Spin waves in the flux-phase description of the $S=1/2$ Heisenberg antiferromagnet

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A so-called "flux-phase" projected-fermion mean-field theory has been shown to give a good account of the ground state and excitations of the $S=\frac{1}{2}$ Heisenberg antiferromagnet on a square lattice. In this paper it is shown that random-phase-approximation spin waves (or paramagnons) of the flux phase have an unusual spectrum, especially near the zone boundary. There is no singularity in the spin-wave density of states at maximum energy, and the small-momentum spin-wave-velocity renormalization is obtained. Noninteracting spin waves are shown to give reasonable description of Raman scattering. It is argued that the conventional picture of strongly interacting, damped Holstein-Primakoff spin waves may in fact be described in terms of less incoherent excitations in this new basis. The flux-phase basis arises through considering the antiferromagnet as the large-U limit of the half-filled Hubbard model. In that model it is suggested that the flux should turn on for $U>U_c \sim 3.1$.

I. INTRODUCTION

The two-dimensional spin-one-half Heisenberg antiferromagnet ($S=\frac{1}{2}$ AFM) has been made widely accessible to experimental study recently by the discovery of a large class of materials possessing large magnetic exchange constants $J \sim O(1000\text{ K})$, namely, the high-T_c oxides. This system is known to have long-range Néel order in the ground state.[1] Holstein-Primakoff (HP) spin-wave theory predicts a correct sublattice magnetization[1] of 60%. In this theory spin waves have a spectrum

$$\omega(k)=2J[1-\gamma^2(k)/16]^{1/2}\ , \quad \gamma(k)=2(\cos k_x+\cos k_y)\ . \tag{1.1}$$

One also obtains this spectrum if one considers a spin-density-wave (SDW) ground state for the large-U Hubbard model.[2]

It is known however that this spectrum is misleading. Higher-order corrections ($1/S$, say, in the HP scheme and calculated in other schemes[1]) produce a spin-wave-velocity renormalization $J \rightarrow Z_c \times J$, $Z_c \sim 1.15-1.2$ and strong damping for zone-boundary spin waves.[3]

Interest in the $S=\frac{1}{2}$ AFM was of course fueled by high-T_c superconductivity and the proposal of Anderson[4] that the large-U Hubbard model described electronic properties of these materials. The $S=\frac{1}{2}$ AFM arises from this model at half-filling and superconductivity appears upon doping. Given this motivation it was natural to try to describe the AFM in terms of the underlying fermions. That allows for a continuous theoretical description linking the doped and insulating states of the Hubbard model.

In mean-field treatments[5] of the Heisenberg model written in terms of constrained electrons a special saddle point (among others) was discovered by Kotliar[6] and Affleck and Marston,[7] which the latter dubbed the "flux phase." In this state the orbital motion of electrons is adjusted as if they were affected by a magnetic flux of $\phi_0/2=hc/2e$ threading each plaquette of the square lattice. If single occupancy is enforced by Gutzwiller projection (P_G) and the resulting state considered as a variational wave function then the numerical work of Zhang *et al.* and Gros[8] shows that indeed this state has a good variational energy.

Our starting point then is the mean-field theory. In Sec. II we describe the flux phase and co-existing flux and spin-density wave phases in detail, explaining how to make spin-wave states and calculating their spectrum. In Sec. III we consider two-magnon Raman scattering. We show that noninteracting spin waves based on the flux phase provide a simple description without need for drastic incoherent scattering effects.

II. FLUX PHASE AND SPIN WAVES

The Hubbard model

$$H=-t\sum_{\langle i,j\rangle,\sigma}(c_i^\dagger c_j+\text{H.c.})+U\sum_i n_{i\uparrow}n_{i\downarrow} \tag{2.1}$$

for $U/t \gg 1$ at half-filling may be canonically transformed and projected onto the nondoubly occupied subspace[9] to become the $S=\frac{1}{2}$ AFM,

$$H^{\text{AFM}}=-J\sum_{\langle i,j\rangle}\sum_{\sigma,\sigma'}c_{i\sigma}^\dagger c_{j\sigma}c_{j\sigma'}^\dagger c_{i\sigma'}\ , \tag{2.2}$$

where $J=4t^2/U$. The mean-field approach assumes a nonzero expectation value for $\chi_{ij}=\langle c_{i\sigma}^\dagger c_{j\sigma}\rangle$, which resembles a link variable of a U(1) lattice gauge field coupled to the remaining fermions:

$$\chi_{ij}=\exp\left[i\int_i^j \mathbf{A}\cdot d\mathbf{l}\right]\ , \tag{2.3}$$

$$H_{\text{eff}}^{afm}=-J\sum_{\langle ij\rangle}\chi_{ij}c_{i\sigma}^\dagger c_{j\sigma}+\frac{1}{J}|\chi_{ij}|^2\ . \tag{2.4}$$

We choose to implement the constraint of one particle per site by Gutzwiller projecting the mean-field fermion many-body wave function. This procedure of Gutzwiller projecting free-fermion states does yield accurate ground-state properties of the large-U Hubbard model. Later we shall give a physical picture to motivate this variational procedure.

It turns out that the best projected mean-field fermion energy[8] for the half-filled case is given by (modulo gauge transformations)

$$\mathbf{A}_{ij}=\frac{\pi}{2}(y_j-y_j)(-1)^{x_i+y_i}\hat{\mathbf{y}} . \tag{2.5}$$

This gauge field is that which is produced by a magnetic flux of $\phi_0/2=hc/2e$ through each plaquette. The effective Hamiltonian becomes

$$H_{\rm eff}^{afm}=\sum_{\mathbf{r}} c_{\mathbf{r}}^{\dagger}(c_{\mathbf{r}+\hat{\mathbf{x}}}+c_{\mathbf{r}-\hat{\mathbf{x}}}+i[c_{\mathbf{r}+\hat{\mathbf{y}}}+c_{\mathbf{r}-\hat{\mathbf{y}}}])+\text{ H.c. }, \tag{2.6}$$

where the even sublattice sites are those for which $x+y=$even integer and odd lattice sites have $x+y=$odd integer.

To construct a variational wave function for the AFM on a lattice of N sites, we place $N/2$ up-spin and $N/2$ down-spin fermions in their kinetic energy ground state on this lattice pierced by magnetic flux and then Gutzwiller project. The resulting variational energy was calculated by Gros *et al.*[8] to be $E\simeq-0.319J$ per link compared with $E\simeq-0.334J$ per link:[1] the lowest known numerical variational energy. Without tuning any parameters we find a wave function having remarkably good energy.

Now let us briefly consider why a Gutzwiller projected double Slater determinant could be a good variational wave function for the antiferromagnet. The point is that minimizing the kinetic energy of fermions induces a exchange hole. Minimizing the kinetic energy of $N/2$ up-spin electrons decreases the nearest-neighbor particle-particle correlation and, since the density is at the commensurate value of $\frac{1}{2}$, increases the amplitude for the up-spin electrons to (locally) be on the same sublattice. Down-spin electrons are likewise correlated so that when the two species are superposed and projected, one finds an enhanced nearest neighbor $\langle S_i^z S_j^z\rangle$. Since the up- and down-spin electrons occupy the same set of single particle states, we automatically have a global spin singlet so that $\langle S_i^x S_j^x\rangle$ and $\langle S_i^y S_y^y\rangle$ are also enhanced.

To be quantitative let us calculate $\langle n_i n_{i+\tau}\rangle$ for half-filled spinless fermions in their kinetic energy ground state with and without flux. τ is a nearest-neighbor vector. Without flux,

$$\langle n_i n_{i+\tau}\rangle \simeq \tfrac{1}{4}-0.0411 . \tag{2.7}$$

The correlation for a random fermion distribution is $\frac{1}{4}$ and -0.0411 is the exchange hole. Now in the case of fermions feeling a uniform flux

$$\langle n_i n_{i+\tau}\rangle \simeq \tfrac{1}{4}-0.0574 . \tag{2.8}$$

The exchange hole is 40% larger.

After Gutzwiller projection numerical calculations show that the energy of a flux state is improved over a state with no flux as follows:

$$\begin{aligned} &E(P_g|\text{free electron}\rangle)=-0.267J \text{ per link },\\ &E(P_g|\text{flux phase}\rangle)=-0.319J \text{ per link }. \end{aligned} \tag{2.9}$$

Given that even our flux state is significantly different in energy from the best known energy, it would seem then that some crucial correlations are being left out of our mean-field state before projection. Gutzwiller projection is actually a very crude operation. It does not generate off-site correlations that are not present before projection. What seems to be missing is the effect of U on nearest-neighbor and longer correlations. If we wish to include that, we must do so *before* projection. What we propose is to include a weak on-site repulsion

$$V\sum_i n_{i\uparrow}n_{i\downarrow} \tag{2.10}$$

as a variational parameter. In mean field, this repulsion may lead to a spin density wave coexisting with the flux order which is known to improve the energy of the flux state.

First let us introduce some notation. Using the relations

$$\begin{aligned} &\sum_{r\text{ even}} \exp(i\mathbf{k}\cdot\mathbf{r})=\frac{N}{2}[\delta(\mathbf{k})+\delta(\mathbf{k}+\mathbf{Q})] ,\\ &\sum_{r\text{ odd}} \exp(i\mathbf{k}\cdot\mathbf{r})=\frac{N}{2}[\delta(\mathbf{k})-\delta(\mathbf{k}+\mathbf{Q})] , \end{aligned} \tag{2.11}$$

where $\mathbf{Q}=(\pi,\pi)$, we define

$$\begin{aligned} &c_e^{\dagger}(\mathbf{k})\equiv[c^{\dagger}(\mathbf{k})+c^{\dagger}(\mathbf{k}+\mathbf{Q})]/\sqrt{2} ,\\ &c_0^{\dagger}(\mathbf{k})\equiv[c^{\dagger}(\mathbf{k})-c^{\dagger}(\mathbf{k}+\mathbf{Q})]/\sqrt{2} . \end{aligned} \tag{2.12}$$

Now consider the flux-phase Hamiltonian with a SDW field m:

$$\begin{aligned} H=&\sum_{\mathbf{r}\text{ even}}\{c_{\mathbf{r}}^{\dagger}[c_{\mathbf{r}+\hat{\mathbf{x}}}+c_{\mathbf{r}-\hat{\mathbf{x}}}+i(c_{\mathbf{r}+\hat{\mathbf{y}}}+c_{\mathbf{r}-\hat{\mathbf{y}}})]+\text{ H.c.}\}\\ &+m_\sigma\left[\sum_{r\text{ even}}c_{\mathbf{r}}^{\dagger}c_{\mathbf{r}}-\sum_{\mathbf{r}\text{ odd}}c_{\mathbf{r}}^{\dagger}c_{\mathbf{r}}\right] , \end{aligned} \tag{2.13}$$

Fourier transforming,

$$H=\sum_{k,\sigma}{}'[c_{e\sigma}^{\dagger}(k)c_{o\sigma}^{\dagger}(k)] \times\begin{bmatrix}\sigma m & 2(\cos k_x+i\cos k_y)\\ 2(\cos k_x-i\cos k_y) & -\sigma m\end{bmatrix} \times\begin{bmatrix}c_{e\sigma}(k)\\ c_{o\sigma}(k)\end{bmatrix} \tag{2.14}$$

with eigenvalues

$$\varepsilon(k)=\pm E_k,\quad E_k\equiv\sqrt{\Gamma_k^2+m^2} , \tag{2.15}$$

where

$$\Gamma_k \equiv \sqrt{\cos^2 k_x + \cos^2 k_y} \ .$$

When $m \to 0$ a notable feature of the spectrum is extrema at $\mathbf{k}=(0,0),(0,\pi)$ and two "Fermi points" at $\mathbf{k}_0^{\pm}=(\pi/2,\pm\pi/2)(\mathrm{mod}\mathbf{Q})$ where the energy goes to zero linearly as $|k-k_0^{\pm}|$. That is, the fermion spectrum is relativistic. The staggered chemical potential looks like a fermion mass. The eigenfunctions are

$$\Psi_{\pm,\sigma}(k)=g(k)[-2(\cos k_x - i\cos k_y)c_{e\sigma}(k) + (\sigma m \mp E_k)c_{o\sigma}(k)]/D_{\mp,\sigma} \ , \quad (2.16)$$

$$c_{e\sigma}(k)=-\left[\frac{\sigma m+E_k}{D_{+,\sigma}}\right]\psi_{+\sigma}(k) + \left[\frac{\sigma m - E_k}{D_{-,\sigma}}\right]\Psi_{-\sigma}(k) \ ,$$
$$c_{o,\sigma}(k)=-\left[\frac{2(\cos k_x - i\cos k_y)}{D_{+,\sigma}}\right]\Psi_{+\sigma}(k) + \left[\frac{2(\cos k_x - i\cos k_y)}{D_{-,\sigma}}\right]\Psi_{-\sigma}(k) \ , \quad (2.17)$$

where

$$D_{\pm,\sigma}=(2\Gamma_K^2+2M^2\pm 2\sigma m E_k)^{1/2} = [2E_k(E_k \pm \sigma m)]^{1/2}$$

and

$$g(k)=2(\cos k_x + i\cos k_y)/\Gamma_k \ .$$

Note that since $m_{\sigma=\uparrow}=-m_{\sigma=\downarrow}$, the sets of states filled by up- and down-spin electrons will not be identical and the overall state (pre and post projection) is not a pure singlet.

Lee and Feng[10] and Gros[8] have done a Monte Carlo calculation with staggered magnetization in the flux phase as a variational parameter. In both cases a best variational energy $-0.332J$ was found for a sublattice magnetization of about 70%. If one allows Néel order with no flux, as was considered by Yokoyama and Shiba,[11] the best variational energy is $-0.321J$ per link with a sublattice magnetization of 84%. The energy is significantly higher than the best Neel states with flux. So at least from this particular variational point of view it is favorable to introduce a magnetic flux.

At this point let us introduce an analytical approximation to Gutzwiller projection which qualitatively reproduces the Monte Carlo results quoted above. In this approximation we focus on two or four sites and calculate the configuration probabilities at these sites *after* Gutzwiller projection in terms of probabilities *before* projection. This approximation is controlled in that we could apply this procedure to larger and larger clusters of sites using multinoninteracting particle correlation functions to get better and better approximations. However we shall show that agreement with Monte Carlo simulations is quite good at our level of approximation. We shall then, with some confidence, assume that using this method to calculate various quantities gives answers accurate to within numerical factors $\sim O(1)$.

Let $P(\cdots)$ be the probability of a spin configuration on two adjacent sites after projection and $P_0(\cdots)$ the probability of some electron configuration (usually of noninteracting electrons) on the same two sites before projection. Let $\uparrow,\downarrow,\Uparrow,\Downarrow$ denote up-spin electrons, down-spin electrons, up-spin holes, and down-spin holes, respectively. Then the probability of having two parallel or antiparallel spins, respectively, on adjacent sites after projection is

$$P(\uparrow\uparrow)=P(\downarrow\downarrow)=P_0(\uparrow\uparrow)\times P_0(\Downarrow\Downarrow) = P_0(\downarrow\downarrow)\times P_0(\Uparrow\Uparrow)=(\tfrac{1}{4}-x)^2 \ ,$$
$$P(\uparrow\downarrow)=P(\downarrow\uparrow)=P_0(\uparrow\Uparrow)\times P_0(\Downarrow\downarrow) = P_0(\downarrow\Downarrow)\times P_0(\Uparrow\uparrow)=(\tfrac{1}{4}+x)^2 \ , \quad (2.18)$$

where, in the absence of SDW say,

$$x=\frac{1}{16N^2}\left[\sum_{\text{occupied}} \varepsilon_k\right]^2 =0.0411 \ \text{no flux} \qquad =0.0574 \ \text{with flux} \ . \quad (2.19)$$

The nearest-neighbor spin-spin correlation is then approximated by

$$\langle S_i^z S_j^z\rangle \simeq \frac{\frac{1}{4}[P(\uparrow\uparrow)+P(\downarrow\downarrow)]-\frac{1}{4}[P(\uparrow\downarrow)+P(\downarrow\uparrow)]}{P(\uparrow\uparrow)+P(\downarrow\downarrow)+P(\uparrow\downarrow)+P(\downarrow\uparrow)} \simeq \frac{-2x}{1+16x^2}$$
$$\simeq -0.080 \ \text{projected without flux} \qquad \simeq -0.109 \ \text{projected flux phase} \ . \quad (2.20)$$

As we are dealing with singlet states our estimate for the projected variational energy is $\langle J\mathbf{S}_i\cdot\mathbf{S}_j\rangle = 3J\langle S_i^z S_j^z\rangle \simeq -0.327J$ for the flux phase, about 3% off from the Monte Carlo value.

To show that this method can be accurate, we now calculate *analytically* the optimal value after Gutzwiller projection of the mass parameter m with respect to the spin Hamiltonian. This method has been extended to estimate also the energy of electron particle-hole excitations after projection. We begin with the density-density correlation

$$\frac{1}{4N}\sum_{i,\tau}\langle n_i n_{i+\tau}\rangle = \frac{1}{N^2}\sum_{k,p,p'}{}'\gamma(p-p')\langle c_e^\dagger(k-p+p')c_e(k)c_0^\dagger(p)c_0(p')\rangle \quad (2.21)$$

and break it up into the direct and exchange pieces. (The prime denotes summation on the reduced Brillouin zone.) The direct piece, which contains terms like

$$\langle \Psi_-^\dagger(k)\Psi_-(k)\Psi_-^\dagger(p)\Psi_-(p)\rangle$$

from the $c_{e,0}$ operators, contributes a term

$$\tilde{a}=\frac{1}{N^2}\sum_{k,p}{}'\left|1-\frac{m}{E_k}\right|\times\left|1+\frac{m}{E_p}\right| . \tag{2.22}$$

The exchange piece, coming from extracted terms like

$$\langle \Psi_-^\dagger(p')\Psi_+(p)\Psi_+^\dagger(p)\Psi_-(p')\rangle$$

gives a contribution

$$\tilde{x}=\frac{1}{16N^2}\left[\sum_p{}'\frac{\Gamma_p^2}{E_p}\right]^2 . \tag{2.23}$$

In the presence of a staggered magnetization $\langle S_i^xS_j^x+S_i^yS_j^y\rangle$ must be calculated separately. For this one can show that

$$\frac{1}{4N}\sum_{i,\tau}\langle c_{i\uparrow}^\dagger c_{i+\tau\uparrow}c_{i+\tau\downarrow}^\dagger c_{i\downarrow}\rangle=\tilde{x} . \tag{2.24}$$

One more ingredient we need is the sublattice magnetization,

$$\begin{aligned}\tilde{b}&=\frac{2}{N}\left[\sum_{i\ \mathrm{odd}}c_{i\uparrow}^\dagger c_{i\uparrow}-\sum_{i\ \mathrm{even}}c_{i\uparrow}^\dagger c_{i\uparrow}\right]\\&=\frac{2}{N}\sum_k{}'[(\Gamma_k^2-(m-E_k)^2)/D_{-\uparrow}^2]\langle\Psi_{-\uparrow}^\dagger(k)\Psi_{-\uparrow}(k)\rangle\\&=\frac{2}{N}\sum_k{}'\frac{m}{E_k} .\end{aligned}\tag{2.25}$$

Defining

$$\tilde{a}=\tfrac{1}{4}-\tfrac{1}{4}\tilde{b}^2$$

and putting all the terms together we have new probabilities

$$P(\uparrow\uparrow)=(\tilde{a}-\tilde{x})^2 ,$$
$$P(\uparrow\downarrow)=(\tfrac{1}{2}+\tfrac{1}{2}\tilde{b}-\tilde{a}+\tilde{x})^2 ,$$
$$P(\downarrow\uparrow)=(\tfrac{1}{2}-\tfrac{1}{2}\tilde{b}-\tilde{a}+\tilde{x})^2 .$$

Our choice for the sign of m favors $\uparrow$ spins on the odd sublattice. We follow a convention that the first arrow in the parentheses $P(\cdots)$ refers to an odd lattice site. The new normalization factor is

$$\begin{aligned}Z&=P(\uparrow\uparrow)+P(\downarrow\downarrow)+P(\uparrow\downarrow)+P(\downarrow\uparrow)\\&=2[(\tilde{a}-\tilde{x})^2+(\tfrac{1}{2}-\tilde{a}+\tilde{x})^2+\tfrac{1}{4}\tilde{b}^2] .\end{aligned}$$

The spin correlations are

$$\langle S_i^zS_j^z\rangle=(2\tilde{a}-\tfrac{1}{2}-2\tilde{x}-\tfrac{1}{2}\tilde{b}^2)/4Z , \tag{2.26}$$

$$\langle S_i^xS_j^x+S_i^yS_j^y\rangle=-\tilde{x}/Z . \tag{2.27}$$

The sublattice magnetization after projection is

$$\frac{2(\frac{1}{2}-\tilde{a}+\tilde{x})\tilde{b}}{Z} . \tag{2.28}$$

In fact the actual numerical computation was carried out extending the above method to four adjacent sites. In this case there are 16 possible spin configurations. The weight of each was computed according to the same procedure as before. For example,

$$\begin{aligned}P\begin{bmatrix}\downarrow & \uparrow\\ \uparrow & \uparrow\end{bmatrix}&=P_0\begin{bmatrix}\Uparrow & \uparrow\\ \uparrow & \uparrow\end{bmatrix}P_0\begin{bmatrix}\downarrow & \Downarrow\\ \Downarrow & \Downarrow\end{bmatrix} ,\\P_0\begin{bmatrix}\Uparrow & \uparrow\\ \uparrow & \uparrow\end{bmatrix}&=2P_0(\Uparrow\uparrow)P_0(\uparrow\uparrow)\\&\quad+P_0\begin{bmatrix}\Uparrow & \\ & \uparrow\end{bmatrix}P_0\begin{bmatrix} & \uparrow\\ \uparrow & \end{bmatrix}\\&\quad-2(\tfrac{1}{2}+\tfrac{1}{2}\tilde{b})^3(\tfrac{1}{2}-\tfrac{1}{2}\tilde{b}) ,\end{aligned}\tag{2.29}$$

where we have chosen the upper-right and lower-left sites as favored by up spins in the presence of a spin-density wave.

The results of our calculation of energy and sublattice magnetization as a function of mass is shown in Fig. 1. For the flux phase, we compute an energy minimum of about $-0.331J$ occurring at $m\approx0.5$. At that point the sublattice magnetization is 60%. These results are in rough agreement with the Monte Carlo results of Lee and Feng, and Gros, confirming the accuracy of our analytical approach. In the uniform phase we found a variational energy minimum of $E=-0.292J$ with a sublattice magnetization of 85%, agreeing roughly with Yokoyama and Shiba.[11] The fact that our simple short-range Gutzwiller projection has such a good energy implies that the flux plus Néel state can obtain almost all of its ground-state energy from adjusting short-range correlations before projection. In this system energy is not sensitive to long-range order. For the same reason it is in a property such as sublattice magnetization that different numerical studies of the AFM in general have the poorest quantitative agreement. Zero-point spin-wave fluctuations make corrections to the ground-state energy in two dimensions which are miniscule but greatly affect sublattice magnetization.

Let us now turn to the calculation of the spin-wave spectrum. Our plan is as follows: we shall first create a

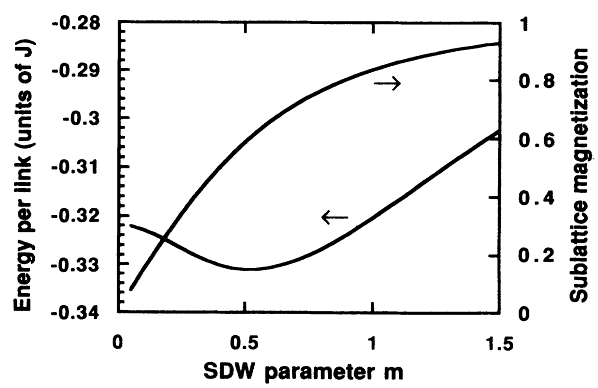

FIG. 1. Gutzwiller projected variational energy and sublattice magnetization of the flux phase as a function of the mass parameter m.

spin wave in the SDW ground state of the flux phase with weak U. (The flux background will be fixed throughout.) The usual RPA-type calculation of the pole of $S^z=\pm 1$ particle-hole Green's function gives a preprojected spin-wave energy spectrum ϵ_q. In addition the residue at ϵ_q gives information about the composition of momentum-q spin waves in terms of plane-wave states. We are assuming that projected spin waves are approximate eigenstates of the large-U Hamiltonian. One indirect check of the assumption is to calculate the effect of P_G on the norm of the spin-wave state.

We begin with the Hamiltonian (2.14) and suppose that there is a weak repulsion

$$\sum_i V n_{i\uparrow} n_{i\downarrow}, \quad V^{-1}=N^{-1}\sum_k{}' E_k^{-1} . \tag{2.30}$$

The weak repulsion is denoted by V to distinguish it from the repulsion U of the physical Hamiltonian (2.1). In our mean-field approach V is chosen to given rise to the appropriate value of m, the SDW staggered potential.

The one-particle bare Green's function is

$$G_0(z)=\sum_{k,n,\sigma}{}' \frac{|k,n,\sigma\rangle\langle k,n,\sigma|}{z-nE(k)} , \tag{2.31}$$

where

$$|k,n,\sigma\rangle=\sqrt{2/N}\left[\sum_{x\text{ even}} e^{ikx}[-2(\cos k_x - i\cos k_y)]/D_{n\sigma}|x \text{ even}\rangle+\sum_{x\text{ odd}} e^{ikx}(\sigma m-nE_k)/D_{n\sigma}|x\text{ odd}\rangle\right] \tag{2.32}$$

is a plane-wave state of momentum k, spin σ in the $n=\pm$(upper/lower) Landau level. The particle-hole Green's function is

$$G_0(z)=\sum_{k,k'}{}' \begin{bmatrix} |k,+1,\sigma;k',-1,\sigma'\rangle \\ |k,-1,\sigma;k',+1,\sigma'\rangle \end{bmatrix}^T \begin{bmatrix} \dfrac{1}{z-E(k)-E(k')} & 0 \\ 0 & -\dfrac{1}{z+E(k)+E(k')} \end{bmatrix} \begin{bmatrix} \langle k,+1,\sigma;k',-1,\sigma'| \\ \langle k,-1,\sigma;k',+1,\sigma'| \end{bmatrix} , \tag{2.33}$$

where primed variables refer to the hole.

We shall consider a $S^z=+1$ spin wave consisting of an up-spin particle and down-spin hole ($\sigma=+1$, $\sigma'=-1$ above). They feel an attractive interaction $-\sum_{x,y}|x,y\rangle V\delta(x,y)\langle x,y|$ where x and y are coordinates of the up particle and down hole, respectively. Using the relation

$$\sum_{i=\text{even}} \langle p,n;p',-n|ii\rangle\langle ii|k,n';k',-n'\rangle=v_n^\dagger(p,p')\tfrac{1}{2}(1+\tau_3)v_{n'}(k,k')\delta(p-p'-k+k') , \tag{2.34}$$

where

$$v_n(p,p')=\sqrt{2/N}\begin{bmatrix} [2(\cos p_x - i\cos p_y)2(\cos p_x'+i\cos p_y')]/D_{-n\uparrow}(p)D_{+n\downarrow}(p') \\ [(m-nE_p)(-m+nE_{p'})]/D_{-n\uparrow}(p)D_{+n\downarrow}(p') \end{bmatrix} \tag{2.35}$$

and also a relation obtained by substituting "even" for "odd" and $(1-\tau_3)$ for $(1+\tau_3)$, the Fourier transform of the interaction V is

$$\sum_{k,k'}{}'\sum_{p,p'}{}'\sum_{n,n'} |k,n,k',-n\rangle v_n^\dagger(k,k')Vv_{n'}(p,p')\langle p,n',p',-n'|\delta(k-k'-p+p') . \tag{2.36}$$

The full propagator is

$$\begin{aligned} \mathrm{Tr}\mathbf{G}(k,k';z)= {} & \mathrm{Tr}\Big[\mathbf{G}_0(k,k';z)-\mathbf{G}_0(k,k';z)\bar{v}(k,k')V\bar{v}^\dagger(k,k')\mathbf{G}_0(k,k';z) \\ & +\mathbf{G}_0(k,k';z)\bar{v}(k,k')V\sum_{p,p'}{}'\bar{v}^\dagger(p,p')\mathbf{G}_0(p,p';z)\bar{v}(p,p')V\bar{v}^\dagger(k,k')\mathbf{G}_0(k,k';z)\cdots\Big] \\ = {} & \mathrm{Tr}\mathbf{G}_0(k,k';z)-\mathrm{Tr}\left[\frac{V\bar{v}^\dagger(k,k')\mathbf{G}_0(k,k';z)\mathbf{G}_0(k,k';z)\bar{v}(k,k')}{1+V\sum_{p,p'}{}'\bar{v}^\dagger(p,p')\mathbf{G}_0(p,p';z)\bar{v}(p,p')}\right] , \end{aligned} \tag{2.37}$$

where

$$\bar{v}^\dagger(p,p'=[v_+(p,p')v_-(p,p')] \tag{2.38}$$

is a 2×2 matrix. Given a total momentum of the particle hole $q=k-k'$, G has poles at $z=\pm\varepsilon_q$ of positive and negative residue, respectively. The smallest z for which $G(k,k-q;z)$ has a pole determines the bound pair or spin-wave excitation energy ε_q. The trace diverges when

$$\det\mathcal{A}=0 , \tag{2.39}$$

where

$$\mathcal{A}=1+V\sum_{p,p'}{}'\bar{v}^{\dagger}(p,p')\mathbf{G}_0(p,p';z)\bar{v}(p,p')\delta(p-p'-q) .$$

In order to calculate the spin-wave energy after Gutzwiller projection, we will need to know the spatial distribution of the relative coordinate of particle and hole for a given spin-wave momentum q. In our analytic projection scheme the spin-wave energy comes from $1/N$ corrections to pre-projection-like spin correlation such as $P_0(\uparrow\uparrow)$ *and* $1/N$ correlations between opposite spins *before* projection $P_0(\uparrow\Downarrow)$ due to the presence of the spin wave. The probability for a bound pair to be in a plane-wave state $|k,+;k-q,-\rangle$ is simply

$$\mathrm{Res}\mathbf{G}(k,+,k-q,-;z)|_{z=\varepsilon_q}=\mathrm{Tr}\frac{V\bar{v}^{\dagger}(k,k')\mathbf{G}_0(k,k';z)\frac{1}{2}(1+\tau_3)\mathcal{A}^{-1}\mathbf{G}_0(k,k';z)\bar{v}(k,k')}{\partial_z \ln \det\mathcal{A}|_{z=\epsilon_q}} , \tag{2.40}$$

$k'=k-q$; $p'=p-q$. This residue may be verified to satisfy the sum rule

$$\sum_k{}' \mathrm{Res}_{z=\varepsilon_q}[\mathbf{G}(k,+;k-q,-;z)-\mathbf{G}(k,-;k-q,+;z)]=1 . \tag{2.41}$$

With the Gutzwiller projection we make use of quantities such as the probability for an $\uparrow$ particle and $\downarrow$ hole to share a site on the even sublattice,

$$\begin{aligned} g_0 &\equiv \mathrm{Res}\frac{2}{N}\sum_{x,y\ \mathrm{even}}\mathbf{G}(x,+;y,-;z)\delta(x-y) \\ &= -V\sum_{k,p}{}'v_+^{\dagger}(p,p-q)\tfrac{1}{2}(1+\tau_3)v_+(k,k-q)\,\mathrm{Tr}\tfrac{1}{2}(1+\tau_3)\mathbf{G}_0(k,k-q;\varepsilon_q)\bar{v}(k,k-q) \\ &\quad\times\frac{\mathcal{A}^{-1}}{\partial_z \ln\det\mathcal{A}|_{z=\varepsilon_q}}\bar{v}^{\dagger}(p,p-q)\mathbf{G}_0(p,p-q;\varepsilon_q) \end{aligned} \tag{2.42}$$

and so on for other diagonal and off-diagonal amplitudes for particle-hole configurations. Any such residues must be divided by the norm of the spin-wave state

$$\sum_k{}'\mathrm{Res}\mathbf{G}(k,+,k-q,-;\varepsilon_q) . \tag{2.43}$$

We have calculated the fraction of the RPA spin wave which survives Gutzwiller projection to be $\gtrsim 50\%$—not too small—ensuring the robustness of our procedure.

The above procedure is quite tedious. But it was useful in confirming[12] the following much simpler, less rigorous derivation of the spin-wave spectrum. In the limit when m is large (i.e., we impose classical Néel order, $V\rightarrow 2m+(4/m)$ and Eq. (2.39) has the solution

$$z(q)=(4/m)\sqrt{1-\gamma^2(q)/16} . \tag{2.44}$$

This is, as expected, the HP spectrum of Eq. (1.1) with $J=4/V=4t^2/U$ as we have set $t=1$. We see therefore that if classical Néel order is imposed, flux phase spin waves continue to HP spin waves. Moreover, the solution of (2.39) has the correct normalization. Thus we guess (and confirm through the more involved, approximate, calculation) that the correct energy after projection in units of J away from the classical Néel state (we use $m=0.5$, the result of our variational calculation) is just the numerical value of the pole of (2.39). Schrieffer *et al.*[2] discuss a similar appearance of an analytical expression for spin wave energy for all U in a SDW theory of the Hubbard model (no flux).

The calculated spectrum is plotted in Fig. 2, along the momentum directions $(0,0)\rightarrow(0,\pi)\rightarrow(\pi,\pi)\rightarrow(0,0)$. The spectrum at $q\rightarrow 0$ shows a spin-wave-velocity renormalization $Z_c\sim 1.20$ relative to the HP value: $\omega\equiv\sqrt{2}Jk\times Z_c$. This agrees with previous work.[1] The high-energy region of the spectrum differs significantly from the HP spectrum. The HP spectrum peaks at $\omega=2J$ for all $\mathbf{q}$ such that $\gamma(\mathbf{q})=0$. The flux-phase spectrum, in the direction $(0,\pi)$, peaks well before $(0,\pi)$ and at a lower energy than at $(\pi/2,\pi/2)$. This peculiar spectrum arises as a result of the peculiar spectrum of the underlying fermions. The density of states does not diverge at the maximum energy. Rather, as plotted in Fig. 3, it has a peak at about $1.8J$. The density of states is rather

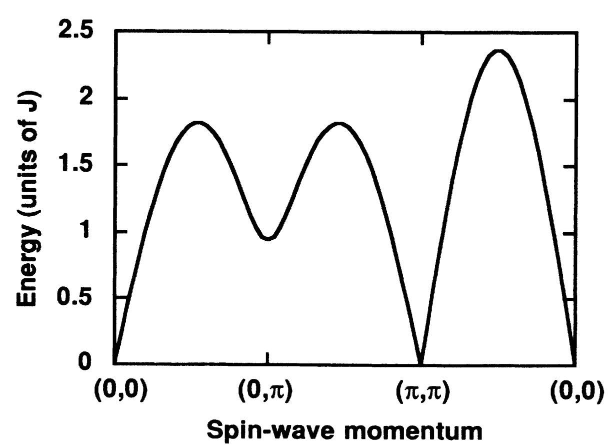

FIG. 2. Spin-wave spectrum from $q=(0,0)$ to $(0,\pi)$ to (π,π) to (0,0).

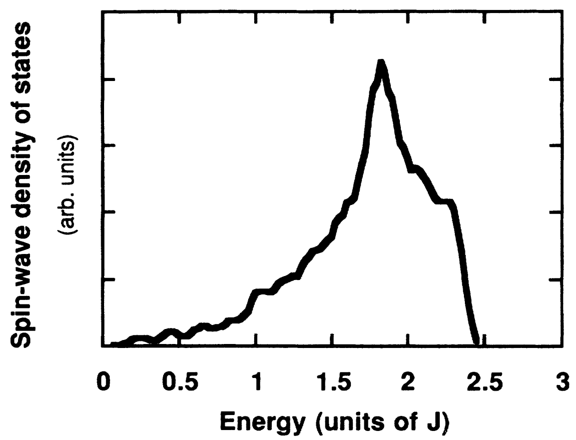

FIG. 3. One-spin-wave density of states. Wiggles are finite-lattice effects.

reminiscent of the single-particle density of states of the flux phase, which was plotted by Hasegawa *et al.*[13] This is consistent with the fact that m is very small compared to the bandwidth and hence does not affect the spectrum of high-energy excitations very much.

One interesting speculation is that if the flux state coexisting with Néel order is indeed the correct fermionic description, Néel order, for large U, on the square lattice is *not* driven by nesting. That is, we imagine that the lattice is slightly doped and move towards half-filling. Before Néel order sets in, there is already a flux order in the doped state. The flux removes any density of states at the nesting vector. Perhaps a flux type of order is a generic picture for real itinerant antiferromagnets like chromium which have large contributions to the large SDW moment from density of states away from any nesting vector present in band structure calculations.[14]

If one supposes that the ground state of the half-filled Hubbard model has a spin-density wave for all values of $U>0$, then an interesting prediction can be made. The existence of flux is incompatible with a spin-density wave if U is too small because of the lack of nesting. In mean field (which overestimates long range order anyway) the minimum U is given by

$$U_c^{-1}=N^{-1}\sum_k{}' \Gamma_k^{-1}, \quad U_c \sim 3.12 \ . \tag{2.45}$$

For $U<U_c$ a flux phase description of the SDW state is not possible.

III. RAMAN SPECTRUM

In Raman scattering[15,16,17] experiments on insulating crystals of high-T_c material a beam of monochromatic light polarized parallel to some axis in the a-b plane is scattered and observed at some other in-plane polarization. The light leaves behind energy but essentially zero momentum. In higher spin antiferromagnets (i.e., $S \geq 1$) observed Raman spectra fit the theoretical curve expected for the creation of two weakly interacting HP magnons of momentum **q** and $-$**q** (Ref. 18). For $S=\frac{1}{2}$, there is a large attraction between two spin waves of spin $+1$ and -1 which shifts the maximum of the Raman spectrum down in energy substantially and also gives rise to a large broadening. Singh *et al.*[19] have calculated the Raman spectrum using an Ising series expansion and shown that the expected spectrum for a $S=\frac{1}{2}$ AFM agrees in detail with observed spectra. Weber and Ford[20] have tried to reproduce experimental data with a phenomenological lifetime broadening model for spin waves. It is claimed here however that such incoherent effects may *not* be needed to explain the high-energy excitations as calculated by Singh *et al.*[19] and measured in experiment.

The Raman spectra for noninteracting spin waves is essentially the density of states for two magnons of momenta $\mathbf{q},-\mathbf{q}$ multiplied by a polarization and momentum-dependent weighting factor. We shall consider two polarizations and their polarization factors:

$$\text{(i)}\ x',y' \text{ polarizaton } f(q)=(\cos q_x-\cos q_y)^2 \ , \quad \text{(ii)}\ x,x \text{ polarization } f(q)=2(\cos q_x)^2 \ . \tag{3.1}$$

(See Ref. 15 for the polarization labeling convention.) In

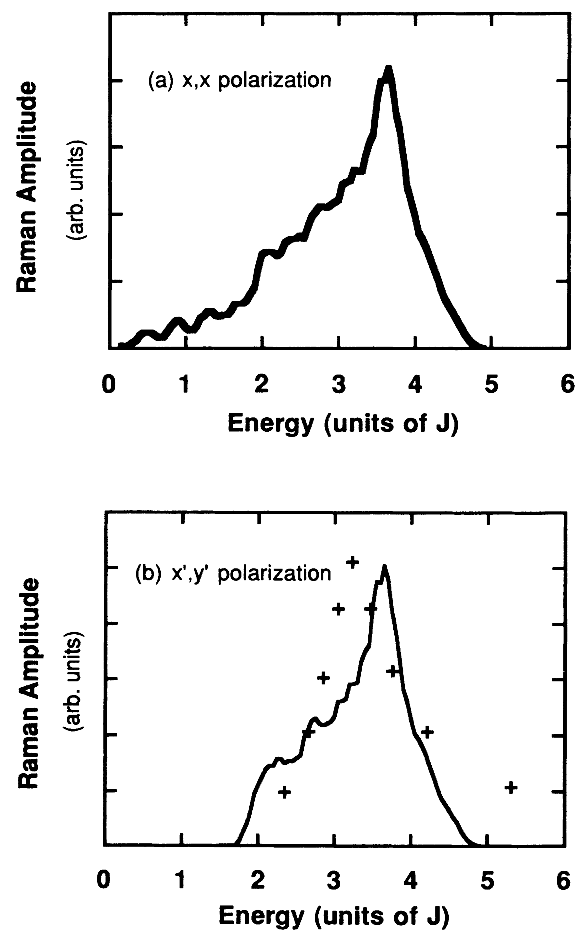

FIG. 4. Raman spectrum for two noninteracting spin waves. (a) x,x polarization, (b) x',y' polarization, crosses are data points from Singh *et al.*

Fig. 4 we plot Raman spectra for the two polarizations. Data extracted from Singh *et al.*[19] by fixing only the amplitude at the maximum are plotted in Fig. 4(b). The energy of the peak and the width are roughly consistent with observed results for x',y' polarization. The energy of the peak calculated here is about 10% high. As Singh *et al.* have emphasized there is a significant resonance enhancement observed with x,x polarization so that comparison with calculated spectra is difficult without knowing the nature of the resonance. In any case the calculated two-magnon spectrum is basically similar for the two polarizations. The only point that should be emphasized is that these spectra are calculated for noninteracting magnons and that the shape and width of the spectrum originates from the underlying fermion spectrum of the flux phase.

IV. CONCLUSIONS

Projected flux-phase paramagnons seem to be a less incoherent description of spin excitations of the $S=\frac{1}{2}$ AFM than Holstein-Primakoff spin waves. In the proposed basis, the "spin waves" have internal structure. That has been calculated elsewhere[12] by considering the residues $\mathbf{G}(i,i,i,i;z)$ and $\mathbf{G}(i,i,i+\tau,i+\tau;z)$ at $z=\varepsilon_q$. It can be shown, for example, that the particle-hole pair is separated by one or more lattice sites about 30% of the time before projection. After projection this figure is reduced to about 5%. Since they are more complicated they seem to be more "relaxed" energetically. The magnetic flux, which simulates the correlated motion of spins carried by fermions in the Hubbard model, also seems to take into account some of the effects of backflow associated with the motion of the spin wave. The single-spin-flip $\sum_x S_x^- \exp(ikx)$ basis may just be a bad basis. it is only because we tried to describe the AFM in terms of electron that we found this a better "flux-phase" basis.

Throughout this paper the mean field χ_{ij} has been kept constant. On the surface this would seem to be an improper assumption. One problem, for example, is that $S^z=0$ (e.g., up-spin particle+up-spin hole) excitations cause spin-dependent fluctuations in χ_{ij}. That breaks spin symmetry, making it very difficult from a technical point of view to ensure the gaplessness of spin wave Goldstone modes. Fortunately, we can take advantage of the fact that U is large. In fact the spin excitations considered here are tightly bound particle-hole pairs with $S^z=\pm 1$ so that they should not contribute to $\Delta\chi_{ij}=\Delta\langle c_{i\sigma}^\dagger c_{j\sigma}\rangle$ which only moves one particle one lattice spacing. Particle-hole excitations with $S^z=0$ or indeed any excitations which affect χ_{ij} are *charged*. Only upon doping are fluctuations in χ_{ij} important and so we must concede that considerations of this paper cannot apply to the doped Hubbard model.

The parameter "$m \sim 0.5$" is very small, viz., $E=\sqrt{4(\cos^2 k_x + \cos^2 k_y)+m^2}$ indicating that high-energy excitations are rather insensitive to the presence of long-range order, even though (because of Gutzwiller projection) the ordered moment is large. In order to produce $m\neq 0$ before projection a minimum value of V is required. That is a consequence of the vanishing density of states of the flux phase. So it is predicted that a flux-phase description is appropriate only above a critical value of the Hubbard U which is about 3.1. It is not clear whether this characteristic of the flux-phase description implies a phase transition. One could calculate the ground-state expectation of the plaquette operator $\mathcal{B}=\chi_{12}\chi_{23}\chi_{34}\chi_{41}$ (where 1,2,3,4 are the vertices of a plaquette) as a function of U near 3.1 and search for an onset of the flux phase as $\mathcal{B}$ crossing over to negative values.

It should be surprising and unexpected that the simple RPA should give such reasonable results. In order to check that the observations in this paper are not merely a coincidence it would be interesting to repeat this calculation on a triangular lattice or in three dimensions. One should also look out for other constrained systems which might be described as the strongly interacting limit of some particle and whose elementary excitations might have an alternative description in this other basis.

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