=\mathcal{A}+|\mathcal{B}|+\frac{\alpha^2\omega^2}{2|\mathcal{B}|}\ . \tag{33}$$

In order to obtain the spin-wave velocity, we now study the response when the momentum transfer $\mathbf{Q}$ is very close to (π,π). Setting $\mathbf{Q}=\pi-\mathbf{q}$, where $qa\ll1$, we expand $\mathcal{A}$ and $\mathcal{B}$ to second order in qa and ω/Δ to obtain

$$\lambda_{\max}=(\mathcal{A}+\mathcal{B})_0+\left[\beta+\frac{\alpha^2}{2\mathcal{B}_0}\right]\omega^2-\gamma q^2a^2 , \tag{34}$$

where β and γ are, respectively, the coefficients of the ω^2 and the q^2a^2 terms in the expansion of $\mathcal{A}+|\mathcal{B}|$. Since we can neglect terms of order ω^2q^2, all the coefficients are evaluated with $\omega,\mathbf{q}\to 0$. The results for the various coefficients, for all values of U/t are

$$(\mathcal{A}+\mathcal{B})_0=\frac{1}{N}\sum_{E_{\mathbf{k}}<E_F}\frac{1}{(\Delta^2+\varepsilon_k^2)^{1/2}}=\frac{1}{U} , \tag{35}$$

$$\beta=\frac{1}{4}\frac{1}{N}\sum_{E_{\mathbf{k}}<E_F}\frac{1}{(\Delta^2+\varepsilon_{\mathbf{k}}^2)^{3/2}}\equiv\frac{x}{4} , \tag{36}$$

$$\alpha=\frac{\Delta}{2}\frac{1}{N}\sum_{E_{\mathbf{k}}<E_F}\frac{1}{(\Delta^2+\varepsilon_{\mathbf{k}}^2)^{3/2}}\equiv\tfrac{1}{2}\Delta x , \tag{37}$$

$$2\mathcal{B}_0=\frac{1}{N}\sum_{E_{\mathbf{k}}<E_F}(1-\Delta^2/E_{\mathbf{k}}^2)\frac{1}{(\Delta^2+\varepsilon_k^2)^{1/2}}\equiv\frac{1}{U}-\Delta^2x , \tag{38}$$

$$\gamma=2t^2\frac{1}{N}\sum_{E_{\mathbf{k}}<E_F}\frac{\sin^2k_x(1-3\varepsilon_{\mathbf{k}}^2/2E_{\mathbf{k}}^2)-\frac{1}{2}\cos^2k_x-\frac{1}{2}\cos k_x\cos k_y}{(\Delta^2+\varepsilon_{\mathbf{k}}^2)^{3/2}}\equiv y . \tag{39}$$

The value $1/U$ of the eigenvalue at $\omega,\mathbf{q}=0$ leads to the cancellation of $O(1)$ terms which ensures a gapless spin-wave spectrum. Substituting the result for the eigenvalue into Eq. (21), we obtain the spectrum of the low-lying, collective excitations:

$$\omega=v_{\mathrm{SW}}q \tag{40}$$

where the spin-wave velocity, v_{SW}, is given below in terms of the quantities defined in Eqs. (35) through (39)

$$v_{\mathrm{SW}}=\left[\frac{2\mathcal{B}_0\gamma}{2\mathcal{B}_0\beta+\alpha^2}\right]^{1/2}a . \tag{41}$$

The spin-wave velocity, as obtained from the preceding expression, is plotted in Fig. 3 as a function of the interaction strength U/t. To get an idea of the magnitude of the spin-wave velocity, we have evaluated the scale factor for $ta=1$ eV Å, which is shown on the right margin of the plot. From their neutron scattering studies, Shirane *et al.*[21] have reported $v_{\mathrm{SW}}>0.4$ eV Å, so that supposing $U/t\approx 5$, our results are somewhat larger than the suggested lower bound.

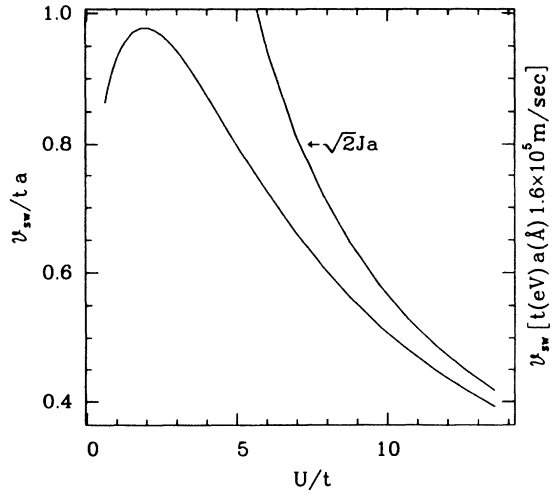

FIG. 3. Spin-wave velocity as a function of the interaction strength with the right-hand scale showing in m/sec for $ta=1$ eV Å.

We now obtain the spin-wave energy in the strong coupling limit ($U/t\gg 1$). In this limit $2\Delta\approx U$, so we can neglect $\varepsilon_{\mathbf{k}}^2$ in comparison with Δ^2 in Eqs. (35) through (39) and we obtain $x=1/2\Delta^3$, $2\mathcal{B}_0=2t^2/\Delta^3$, and $\gamma=t^2/4\Delta^3$. Substituting these in Eq. (41) for the spin-wave velocity, we obtain

$$v_{\mathrm{SW}}=\sqrt{2}Ja , \tag{42}$$

where $J=4t^2/U$ is the nearest-neighbor exchange term obtained in the spin-$\frac{1}{2}$ Heisenberg Hamiltonian to which the Hubbard model can be canonically mapped in the strong-coupling limit. In fact, the quantization of antiferromagnons in the Heisenberg model of localized spins leads to precisely the same value for the spin-wave velocity within the linear approximation.[16,22] The spin-wave velocity in the strong-coupling limit is also shown in Fig. 3. Comparison with the general result shows that the discrepancy is about 15% at $U/t=8$, where the interaction strength is equal to the free-particle bandwidth.

The full $\mathbf{Q}$ dependence of the spin-wave mode can be obtained in the large U/t limit if we retain terms only up to order $1/\Delta^3$ in the quantities $\mathcal{A}$, $\mathcal{B}$, and α. We obtain

$$\mathcal{A}=\frac{1}{U}-\frac{1}{N}\sum_{E_{\mathbf{k}}<E_F}\frac{\varepsilon_{\mathbf{k}-\mathbf{Q}}^2}{2\Delta^3} , \tag{43}$$

$$\mathcal{B}=\frac{1}{N}\sum_{E_{\mathbf{k}}<E_F}\frac{\varepsilon_{\mathbf{k}}\varepsilon_{\mathbf{k}-\mathbf{Q}}}{2\Delta^3} , \tag{44}$$

$$\alpha=\frac{1}{4\Delta^2} . \tag{45}$$

Evaluation of the sum over states is easily done and yields

$$\mathcal{A}=1/U-t^2/\Delta^3$$

and

$$\mathcal{B}=(t^2/2\Delta^3)(\cos Q_x a+\cos Q_y a) .$$

Substituting the eigenvalue,

$$\lambda=\mathcal{A}+[\mathcal{B}^2+(\alpha\omega)^2]^{1/2} ,$$

into Eq. (21) for the spin-wave mode, we obtain

$$\omega=2J(1-\gamma_Q^2)^{1/2} , \tag{46}$$

where

$$\gamma_Q=(\tfrac{1}{2})(\cos Q_x a+\cos Q_y a) .$$

This expression for the full Q dependence of the spin-wave energy in the strong-coupling limit is also in agreement with the result obtained starting with the Heisenberg model of localized spins.[16,22] We should note that results obtained by Schrieffer *et al.*[23] for the spin-wave velocity in the strong-coupling limit differ from ours by a factor of 2. We have also obtained the spin-wave velocity numerically, as described in the following section, and find it to be in agreement with our result just given.

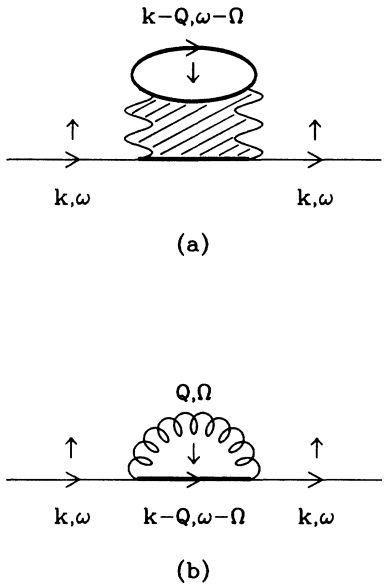

FIG. 4. (a) Diagrammatic representation for the self-energy correction at the one-loop level due to transverse spin fluctuations. (b) This may be viewed as arising from virtual emission and absorption of a spin-wave boson (spin 1) accompanied by spin flips.

IV. QUANTUM FLUCTUATIONS IN AN ANTIFERROMAGNET

The sublattice magnetization (or the gap parameter) is, among other properties of the antiferromagnet obtained in the Hartree-Fock approximation, sensitive to quantum fluctuations about the Hartree-Fock ground state. The lowest-lying quantum fluctuations are the collective spin-wave modes that represent transverse spin fluctuations. These transverse spin fluctuations involve spin-flip processes and therefore necessarily affect the spin densities and hence the magnetization that was obtained in the Hartree-Fock ground state. Figure 4(a) diagrammatically shows the self-energy correction from transverse spin fluctuations. This one-loop process may be viewed as representing correction to a quasiparticle state arising from the virtual emission and absorption of a spin-wave boson (spin 1) accompanied by spin flips [Fig. 4(b)]. The spin-wave propagator is thus related to the effective interaction in the antiparallel-spin channel. Since the spin-wave stiffness, and hence the characteristic energy scale for the spin-wave excitations, decreases inversely with U in the large U/t limit, we expect the effect of spin fluctuations to become more and more pronounced with increasing U/t.

There are, in addition, other virtual processes in which the spin is not flipped and which involve an effective interaction in the parallel-spin channel. The effective interaction in the parallel-spin channel involves $\chi_0^{\sigma\sigma}(\mathbf{Q},\omega)$, which does not admit to a low-lying spin-wave mode. In the large U/t limit such processes contribute only to order $(t/U)^2$ and are, therefore, not important.

We consider the one-loop correction to the sublattice magnetization (or the gap parameter) arising from transverse spin fluctuations. In terms of the self-energy corrections, the one-particle Green's function is

$$G^\sigma(\mathbf{k},\omega)=\frac{1}{[G^\sigma_{\rm HF}(\mathbf{k},\omega)]^{-1}-\Sigma^\sigma(\mathbf{k},\omega)} . \tag{47}$$

Since

$$[G^\sigma_{\rm HF}(\mathbf{k},\omega)]^{-1}=\omega-H^\sigma_{\rm HF} ,$$

the self-energy correction effectively renormalizes the HF Hamiltonian. We now study the self-energy correction due to the transverse spin fluctuations. This self-energy correction arises from the amplitude for a particle in the occupied band to undergo a virtual spin-flip transition into, and back from, the upper hole band, accompanied with the emission and reabsorption of a spin wave. In real space we have

$$\Sigma^\sigma_{\rm SF}(\mathbf{r},\mathbf{r}';\omega)=\int\frac{d\Omega}{2\pi i}U^{\uparrow\downarrow}_{\rm eff}(\mathbf{r},\mathbf{r}';\Omega)G^{-\sigma}(\mathbf{r},\mathbf{r}';\omega-\Omega) , \tag{48}$$

where $U^{\uparrow\downarrow}_{\rm eff}(\mathbf{r},\mathbf{r}';\Omega)$ is the effective interaction in the antiparallel-spin channel. Fourier transformation, with $\mathbf{r}$ and $\mathbf{r}'$ belonging to a fixed pair of sublattices, leads to the self-energy matrix, $\Sigma^\sigma_{\rm SF}(\mathbf{k},\omega)$ in the sublattice basis,

$$\Sigma^\sigma_{\rm SF}(\mathbf{k};\omega)=\frac{1}{N}\sum_{\mathbf{Q}}\int\frac{d\Omega}{2\pi i}[U^{\uparrow\downarrow}_{\rm eff}(\mathbf{Q},\Omega)G^{-\sigma}(\mathbf{k}-\mathbf{Q};\omega-\Omega)] +\sigma_3[U^{\uparrow\downarrow}_{\rm eff}(\mathbf{Q},\Omega)G^{-\sigma}(\mathbf{k}-\mathbf{Q}+\pi;\omega-\Omega)]\sigma_3 . \tag{49}$$

The matrix $[U^{\uparrow\downarrow}_{\rm eff}G^{-\sigma}]$ in Eq. (49) is obtained by multiplying, element by element, the two matrices $[U^{\uparrow\downarrow}_{\rm eff}]$ and

$[G^{-\sigma}]$, i.e.,

$$[U_{\text{eff}}^{\uparrow\downarrow}G^{-\sigma}]_{ij}=[U_{\text{eff}}^{\uparrow\downarrow}]_{ij}[G^{-\sigma}]_{ij} .$$

In the sublattice basis, $[U_{\text{eff}}^{\uparrow\downarrow}(\mathbf{Q},\Omega)]$, the effective interaction in the antiparallel-spin channel, is given by

$$U_{\text{eff}}^{\uparrow\downarrow}(\mathbf{Q},\Omega)=U^2\frac{[\chi_0^{-+}(\mathbf{Q},\Omega)]}{[1-U\chi_0^{-+}(\mathbf{Q},\Omega)]} . \tag{50}$$

In Eq. (49) if the self-energy correction is to a particle state, then the intermediate state represented by $G^{-\sigma}(\mathbf{k}-\mathbf{Q};\omega-\Omega)$ should be a hole state and vice versa. This is because the self-energy is derived from the transverse susceptibility which is a particle-hole propagator. That the intermediate state should lie on the opposite side of the Fermi surface is, therefore, merely a consequence of the Pauli exclusion principle. Now for any value of $\mathbf{Q}$, one and only one of $\mathbf{k}-\mathbf{Q}$ or $\mathbf{k}-\mathbf{Q}+\boldsymbol{\pi}$ lies on one particular side of the MBZ. Furthermore, owing to the manner in which the Green's function transforms under translation by $\boldsymbol{\pi}$, the matrix elements are identical whether the residue is obtained from $G^{-\sigma}(\mathbf{k}-\mathbf{Q},\omega-\Omega)$ or $G^{-\sigma}(\mathbf{k}-\mathbf{Q}-\boldsymbol{\pi},\omega-\Omega)$. The net result is that the sum over $\mathbf{Q}$ can be done without any restriction.

We briefly sketch out the evaluation of the self-energy at the one-loop level in the strong-coupling limit as this can be done without taking recourse to numerically evaluating the sums over states. In this limit the bandwidth is negligible in comparison to the band gap and the energy denominators $|E_{\mathbf{k}-\mathbf{Q}}^{\pm}-E_k^{\mp}|\approx 2\Delta$ can be taken outside the sum over $\mathbf{Q}$.

In the strong-coupling limit, the full RPA susceptibility can be written as

$$\chi^{-+}(\mathbf{Q},\Omega)=-\frac{1}{2}\begin{vmatrix} 1-\frac{\Omega}{2J} & \gamma_{\mathbf{Q}} \\ \gamma_{\mathbf{Q}} & 1+\frac{\Omega}{2J}\end{vmatrix}\frac{1}{\sqrt{1-\gamma_{\mathbf{Q}}^2}}\left[\frac{1}{\Omega-2J(1-\gamma_{\mathbf{Q}}^2)^{1/2}}-\frac{1}{\Omega+2J(1-\gamma_{\mathbf{Q}}^2)^{1/2}}\right] . \tag{51}$$

In this form the spin susceptibility represents a propagator with advanced and retarded components. The pole with positive spin-wave energy represents rotation in spin space of an electron sitting on the right sublattice. For hole states which represent electrons sitting on the wrong sublattice, rotation of spin leads to a lowering of energy. Such collective modes are represented by the pole with negative spin-wave energy.

Since $G^{-\sigma}(\mathbf{k}-\mathbf{Q},\omega-\Omega)$ is diagonal in the strong-coupling limit, in view of Eq. (48) the self-energy matrix is also diagonal. Consider the self-energy correction for $\uparrow$-spin particle states at the top of the occupied band ($\omega=-\Delta$). In this case $G^{\downarrow}(\mathbf{k}-\mathbf{Q}-\boldsymbol{\pi},\omega-\Omega)$, which must represent a $\downarrow$-spin hole state, has an amplitude 1 on the $\uparrow$-spin sublattice only, with an energy denominator of -2Δ. This intermediate state arises from rotating the spin of a $\uparrow$-electron the right sublattice. In the integration over Ω, contribution therefore comes from the pole with a positive spin-wave energy. For the self-energy component on the $\uparrow$-spin sublattice we obtain

$$\Sigma_{\text{SF}}^{\uparrow\uparrow}=\frac{1}{N}\sum_{\mathbf{Q}}\left[\frac{1}{(1-\gamma_{\mathbf{Q}}^2)^{1/2}}-1\right]\Delta=(J_2-1)\Delta , \tag{52}$$

where following Anderson,[15] we have used J_2 to denote the two-dimensional sum

$$J_2=\frac{1}{N}\sum_{\mathbf{Q}}\frac{1}{\sqrt{1-\gamma_{\mathbf{Q}}^2}}=1.393 . \tag{53}$$

Similarly the self-energy correction for an $\uparrow$-spin electron on the $\downarrow$-spin sublattice ($\omega=\Delta$) is determined. This represents the self-energy correction for a hole state and therefore the intermediate $\downarrow$-spin state must be a particle state. Rotation of an $\uparrow$-spin on the $\downarrow$-spin sublattice leads to a lowering in the energy and therefore in the Ω integration we pick the pole with a negative spin-wave energy. We obtain

$$\Sigma_{\text{SF}}^{\downarrow\downarrow}=-(J_2-1)\Delta . \tag{54}$$

The gap parameter is thus reduced due to the transverse spin fluctuations by an amount equal to (J_2-1) times the HF value. In fact, in D dimensions the fractional reduction will be (J_D-1), which vanishes as $D\to\infty$, confirming that the HF result is exact in infinite dimensions.

Adding the self-energy correction to the HF Hamiltonian, the renormalized gap parameter, Δ_{SF}, in two dimensions is simply given by $\Delta_{\text{SF}}/\Delta_{\text{HF}}=(2-J_2)$. And, therefore, the renormalized sublattice magnetization, m_{SF}, related to the gap parameter by $2\Delta_{\text{SF}}=m_{\text{SF}}U$, is given by

$$\frac{m_{\text{SF}}}{m_{\text{HF}}}=(2-J_2)=0.607 . \tag{55}$$

The sublattice magnetization is therefore reduced by about 60% of its HF or saturation value by the zero point, quantum spin fluctuations. This result for the sublattice magnetization is in very good agreement with the recent Monte Carlo studies,[14] and in exact agreement with the spin-wave analysis results[15,16] and the mean-field result[24] within the Schwinger boson theory,[25] of the Heisenberg model. This indicates significantly that HF together with the zero-point spin fluctuations due to spin waves is able to account for the physics of the Hubbard model even in the strong-coupling limit.

V. COLLECTIVE EXCITATIONS IN THE SPIN-BAG GROUND STATE

Spin waves are the low-lying collective excitations about the Hartree-Fock ground state of a half-filled-band antiferromagnet, and in the last two sections we discussed their nature and consequences on the sublattice magnetization. In an effort to understand the properties of a doped antiferromagnet, we start, in this section, with the spin-bag ground state with precisely one hole, the nature of which has been discussed in detail in Sec. II, and study the nature of collective excitations about this self-consistent ground state. We explicitly establish that the spin-bag ground state admits to the Goldstone mode and show that the single hole appreciably reduces the energy of some collective modes by mixing the modes of the half-filled-band system.

That the spin-bag state admits to a Goldstone mode is significant because it is not necessarily true that a self-consistent solution should represent a ground state. In fact, as we show in the last section, within the rigid-band approximation, a system with a finite density of holes has a commensurate spin-density-wave solution which is self-consistent, but nonetheless has no stable Goldstone mode. The static susceptibility in this state actually diverges for a small $\mathbf{Q}$ indicating an instability towards an incommensurate structure. The commensurate spin-density-wave state must, therefore, represent an unstable saddle point solution of the free energy.

We start by evaluating the zeroth-order transverse spin susceptibility matrix in the spin-bag ground state using the numerically obtained wave functions and energy eigenvalues, $\{|\phi_{l\sigma}\rangle, E_{l\sigma}\}$, representing the self-consistent solution of the Hartree-Fock Hamiltonian. The procedure used in the unrestricted Hartree-Fock method described earlier in Sec. II. This section addresses the intermediate-coupling limit wherein the interaction strength is of the same order as the bandwidth. Therefore, as determined in Sec. II, for $U/t<20$, we only need to consider the spin-diagonal terms in the Hartree-Fock Hamiltonian. The Hamiltonian matrix is thus real, symmetric and yields real eigenfunctions. Using i,j to refer to two sites in the system, the matrix element $[\chi_0^{-+}(\omega)]_{ij}$ is obtained from

$$[\chi_0^{-+}(\omega)]_{ij}=\sum_{E_{l\uparrow}>E_F}^{E_{m\downarrow}<E_F}\frac{\phi^i_{l\uparrow}\phi^j_{l\uparrow}\phi^i_{m\downarrow}\phi^j_{m\downarrow}}{E_{l\uparrow}-E_{m\downarrow}-\omega}+\sum_{E_{m\downarrow}>E_F}^{E_{l\uparrow}<E_F}\frac{\phi^i_{l\uparrow}\phi^j_{l\uparrow}\phi^i_{m\downarrow}\phi^j_{m\downarrow}}{E_{m\downarrow}-E_{l\uparrow}+\omega}\ . \tag{56}$$

The particle-hole (Stoner-type) excitations are explicitly given by the poles in the preceding expression. For example, the pole at $E_{l\uparrow}-E_{m\downarrow}-\omega=0$ represents a spin-flip excitation of a $\downarrow$-spin electron across the Fermi level. The second term similarly represents an emission (deexcitation) process.

The full susceptibility at the RPA level is then given, in matrix form, by

$$\chi^{-+}(\omega)=\frac{\chi_0^{-+}(\omega)}{1-U\chi_0^{-+}(\omega)}\ . \tag{57}$$

The matrix expression on the right-hand side can be expanded in terms of the eigenvalues and eigenvectors of $\chi_0^{-+}(\omega)$ and we obtain,

$$\chi^{-+}(\omega)=\sum_\lambda\frac{|\Phi_\lambda(\omega)\rangle\langle\Phi_\lambda(\omega)|}{1-U\lambda(\omega)}\ . \tag{58}$$

The preceding form is nothing but a propagator representation for the transverse spin excitations. All the information regarding the nature of these collective excitations about the ground state is contained in the eigensolutions $\{|\Phi_\lambda(\omega)\rangle,\lambda(\omega)\}$. In fact, the eigenfunctions, $|\Phi_\lambda\rangle$, represent the wave functions of the collective modes, while the collective-modes energies are given by the poles at $1-U\lambda(\omega)=0$. By looking at the nature of these modes in the spin-bag ground state, and by comparing with the modes present in the half-filled-band case, we are able to determine how the collective modes are affected by the presence of the spin bag.

In the following we discuss our results for the nature of the collective excitation modes, as given by the eigensolutions, $\{|\Phi_\lambda(\omega)\rangle,\lambda(\omega)\}$, obtained in the spin-bag ground state on a 10×10 lattice system for $U/t=5$—a situation representative of the intermediate-coupling regime. In the static limit ($\omega=0$), we find that the largest eigenvalue (in units of t) is precisely $\frac{1}{5}$. This implies that, as for the half-filled-band case, the spectrum of the collective excitations in the spin-bag ground state remains perfectly gapless. Also the mode represented by this largest eigenvalue is actually a Goldstone mode, corresponding to a rigid rotation of the magnetization direction, and therefore costing no energy. We now explicitly show that the nature of $|\Phi_{\lambda_{\max}}(0)\rangle$, the mode corresponding to this largest eigenvalue, is indeed consistent with its interpretation as a Goldstone mode.

We start by defining local spin vectors, $\mathbf{S}_i$, at every site as the ground-state expectation value of the Pauli-spin operator

$$\mathbf{S}_i=\langle\Psi_G|a^\dagger_{i\mu}\boldsymbol{\sigma}_{\mu\nu}a_{i\nu}|\Psi_G\rangle\ . \tag{59}$$

When there are only spin-diagonal terms in the Hartree-Fock Hamiltonian (as for $U/t=5$), all the local spin vectors are directed along the z axis, with their magnitudes equal to the difference in the local electronic spin densities. We now describe these local spins using a spinor representation—$\binom{1}{0}$ for a spin pointing up and $\binom{0}{1}$ for a spin pointing down, both with an am amplitude of $\sqrt{S_i}$ to give the appropriate magnitude. Now a spin-wave mode being a transverse excitation will result in a rotation in spin space of every individual spinor, which can then be expressed in terms of rotation angles,

$$\begin{bmatrix}\varphi_{i\uparrow}\\ \varphi_{i\downarrow}\end{bmatrix}=\sqrt{S_i}\begin{bmatrix}\cos\theta_i/2\\ i\sin\theta_i/2\end{bmatrix}\ . \tag{60}$$

The difference in the densities of the two components of a spinor yields for the z component $S_i\cos\theta_i$, consistent with the classical picture of a spin tilted by an angle θ_i with respect to the z axis. Now the amplitude of the collective mode, $|\Phi_\lambda\rangle$, at site i is simply the expectation value of the spin lowering (or raising) operator because a

spin-wave boson with up (or down) spin is actually created by this operator. Therefore, $|\Phi_\lambda\rangle$ is just the product $\varphi^*_{i\uparrow}\cdot\varphi_{i\downarrow}$ which, from Eq. (60), is proportional to $S_i\sin\theta_i$. In Figs. 5(a) through (e) we have shown, the collective-mode amplitude $|\Phi_\lambda\rangle$ and the ratio, Φ^i_λ/S_i, of this amplitude to the local magnetization, on each lattice site, respectively, in terms of size and orientation of arrows (relative to the vertical), with fixed scale factors.

We observe that for the collective mode corresponding to the largest eigenvalue (energy=0), this ratio, $\Phi^i_{\lambda_{\max}}/S_i$, is independentof the site i. This is clearly seen in Fig. 5(a) which shows that though the amplitude itself of this wave function (arrow sizes) decreases in the vicinity of the spin bag near the lattice center, its ratio to the local magnetization (arrow orientations) remains constant. This establishes that the rotation angles are identical for every site and, therefore, that the collective mode represented by the largest eigenvalue is indeed a Goldstone mode.

Before discussing the nature of the other wave functions, we digress a little and consider the half-filled-band case first. The eigenfunctions of the zeroth-order susceptibility matrix, $[\chi_0^{-+}(\omega)]$, can be expressed in the following form in the sublattice basis

$$\Phi_{\mathbf{k}}(\mathbf{r})=\left[\frac{2}{N}\right]^{1/2}\begin{bmatrix}\alpha_{\mathbf{k}}\\ \beta_{\mathbf{k}}\end{bmatrix}e^{-i\mathbf{k}\cdot\mathbf{r}}\ . \tag{61}$$

It is straightforward to verify that $\Phi_{\mathbf{k}}(\mathbf{r})$ is indeed an eigenfunction of χ_0^{-+} provided $\binom{\alpha_{\mathbf{k}}}{\beta_{\mathbf{k}}}$ is an eigenvector of $\chi_0^{-+}(\mathbf{k})$. The spin-wave amplitude in the half-filled case is, therefore, simply given by a superposition of plane waves, just like the eigenfunctions of the HF Hamiltonian itself. In a finite system with periodic boundary conditions, the spatial dependence will be given by $\cos(k_x x+k_y y)$ and $\sin(k_x x+k_y y)$, with k_x and k_y given by multiplies of $\pm\pi/L$.

A general feature of the wave functions, Φ_λ, is that they come in two distinct parity states. States with even parity have wave functions symmetric with respect to inversion about the spin-bag site. By comparison with the half-filled-band case, also studied for a 10×10 lattice system with periodic boundary condition, we find that the nature and energy of these modes are essentially unchanged from the above-mentioned cosine modes for the half-filled-band system. There also exist, in the spin-bag ground state, modes with odd parity with change sign under inversion with respect to the spin-bag site

$$\Phi_\lambda(-\mathbf{r})=-\Phi_\lambda(\mathbf{r})\ . \tag{62}$$

These odd-parity modes in the spin-bag ground state differ, in structure as well as energy, rather substantially from the sine modes of the half-filled-band system which they replace.

From the preceding discussion given in terms of rotation angles, the collective-mode amplitude at a site is proportional to the local magnetization times the sine of the rotation angle at that site. Since the local magnetization on sites $\mathbf{r}$ and $-\mathbf{r}$ are identical, both sites being on the same sublattice, the difference in sign of the collective-mode amplitudes translates into the two rotation angles having opposite sign. Odd-parity collective modes, therefore, correspond to excitations in the system which result in nearby local spins on the *same sublattice* being tilted in opposite directions.

Figure 5(b) shows one of the two degenerate eigenfunctions which correspond to the second largest eigenvalue and is representative of the odd-parity state already discussed. As is clearly evident, there exists a vertical domain boundary passing through the spin-bag site which separates regions of opposite tilt. Thus as one crosses the domain boundary from left to right, there is an abrupt change in the direction of orientation of the local spins brought about by this mode. In the other symmetrical member of this state the domain boundary is horizontal. These two states appear in the spin-bag ground state in place of the sine wave functions of the half-filled-band system. The two states shown in Figs. 5(c) and (d), which are examples of even parity states and which correspond to the next two (nearly equal) eigenvalues (in decreasing order), are essentially unchanged in nature and in their energies from the cosine states of the half-filled-band system.

We next look at the energy of this collective mode (corresponding to the second largest eigenvalue) which is the energy for which $1-U\lambda(\omega)=0$ is satisfied. This energy corresponds to the lowest excitation energy in the spectrum of the collective modes. For $U/t=5$ and for the 10×10 lattice system, we find $\omega^1|_{\text{collective}}=0.35t$. For a half-filled-band, 10×10 lattice system with $U/t=5$, on the other hand, we find the lowest excitation energy of the spin wave to be $0.47t$, which is, for $Q_x a$ (or $Q_y a)=2\pi/10$, $Q_y a$ (or $Q_x a)=0$, consistent with our analytical result using a spin-wave velocity of $0.8ta$ at $U/t=5$ from Fig. 3. Thus a single hole causes considerable softening of the collective-excitation spectrum, making the system more susceptible to quantum fluctuation effects.

The wave function itself for this first collective excitation is shown in Fig. 5(e). Two features are noteworthy. The amplitude of this collective mode is localized near the spin-bag site with the maximum amplitude on two nearest-neighbor sites on opposite sides. Moreover, this mode has an odd parity, so that the sign of the amplitudes are opposite on these two sites (belonging to the same sublattice). In the other member of the degenerate pair, the wave function is identical except for a rigid rotation by a right angle. Recalling that opposite signs translate into opposite tilts of the local spin vectors, if we take an appropriate combination of these two degenerate modes, we are led to a picture wherein this collective mode induces, in the ground state, a twist in the spin directions about the spin-bag site.

In view of the substantial softening, by a single spin bag, of the collective-excitation spectrum of odd-parity modes, it should be of great interest to see how the energy of these modes scales with increasing system size and increasing hole number. The scaling with size should go as $1/L$, just as for the modes in the half-filled-band case for which the energy of low-lying modes goes as $Q\approx\pi/L$. If for a fixed system size the energy decreases linearly with increasing hole number, which should be

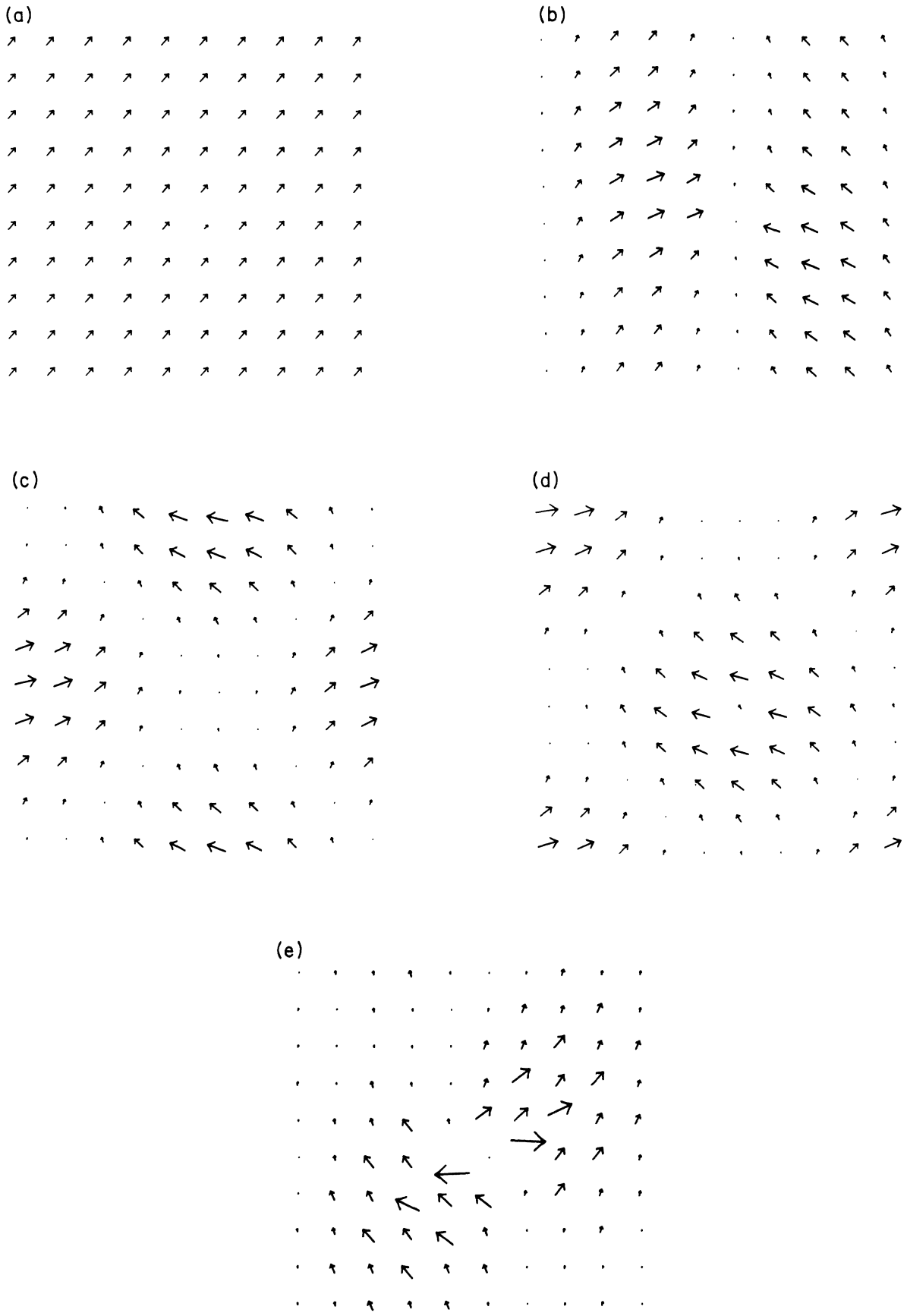

FIG. 5. (a)–(e) The collective-mode amplitudes, Φ_λ^i, and the ratio, Φ_λ^i/S_i, of this amplitude to the total magnetization on each lattice site, shown respectively in terms of arrow size and orientation (with respect to vertical) with fixed scale factors.

reasonable for small hole concentrations, then for a *fixed hole concentration,* the energy will scale as $1/L^2$. This drastic reduction in the energy of the low-lying, odd-parity collective modes, compared with the corresponding energies in the half-filled-band system, will lead to enhanced quantum fluctuations to the extent that long-range commensurate antiferromagnetic order may be wiped out. This issue of scaling with system size and hole number is presently under investigation.

VI. FINITE DENSITY OF HOLES: THE RIGID-BAND APPROXIMATION

As we pointed out in the previous section, a self-consistent solution does not necessarily represent a local minimum in the free energy. It represents rather an extremum and the only way to determine whether the extremum corresponds to a maximum or a minimum is to examine the nature of excitations around the self-consistent state. We present, in this final section, a commensurate spin-density-wave solution as an example of a self-consistent solution for a finite fraction of holes which actually represents a maximum and exhibits an instability towards an incommensurate structure.

In this section we study the nature of excitations in a system which has a finite fraction of holes. We shall work in the "rigid-band approximation" in which the band structure is assumed to be similar to that obtained in the half-filled-band case. It should be pointed out, however, that it is the gap parameter for this system with a finite fraction of holes, which, obtained self-consistently, is used to obtain the bands. The Fermi level, in this case, will lie inside the lower band to account for the less-than-half filling. The added holes are, therefore, effectively assumed to be in quasiparticle states of the system with a commensurate spin-density-wave structure and occupy states in the lower band that lie above the Fermi level. That such a state is indeed self-consistent can be shown easily. As long as the total electronic density on every site is constant, the analysis for the half-filled-band case can be carried through and one arrives at the same self-consistency condition

$$\frac{1}{U}=\frac{1}{N}\sum_{E_{\mathbf{k}}<E_F}\frac{1}{E_{\mathbf{k}}} . \tag{63}$$

There is, however, a difference from the half-filled-band case in that the preceding condition is not satisfied for arbitrarily small values of U. If the Fermi level is within the lower band, the right-hand side of the preceding equation never diverges, rather it is bounded from above roughly by $1/|\varepsilon_{\mathbf{k}_F}|$, the inverse of the free-particle energy on the Fermi surface. Therefore, a self-consistent solution with a nonzero sublattice magnetization is not possible if U is much smaller than $|\varepsilon_{\mathbf{k}_F}|$. In terms of the doping $x=1-n$ which represents the deviation from half filling and is related to $\varepsilon_{\mathbf{k}_F}$ by

$$x\approx\frac{|\varepsilon_{\mathbf{k}_F}|}{t}\ln\frac{t}{|\varepsilon_{\mathbf{k}_F}|} \tag{64}$$

the critical interaction strength, $U_c/t\approx x$.

Since the Fermi level now lies inside the band (instead of in the middle of the band gap as in the half-filled-band case), we expect there to be intraband processes present as well as the interband ones in the spin susceptibility. The intraband processes also include particle-hole excitations across the Fermi level—these excitations being represented by poles in the zeroth-order spin susceptibility. These particle-hole excitations are analogous to the Stoner excitations in a ferromagnet. Within our rigid-band approximation with a finite fraction of holes, these *p-h* excitations will form the gapless branch corresponding to intraband excitations within the lower band itself. In this section we shall, however, focus on the collective excitations arising from the intraband plus the interband processes. A particularly relevant issue is the stability of the self-consistent HF ground state against these collective excitations.

Inverse Fourier transformation of $\chi^{-+}(\mathbf{r},\mathbf{r}';\omega)$ explicitly leads to intraband and interband pieces in the total spin susceptibility

$$\chi^{-+}(\mathbf{r},\mathbf{r}';\omega)=\frac{1}{N}\sum_{\mathbf{Q}}[\chi^{-+}_{\text{intra}}(\mathbf{Q},\omega)+\chi^{-+}_{\text{inter}}(\mathbf{Q},\omega)]e^{-i\mathbf{Q}\cdot(\mathbf{r}-\mathbf{r}')} \tag{65}$$

where $\chi^{-+}_{\text{intra}}(\mathbf{Q},\omega)$ and $\chi^{-+}_{\text{inter}}(\mathbf{Q},\omega)$ are given by expressions similar to Eq. (26) with the condition that the quasiparticle energies for momentum $\mathbf{k}-\mathbf{Q}$ are to be taken with $+/-$ sign in the interband/intraband susceptibilities, explicitly (and implicitly in the quasiparticle amplitudes). Owing to the antisymmetry of the energy denominators, the condition that $\mathbf{k}-\mathbf{Q}$ be outside the Fermi surface can be overlooked in the intraband piece. We first study the static limit of the intraband susceptibility. Substituting the quasiparticle amplitudes in the expression for the susceptibility, we obtain the two eigenvalues,

$$\lambda_{\text{intra}}(\mathbf{Q},\omega=0)=\frac{1}{\Delta}\frac{1}{N}\sum_{\mathbf{k}}''\left[\frac{\varepsilon_{\mathbf{k}-\mathbf{Q}}+\varepsilon_{\mathbf{k}}}{\varepsilon_{\mathbf{k}-\mathbf{Q}}-\varepsilon_{\mathbf{k}}},\frac{\varepsilon_{\mathbf{k}-\mathbf{Q}}-\varepsilon_{\mathbf{k}}}{\varepsilon_{\mathbf{k}-\mathbf{Q}}+\varepsilon_{\mathbf{k}}}\right] , \tag{66}$$

where $\sum_{\mathbf{k}}''$ indicates that the sum is over all $\mathbf{k}$ such that $E_{\mathbf{k}}<E_F$, $E_{\mathbf{k}-\mathbf{Q}}>E_F$, and $\mathbf{k}-\mathbf{Q}$ lies between the Fermi surface and the surface obtained by shifting the Fermi surface by π [see Fig. 6]. We have also used $E_{\mathbf{k}-\mathbf{Q}}-E_{\mathbf{k}}\approx(\varepsilon^2_{\mathbf{k}-\mathbf{Q}}-\varepsilon^2_{\mathbf{k}})/2\Delta$ which is valid for $\varepsilon_{\mathbf{k}_F}<\Delta$, i.e., when the Fermi surface is very close to the top of the band (low density of holes). In the limit $\mathbf{Q}\to 0$, the second eigenvalue vanishes and the first one is obtained in terms of $N(\varepsilon_F)$, the free-particle density of states at the Fermi level

$$\lambda^1_{\text{intra}}(\mathbf{Q}\to 0,\omega=0)=\frac{2\varepsilon_F}{\Delta}N(\varepsilon_F) . \tag{67}$$

The eigenvectors are, respectively, $(2^{-1})^{1/2}\binom{1}{1}$ and $(2^{-1})^{1/2}\binom{1}{-1}$. In view of the only logarithmically diverging density of states as $\varepsilon_F\to 0$, the eigenvalue vanishes as $\varepsilon_F\to 0$, or as the doping $x\to 0$. This physically means the amplitude for intraband $\uparrow$ particle-$\downarrow$ hole excitations across the Fermi level vanishes as $\varepsilon_F\to 0$. This is because as the Fermi level approaches the top of the valence

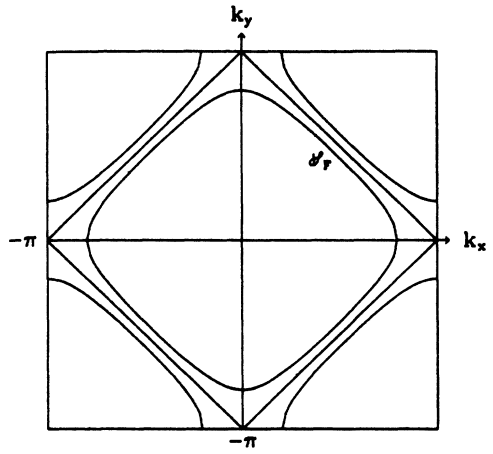

FIG. 6. The Brillouin zone showing the Fermi surface inside the lower band for a system with a finite density of holes in the self-consistent state within the rigid-band approximation.

band, the quasiparticle amplitudes for valence-band states very close to the Fermi level tend to vanish on one or the other sublattice, depending on the spin.

For the static interband susceptibility itself, in the $\mathbf{Q}\to 0$ limit we find the eigenvalues as before,

$$\lambda_{\text{inter}}(\mathbf{Q}\to 0,\omega=0)=\frac{1}{N}\sum_{\mathbf{E_k}<E_F}\frac{1}{E_{\mathbf{k}}}\left[1,\frac{\Delta^2}{E_{\mathbf{k}}^2}\right] \tag{68}$$

with the same eigenvectors respectively as before. Using the self-consistency condition, the larger eigenvalue corresponding to the eigenvector $(2^{-1})^{1/2}\binom{1}{1}$ is simply $1/U$. The total eigenvalue, corresponding to this common eigenvector, of the spin susceptibility is, therefore, the sum

$$\lambda(\mathbf{Q}\to 0,\omega=0)=\frac{1}{U}+\frac{2\varepsilon_F}{\Delta}N(\varepsilon_F)\ . \tag{69}$$

Substituting this value in the RPA expression for the spin susceptibility, we immediately note the absence of a stable Goldstone mode. In fact, the susceptibility comes out to be *negative* (diamagnetic), already an indication that the HF state we were working with may actually not be the true ground state but rather a saddle point corresponding to a local maximum in the free energy. A slight perturbation via an external magnetic field, for example, or due to internal quantum fluctuations, is sufficient to topple the system from this unstable saddle point to a state with lower magnetization—and hence the negative susceptibility.

To examine the nature of the instability in the static limit, we study the spin response for a small, nonzero $\mathbf{Q}$. For small doping concentrations we do not expect significant changes in the interband piece of the spin susceptibility from the half-filled case studied earlier. We found, as discussed in Sec. III [Eq. (34)], that in the static limit the larger eigenvalue goes as $1/U-\gamma\mathbf{Q}^2a^2$, with γ given in Eq. (39). The intraband piece will also have a $\mathbf{Q}$ dependence which, however, can be neglected in comparison to that of the interband piece provided $\varepsilon_F N(\varepsilon_F)\Delta$ is small compared to γ.

Substituting the eigenvalue for small Qa, obtained above in the limit $\varepsilon_F\to 0$, in the RPA expression for the full spin susceptibility, we find that the static susceptibility diverges at a new wave vector, $Q(x)$, which depends on the hole concentration x and is given by

$$Q(x)=\left[\frac{2\varepsilon_F N(\varepsilon_F)^{1/2}}{\gamma\Delta}\right]^{1/2}a^{-1}\ . \tag{70}$$

Since the free-particle density of states, $N(\varepsilon_F)$, diverges as $\ln(t/\varepsilon_F)$, in view of Eq. (64), we find that $[Q(x)a]^2$ is proportional to x.

The self-consistent commensurate SDW state within the rigid-band approximation is thus unstable with respect to collective excitations toward the formation of a two-dimensional incommensurate structure. The wave vector of this incommensurate structure, as projected from the instability in the commensurate SDW state, is proportional to the linear hole density. Whether this incommensurate state is a true HF ground state remains to be seen explicitly (see Ref. 6 for study of various self-consistent incommensurate HF states). In Ref. 4 it is argued that, for a finite concentration of holes, a 1D incommensurate state has a lower HF energy relative to both the commensurate SDW state and an incommensurate 2D state.[26] The argument against the 2D incommensurate structure relies on weak coupling and needs to be reexamined for arbitrary U/t.

VII. CONCLUSIONS

In this paper we have developed a systematic procedure for studying the consequences of holes doped in an antiferromagnet in the intermediate coupling regime. Starting with the half-filled-band case, we have developed a matrix formulation in the sublattice-basis representation, which has the advantage that the RPA forms for all expressions are retained. We have obtained the spectrum of the collective spin-wave excitations about the HF ground state for all values of U/t and find that in the strong-coupling limit, the full $\mathbf{Q}$ dependence of the spin-wave energy is exactly identical to the result obtained from the corresponding spin-$\frac{1}{2}$ Heisenberg model of localized spins (to which the Hubbard model can be mapped in this limit with a nearest-neighbor exchange term of $J=4t^2/U$).

We have also evaluated the one-loop correction to the sublattice magnetization representing the effects of quantum spin fluctuations about the HF state due to virtual emission and absorption of spin waves. In the limit of $U/t\to\infty$ we find that the sublattice magnetization is reduced to 0.6. The zero-point quantum spin fluctuations therefore reduce the sublattice magnetization to 60% of its HF or saturation value, a result which is in excellent agreement with the Monte Carlo studies and linear spin-wave analysis of the Heisenberg model. This indicates that HF plus a self-consistent treatment of the transverse spin fluctuations is able to account for the physics of the half-filled-band Hubbard model even in the strong-coupling limit.

As a first step toward applying this systematic pro-

cedure to the problem of holes doped in an antiferromagnet, we have made a detailed numerical study of the HF ground state with precisely one hole which gets self-consistently trapped by the spin polarization it induces. At the HF level translational symmetry is thus spontaneously broken by the localized hole. The question of how the hole may become mobile when quantum fluctuations (via the self-energy) are incorporated is presently under investigation. We have shown that in the intermediate- and strong-coupling limits, an important role in the stabilization of the spin-bag ground state with, say, one $\uparrow$-spin hole is played by the delocalization of $\downarrow$-spin electrons in the vicinity of the spin bag, leading to the formation of a five-site ferromagnetic core.

When the spin-flip terms (arising from the most general linearization of the Hubbard term) are included in the one-particle HF Hamiltonian, our self-consistent study shows that, starting with a seed for the spin-flip terms around the spin bag, the spin-flip terms iterate toward zero when $U/t < 20$, whereas they grow slowly but relentlessly for $U/t > 20$. This instability of the spin-diagonal HF ground state indicates an onset, at $U/t \approx 20$, of a tendency towards angular fluctuations in the local spin directions around the spin-bag site.

We have also examined the nature and energies of the collective excitations about the self-consistent spin-bag ground state with precisely one hole in a 10×10 lattice system for $U/t = 5$ which is representative of the intermediate-coupling regime. We explicitly show that this spin-bag state admits to a stable Goldstone mode confirming the local stability of the HF state. We find that the nature and energy of the even-parity modes (symmetric under inversion about the spin-bag site) are essentially unchanged from the corresponding cosine modes of the half-filled-band system. On the other hand, odd-parity modes (which replace the sine modes of the half-filled-band system) are strongly affected, both in their nature as well as in energy, by the single hole. The energy of the first collective excitation, for example, is reduced by about 30% relative to the corresponding energy in the half-filled-band case. Also the wave function of this collective excitation is localized around the spin-bag site and represents a mode that induces a twist in the local spin directions about the spin-bag site.

Finally, going to a finite density of holes, we have examined the self-consistent HF state obtained in the rigid-band approximation. In this state the holes occupy quasiparticle states from the top of the valence band of a half-filled-band system, with the gap parameter being self-consistently determined from the finite hole-density system. We find that this self-consistent HF ground state within the rigid-band approximation is unstable with respect to collective excitations toward the formation of a two-dimensional incommensurate structure.

In view of the instability of the commensurate SDW state with extended holes, we have initiated an investigation of the self-consistent state with many holes in order to determine the nature of the HF ground state at finite hole density. As a first step we have studied the interaction between two holes. For $U/t = 5$, which is representative of the intermediate-coupling regime, we find that the interaction between two holes is repulsive irrespective of their spins. Together with our result in the strong-coupling regime, discussed in Sec. II, the interaction is therefore repulsive all the way down to the intermediate-coupling regime.

This suggests that in the intermediate-coupling regime the spin bags will tend to form a lattice arrangement to minimize the interaction energy. Furthermore, we find that for $U/t = 5$ the HF ground-state energy with two parallel-spin holes is slightly smaller than that with two antiparallel-spin holes. At the HF level the picture which emerges for the ground state is therefore one in which spin bags due to parallel-spin holes are arranged in a regular lattice. The commensurate SDW is thus spoiled to some extent not only by modulations in the SDW amplitude but also due to presence of the ferromagnetic cores. Naturally, the next step is to study quantum fluctuations around such a mean-field state. This should shed some light on the way in which the physics of the Hubbard model evolves as one goes from weak to strong coupling, and also possibly result in a quantitatively useful calculational scheme in the intermediate coupling regime. The results presented in this paper indicate that the HF solution and the concept of the spin bag plus self-consistent quantum fluctuations provide a useful tool in this quest, as originally proposed by Schrieffer, Wen and Zhang.[12]

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[1]W. F. Brinkman and T. M. Rice, Phys. Rev. B **2**, 1324 (1970).
[2]B. I. Shraiman and E. D. Siggia, Phys. Rev. Lett. **62**, 1564 (1989).
[3]C. Kane, P. Lee, and N. Read, Phys. Rev. B **39**, 6880 (1989).
[4]H. J. Schulz (to be published).
[5]C. Jayaprakash (to be published).
[6]D. Poilblanc and T. M. Rice (to be published).
[7]B. I. Shraiman and E. D. Siggia, Phys. Rev. Lett. **61**, 467 (1988).
[8]S. A. Trugman, Phys. Rev. B **37**, 1597 (1988).

[9]K. Huang and E. Manousakis, Phys. Rev. B **36**, 8302 (1987).
[10]E. Kaxiras and E. Manousakis, Phys. Rev. B **37**, 657 (1988).
[11]S. Trugman (to be published).
[12]J. R. Schrieffer, X-G. Wen, and S.-C. Zhang, Phys. Rev. Lett. **60**, 944 (1988); E. W. Fenton, *ibid.* **61**, 2813 (1988); J. R. Schrieffer, X-G. Wen and S.-C. Zhang, *ibid.* **61**, 2814 (1988).
[13]E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. **20**, 1445 (1968).
[14]J. D. Reger and A. P. Young, Phys. Rev. B **37**, 5978 (1988).
[15]P. W. Anderson, Phys. Rev. **86**, 694 (1952).
[16]T. Oguchi, Phys. Rev. **117**, 117 (1960).
[17]W. P. Su, Phys. Rev. B **37**, 9904 (1988).
[18]W. P. Su and X. Y. Chen, Phys. Rev. B **38**, 8879 (1988).
[19]H.-C. Choi and E. J. Mele, Phys. Rev. B **38**, 4540 (1988).
[20]Y. Nagaoka, Phys. Rev. **147**, 392 (1966).
[21]G. Shirane, Y. Endoh, R. J. Birgeneau, M. A. Kastner, Y. Hidaka, M. Oda, M. Suzuki, and T. Murakami, Phys. Rev. Lett. **59**, 1613 (1987).
[22]D. C. Mattis, *The Theory of Magnetism* (Springer-Verlag, Berlin, 1981), Vol. I.
[23]J. R. Schrieffer, X.-G. Wen, and S.-C. Zhang, Phys. Rev. B **39**, 11 663 (1989).
[24]J. E. Hirsch and S. Tang, Phys. Rev. B **39**, 2850 (1989).
[25]A. Auerbach and A. Arovas, Phys. Rev. Lett. **61**, 617 (1988).
[26]On a more general note, a one dimensional incommensurate state (an array of domain walls) is unlikely in the presence of long-range Coulomb forces. J. R. Schrieffer (private communication).