Motion of a single hole in a quantum antiferromagnet

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We formulate a quasiparticle theory for a single hole in a quantum antiferromagnet in the limit that the Heisenberg exchange energy is much less than the hopping matrix element, $J \ll t$. We consider the ground state of the spins to be either a quantum Néel state or a *d*-wave resonating-valence-bond (RVB) state. We show in a self-consistent perturbation theory that the hole spectrum is strongly renormalized by the interactions with spin excitations. The hole can be described by a narrow quasiparticle band located at an energy of order $-t$ with a quasiparticle residue of order J/t and a bandwidth of order J. Above the quasiparticle band is an incoherent band of width of order t. Our results indicate that the energy scale for any coherent phenomenon involving the holes is δJ, where δ is the doping concentration. In the Néel state we perform a spin-wave expansion on an anisotropic Heisenberg model. In the Ising limit we reproduce previously known results and then expand perturbatively about that limit. In this expansion we find that the holes have a quasiparticle residue of J_z/t and a bandwidth of $J_\perp$. In the Heisenberg limit we employ a "dominant pole" approximation in which we ignore contributions to the self-energy from the incoherent part of the hole spectrum. A similar technique is used to study the *d*-wave RVB state. The relevance of our results to recent optical experiments is discussed.

I. INTRODUCTION

Since the discovery of superconductivity in the rare-earthy-based copper oxides[1] there has been growing interest in strongly correlated electronic systems. Anderson[2] has suggested that the physics of these materials is contained in a two-dimensional, large-U, single-band Hubbard model. In the large U limit, the Hubbard model may be transformed into the model Hamiltonian[3]

$$H = -t \sum_{\langle i,j \rangle} c_{i\sigma}^{\dagger} c_{j\sigma} + \text{H.c.} + J \sum_{\langle i,j \rangle} (\mathbf{s}_i \cdot \mathbf{s}_j - n_i n_j) \tag{1.1}$$

acting on the space with no doubly occupied sites, with $\mathbf{s}_i$ the electron spin and n_i the electron number. We have left out the pair-hopping term which is unimportant near half-filling.

At half-filling, this model reduces to a two-dimensional antiferromagnetic Heisenberg model, where the spins interact via the superexchange mechanism. Neutron scattering experiments[4] on undoped La_2CuO_4 have demonstrated the existence of long-range Néel order, and have indicated that the antiferromagnetic exchange energy $J \approx 0.1$ eV. The nature of the ground state and excitations of the two-dimensional Heisenberg model is a subject of intense current interest.

Many of the fascinating properties of these materials emerge when they are doped. The holes are now widely believed to be the charge carriers in these materials, and the presence of superconductivity depends crucially on their concentration. In order to understand the superconducting and normal-state properties of these materials it is of great importance to understand the holes.

When the doping concentration δ is large, such that $\delta t \gg J$, it has been shown[5] that a Fermi-liquid description with a Fermi surface containing $1+\delta$ holes in accordance with Luttinger's theorem is a good starting point. Here we are concerned with the opposite limit, $\delta t \ll J$, where the Fermi-liquid theory is expected to break down. In particular, this paper deals with the $\delta \to 0$ limit, and we discuss the motion of a single hole in an antiferromagnetic background.

The presence of holes poses two questions: (1) How will the holes affect the background spin configuration? In particular, for a given concentration of holes, what will the ground state and excitations of the spins be? (2) What are the properties (i.e., mass lifetime, . . .) of the holes which are inbedded in this spin state? By treating the $\delta \to 0$ limit, we forego the first question. The properties of a hole depend on the ground state and excitations of the model at half-filling. We will consider two types of ground states for the spins at half-filling: a quantum Néel state and a *d*-wave resonating-valence-bond state.[6,7]

The important feature which we would like to emphasize is that the holes are very strongly coupled to the excitations of the spins. In the Hamiltonian (1.1), a hole can hop with rate t, which has been estimated to be 1 eV.[8] But when it does so it disturbs the local spin configuration.[9] The typical energy for such disturbances in $J \approx 0.1t$. Each hole will thus be surrounded by a cloud of spin excitations. In order to treat the holes correctly, it is necessary to construct a quasiparticle theory for them.

Our general approach is to select a ground state for the spin configuration, classify its excitations and then determine how a hole will couple to these excitations when it hops. We calculate the hole propagator diagrammatically. Naive expansion in terms of the hopping interaction, however, will not yield a sensible result because we are in the strong-coupling regime $t \gg J$. Diagrams with more interactions will typically be higher order in t/J.

We consider the limit $J \ll t$ and obtain a self-consistent perturbation theory, in which an infinite class of "noncrossing" diagrams are summed. That is, we consider the self-energy corresponding to the diagram shown in Fig. 1 where the wavy line represents a spin excitation and the double line is the exact hole propagator. Summing the "noncrossing" diagrams is equivalent to ignoring corrections to the hole spin excitation vertex, and is the central approximation in this paper. We do not expect that this will qualitatively charge our results. We will address this issue in Appendix A.

Since the energy scale in this problem is $J \approx 1000$ K, we adopt the zero-temperature formalism. When the self-energy depicted in Fig. 1 is evaluated, we obtain a self-consistent integral equation for the hole propagator

$$G(\mathbf{k},w)=\frac{1}{\omega-\sum_q f(\mathbf{k},\mathbf{q})G(\mathbf{k}-\mathbf{q},\omega-E_{\mathbf{q}})}\ , \tag{1.2}$$

where $f(\mathbf{k},\mathbf{q})$ contains information about the coupling of the holes to the spin excitations and is of the order t^2, since it involves two hopping events. $E_{\mathbf{q}}$ is the energy of the spin excitations, which is of order J. The situation will be slightly more complicated when we consider the RVB state, but the general features remain the same.

The quantity which we are interested in knowing is the spectral function $A(\mathbf{k},\omega)\equiv(1/\pi)\mathrm{Im}G(\mathbf{k},\omega)$, which describes the spectrum of energies of the hole excitations. If the spectral function has a sharp peak as a function of ω, then we may think of this peak as describing a coherent excitation, or quasiparticle. The positions of these quasiparticle peaks as a function of momentum will determine the quasiparticle mass. If there is no such peak in the spectral function, then the hole is completely incoherent, and a particlelike description of its motion is not valid.

Equation (1.2) is a very complicated integral equation, which can only be solved in the simplest cases. We will examine such cases in the next section. One may develop some intuition for how the solutions behave by considering the following arguments. Since at zero temperature the only mechanism for scattering of the hole is the creation of spin excitations, holes may only scatter into states with lower energy. Therefore, if the density of low-energy spin excitations is small, there should be a well-defined state at the bottom of the hole spectrum which has an infinite lifetime. At higher energies, scattering will dominate. The picture thus emerges of a sharp quasiparticle peak at the bottom of a broad, multiple spin excitation background.

This self-consistent perturbation theory for the hole propagator has also been considered in Ref. 10. The integral equation (1.2) was solved numerically in one dimension for the case of the Néel state, and a quasiparticle peak was seen below an incoherent background. As we shall explain in Sec. II C, however, there are some subtleties associated with one dimension, and in that case the spectrum is entirely incoherent. In two dimensions, though, we will show that there is a quasiparticle peak.

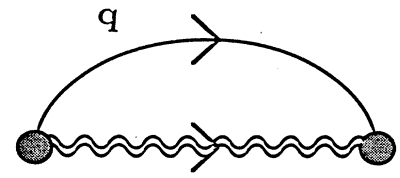

FIG. 1. Self-energy diagram considered in the noncrossing approximation of the hole propagator. The double wavy line represents the exact hole propagator and the solid line is the propagator for spin excitations. The shaded circle is a hole-spin vertex, which is of order t.

We are interested in obtaining information about this quasiparticle peak. In particular we would like to know its weight relative to the background and its dispersion (or mass). This can be done by writing the propagator as

$$G(\mathbf{k},\omega)=\frac{a_{\mathbf{k}}}{\omega-\omega_{\mathbf{k}}}+G_{\mathrm{inc}}(\mathbf{k},\omega)\ . \tag{1.3}$$

The following are self-consistent expressions for the quasiparticle residue and the position of the pole:

$$a_{\mathbf{k}}=\frac{1}{1-\frac{\partial\Sigma}{\partial\omega}(\mathbf{k},\omega_{\mathbf{k}})},\quad \omega_{\mathbf{k}}=\Sigma(\mathbf{k},\omega_{\mathbf{k}})\ . \tag{1.4}$$

In order to examine the shape of the quasiparticle band, it is important to keep track of the fact that there is implicit dependence of the self-energy on $\omega_{\mathbf{k}}$. Thus, for instance, the mass at the bottom of the band will be renormalized by the quasiparticle residue, $a_{\mathbf{k}}$,

$$\begin{aligned}\frac{1}{m_{ij}}&\equiv\frac{\partial^2}{\partial k_i\partial k_j}\omega_{\mathbf{k}}\\&=\frac{\partial^2}{\partial k_i\partial k_j}\Sigma(\mathbf{k},\omega)+\frac{\partial\Sigma}{\partial\omega}(\mathbf{k},\omega)\frac{\partial^2}{\partial k_i\partial k_j}\omega_{\mathbf{k}}|_{\omega=\omega_{\mathbf{k}}}\\&=a_{\mathbf{k}}\frac{\partial^2}{\partial k_i\partial k_j}\Sigma(\mathbf{k},\omega)|_{\omega=\omega_{\mathbf{k}}}\ .\end{aligned} \tag{1.5}$$

Thus, as in Fermi-liquid theory, if the self-energy is a rapidly varying function of ω then the residue of the quasiparticle pole will be decreased, and its effective mass will be increased.

Before going into specific details, we first give a rough estimate of the quasiparticle residue. We express the real part of the self-energy in terms of its imaginary part, $\Gamma(\mathbf{k},\omega)=(1/\pi)\mathrm{Im}\Sigma(\mathbf{k},\omega)$, via the Kramers-Kronig relation,

$$a_{\mathbf{k}}=\frac{1}{1+\int dy\frac{\Gamma(\mathbf{k},y)}{(y-\omega_{\mathbf{k}})^2}}\ . \tag{1.6}$$

$\Gamma(\mathbf{k},y)$ may be thought of as a scattering rate for states at momentum **k** and energy y. At low temperatures, holes may only scatter by creating spin excitations, which have a typical energy of J. Moreover, we shall see that in the spin states which we consider, the density of low-energy spin excitations vanishes like a power of their energy. Therefore, for $y-\omega_{\mathbf{k}} \ll J$, we expect $\Gamma(\mathbf{k},y)$ to vanish like a power of $y-\omega_{\mathbf{k}}$. In two dimensions, this power is sufficient to cut off the divergence in the integral. For $y-\omega_{\mathbf{k}}$ comparable or greater than J, we expect scattering to dominate and $\Gamma(\mathbf{k},y)\approx t$. A schematic portrait of $\Gamma(\mathbf{k},y)$ is shown in Fig. 2. Given this form of $\Gamma(\mathbf{k},y)$ we can estimate the residue for $J \ll t$ to be

$$a_{\mathbf{k}} \approx \frac{1}{1+\int_J^\infty dy \frac{t}{y^2}} \approx \frac{J}{t} . \tag{1.7}$$

The effective mass of these quasiparticles can be estimated from Eq. (1.5). Though the self-energy has a singular frequency dependence in the $J \to 0$ limit, we will argue that it is not a singular function of **k** in that limit. Therefore, its derivative with respect to **k** in (1.5) may be evaluated in the $J=0$ limit and must depend only on t. Thus, the mass of the hole will be enhanced from the noninteracting band mass by a factor of t/J.

The enhanced quasiparticle mass is consistent with recent optical data,[11] in which the Drude peak in the conductivity indicates a mass enhancement of order 10. Furthermore, we shall argue that the broad feature observed at higher energies may be associated with the incoherent part of the hole spectrum.

The remainder of this paper is organized as follows. In Sec. II we investigate hole motion in a quantum Néel state by formulating a large S expansion of the spin interaction. We first consider the simplified case of an Ising spin interaction and compare our results to the work of previous authors. We then demonstrate the effects of the Heisenberg spin interaction by expanding perturbatively about the Ising limit. We then treat the Heisenberg limit by considering the self-consistent equations for the quasiparticle pole discussed above. In Sec. III we analyze hole motion in a particular version of the resonating valence bond state, using the same technique. Finally, in Sec. IV, we discuss the conductivity, $\sigma(\omega)$, and the relevance of our results to some recent optical experiments.[11]

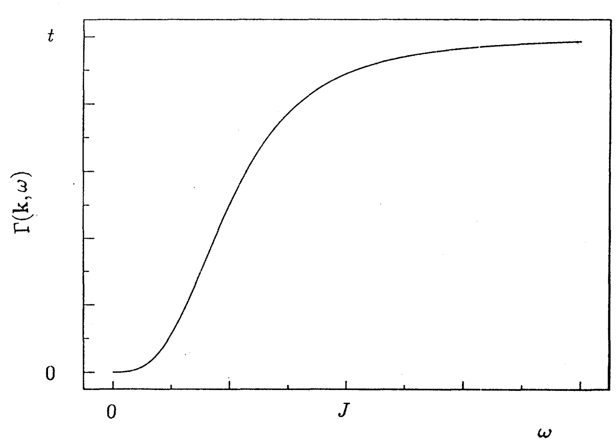

FIG. 2. A schematic portrait of the imaginary part of the self-energy, $\Gamma(\mathbf{k},\omega)$ as a function of ω.

II. HOLE MOTION IN A NÉEL STATE

A. Effective Hamiltonian

In this section we examine the motion of a hole in a half-filled Hubbard model, assuming that the ground state at half-filling can be described by a Néel state with spin-wave excitations. Our motivation for considering such a state lies in the fact that undoped La_2CuO_4 has been shown to posess Néel order,[4] and simple spin-wave theory has done quite well in predicting ground-state energy and magnetization in the Heisenberg antiferromagnet.[12,13]

Numerous authors have considered this problem.[9,10,14–18] One line of attack is based on the retraceable path approximation of Brinkman and Rice.[9] They considered the Ising limit and the basic idea is that as a hole hops in a Néel state, it will scramble the spin configuration, creating a "string" of overturned spins along its path. In order to return the spin configuration to its original state, Brinkman and Rice argued that to a good approximation, one can consider only paths in which the hole retraces its path back to the origin, thereby returning all of the spins to their original positions. They found that in the $J=0$ limit (ignoring the spin dynamics), that the hole is described by an incoherent band, which is somewhat narrower than the noninteracting band.

The case of finite J has been considered by Bulaevskii, Nagaev, and Khomskii[14] and Shraiman and Siggia.[17] They considered the Ising limit of the spin interaction in which the quantum fluctuations are turned off. In this case, each time a hole hops, the "string" which it creates costs a finite energy J_z, since there are bonds which are left unsatisfied. The hole can then be viewed as if it were a particle in a linear potential. They find that there is a bound state with an energy which is of the order $t(J_z/t)^{2/3}$ above the Brinkman Rice band edge, and has a spatial extent which scales like $J_z^{-1/6}$.

In this Ising limit, the holes are infinitely massive in the retraceable path approximation, since they are bound to their original position by a "string." If we include $J_\perp$, the spins will no longer be in an eigenstate of the Hamiltonian, and quantum fluctuations will allow pairs of spins to spontaneously flip, thereby relaxing the "strings," and allowing the holes to be mobile.[17] Furthermore, if one includes paths that have closed loops, the hole may hop by going around a loop one and a half times and return the spins to their original positions.[18] Such effects of $J_\perp$ have been included in the partial diagonalization studies of Trugman[18] and the variational studies of Sachdev.[16] Both authors find evidence that the mass of the holes is large when $J \ll t$.

Our approach of summing noncrossing diagrams is similar in spirit to the retraceable path approximation of Brinkman and Rice.[9] The retraceable path approximation ignores processes where the hole goes around a closed loop, returning the spins to their original configuration in a different order than that in which they were flipped. By omitting crossed diagrams, we ignore processes in which the spin excitations are absorbed in a different order than that in which they were created. We do, however, allow for the fact that the spin excitations may propagate, so that the hole trajectory need not follow a retraceable path, and the holes may be mobile. Since the hole must absorb every spin excitation which it emits, it must hop an even number of times in order to return the spins to their original configuration. Thus, a hole is associated with a single sublattice.

We consider a more general anisotropic version of the Hamiltonian (1.1) where we include two interaction parameters J_z and $J_\perp$, with a ratio we define as $\alpha \equiv J_\perp / J_z$,

$$H = -t \sum_{\langle i,j \rangle} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{\langle i,j \rangle} c_{i\alpha}^\dagger c_{i\beta} c_{j\gamma}^\dagger c_{j\delta} [J_z \sigma_{\alpha\beta}^z \sigma_{\gamma\delta}^z + J_\perp (\sigma_{\alpha\beta}^x \sigma_{\gamma\delta}^x + \sigma_{\alpha\beta}^y \sigma_{\gamma\delta}^y)] , \tag{2.1}$$

with the constraint of no double occupancy. We have omitted the density terms in Eq. (2.1), since near half-filling they will have no effect. We consider this anisotropic model because in the limit $\alpha = 0$, the calculations are tractable, and we can compare our results with those of Brinkman and Rice,[9] Bulaevskii, Nagaev, and Khomskii[14] and Shraiman and Siggia.[17] Furthermore, we can perform a perturbative expansion in α and analyze the effects of a finite $J_\perp$. We will treat the Heisenberg limit, $\alpha = 1$ using a "dominant pole" approximation, where the contribution of the incoherent part of the hole spectrum to the self-energy is ignored.

Our approach is to formulate a $1/S$ expansion of the spin part of the Hamiltonian (2.1), which in lowest order yields an effective Hamiltonian which is expressed in terms of Holstein-Primakoff[19] spin-wave operators. We then introduce holes and determine how they couple to these spin waves.

Away from half-filling, one must carefully treat the inequality constraint of no double occupancy. A powerful method for doing this is to enlarge the Hilbert space by introducing new operators to keep track of unoccupied sites (holes) and occupied sites (spins).[20] The inequality constraint then becomes the equality constraint that on each site the number of holes plus the number of spins is unity. The electron creation operators are replaced by a spin creation operator and a hole annihilation operator. In order to preserve the fermion commutation rules for the electrons, one operator must obey Bose statistics and the other must obey Fermi statistics. We have the freedom, however, to choose which is which. In this section, in order to facilitate a large S expansion in terms of spin-wave operators, we represent the spins by boson operators and holes by fermion operators. We therefore express the electron operators in the "slave fermion" representation, $c_{i\sigma}^\dagger = f_i b_{i\sigma}^\dagger$, subject to the constraint that $f_i^\dagger f_i + b_{i\sigma}^\dagger b_{i\sigma} = 1$ on each site.

We can express the Hamiltonian as,

$$\begin{aligned} H = -t &\sum_{\langle i,j \rangle} f_i b_{i\sigma}^\dagger b_{j\sigma} f_j^\dagger \\ &+ \sum_{\langle i,j \rangle} b_{i\alpha}^\dagger b_{i\beta} b_{j\gamma}^\dagger b_{j\delta} [J_z \sigma_{\alpha\beta}^z \sigma_{\gamma\delta}^z + J_\perp (\sigma_{\alpha\beta}^x \sigma_{\gamma\delta}^x + \sigma_{\alpha\beta}^y \sigma_{\gamma\delta}^y)] \\ &+ \sum_i \lambda_i (f_i^\dagger f_i + b_{i\sigma}^\dagger b_{i\sigma} - 1) , \end{aligned} \tag{2.2}$$

where λ_i is a Lagrange multiplier which constrains us to the subspace in which there is one object on each site.

Consider first the case of exact half-filling. In that case, the constraint requires that there be no fermions, so the Hamiltonian reduces to the pure Heisenberg Hamiltonian expressed in terms of Schwinger bosons,

$$\begin{aligned} H = - &\sum_{\langle i,j \rangle} b_{i\alpha}^\dagger b_{i\beta} b_{j\gamma}^\dagger b_{j\delta} [J_z \sigma_{\alpha\beta}^z \sigma_{\gamma\delta}^z \\ &\qquad + J_\perp (\sigma_{\alpha\beta}^x \sigma_{\gamma\delta}^x + \sigma_{\alpha\beta}^y \sigma_{\gamma\delta}^y)] \\ &+ \sum_i \lambda_i (b_{i\sigma}^\dagger b_{i\sigma} - 1) . \end{aligned} \tag{2.3}$$

We may generalize the Schwinger boson spin representation to large S by replacing the constraint by

$$b_{i\uparrow}^\dagger b_{i\uparrow} + b_{i\downarrow}^\dagger b_{i\downarrow} = 2S , \tag{2.4}$$

so that there are now $2S$ spin-$\frac{1}{2}$ Schwinger bosons on each site. Our approach is to consider large S, in which we can formulate a consistent $1/S$ spin wave expansion. As in usual treatments of antiferromagnets, we divide the lattice into two sublattices labeled by 1 and 2, and Hamiltonian in (2.3) may be written

$$\begin{aligned} H = - &\sum_{\langle i,j \rangle} \tfrac{1}{4} J_z (2b_{1i\uparrow}^\dagger b_{1i\uparrow} - 2S)(2b_{2j\downarrow}^\dagger b_{2j\downarrow} - 2S) \\ &- \tfrac{1}{2} J_\perp (b_{1i\uparrow}^\dagger b_{1i\downarrow} b_{2j\downarrow}^\dagger b_{2j\uparrow} + b_{1i\downarrow}^\dagger b_{1i\uparrow} b_{2j\uparrow}^\dagger b_{2j\downarrow}) \\ &+ \sum_i \lambda_{1i} (b_{1i\uparrow}^\dagger b_{1i\uparrow} + b_{1i\downarrow}^\dagger b_{1i\downarrow} - 2S) \\ &+ \sum_j \lambda_{2j} (b_{2j\uparrow}^\dagger b_{2j\uparrow} + b_{2j\downarrow}^\dagger b_{2j\downarrow} - 2S) . \end{aligned} \tag{2.5}$$

In the large S limit we may consider mean-field theory in the Schwinger bosons and the Lagrange multipliers, which is equivalent to a saddle-point expansion of a functional integral. A stable mean-field solution occurs when

$$\begin{aligned} &b_{1i\uparrow} = b_{2j\downarrow} = 0 , \\ &b_{1i\downarrow} = b_{2j\uparrow} = \sqrt{2S} , \\ &\lambda_{1i} = \lambda_{2j} = 0 . \end{aligned} \tag{2.6}$$

This mean-field corresponds to a Néel state. On the 1 sublattice, the spin points down, since there are $2S$ "down" Schwinger bosons and no "up" Schwinger bosons. On the 2 sublattice, the spins point up.

If we expand to quadratic order about this saddle point, we obtain an effective Hamiltonian,

$$H=\sum_{\langle i,j\rangle} SJ_z(b_{1i\uparrow}^\dagger b_{1i\uparrow}+b_{2j\downarrow}^\dagger b_{2j\downarrow}) +SJ_\perp(b_{1i\uparrow}^\dagger b_{2j\downarrow}^\dagger+b_{1i\uparrow}b_{2j\downarrow}) . \quad (2.7)$$

Note that the fluctuations in $b_{1i\downarrow}$, $b_{2j\uparrow}$, λ_{1i}, and λ_{2j} do not appear in quadratic order. This is precisely the Hamiltonian for Holstein-Primakoff spin waves. What we have done is identify the Holstein-Primakoff spin-wave operators with the creation operators for the Schwinger bosons to lowest order in $1/S$.

This Hamiltonian is easily diagonalized by Fourier and Bogoliubov transformation, and we obtain the Holstein-Primakoff Hamiltonian,

$$H=zJ_z\sum_{\mathbf{k}}(1-\alpha^2\gamma_{\mathbf{k}}^2)^{1/2}\beta_{\mathbf{k}}^\dagger\beta_{\mathbf{k}} , \quad (2.8)$$

where we have absorbed a factor of 2S into J_z and $\alpha=J_\perp/J_z$, z is the coordination number ($z=4$ on the square lattice), $\gamma_{\mathbf{k}}=1/z\sum_\delta e^{i\mathbf{k}\cdot\delta}$, and

$$b_{\mathbf{k}}=\sum_{i\in 1} b_{1i\uparrow}e^{i\mathbf{k}\cdot\mathbf{r}_i}+\sum_{j\in 2} b_{2j\downarrow}e^{i\mathbf{k}\cdot\mathbf{r}_j} ,$$

$$\begin{bmatrix}\beta_{\mathbf{k}}\\ \beta_{-\mathbf{k}}^\dagger\end{bmatrix}=\begin{bmatrix}u_{\mathbf{k}} & -v_{\mathbf{k}}\\ -v_{\mathbf{k}} & u_{\mathbf{k}}\end{bmatrix}\begin{bmatrix}b_{\mathbf{k}}\\ b_{-\mathbf{k}}^\dagger\end{bmatrix} ,$$

$$u_{\mathbf{k}}=\left[\frac{1+(1-\alpha^2\gamma_{\mathbf{k}}^2)^{1/2}}{2(1-\alpha^2\gamma_{\mathbf{k}}^2)^{1/2}}\right]^{1/2} , \quad (2.9)$$

$$v_{\mathbf{k}}=-(\mathrm{sgn}\gamma_{\mathbf{k}})\left[\frac{1-(1-\alpha^2\gamma_{\mathbf{k}}^2)^{1/2}}{2(1-\alpha^2\gamma_{\mathbf{k}}^2)^{1/2}}\right]^{1/2} .$$

The ground state of this Hamiltonian is a Néel state with quantum fluctuations. It may be expressed in terms of the classical Néel state as,

$$|0\rangle=\exp\left[-\sum_k\frac{v_{\mathbf{k}}}{u_{\mathbf{k}}}b_{\mathbf{k}}^\dagger b_{-\mathbf{k}}^\dagger\right]|N\rangle , \quad (2.10)$$

where $|N\rangle$ is the classical Néel state. It is important to remember that even in the $J_z\to 0$ limit, this ground state depends on α. Though the operator in the exponent of (2.10) does not appear to conserve spin, it actually does because the form of $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ ensure that the two b's lie on opposite sublattices.

Next we consider the addition of holes. In this case, we must generalize our identification of the electron operators to large S. One possibility is to consider spin S electrons. In that case, since we would like to express the spin to the electron in terms of the Schwinger bosons, we must identify the electron in the m spin channel as,

$$c_{im}^\dagger=\frac{1}{\sqrt{(S+m)!(S-m)!}}f_i b_{i\uparrow}^{\dagger S+m}b_{i\downarrow}^{\dagger S-m} . \quad (2.11)$$

Thus, an electron is composed of a fermion and $2S$ Schwinger bosons. Unfortunately, if we use this identification, the fermion couples to $2S$ bosons and it turns out that there is no sensible $1/S$ expansion for the hole propagator.

An alternative procedure, since we are really interested in $S=\frac{1}{2}$, is to interpret the holes to be sites which have spin $S-\frac{1}{2}$. Thus, a site without a "hole" will have $2S$ Schwinger bosons, while a site with a hole will have $2S-1$ Schwinger bosons. The hopping part of the Hamiltonian will involve the interchange of a hole operator with a single Schwinger boson on nearest-neighbor sites, and will look exactly like the hopping part of the spin-$\frac{1}{2}$ Hamiltonian (2.2). The only difference is that in this case we are constrained to a different sector of the Hilbert space in which $f_i^\dagger f_i+b_{i\uparrow}^\dagger b_{i\uparrow}+b_{i\downarrow}^\dagger b_{i\downarrow}=2S$. When S is large, the presence of a "hole" is a small perturbation on the spin state, so that a large S expansion for the hole propagator exists.

For large S, we may replace $b_{1i\downarrow}$ and $b_{2j\uparrow}$ by $\sqrt{2S}$. The hopping Hamiltonian is then expressed in terms of the fluctuations in $b_{1i\uparrow}$ and $b_{2j\downarrow}$. If we absorb $\sqrt{2S}$ into t, this becomes,

$$\begin{aligned}H_t&=-t\sum_{\langle i,j\rangle}f_if_j^\dagger(b_{1i\uparrow}+b_{2j\downarrow})+\text{H.c.}\\&=-zt\sum_{\mathbf{k},\mathbf{q}}f_{\mathbf{k}}f_{\mathbf{k}-\mathbf{q}}^\dagger(\gamma_{\mathbf{k}-\mathbf{q}}b_{\mathbf{q}}^\dagger+\gamma_{\mathbf{k}}b_{-\mathbf{q}})+\text{H.c.}\\&=-zt\sum_{\mathbf{k},\mathbf{q}}f_{\mathbf{k}}f_{\mathbf{k}-\mathbf{q}}^\dagger(u_{\mathbf{q}}\gamma_{\mathbf{k}-\mathbf{q}}\beta_{\mathbf{q}}+v_{\mathbf{q}}\gamma_{\mathbf{k}}\beta_{-\mathbf{q}}^\dagger)+\text{H.c.}\end{aligned} \quad (2.12)$$

Thus, we have an effective Hamiltonian in which holes may hop by emitting or absorbing spin waves.

Given the effective Hamiltonian (2.12), we would like to calculate the spectral function for a single hole. The true hole propagator depends on the electron operators $c_{ik\sigma}^\dagger=f_ib_{i\sigma}^\dagger$,

$$G_{\sigma\sigma'}(i,j,\omega)=\int_{-\infty}^{\infty}dt\, e^{i\omega t}\langle T[f_i(t)b_{i\sigma}^\dagger(t)b_{j\sigma'}(0)f_j^\dagger(0)]\rangle . \quad (2.13)$$

If we consider the dominant contribution in our $1/S$ expansion, the boson operators are replaced by $\sqrt{2S}$ when the spin is up on the 1-sublattice and down on the 2-sublattice. We therefore focus on the f propagator,

$$G(i,j,\omega)=\int_{-\infty}^{\infty}dt\, e^{i\omega t}\langle T[f_i(t)f_j(0)^\dagger]\rangle . \quad (2.14)$$

This fermion propagator is useful for calculating physical quantities such as the conductivity. We will argue that the low-frequency conductivity may be represented by a bubble diagram involving these fermion propagators. Implicit in this way of looking at the holes is the assumption that the spin of the hole decouples, so that we may regard the hole as spinless.

We proceed to construct the self-consistent perturbation theory discussed in the Introduction. The self-energy depicted in Fig. 1 may be written as,

$$\Sigma(\mathbf{k},\omega)=\sum_q f(\mathbf{k},\mathbf{q})G(\mathbf{k}-\mathbf{q},\omega-E_{\mathbf{q}}) , \quad (2.15)$$

where,

$$f(\mathbf{k},\mathbf{q})=z^2t^2|\gamma_{\mathbf{k}-\mathbf{q}}u_{\mathbf{q}}+\gamma_{\mathbf{k}}v_{\mathbf{q}}|^2 . \quad (2.16)$$

We obtain the following integral equation for the hole propagator:[10]

$$G(\mathbf{k},\omega)=\frac{1}{\omega-\sum_{q} f(\mathbf{k},\mathbf{q})G(\mathbf{k}-\mathbf{q},\omega-E_{\mathbf{q}})} . \tag{2.17}$$

In the remainder of this section we will discuss some limiting cases, in which this equation is exactly soluble, and make connection to the work of Brinkman and Rice,[9] Nagaev, and Khomskii[14] and Shraiman and Siggia.[17] We will then go on to discuss the general case using the dominant pole approximation.

B. Expansion about Ising limit

We consider an expansion about the Ising, or $\alpha=0$ limit of the model (2.1). In that case, we may expand the coupling factor as,

$$\begin{aligned} f(\mathbf{k},\mathbf{q})&=z^2t^2[\gamma_{\mathbf{k}-\mathbf{q}}^2-\alpha\gamma_{\mathbf{k}}\gamma_{\mathbf{q}}\gamma_{\mathbf{k}-\mathbf{q}} \\ &\quad+\tfrac{1}{4}\alpha^2\gamma_{\mathbf{q}}^2(\gamma_{\mathbf{k}}^2+\gamma_{\mathbf{q}}^2)+\cdots] , \\ E_{\mathbf{k}-\mathbf{q}}&=zJ_z(1-\tfrac{1}{2}\alpha^2\gamma_{\mathbf{k}-\mathbf{q}}^2+\cdots) . \end{aligned} \tag{2.18}$$

1. *Ising limit* $\alpha=0$

We first consider the Ising limit, $\alpha=0$. In that case, the Hamiltonian is purely classical, in that the spin interaction does not admix different spin states. The spin excitations in such a model will not propagate. It is clear from (2.18) that their energy is dispersionless, and corresponds to breaking z bonds. As a hole propagates, it will leave behind a trail of flipped spins, so that there is a very restricted set of paths which the hole can take which leave the spin configuration unaltered.

For $\alpha=0$, it is clear from (2.17) and (2.18) that $G(\mathbf{k},\omega)$ will be independent of $\mathbf{k}$, so our integral equation becomes (using $\sum_{\mathbf{k}}\gamma_{\mathbf{k}}^2=1/z$),

$$G(\omega)=\frac{1}{\omega-zt^2G(\omega-J_z)} . \tag{2.19}$$

Consider first the case $J_z=0$. In that case G can be evaluated exactly as

$$G(\omega)=\frac{\omega-\sqrt{\omega^2-4zt^2}}{2zt^2} . \tag{2.20}$$

The spectral function is

$$A(\omega)\equiv\frac{1}{\pi}\mathrm{Im}G(\omega)=\frac{\sqrt{4zt^2-\omega^2}}{2\pi zt^2} \quad \text{for } \omega<2\sqrt{zt} \tag{2.21}$$

as shown in Fig. 3(a).

This result is similar to the result of the retraceable path approximation of Brinkman and Rice.[9] It describes an incoherent band. The band edge is at $\omega_0=-2\sqrt{zt}$, as opposed to $-2\sqrt{z-1}t$ in Brinkman-Rice. This discrepancy is a result of the fact that in our picture we include certain hops which Brinkman and Rice would say are double counted. Consider the diagrams shown in Fig. 4. Both diagrams correspond to a hole hopping from site i to i' to i to i' and back to i, so they both correspond to the same physical process and should not both be counted. Brinkman and Rice therefore enforce the constraint

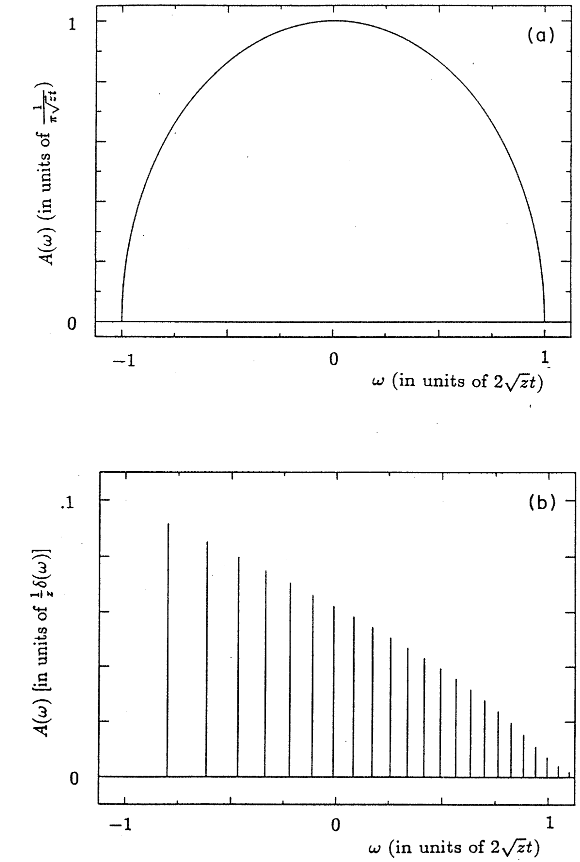

FIG. 3. Hole spectral function in the $J_\perp=0$ limit. (a) The limit $J_z=0$. (b) $J_z/t=0.1$. The vertical lines represent delta functions with weight specified by their height.

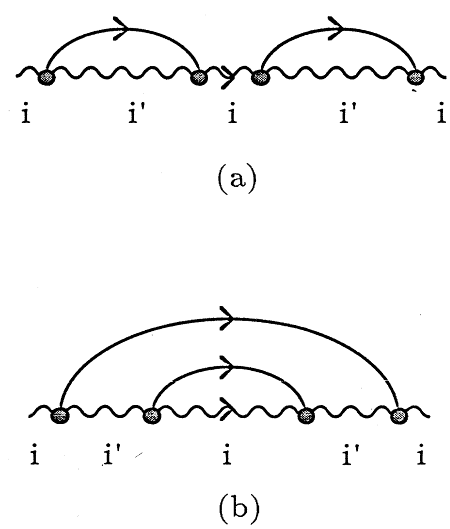

FIG. 4. Two contributions to the self-energy which are overcounted in our large S expansion. In both processes, the hole hops from site i to i' to i to i' and back to i. For $S=\frac{1}{2}$, (b) should not be counted.

that in the second diagram the hole cannot return to i. Hence, it can only go $z-1$ places, which leads to the band edge at $-2\sqrt{z-1}t$.

In our picture, these two processes are different, since the intermediate case in Fig. 4(a) has no spin excitations present, while that in Fig. 4(b) has two spin excitations present. The discrepancy has to do with our large S treatment of the spin excitations. Since we have spin S on each site, it is possible to have up to $2S$ localized spin-$\frac{1}{2}$ excitations on each site. For spin $\frac{1}{2}$ there can be at most one.

It is important to emphasize that the $J_z=0$ limit of the hole propagator still depends on α. This is because for arbitrarily small J_z, the ground state will contain different amounts of spin fluctuations depending on α. The case which Brinkman and Rice consider is the classical Néel state with no spin fluctuations, and corresponds to $\alpha=0$. For $\alpha>0$, the spectral function will in general be $\mathbf{k}$ dependent and the band edge need not be at $2\sqrt{z-1}t$.

We next consider the case where J_z is small but finite. In that case, it costs an energy J_z to hop by creating a spin excitation. This situation has been considered by Bulaevskii, Nagaev, and Khomskii[14] and Shraiman and Siggia[17] using a technique similar to that of Brinkman and Rice.[9] The essence of their argument is that the further a hole hops, the more spins it has left turned over and hence the higher the energy cost. For small J_z, they adopted a continuum limit in which the hole can be viewed as if it were a particle in a linear potential described by the Hamiltonian,

$$H=-\sqrt{z-1}t\frac{\partial^2}{\partial x^2}+J_z x-2\sqrt{z-1}t \ . \tag{2.22}$$

The J_z dependence can be scaled out, and there are discrete levels at energies

$$E_n=\left[\frac{J_z}{t}\right]^{2/3} t a_n-2\sqrt{z-1}t \ , \tag{2.23}$$

where a_n are the eigenvalues of a dimensionless Airy-like equation. The lowest eigenvalues are separated by an energy of the order $t(J_z/t)^{2/3}$. Like $J_z=0$ case, our theory will predict z in place of $z-1$ for the same reasons as described above.

For finite J_z, Eq. (2.19) cannot be solved analytically, however, it is quite easy to obtain a numerical solution. The spectral function for $J_z=0.1t$ is shown in Fig. 3(b). The continuum in the Brinkman-Rice $J=0$ limit is split into a series of sharp delta functions. Near the bottom of the spectrum, the peaks have a weight very closely equal to J_z/t, and they are separated by an amount which is proportional to $t(J_z/t)^{2/3}$.

One can understand the low-energy behavior by considering the dominant pole approximation. Suppose that near the pole,

$$G(\omega)=\frac{a_0}{\omega-\omega_0}+C_0 \ . \tag{2.24}$$

Then, substituting this into Eq. (2.19) and (1.4), we can calculate the residue and location of the pole,

$$a_0=\frac{1}{1-zt^2\dfrac{\partial G}{\partial\omega}(\omega_0-J_z)}\approx\frac{1}{1+zt^2\dfrac{a_0}{J_z^2}} \ , \tag{2.25a}$$

$$\omega_0=-\frac{a_0}{J_z}+C_0 \ . \tag{2.25b}$$

The dominant pole approximation cannot tell us the value of ω_0, but from the $J_z=0$ limit, we know that it must be close to $-2\sqrt{zt}$. If J_z is small, we obtain from Eq. (2.25a) that $a_0=J_z/\sqrt{zt}$. Furthermore, if the weight of the lowest poles is proportional to J_z, their separation must be proportional to $J_z^{2/3}$ in order to reproduce the square-root band edge in the $J_z=0$ limit. This agrees well with our numerical results.

In writing Eq. (2.25), we have ignored contributions to the self energy from the other poles. This is valid for the lowest pole, since the other poles are $O(t(J_z/t)^{2/3})$ away in energy, so that their contribution to $\partial\Sigma/\partial\omega$ is proportional to $(J_z/t)^{-1/3}$, which is small compared with $(J_z/t)^{-1}$ when $J_z \ll t$.

2. Lowest order in α

We now consider slight deviations from the Ising limit perturbatively. When $J_\perp$ is finite, the spins are no longer in exact eigenstates of the Hamiltonian so they can spontaneously flip. In this way, "strings" of flipped spins generated when the hole hops can relax, thereby allowing the hole to propagate.

We first consider the $J_z=0$ limit, to first order in α. In this case, we expect a spectrum which resembles the incoherent Brinkman-Rice[9] spectrum. To first order in α, with $J_z=0$, the equation reads,

$$G(\mathbf{k},\omega)=\frac{1}{\omega-z^2t^2\sum_q(\gamma_{\mathbf{q}}^2-\alpha\gamma_{\mathbf{k}}\gamma_{\mathbf{q}}\gamma_{\mathbf{k}-\mathbf{q}})G(\mathbf{q},\omega)} \ . \tag{2.26}$$

We can solve this equation to lowest order in α, and we find that away from the band edge,

$$G(\mathbf{k},\omega)=G^0(\omega)-\alpha t^2 G^0(\omega)^3\left[(z-2)\gamma_{\mathbf{k}}^{(2)}+\gamma_{\mathbf{k}}^{(3)}+\frac{1-(z-1)^2t^2G^0(\omega)^2}{1-zt^2G^0(\omega)^2}\right] , \tag{2.27}$$

where, $\gamma_{\mathbf{k}}^2=\frac{1}{2}[\cos(k_x+k_y)+\cos(k_x-k_y)]$ and $\gamma_{\mathbf{k}}^{(3)}=\frac{1}{2}(\cos 2k_x+\cos 2k_y)$ are the cubic harmonics for second- and third-nearest-neighbor hopping. The spectral function for two values of $\mathbf{k}$ are shown (extrapolated to $\alpha=1$) in Fig. 5. The perturbation theory breaks down close to the band edge, where ImG is small. The fact that the perturbation is negative near the band edges indicates that the band edge moves inward, so that it is at an energy higher than $\omega_0=-2\sqrt{z}t$.

When J_z is finite, we saw that for $\alpha=0$ the spectrum is

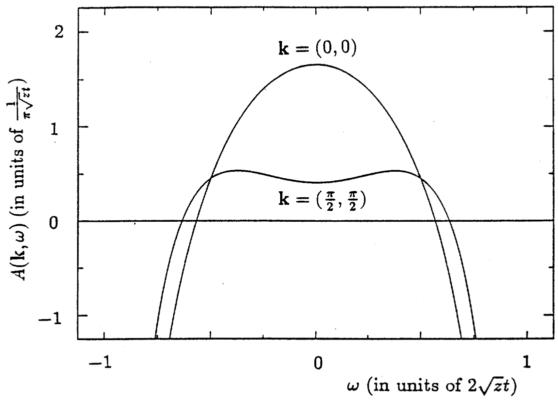

FIG. 5. Hole spectral function, $A(\mathbf{k},\omega)$ obtained from the perturbation in small $\alpha \equiv J_\perp / J_z$, extrapolated to $\alpha=1$, and shown as a function of ω for two values of $\mathbf{k}$.

split into discrete poles. Making α finite affects the spectrum in two ways. First, it adds dispersion to the lowest poles with a bandwidth of the order $J_\perp$. Second, the higher poles will be smeared out, and spectral weight will appear at an energy J_z above the lowest pole [as opposed to $t(J_z/t)^{2/3}$].

The nature of the lowest poles is most easily examined by considering the dominant pole approximation, which gave a very good description of the $\alpha=0$ limit. Therefore, we write,

$$G(\mathbf{k},\omega)=\frac{a_\mathbf{k}}{\omega-\omega_\mathbf{k}}+C_\mathbf{k} \, . \tag{2.28}$$

To first order in α, the self-consistent equations for $a_\mathbf{k}$ and $\omega_\mathbf{k}$ read,

$$a_\mathbf{k}=\frac{1}{1+z^2t^2\sum_\mathbf{q}(\gamma_\mathbf{q}^2-\alpha\gamma_\mathbf{k}\gamma_{\mathbf{k}-\mathbf{q}}\gamma_\mathbf{q})\frac{a_\mathbf{q}}{(\omega_\mathbf{k}-\omega_\mathbf{q}-J_z)^2}} \, ,$$
$$\omega_\mathbf{k}=z^2t^2\sum_\mathbf{q}(\gamma_\mathbf{q}^2-\alpha\gamma_\mathbf{k}\gamma_{\mathbf{k}-\mathbf{q}}\gamma_\mathbf{q})\left[\frac{a_\mathbf{q}}{\omega_\mathbf{k}-\omega_\mathbf{q}-J_z}+C_\mathbf{q}\right] . \tag{2.29}$$

The dominant pole approximation cannot tell us the position of the band, however, it can tell us about its shape. When α is small, we expect that $\omega_\mathbf{k}-\omega_\mathbf{q} \ll J_z$, so that we may expand $\omega_\mathbf{k}-\omega_{\mathbf{k}'}$ to lowest order in α,

$$\omega_k-\omega_{\mathbf{k}'}=z^2t^2\sum_\mathbf{q}\left[-\gamma_\mathbf{q}^2\frac{a_\mathbf{q}}{J^2}(\omega_\mathbf{k}-\omega_{\mathbf{k}'})-\alpha\gamma_\mathbf{q}^2(\gamma_\mathbf{k}^2-\gamma_{\mathbf{k}'}^2)\left[-\frac{a_0}{J}+C_0\right]\right]$$
$$=-\frac{\alpha z t^2(\gamma_\mathbf{k}^2-\gamma_{\mathbf{k}'}^2)\left[-\frac{a_0}{J}+C_0\right]}{1+zt^2\frac{a_0}{J^2}} \, . \tag{2.30}$$

a_0 and C_0 are the $\alpha=0$ limits of $a_\mathbf{k}$ and $C_\mathbf{k}$. From the $J_\perp=0$ limit we know that $-a_0/J+C_0=-2\sqrt{z}t$, so we find,

$$\omega_\mathbf{k}-\omega_{\mathbf{k}'}=2\alpha J_z(\gamma_\mathbf{k}^2-\gamma_{\mathbf{k}'}^2) \, . \tag{2.31}$$

Thus, there is a band with a width $2J_\perp$. The quasiparticle residue of these peaks, however will still be of the order J_z/t. Note that it was important to account for the strong dependence of the self-energy on frequency. Had it been ignored, we would have expected the bandwidth to be αt. The bottom of the band is degenerate in this approximation, and is at the points where $\gamma_\mathbf{k}^2=0$, which lie on a square corresponding to a half-filled Brillouin zone.

We may also ask what happens to the rest of the hole spectrum. For $\alpha=0$ there was a series of sharp delta functions separated by an energy $\approx t(J_z/t)^{2/3}$. In order to see what happens for $\alpha>0$, we iterate the integral equation by inserting Eq. (2.28) into the right-hand side of Eq. (2.26). The self-consistency of the dominant pole approximation ensures that the pole will remain unchanged, however, there will be new contributions as well. The iterated spectral function can be written,

$$A(\mathbf{k},\omega)=\frac{\Gamma(\mathbf{k},\omega)}{(\omega-\omega_\mathbf{k})^2\left[1+z^2t^2\sum_\mathbf{q}(\gamma_\mathbf{q}^2-\alpha\gamma_\mathbf{k}\gamma_{\mathbf{k}-\mathbf{q}}\gamma_\mathbf{q})\frac{a_\mathbf{q}}{(\omega-\omega_\mathbf{q}-J_z)(\omega_\mathbf{k}-\omega_\mathbf{q}-J_z)}\right]^2+\Gamma(\mathbf{k},\omega)^2} \, , \tag{2.32}$$

where,

$$\Gamma(\mathbf{k},\omega)=z^2t^2\sum_\mathbf{q}(\gamma_\mathbf{q}^2-\alpha\gamma_\mathbf{k}\gamma_{\mathbf{k}-\mathbf{q}}\gamma_\mathbf{q})a_{\mathbf{k}-\mathbf{q}}\delta(\omega-\omega_\mathbf{q}-J_z) \, . \tag{2.33}$$

If the lowest pole is at ω_0, then there is clearly no spectral weight (besides the poles) up to an energy ω_0+J_z. However at that energy, $\Gamma(\mathbf{k},\omega)$ becomes finite, so there will be spectral weight there. The amount of weight there will be of order α^2, since when α is small the denominator will be large at $\omega=\omega_0+J_z$. If we iterate the integral equation further, these features will remain. However, higher-energy spectral weight will emerge. This will smear out the higher poles in the Bulaevskii, Nagaev, and Khomskii,[14] Shraiman-Siggia[17] spectrum.

Thus, to lowest order in α, we have a quasiparticle band with a width $J_\perp$, and there is incoherent spectral weight separated by a gap of order J_z. If we go to higher order in α, we do not expect these qualitative features to change. Larger α will introduce higher harmonics into the band structure, and break the degeneracy of the band minima. Also, the gap to spin excitations will decrease from its $\alpha=0$ value of J_z, so there will be a smaller gap to the incoherent background. When $\alpha \to 1$, the gap to spin excitations disappears. In the next section we will discuss the hole spectrum in that limit.

C. Heisenberg model in the dominant pole approximation

In the previous sections, we have seen that near the Ising limit, the hole spectrum has a well-defined quasiparticle peak which has a spectral weight comparable to J_z/t and a bandwidth of $J_\perp$. This peak is well described by the dominant pole approximation in which we ignore the effects of the incoherent part of the spectrum and consider only a single quasiparticle pole. The validity of ignoring the incoherent part was justified by the fact that there is a gap in the spin excitation spectrum of order $t(J_z/t)^{2/3}$, so that the dominant contribution to $\partial\Sigma/\partial\omega$ comes from the pole.

In this section we investigate the case where $J_\perp = J_z \equiv J$, so that there is no gap to the spin excitations. The low-energy spin excitations have a linear dispersion and in two dimensions a linear density of states. We will argue that even though there is no gap, the fact that there is a small density of states of low-lying spin excitations implies that a well-defined quasiparticle exists. We can get qualitative information about the low-energy structure of the hole spectrum by considering the dominant pole approximation. In this case the contributions from the pole and from the incoherent part have comparable magnitudes, so that by ignoring the incoherent part, we are losing numerical factors, but not qualitative features.

The existence of a quasiparticle pole depends crucially on the density of states of low-lying excitations which can couple to the hole. When there are many such excitations, there will be too much scattering and the entire spectrum will be incoherent. However, as we shall show, when there are very few low-lying spin excitations, there is very little phase space available for the hole to scatter, so that the low-energy states of the hole can have a long lifetime.

We now consider the self-consistent equations of the dominant pole approximation. We write the hole propagator as,

$$G(\mathbf{k},\omega)=\frac{a_{\mathbf{k}}}{\omega-\omega_{\mathbf{k}}+i\Gamma_{\mathbf{k}}}+\int dy\frac{A_{\text{inc}}(\mathbf{k},y)}{\omega-y} \ . \qquad (2.34)$$

We may then solve for the parameters which describe the pole,

$$\omega_{\mathbf{k}}=\sum_{\mathbf{q}} f(\mathbf{k},\mathbf{q})\mathrm{Re}G(\mathbf{k}-\mathbf{q},\omega_{\mathbf{k}-\mathbf{q}}-E_{\mathbf{q}}) \ , \qquad (2.35a)$$

$$\Gamma_{\mathbf{k}}=\sum_{\mathbf{q}} f(\mathbf{k},\mathbf{q})\mathrm{Im}G(\mathbf{k}-\mathbf{q},\omega_{\mathbf{k}-\mathbf{q}}-E_{\mathbf{q}}) \ , \qquad (2.35b)$$

$$a_{\mathbf{k}}=\frac{1}{1-\sum_{\mathbf{q}} f(\mathbf{k},\mathbf{q})\frac{\partial}{\partial\omega}\mathrm{Re}G(\mathbf{k}-\mathbf{q},\omega_{\mathbf{k}-\mathbf{q}}-E_{\mathbf{q}})} \ . \qquad (2.35c)$$

Let us first consider the quasiparticle lifetime $\Gamma_{\mathbf{k}}$. Suppose we are at the lowest-energy pole of the hole spectrum at $\omega_{\mathbf{k}^*}$. Then, since $\Gamma_{\mathbf{k}^*}$ depends on the hole spectral function at energies less than $\omega_{\mathbf{k}^*}$, it necessarily vanishes. This is because there are no lower-energy states to which the hole can scatter. Thus, if there is a pole at the bottom of the spectrum, it will have infinite lifetime. This is a very general statement, and as we will discuss in Appendix A, it is independent of the noncrossing approximation for the self-energy.

We might expect that if we increase the energy slightly, that the lifetime would be finite. However if the band has quadratic dispersion, then since the spin excitations have linear dispersion, conservation of energy and momentum forbids scattering to the lower-energy states by single or multiple spin wave excitations. This will be true as long as the hole velocity, dE/dk is less than the spin-wave velocity. Therefore, $\Gamma_{\mathbf{k}}=0$ for all of the low-energy poles. There will be a critical energy when the hole velocity and the spin-wave velocity will be equal, and above that energy, the holes may scatter, and will have a finite lifetime. However, since we are interested in the low-energy poles, we can set $\Gamma_{\mathbf{k}}=0$.

Next we consider the quasiparticle residue $a_{\mathbf{k}}$. Since the contribution from the incoherent part in the denominator of (2.35c) is necessarily positive, we can make the following upper bound for the residue:

$$a_{\mathbf{k}} \le \frac{1}{1+t^2\sum_{\mathbf{q}} f(\mathbf{k},\mathbf{q})\frac{a_{\mathbf{k}-\mathbf{q}}}{(\omega_{\mathbf{k}}-\omega_{\mathbf{k}-\mathbf{q}}-E_{\mathbf{q}})^2}} \ . \qquad (2.36)$$

Consider first the pole at the bottom of the spectrum, where $\omega_{\mathbf{k}}=0$ in the $J=0$ limit. The integral in the denominator will be dominated by its $\mathbf{q}=0$ limit. From Eq. (2.16), the limiting behavior for small $\mathbf{q}$ is, $f(\mathbf{k},\mathbf{q})=|\mathbf{q}|(\gamma_{\mathbf{k}}-\hat{q}\cdot\nabla\gamma_{\mathbf{k}})^2$, which means that the hole couples weakly to the long wavelength spin waves. If the mass at the bottom of the band is m^*, then

$$a_{\mathbf{k}^*} \le \frac{1}{1+t^2\sum_{\mathbf{q}} |\mathbf{q}|\frac{a_{\mathbf{k}^*}}{\left[\frac{\mathbf{q}^2}{2m^*}\right]^2}} \ . \qquad (2.37)$$

The integral in the denominator is divergent in dimensions three or less. Thus, in the case of interest, $d=2$, $a_{\mathbf{k}^*}=0$. The fact that the pole cannot exist is a result of the fact that it is too easy for the hole to scatter, due to the large density of states at the bottom of a parabolic band. In addition, the vanishing spectral weight implies an infinite mass, so that there will not be any finite-residue poles in the $J=0$ limit. Thus, we expect a broad, incoherent continuum spectrum similar to the Brinkman-Rice spectrum examined earlier, except for the fact that it will be momentum dependent.

We may now ask whether a pole may exist when J is small but finite. In this case, the divergence in Eq. (2.37) is cut off by the linear spin-wave dispersion $E_{\mathbf{q}}$,

$$a_{\mathbf{k}^*} \le \frac{1}{1+t^2\sum_{\mathbf{q}} |\mathbf{q}| \frac{a_{\mathbf{k}^*}}{\left[J|\mathbf{q}|+\frac{q^2}{2m^*}\right]^2}} . \tag{2.38}$$

This integral is convergent in dimensions greater than one. In one dimension, there can be no pole with finite residue, even for finite J. (Note, however, that if a finite lifetime is inserted by hand that this logarithmic divergence will be cut off, yielding a finite residue.[10]) In two dimensions, the integral is not singular so that a convergent result may be obtained. We may estimate the small J singularity in two dimensions of the integral to be

$$\sum_{\mathbf{q}} \frac{|\mathbf{q}|a_{\mathbf{k}^*}}{\left[J|\mathbf{q}|+\frac{\mathbf{q}^2}{2m^*}\right]^2} \approx \frac{m^* a_{\mathbf{k}^*}}{J} . \tag{2.39}$$

Furthermore, we will show that the mass at the bottom of the band is $m^*=m/a_{\mathbf{k}^*}$, where m depends only on t. Thus, the integral is of the order t/J, so that $a_{\mathbf{k}^*} \le J/t$.

At this point we have an upper bound for the spectral weight, which we derived by omitting the contribution from the incoherent part of the spectrum. In Appendix A we will argue that the incoherent contribution in the denominator of (2.35c) will not be larger than t/J, so that the qualitative result that $a_{\mathbf{k}} \approx J/t$ remains true.

Let us now consider the shape of the quasiparticle band. The positions of the peaks are given by

$$\omega_{\mathbf{k}} = t^2 \sum_{\mathbf{q}} f(\mathbf{k},\mathbf{q}) \mathrm{Re} G(\mathbf{k}-\mathbf{q}, \omega_{\mathbf{k}} - E_{\mathbf{q}}) . \tag{2.40}$$

This self-consistent equation is rather subtle, since there is implicit dependence on $\omega_{\mathbf{k}}$ on the right-hand side, which has a crucial effect. If we calculate the slope of $\omega_{\mathbf{k}}$, for instance, from the arguments given in the Introduction,

$$\nabla_{\mathbf{k}}\omega_{\mathbf{k}} = a_{\mathbf{k}} t^2 \sum_{\mathbf{q}} \nabla_{\mathbf{k}} f(\mathbf{k},\mathbf{q}) G(\mathbf{k}-\mathbf{q}, \omega - E_{\mathbf{q}})|_{\omega=\omega_{\mathbf{k}}} . \tag{2.41}$$

If J is very small, then we may consider the $J=0$ limit of the right-hand side, which can be written (after substituting $\mathbf{q}\to\mathbf{k}-\mathbf{q}$ in the sum)

$$\nabla_{\mathbf{k}}\omega_{\mathbf{k}} = a_{\mathbf{k}} t^2 \sum_{\mathbf{q}} [\nabla_{\mathbf{k}} f(\mathbf{k},\mathbf{k}-\mathbf{q})] G^0(\mathbf{q},\omega_0) , \tag{2.42}$$

where $G^0(\mathbf{q},\omega_0)$ is the $J=0$ limit hole propagator, (which we expect to resemble the incoherent Brinkman-Rice spectrum) evaluated at its lower band edge, ω_0. Since there are no poles at $J=0$, we know that $G^0(\mathbf{q},\omega_0) \approx O(1/t)$ and is a smooth function of q. It should also be negative, since there is no spectral weight below ω_0.

Thus, the band becomes flatter in the $J=0$ limit because the residue $q_{\mathbf{k}} \approx J/t$, and the quasiparticle mass will be enhanced by a factor t/J. We can also write the mass at the bottom of the band (where $\nabla_{\mathbf{k}}\omega_k=0$) as,

$$\frac{1}{m_{ij}} \equiv \frac{\partial^2}{\partial k_i \partial k_j}\omega_{\mathbf{k}} = a_{\mathbf{k}} t^2 \sum_{\mathbf{q}} \left[\frac{\partial^2}{\partial k_i \partial k_j} f(\mathbf{k},\mathbf{k}-\mathbf{q})\right] G^0(\mathbf{q},\omega_0) . \tag{2.43}$$

The reason why naively taking the $J=0$ limit of Eq. (2.40) is incorrect is that for small J, the frequency dependence of the self-energy becomes singular ($\partial\Sigma/\partial\omega\to\infty$) at the band edge, so that it is important to account for the implicit frequency dependence before the $J=0$ limit is taken.

We can identify the position of the band minimum by examining the zeros of $\nabla_{\mathbf{k}}\omega_{\mathbf{k}}$ in Eq. (2.42). Though we do not know the precise form of $G(\mathbf{q},\omega_0)$, we know that it must be negative and have the full cubic symmetry. Given the form of $f(\mathbf{k},\mathbf{k}-\mathbf{q})$, this allows us to say that $\nabla_{\mathbf{k}}\omega_{\mathbf{k}}=0$ at the points (0,0), (π,π), $(\pm\pi/2,\pm\pi/2)$, $(0,\pi)$, and $(\pi,0)$ in the Brillouin zone. We numerically plugged various plausible forms for $G^0(\mathbf{q},\omega)$ into Eq. (2.43). We found that independent of which forms we tried, the band minimum was at $(\pm\pi/2,\pm\pi/2)$, and that the mass is heavier along the direction towards $(0,\pi)$ than in the direction towards (0,0). This is in good agreement with the results of Trugman.[18]

We now consider the behavior of the spectral function at energies higher than the lowest pole. In general, we may express the spectral function in terms of the self-energy as,

$$A(\mathbf{k},\omega) = \frac{\Gamma(\mathbf{k},\omega)}{(\omega-\omega_{\mathbf{k}})^2\left[1-\mathrm{Re}\frac{\Sigma(\mathbf{k},\omega)-\Sigma(\mathbf{k},\omega_{\mathbf{k}})}{\omega-\omega_{\mathbf{k}}}\right]^2+\Gamma(\mathbf{k},\omega)^2} , \tag{2.44}$$

where $\Gamma(\mathbf{k},\omega) \equiv 1/\pi \mathrm{Im}\Sigma(\mathbf{k},\omega)$. In the noncrossing approximation, we write,

$$\Gamma(\mathbf{k},\omega) = t^2 \sum_{\mathbf{q}} f(\mathbf{k},\mathbf{q}) A(\mathbf{k}-\mathbf{q}, \omega - E_{\mathbf{q}}) . \tag{2.45}$$

For $\omega-\omega_{\mathbf{k}} \ll J$, the dominant contribution to $\Gamma(\mathbf{k},\omega)$ will come from the pole in $A(\mathbf{k},\omega)$. Furthermore, there will only be a contribution when $\mathbf{q}$ is very small, so that $E_{\mathbf{q}} \ll J$. We may thus write,

$$\Gamma(\mathbf{k},\omega) = t^2 \sum_{\mathbf{q}} |\mathbf{q}| a_{\mathbf{k}-\mathbf{q}} \delta\left[\omega - \frac{(\mathbf{k}-\mathbf{q})^2}{2m^*} - J|\mathbf{q}|\right] . \tag{2.46}$$

In two dimensions, we find that

$$\Gamma(\mathbf{k},\omega) \approx t^2 \frac{a_{\mathbf{k}}}{J}\left[\frac{\omega-\omega_{\mathbf{k}}}{J}\right]^2 . \tag{2.47}$$

Thus, for $\omega-\omega_{\mathbf{k}} \ll J$, $\Gamma(\mathbf{k},\omega)\propto(\omega-\omega_{\mathbf{k}})^2$. Furthermore, if we extrapolate this expression to $\omega\approx J$, we find $\Gamma(\mathbf{k},\omega_{\mathbf{k}}+J)\approx t$, as shown in Fig. 2. Since in this limit the quantity in the brackets in Eq. (2.44) becomes $(1-\partial\Sigma/\partial\omega)^2=a_{\mathbf{k}}^{-2}$, the spectral function may be written,

$$A(\mathbf{k},\omega)\approx t^2\frac{a_{\mathbf{k}}^3}{J^3}\approx\frac{1}{t}\ . \tag{2.48}$$

Thus, slightly above the pole, the incoherent part of the spectral function is a constant of order $1/t$.

We have shown that there is a quasiparticle peak with spectral weight J/t and mass enhancement t/J below an incoherent background. From our intuition gained from the $J_\perp$ expansion, we expect that this peak will be at an energy of the order $-4t$ and that the incoherent band will have a width proportional to t.

III. HOLE MOTION IN AN RVB STATE

In the preceding section we studied the motion of holes in a state which is described by a Néel state, with Holstein-Primakoff spin-wave excitations. Another possible ground state for spin $\frac{1}{2}$, which has received a great deal of attention lately is the resonating-valence-bond state originally proposed by Anderson.[2] Our approach to treating the hole motion in this state will be the same as our approach to the Néel state. We will examine the spin excitations at the mean-field level of the model at half-filling, and then determine how a hole will couple to these excitations. By neglecting vertex corrections, we obtain a self-consistent integral equation for the hole propagator which can be analyzed using the self-consistent pole techniques developed in the previous section.

In the original mean-field theory of the RVB state, Baskaran, Zou, and Anderson[21] decoupled the magnetic interaction in the particle-particle channel by introducing an s-wave order parameter $\Delta_{\mathbf{k}}=\Delta(\cos k_x+\cos k_y)$ which describes an RVB state with a "pseudo-Fermi surface" of low-lying excitations. It was subsequently shown by Kotliar[22] that at zero temperature, the stable mean-field solution is a state with an order parameter with mixed symmetry, $\Delta_{\mathbf{k}}=\Delta(\cos k_x+i\cos k_y)$. In this state the gap vanishes only at four points in Brillouin zone. Affleck and Marston[23] developed a mean-field theory based on a two sublattice particle-hole decoupling of the magnetic interaction and found that the "flux" phase was stable at half-filling and has the same excitation spectrum as Kotliar's[22] mixed state. It was then shown by Affleck, Hsu, and Anderson[24] that these two solutions were related by a local SU(2) gauge symmetry, which is essentially a result of the particle-hole symmetry of the half-filled Hubbard model.

Away from half-filling, particle-hole symmetry and hence the SU(2) gauge symmetry is broken, so that a particular solution will be chosen. Kotliar and Liu[6] and Zhang, Gross, Rice, and Shiba[7] have independently shown that the stable translationally invariant mean-field solution near half-filling is a state with a combination of d-wave particle-particle paring and s-wave particle-hole pairing. This particular mean-field solution is chosen away from half-filling because it allows the holes to gain the most kinetic energy by maximizing the "bare-hopping" probability of the holes. We will examine the hole motion in this state.

Kotliar and Liu[6] cast the problem in terms of a slave boson Hamiltonian, in which an additional field is introduced to keep track of unoccupied sites. We adopt this approach, since it leads naturally to the treatment of holes. Thus, as in Sec. II, we express the electron operator as a product of two operators. In this case, however, we represent the spin by a fermion operator and the hole by a boson operator. We write $c_{i\sigma}^\dagger=b_i f_{i\sigma}^\dagger$, and impose the constraint $b_i^\dagger b_i+f_{i\sigma}^\dagger f_{i\sigma}=1$. The slave boson Hamiltonian is then,

$$\begin{aligned}H=&-t\sum_{\langle i,j\rangle} b_i f_{i\sigma}^\dagger f_{j\sigma} b_j^\dagger\\&+J\sum_{\langle i,j\rangle} f_{i\alpha}^\dagger f_{i\beta} f_{j\gamma}^\dagger f_{j\delta}(\sigma_{\alpha\beta}\cdot\sigma_{\gamma\delta}-1)\\&+\sum_i \lambda_i(b_i^\dagger b_i+f_{i\sigma}^\dagger f_{i\sigma}-1)\ .\end{aligned} \tag{3.1}$$

At half-filling (when there are no bosons), this Hamiltonian represents a Heisenberg model, with the spins expressed in the fermion representation. The spin interaction is then simultaneously factorized in the particle-particle and particle-hole channels. At half-filling the mean-field equations admit a class of solutions which are related by SU(2) particle-hole transformations. A slight deviation from half-filling will single out one of these solutions. At half-filling, the mean-field Hamiltonian corresponding to this solution is

$$H=-CJ\sum_{\mathbf{k},\sigma}\gamma_{\mathbf{k}}^s f_{\mathbf{k}\sigma}^\dagger f_{\mathbf{k}\sigma}+\gamma_{\mathbf{k}}^d f_{\mathbf{k}\sigma} f_{-\mathbf{k}-\sigma}+\text{H.c.}, \tag{3.2}$$

where $C\approx 2$, and $\gamma_{\mathbf{k}}^s=\frac{1}{2}(\cos k_x+\cos k_y)$ and $\gamma_{\mathbf{k}}^d=\frac{1}{2}(\cos k_x-\cos k_y)$ are the s- and d-wave nearest-neighbor cubic harmonics. This may then be diagonalized by Bogoliubov transformation yielding,

$$H=\sum_{\mathbf{k},\sigma}E_{\mathbf{k}}\beta_{\mathbf{k}\sigma}^\dagger\beta_{\mathbf{k}\sigma}\ , \tag{3.3}$$

where

$$\begin{aligned}E_{\mathbf{k}}&=CJ(\gamma_{\mathbf{k}}^{s2}+\gamma_{\mathbf{k}}^{d2})^{1/2}\\&=CJ\sqrt{\tfrac{1}{2}(\cos^2 k_x+\cos^2 k_y)}\ ,\end{aligned}$$

and

$$\begin{aligned}&\begin{bmatrix}\beta_{\mathbf{k}\uparrow}\\ \beta_{-\mathbf{k}\downarrow}^\dagger\end{bmatrix}=\begin{bmatrix}u_{\mathbf{k}}^* & -v_{\mathbf{k}}\\ v_{\mathbf{k}}^* & u_{\mathbf{k}}\end{bmatrix}\begin{bmatrix}f_{\mathbf{k}\uparrow}\\ f_{-\mathbf{k}\downarrow}^\dagger\end{bmatrix},\\&u_{\mathbf{k}}=\frac{1}{\sqrt{2}}\left[1-\frac{\gamma_{\mathbf{k}}^s}{E_{\mathbf{k}}}\right]^{1/2},\\&v_{\mathbf{k}}=(\sin\gamma_{\mathbf{k}}^d)\frac{1}{\sqrt{2}}\left[1+\frac{\gamma_{\mathbf{k}}^s}{E_{\mathbf{k}}}\right]^{1/2}.\end{aligned} \tag{3.4}$$

The hopping part of the Hamiltonian is then,

$$H_t=-4t\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}}\gamma_{\mathbf{k}-\mathbf{k}'}b_{\mathbf{k}}f_{\mathbf{k}'\sigma}^\dagger f_{\mathbf{k}'-\mathbf{q}\sigma}b_{\mathbf{k}-\mathbf{q}}^\dagger\ . \tag{3.5}$$

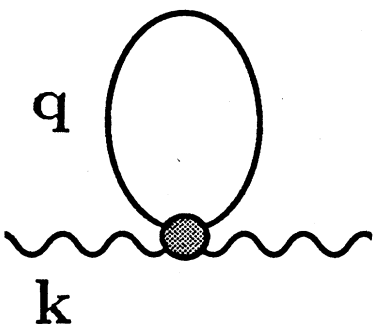

FIG. 6. Hole self-energy diagram in the d-wave RVB state which is responsible for the bare-hopping term.

This hopping Hamiltonian is different from that which we considered in the previous section because the hole couples to two spin excitations when it hops. This introduces the new feature of a "bare-hopping term" in which a boson can hop from one site to another without changing the spin configuration. The bare-hopping (BH) term arises from a self-energy contribution shown in Fig. 6.

$$\Sigma^{\rm BH}(\mathbf{k},\omega)=-Ct\sum_{\mathbf{k}'}\gamma_{\mathbf{k}-\mathbf{k}'}\times 2|v_{\mathbf{k}'}|^2=-t_b\gamma_{\mathbf{k}}\ , \qquad (3.6)$$

where $v_{\mathbf{k}}$ is defined above, and $t_b\approx t/3$. The bare-hopping term allows a hole to hop a single time while keeping the spin state unchanged. Thus, unlike in the Néel state, the hole will not be associated with a single sublattice.

Based on this mean-field theory we would expect a boson bandwidth of $2t_b$, so that holes would have a kinetic energy of $-t_b$, and a band minimum at $\mathbf{k}=0$. Indeed, the reason that this solution is favored in mean-field theory is that it has the largest bare-hopping term among translationally invariant states so that the holes may acquire the greatest kinetic energy. It is also possible to consider the nontranslationally invariant decouplings. For example, Affleck and Marston's flux phase[23] is a two sublattice decoupling in the particle-hole channel. The magnitude of the bare-hopping matrix element is larger than that for the d-wave state by $\sqrt{2}$. On the other hand, due to the two-sublattice nature of the band structure, the boson bandwidth in this case turns out to be the same as that in the d-wave translationally invariant state.

However, we shall now argue that fluctuations about the mean-field theory are very important, and provide an additional source for kinetic energy of the holes of the same order of magnitude as the mean-field theory, i.e., of

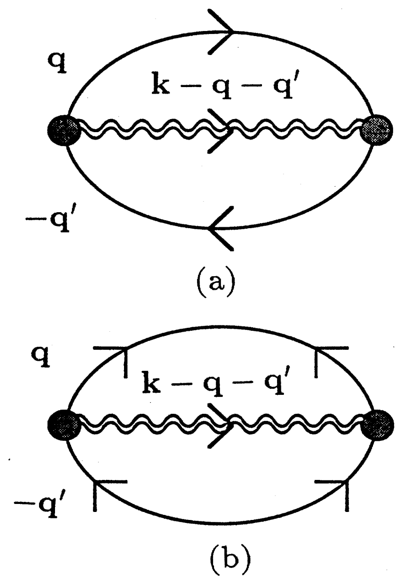

FIG. 7. Self-energy diagrams considered in the noncrossing approximation of the hole propagator in the d-wave RVB state. The double wavy line is the exact hole propagator, and the solid lines are propagators for the spin excitations.

order t. Since the holes are very strongly coupled to the spin excitations, it is important to consider the quasiparticle hole, which is dressed by a cloud of spin excitations. We anticipate a picture similar to that in Sec. II, where there is a quasiparticle peak at the bottom of an incoherent band of width t.

As in the previous section, we calculate the propagator for the spinless hole operator b,

$$G(i,j,\omega)=\int_{-\infty}^{\infty}dt\, e^{i\omega t}\langle T[b_i(t)b_j^\dagger(0)]\rangle\ . \qquad (3.7)$$

Though this is not physically meaningful by itself, since one cannot remove an electron without removing a spin, it is useful for calculating physical quantities. For instance, the conductivity involves the creation of particle-hole pairs, and it is possible for the spins of the particle and hole to be absorbed as a singlet into the background spin state.

As in the previous section we consider a self-consistent perturbation theory in which vertex corrections are ignored, so that we consider corrections to the self-energy of the form shown in Fig. 7. At zero temperature, these diagrams can be evaluated to give the self-consistent integral equation for the hole propagator,

$$G(\mathbf{k},\omega)=\frac{1}{\omega+t_b\gamma_{\mathbf{k}}-t^2\sum_{\mathbf{q},\mathbf{k}'}f(\mathbf{k},\mathbf{k}',\mathbf{q})G(\mathbf{k}-\mathbf{q},\omega-E_{\mathbf{k}'}-E_{\mathbf{q}-\mathbf{k}'})}\ , \qquad (3.8)$$

where

$$f(\mathbf{k},\mathbf{k}',\mathbf{q})=16|\gamma_{\mathbf{k}-\mathbf{k}'}u_{\mathbf{k}'}v_{\mathbf{k}'-\mathbf{q}}-\gamma_{\mathbf{k}+\mathbf{k}'-\mathbf{q}}u_{\mathbf{k}'-\mathbf{q}}v_{\mathbf{k}'}|^2\ . \qquad (3.9)$$

We first show that in the $J=0$ limit, the hole spectrum is completely incoherent, as it was in the previous section. In that case, the spin excitations cost zero energy. Suppose the lowest pole is at $\omega_{\mathbf{k}}$. We may write its residue as,

$$a_{\mathbf{k}^*}=\frac{1}{1-t^2\sum_{\mathbf{q},\mathbf{k}'}f(\mathbf{k}^*,\mathbf{k}',\mathbf{q})\frac{\partial}{\partial\omega}G(\mathbf{k}^*-\mathbf{q},\omega_{\mathbf{k}})} . \quad (3.10)$$

We show that this residue must vanish by considering the following upper bound, in which we keep only the pole part of $G(\mathbf{k},\omega)$.

$$a_{\mathbf{k}^*}\le\frac{1}{1+t^2\sum_{\mathbf{q},\mathbf{k}'}f(\mathbf{k}^*,\mathbf{k}',\mathbf{q})\frac{a_{\mathbf{k}^*-\mathbf{q}}}{\left[\frac{q^2}{2m^*}\right]^2}} . \quad (3.11)$$

The integral in the denominator will be dominated by its small $\mathbf{q}$ limit. If $\mathbf{k}^*$ is somewhere other than (0,0), $(0,\pi)$, $(\pi,0)$, or (π,π) $[(\pi/2,\pi/2)$, for instance], then we can see from (3.9) that $\sum_{\mathbf{k}'}f(\mathbf{k}^*,\mathbf{k}',\mathbf{q})$ is of order unity for small $\mathbf{q}$. In that case the integral in the denominator is divergent in dimensions four or less. If $\mathbf{k}^*$ is at one of those four points, then $\sum_{\mathbf{k}'}f(\mathbf{k}^*,\mathbf{k}',\mathbf{q})$ is of order q^2 for small $\mathbf{q}$, and the integral is logarithmically divergent in two dimensions.

Since this upper bound vanishes, there can be no finite residue poles in the $J=0$ limit. We expect the hole spectrum to be an incoherent, $\mathbf{k}$-dependent band with width of the order t. In mean-field theory we would have expected a coherent boson band with a width $2t_b$. By including the strong interactions of the bosons with the spin excitations, we have shown that fluctuations destroy the coherence.

We now proceed to consider finite J, and to show that a sharp quasiparticle band does exist with a residue of the order J/t and a mass enhancement of t/J. As in the previous section, suppose that

$$G(\mathbf{k},\omega)=\frac{a_{\mathbf{k}}}{\omega-\omega_{\mathbf{k}}+i\Gamma_{\mathbf{k}}} . \quad (3.12)$$

We will omit the incoherent contribution in this treatment, since due to arguments similar to those given in the previous section, they will not alter the qualitative features.

We first consider the lifetime $\Gamma_{\mathbf{k}}$:

$$\Gamma_{\mathbf{k}}=t^2\sum_{\mathbf{q},\mathbf{k}'}f(\mathbf{k},\mathbf{k}',\mathbf{q})A(\mathbf{k}-\mathbf{q},\omega_{\mathbf{k}}-E_{\mathbf{k}'}-E_{\mathbf{q}-\mathbf{k}'}) . \quad (3.13)$$

As in the Néel state, since the hole dispersion is quadratic, while the spin excitation dispersion is linear in the d-wave state near half-filling, conservation of energy and momentum forbids scattering as long as the hole velocity $\nabla_{\mathbf{k}}\omega_{\mathbf{k}}$ is less than the spin excitation velocity, $\nabla_{\mathbf{k}}E_{\mathbf{k}}$. Thus, $\Gamma(\mathbf{k},\omega)=0$ for the low-lying poles, and as in the previous section, we shall henceforth omit it.

The quasiparticle weight must be determined self-consistently from

$$a_{\mathbf{k}}=\frac{1}{1+t^2\sum_{\mathbf{q},\mathbf{k}'}f(\mathbf{k},\mathbf{k}',\mathbf{q})\frac{a_{\mathbf{k}-\mathbf{q}}}{(\omega_{\mathbf{k}}-E_{\mathbf{k}'}-E_{\mathbf{q}-\mathbf{k}'})^2}} . \quad (3.14)$$

The sum in the denominator is convergent for small $\mathbf{q}$, because the region in phase space in which the integrand diverges is very small. This is a result of the small density of states of low-energy spin excitations. When $J\to0$ we have seen that the integral is divergent. Finite J will cut off this divergence. We may estimate the singular behavior of the integral in the $J=0$ limit to be [assuming the position of the band minimum is such that $f(\mathbf{k}^*,\mathbf{k}',\mathbf{q})$ is of order unity for small $\mathbf{q}$]

$$t^2\sum_{\mathbf{k}',\mathbf{q}}\frac{f(\mathbf{k}^*,\mathbf{k}',\mathbf{q})a_{\mathbf{k}^*-\mathbf{q}}}{\left[\frac{q^2}{2m^*}-J|\mathbf{k}'|-J|\mathbf{k}'-\mathbf{q}|\right]^2}\propto\frac{a_{\mathbf{k}^*}t^2m^*}{J} . \quad (3.15)$$

Furthermore, as we will see, we can say in general that $m^*=(1/a_{\mathbf{k}})m$, where m is the noninteracting band mass, which depends only on t. Therefore, the denominator in equation (3.14) is of order t/J, so that $a_{\mathbf{k}^*}\propto J/t$ for $J\ll t$. Thus, as in the case of the Néel state, there exists a quasiparticle peak with a weight of the order J/t. If the band minimum is at (0,0), $(0,\pi)$, $(\pi,0)$, or (π,π), then $f(\mathbf{k}^*,\mathbf{k}',\mathbf{q})\propto q^2$, and finite J will cut off the logarithmic divergence in the denominator of (3.14), and we find

$$a_{\mathbf{k}^*}\approx\frac{1}{1+\frac{1}{a_{\mathbf{k}^*}}\ln\frac{a_{\mathbf{k}^*}t}{J}} . \quad (3.16)$$

This is clearly only consistent if $a_{\mathbf{k}^*}$ is proportional to J/t in the $J\to0$ limit.

The dispersion of the boson band is given by

$$\omega_{\mathbf{k}}=-t_b\gamma_{\mathbf{k}}+t^2\sum_{\mathbf{q},\mathbf{k}'}f(\mathbf{k},\mathbf{k}',\mathbf{q})G(\mathbf{k}-\mathbf{q},\omega_{\mathbf{k}}-E_{\mathbf{k}'}-E_{\mathbf{q}-\mathbf{k}'}) . \quad (3.17)$$

As in the case of the Néel state, we may write the mass at the bottom of the band as,

$$\frac{1}{m_{ij}}\equiv\frac{\partial^2}{\partial k_i\partial k_j}\omega_{\mathbf{k}}$$
$$=a_{\mathbf{k}}\frac{\partial^2}{\partial k_i\partial k_j}\left[-t_b\gamma_{\mathbf{k}}+t^2\sum_{\mathbf{q},\mathbf{k}'}f(\mathbf{k},\mathbf{k}',\mathbf{k}-\mathbf{q})G^0(\mathbf{q},\omega_0)\right] , \quad (3.18)$$

where $G^0(\mathbf{q},\omega_0)\approx-1/t$ is $J=0$ limit with band edge at ω_0. Thus, we see that both the "bare-hopping term" and the self-consistent terms are renormalized by the quasiparticle residue, leading to an effective mass which is enhanced by t/J.

Above the quasiparticle peaks, there will be an incoherent background. We may estimate its low-energy behavior by interating the integral equation. As in Sec. II we write

$$A(\mathbf{k},\omega)=\frac{\Gamma(\mathbf{k},\omega)}{(\omega-\omega_{\mathbf{k}})^2\left[1-\dfrac{\Sigma(\mathbf{k},\omega)-\Sigma(\mathbf{k},\omega_{\mathbf{k}})}{\omega-\omega_{\mathbf{k}}}\right]^2+\Gamma(\mathbf{k},\omega)^2}, \tag{3.19}$$

where now the noncrossing approximation yields,

$$\Gamma(\mathbf{k},\omega)=t^2\sum_{\mathbf{k}',\mathbf{q}} f(\mathbf{k},\mathbf{k}',\mathbf{q})A(\mathbf{k}-\mathbf{q},\omega-E_{\mathbf{k}'}-E_{\mathbf{q}-\mathbf{k}'}) . \tag{3.20}$$

As in Sec. II we may obtain the behavior for $\omega-\omega_{\mathbf{k}}\ll J$, in which the only contributions come when $\mathbf{k}'$ and $\mathbf{q}-\mathbf{k}'$ are near the zeros of the spin excitation spectrum. We find that

$$\Gamma(\mathbf{k},\omega)\approx t^2\frac{a_{\mathbf{k}}}{J}\left[\frac{\omega-\omega_{\mathbf{k}}}{J}\right]^3 , \tag{3.21}$$

and

$$A_{\text{inc}}(\mathbf{k},\omega)\approx t^2\frac{a_{\mathbf{k}}^3}{J^3}\left[\frac{\omega-\omega_{\mathbf{k}}}{J}\right]\approx\frac{1}{t}\left[\frac{\omega-\omega_{\mathbf{k}}}{J}\right] . \tag{3.22}$$

Thus we see that as in the Néel state, the hole spectrum in this RVB state has a quasiparticle band of width J at the bottom of an incoherent spectrum. Note that this is drastically different from the mean-field prediction of a coherent band whose width is of order t.[6,7] The strong coupling with the spin excitations causes this bandwidth to be renormalized. In fact, once these fluctuations are included, it is not even clear that maximizing the bare-hopping term necessarily gives the most energetically favorable state. Via the interactions with the spins alone, the holes are able to acquire a kinetic energy of order t, whether there is a "bare-hopping term" or not.

IV. OPTICAL PROPERTIES

In this section we discuss the relevance of our results to optical experiments. Recent reflectivity measurements have probed the frequency-dependent conductivity, $\sigma(\omega)$.[11] A Drude peak is observed with an integrated area which corresponds to an effective-mass enhancement of 10, assuming that the carrier density is the hole density due to doping. At higher frequencies, there is a broad feature which is peaked at 0.2 eV.

The large mass enhancement follows naturally from the t/J mass enhancement predicted by our theory. In addition, we would like to identify the observed broad peak with the incoherent background in the hole spectrum.

We now describe the conductivity predicted by our theory. Details of the diagrammatic calculation may be found in Appendix B. We will assume that the density of holes is very small, so that they will not interact, and their spectrum will be like that of a single hole. The conductivity, $\sigma(\omega)$ is a measure of the excited states with energy ω which couple to the current. In Appendix B we will show that for $\omega\ll J$ we may write $\sigma(\omega)$ in terms of the hole spectral function $A(\mathbf{k},\omega)$ and the current vertex function $C(\mathbf{k},\Omega,\omega)$,

$$\sigma(\omega)\approx\sum_{\mathbf{k}}\int d\Omega\frac{n(\Omega)-n(\Omega+\omega)}{\omega}C(\mathbf{k},\Omega,\omega)^2A(\mathbf{k},\Omega)\times A(\mathbf{k},\Omega+\omega) , \tag{4.1}$$

where $n(\Omega)$ is the thermal occupation number for a density of δ carriers. When evaluated on shell near the bottom of the band, $C(\mathbf{k},\Omega=\omega_{\mathbf{k}},\ \omega=0)\approx(e/m)(k-k^*)$, where $\mathbf{k}^*$ is the position of the band minimum and m is the bare hole mass ($m\approx1/t$). At frequencies comparable or larger than J, there will be additional, more complicated contributions to $\sigma(\omega)$ which include spin excitations.

The Drude peak in the conductivity follows from the consideration of the quasiparticle peaks in the spectral function, $A(\mathbf{k},\omega)$. If we omit the incoherent part of A, then (4.1) may be written as,

$$\sigma_D(\omega)\approx\delta(\omega)\sum_{\mathbf{k}}-\frac{\partial n}{\partial\omega}(\omega_{\mathbf{k}})\frac{e^2}{m^2}(k-k^*)^2a_{\mathbf{k}}^2 . \tag{4.2}$$

The sum over k may be converted into an integral over energy. The density of states in two dimensions is a constant $m^*=m/a_{\mathbf{k}*}$, so

$$\sigma_D(\omega)\approx\delta(\omega)\frac{e^2}{m^*}\int d\Omega-\omega\frac{\partial n}{\partial\omega} . \tag{4.3}$$

This may then be integrated by parts, and using the fact that the hole concentration is δ we find

$$\sigma^d(\omega)\approx\frac{\delta e^2}{m^*}\delta(\omega) , \tag{4.4}$$

where m^* is the effective mass which is enhanced by t/J.

The weight of this peak is consistent with the observed behavior. Note, however, that it has zero width. This is because the quasiparticle peaks are sharp at zero temperature. At present we do not have an explanation of the peculiar linear temperature dependence of the DC conductivity.

At finite frequency, the incoherent part will become important. For $\omega\ll J$ and $T\ll J$ the occupation factors in Eq. (4.1) will keep Ω close to $\omega_{\mathbf{k}^*}$, so that it is reasonable to keep only the pole part of $A(\mathbf{k},\Omega)$ in (4.1), while keeping the incoherent part of $A(\mathbf{k},\Omega+\omega)$, so that we may write,

$$\sigma(\omega)\approx\sum_{\mathbf{k}}\frac{n(\omega_{\mathbf{k}})-n(\omega_{\mathbf{k}}+\omega)}{\omega}C(\mathbf{k},\omega_{\mathbf{k}},\omega)^2a_{\mathbf{k}}A(\mathbf{k},\omega_{\mathbf{k}}+\omega). \tag{4.5}$$

Since we do not precisely know the form of $C(\mathbf{k},\omega_{\mathbf{k}},\omega)$ for finite frequencies, it is difficult to get a reliable expression for $\sigma(\omega)$. However, if the density of carriers is small, the structure of $\sigma(\omega)$ will be similar to the structure of $A(\mathbf{k}^*,\omega_{\mathbf{k}^*}+\omega)$.

In Ref. 11, $\sigma(\omega)$ was analyzed in terms of a frequency dependent effective mass and effective scattering rate,

$$\sigma(\omega)=\frac{\delta e^2}{m}\frac{\Gamma(\omega)}{\omega^2\left[\frac{m^*(\omega)}{m}\right]^2+\Gamma(\omega)^2} . \qquad (4.6)$$

To the extent that the structure of $\sigma(\omega)$ is that of $A(\mathbf{k}^*,\omega)$, we may identify the effective scattering rate $\Gamma(\omega)$ in (4.5) with the imaginary part of the self-energy $\Gamma(\mathbf{k}^*,\omega)$. At low frequency and temperature, $\Gamma(\omega)$ appears to grow like a power of ω and increases rapidly up to a frequency corresponding to roughly 0.1 eV, where it levels off at a value corresponding to roughly 0.8 eV. If we identify $J\approx0.1$ eV and $t\approx0.8$ eV, then this is precisely the behavior which we have suggested for $\Gamma(\mathbf{k}^*,\omega)$ in Fig. 2.

At frequencies comparable or greater than J, Eq. (4.1) must be modified in order to include spin excitations. We may expect, however, that the qualitative features in (4.4) remain. In particular, there will be a broad feature in $\sigma(\omega)$ which decays like $1/\omega$ for $J<\omega<t$, since the incoherent spectrum extends up to an energy of order t.

Thus, we see that the qualitative features of the low-temperature ac conductivity are consistent with our picture of a renormalized quasiparticle band beneath a broad incoherent spectrum.

V. CONCLUSION

We have developed a quasiparticle theory for the motion of a single hole in an antiferromagnetic background, in which the ground state of the spins is described either by a quantum Néel state or a d-wave RVB state. By considering the $J \ll t$ limit, we have shown in a self-consistent perturbation theory that interactions with spin excitations strongly renormalize the hole spectrum.

We found a quasiparticle band which is at an energy of the order $-t$ and has an effective-mass enhancement of t/J. The origin of this mass enhancement lies in the strong frequency dependence of the self-energy, which renormalizes the residue and the mass of the quasiparticles. In this picture, the hole gains a kinetic energy of the order t when it delocalizes by surrounding itself with spin excitations. The mobility of these quasiparticles, however, is diminished by this cloud of spin excitations.

The existence of the quasiparticle poles depends crucially on the vanishing density of states of low-energy spin excitations which couple to the holes. In the Néel state, the hole couples to a single spin wave which has linear dispersion with an interaction strength which vanishes linearly with $\mathbf{q}$. The density of states of low-energy excitations is then proportional to E^2. In the d-wave RVB state, the hole couples to two spin excitations, whose energies have four-point zeros in the Brillouin zone. In this case the density of states of excitations coupling to the holes is proportional to E^3. In both cases, this density of states is sufficiently small that the scattering rate vanishes quickly enough to have a coherent quasiparticle pole. In the original s-wave RVB state,[21] the spin excitations have a "pseudo-Fermi surface" and hence a constraint density of states at low energy. The scattering rate would therefore not vanish at low energies, and the coherence of the quasiparticles would be lost.

The large mass enhancement in our theory is consistent with the observed weight of the Drude peak in the ac conductivity.[11] Our theory also predicts a broad peak with a typical frequency comparable to J, and extending out to a frequency of the order t. This broad feature is a consequence of multiple spin excitations and the incoherent part of the hole spectrum.

Since there are very few low-lying spin excitations, the quasiparticle states below a certain energy have infinite lifetime. This is in contrast to theories in which a hole scatters off spin excitations with a pseudo-Fermi surface.[25] Our theory has nothing to say about the intriguing linear temperature dependence of the dc resistivity.

An important lesson to be learned from our work is that is is necessary to include fluctuations about mean-field theory in order to have a complete description of the holes. In mean-field theories of the RVB state,[6,7] introduction of holes favors states which have the largest bare-hopping probability for the holes, so that the holes may gain the most kinetic energy. We have found, however, that by including the interactions of the holes with spin excitations, the holes may gain a comparable kinetic energy, whether there is a bare-hopping term or not. Thus, it is not clear which mean-field solution is the appropriate starting point when holes are added. More quantitative information is necessary before that can be decided.

There remain many unanswered questions regarding the motion of holes in an antiferromagnet. In our theory, we have implicitly assumed that the spin decouples from the hole, so that we may treat the hole as a spinless entity. It remains to be shown, however, whether or not some spin is bound to the hole.

By considering the motion of a single hole, we have avoided the question of the hole statistics. Even though at first sight, our slave boson and slave fermion decouplings appear to specify formally the hole statistics, that the situation is more complex can be seen from the following example. Even though the RVB state has been discussed in a "slave boson" type of decoupling, Arovas and Auerbach[26] have performed an RVB type of decoupling of the Heisenberg model in the Schwinger boson representation. The natural generalization of that to include holes involves the introduction of "slave fermions." We are currently studying this model, but it is clear that the general picture of a quasiparticle with a mass enhancement of t/J remains the same.

We recall that the original suggestion of Baskaran, Zou, and Anderson[21] was that the presence of the holes favors the RVB state because the kinetic energy gained is greater. That point has been disputed by Lederer and Takahashi,[27] and our studies support their argument that the kinetic energy of a hole in the RVB state or the Néel state are both of order t and that it is a subtle question to decide which is more stable. Baskaran, Zou, and Anderson also proposed that the holes are bosons with a bandwidth t which undergoes Bose-Einstein condensation.[21] That would place the effective condensation temperature at $\approx \delta t$ in two dimensions. While our study cannot decide the issue of the statistics of the holes, we can nevertheless conclude that any coherent phenomenon involving the holes, whether it is Bose-Einstein condensation or pairing between fermions involves an energy of order δJ, which brings the temperatures scale much closer to the experimentally observed transition temperatures.

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APPENDIX A

In this appendix, we present some general arguments regarding the quasiparticle residue of the holes without making the noncrossing approximation for the self-energy. If there is a pole at $\omega_{\mathbf{k}}$, we may write its residue as,

$$a_{\mathbf{k}} = \frac{1}{1 - \frac{\partial \Sigma}{\partial \omega}(\mathbf{k}, \omega_{\mathbf{k}})} . \tag{A1}$$

We may express the self-energy in terms of its imaginary part, $\Gamma(\mathbf{k},\omega) = 1/\pi \mathrm{Im}\Sigma(\mathbf{k},\omega)$ as a spectral representation and write,

$$a_{\mathbf{k}} = \frac{1}{1 + \int dy \frac{\Gamma(\mathbf{k},y)}{(\omega_{\mathbf{k}} - y)^2}} . \tag{A2}$$

$\Gamma(\mathbf{k},y)$ may be thought of as the inverse lifetime of a state at momentum $\mathbf{k}$ and energy y. It depends on the density of states into which a particle at $\mathbf{k}$ and y may scatter. At low temperatures the only way in which a hole can scatter is to create spin excitations, while lowering its energy. Since there are very few low-lying spin excitations, we expect that for energies slightly above the lowest-hole energies, $\Gamma(\mathbf{k},y)$ will be small.

We may write a formal expression for $\Gamma(\mathbf{k},y)$ using the Landau-Cutkosky rule,[28] which is essentially a generalized Fermi's golden rule,

$$\Gamma(\mathbf{k},y) = \sum_{N=1}^{\infty} \sum_{\mathbf{q}_1,\ldots,\mathbf{q}_N} |V(\mathbf{k},y,\{\mathbf{q}\},\{E_{\mathbf{q}}\})|^2 \times A\left[\mathbf{k} - \sum_{i=1}^{N} \mathbf{q}_i, y - \sum_{i=1}^{N} E_{q_i}\right] . \tag{A3}$$

Equation (A3) is a sum over all possible states into which the hole may scatter involving any number N of spin excitations with momenta $\{\mathbf{q}\}$ and energy $\{E_{\mathbf{q}}\}$. $V(\mathbf{k},y,\{\mathbf{q}\},\{E_{\mathbf{q}}\})$ is the exact vertex function for the creation of N spin excitations.

If we measure y relative to the lowest energy in the band, then for $y \ll J$, there will be very few states into which the hole may scatter, due to the small density of states of low-lying spin excitations. The density of excited states with more than one spin excitation present will be a higher power of y/J, so that we may get the low-energy behavior by considering only a single-spin excitation. We assume the vertex functions for multiple spin excitations are not singular as ω goes to 0,

$$\Gamma(\mathbf{k},y) = \sum_{\mathbf{q}} |V(\mathbf{k},y,\mathbf{q},E_{\mathbf{q}})|^2 A(\mathbf{k}-\mathbf{q}, y - E_{\mathbf{q}}) . \tag{A4}$$

The dominant contribution will come from the pole,

$$\Gamma(\mathbf{k},y) = \sum_{\mathbf{q}} |V(\mathbf{k},y,\mathbf{q},E_{\mathbf{q}})|^2 a_{\mathbf{k}-\mathbf{q}} \delta(y - \omega_{\mathbf{k}-\mathbf{q}} - E_{\mathbf{q}}) . \tag{A5}$$

Provided there is no singularity in V when $y \to 0$, $\Gamma(\mathbf{k},y)$ will go as a power of y for small y. As we saw in Sec. II, in the Néel state $\Gamma(\mathbf{k},y) \propto y^2$. (Note that since the bare vertex vanishes for $\mathbf{q}=0$ in this case, so must the dressed vertex.) In Sec. III we saw that in the RVB state, where there are actually two spin excitations created, $\Gamma(\mathbf{k},y) \propto y^3$. Therefore, the $y=0$ divergence in the integral in (A2) is cut off, so that the resulting residue may be finite.

In order to calculate the residue, we need to know $\Gamma(\mathbf{k},y)$ for larger values of y. This is very difficult, since in general, $\Gamma(\mathbf{k},y)$ depends on the exact vertex functions and includes multiple spin excitations. We may say with certainty however that

$$\Gamma(\mathbf{k},y) \geq \sum_{\mathbf{q}} |V(\mathbf{k},y,\mathbf{q},E_{\mathbf{q}})|^2 A(\mathbf{k}-\mathbf{q}, y - E_{\mathbf{q}}) \geq \sum_{\mathbf{q}} |V(\mathbf{k},y,\mathbf{q},E_{\mathbf{q}})|^2 a_{\mathbf{k}-\mathbf{q}} \delta(y - \omega_{\mathbf{k}-\mathbf{q}} - E_{\mathbf{q}}) \tag{A6}$$

since the terms involving higher numbers of spin excitations are positive definite. We may then an upper bound for the quasiparticle residue as,

$$a_{\mathbf{k}} \leq \frac{1}{1 + \sum_{\mathbf{q}} a_{\mathbf{k}-\mathbf{q}} \frac{|V(\mathbf{k},\omega_{\mathbf{k}},\mathbf{q},E_{\mathbf{q}})|^2}{(\omega_{\mathbf{k}} - \omega_{\mathbf{k}-\mathbf{q}} - E_{\mathbf{q}})^2}} . \tag{A7}$$

The dressed vertex function contains many diagrams and cannot be evaluated exactly. However, if we consider the $J=0$ limit, V must be of order t (provided the coefficient is not zero, which is unlikely, since in that case the self-energy would be zero). It is therefore reasonable to suppose that for $J \ll t$, V is of order T and is not qualitatively different from the bare vertex. This is the essence of the noncrossing approximation in which vertex corrections are ignored. If we accept this assumption, then the upper bound for the quasiparticle residue discussed in the text follows.

In order to replace the inequality $a_{\mathbf{k}} < J/t$ by equality, we must show that the denominator of (A2) is not larger than t/J. Since for $y \ll J$, $\Gamma(\mathbf{k},y)$ goes to zero at least as fast as y^2, the integral in the denominator is effectively cut off by J, and may be written as

$$\int_J^\infty \frac{\Gamma(\mathbf{k},y)}{y^2} \; . \tag{A8}$$

When $y \approx J$, we know from (A6) that $\Gamma(\mathbf{k},y)$ is at least of order t. In the $J=0$ limit, the only way it could be larger is if $\Gamma(\mathbf{k},y)$ diverged at the band edge. This, however, is unlikely. There is no reason to expect scattering to be much stronger at the bottom of the band. Therefore, we contend that $\Gamma(\mathbf{k},y)$ may be qualitatively described by the picture in Fig. 2, where for $y \ll J$, it grows as a power until $y \approx J$, where it has a value of the order t. In that case the residue may be written as

$$a_{\mathbf{k}} \approx \frac{1}{1+\int_J^\infty dy(t/y^2)} \approx \frac{J}{t} \; . \tag{A9}$$

This argument also shows that the incoherent part of the hole spectrum does not qualitatively change the results of Secs. II C and III, which were based on the dominant pole approximation.

APPENDIX B

In this appendix we consider the conductivity, $\sigma(\omega)$, in the context of our quasiparticle theory. We will consider both the Néel state and the RVB state discussed in the text.

The conductivity may be expressed in terms of a current-current correlation function and evaluated diagrammatically. The current operator may be expressed in terms of the electron operators as,

$$\begin{aligned} j_\mu(\mathbf{q}) &= \sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i}\frac{1}{2i}t(c^\dagger_{i+\mu,\sigma}c_{i,\sigma}-c^\dagger_{i,\sigma}c_{i+\mu,\sigma}) \\ &= \sum_{\mathbf{k}} c^\dagger_{\mathbf{k}+\mathbf{q},\sigma}c_{\mathbf{k},\sigma}\frac{t}{2}\sin(2\mathbf{k}+\mathbf{q}) \; . \end{aligned} \tag{B1}$$

As in the text, we replace the electron operators in terms of their slave boson or slave fermion representations. In the case of the Néel state, we make the replacement $c^\dagger_{i\sigma} \to f_i b^\dagger_{i\sigma}$. Since the two electron operators are on opposite sublattices, one of the b operators will contribute $\sqrt{2S}$ in our large S expansion, while the other will be a Holstein-Primakoff spin-wave operator. We may then write the current operator in this state as,

$$\begin{aligned} j_\mu^{\text{Néel}} = t\sum_{\mathbf{k},\mathbf{k}'} f_{\mathbf{k}} f^\dagger_{\mathbf{k}'}[&b_{\mathbf{q}+\mathbf{k}-\mathbf{k}'}\sin(2\mathbf{k}'+\mathbf{q}) \\ &+b_{-\mathbf{q}-\mathbf{k}+\mathbf{k}'}\sin(2\mathbf{k}+\mathbf{q})] \; . \end{aligned} \tag{B2}$$

In the RVB state, we make the substitution $c^\dagger_{i\sigma} \to b_i f^\dagger_{i\sigma}$ and we find

$$j_\mu^{\text{RVB}} = t\sum_{\mathbf{k},\mathbf{k}',\mathbf{q}} \mathrm{f}_{\mathbf{k}}\mathrm{f}^\dagger_{\mathbf{q}'}\mathrm{b}^\dagger_{\mathbf{k}'+\mathbf{k}+\mathbf{q}}\mathrm{b}_{\mathbf{k}'+\mathbf{q}'}\sin(2\mathbf{k}'+\mathbf{q}) \; . \tag{B3}$$

Thus, both current operators involve the creation and anihilation of the "holes" and the creation or anihilation of the spin excitations.

As in the previous appendix, we may organize the diagrammatic expansion of the conductivity in terms of the intermediate states which may occur between the current vertices. If the temperature and frequency are both much less than J, then since the density of low-energy spin excitations is small, the dominant contribution will come from the intermediate state in which there are no spin excitations directly excited. This corresponds to diagrams of the type shown in Fig. 8.

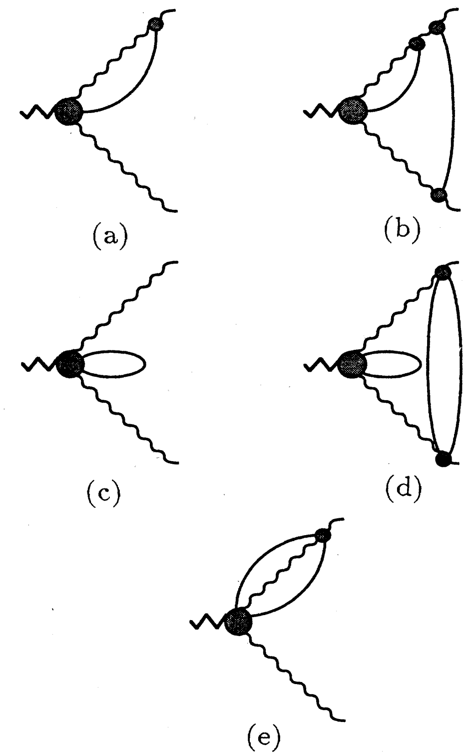

FIG. 8. Several diagrams which contribute to the dressed current vertex. (a) and (b) arise in the Néel state, and (c)–(e) arise in the d-wave RVB state. The large shaded circle is the bare current vertex, the wavy line is the hole propagator, and the solid lines are the spin excitation propagators.

We may write the general finite temperature, finite frequency conductivity as,

$$\sigma(\omega) = \sum_{\mathbf{k}} \int d\Omega \frac{n(\omega)-n(\omega+\Omega)}{\omega} L(\omega,\Omega,\mathbf{k}) \; , \tag{B4}$$

where $n(\omega)$ is the thermal occupation number, which for the limits we consider is a Boltzman distribution, and $L(\omega,\Omega,\mathbf{k})$ is a spectral function for the current-current Green's function, which may be expanded in terms of intermediate states using the Landau-Cutkosky rule,[28]

$$L(\omega,\Omega,\mathbf{k}) = |C(\omega,\Omega,\mathbf{k})|^2 A(\mathbf{k},\Omega)A(\mathbf{k},\Omega+\omega)+\dots \; , \tag{B5}$$

where $A(\mathbf{k},\Omega)$ is the hole spectral function and $C(\omega,\Omega,\mathbf{k})$ is the exact dressed current vertex with two external hole legs. The remaining terms in (B5) will have intermediate states which contain spin excitations, however, at low frequency their contributions will be small, and will be ignored.

The current vertex, C, will in general be the sum of many diagrams, and is difficult to evaluate in general. At zero frequency we may appeal to the Ward identity which states that

$$C(\omega=0,\Omega,\mathbf{k})=e\nabla_{\mathbf{k}}G^{-1}(\mathbf{k},\omega)=e\nabla_{\mathbf{k}}\Sigma(\mathbf{k},\omega) \ . \tag{B6}$$

Since $\nabla_{\mathbf{k}}\Sigma(\mathbf{k},\omega)$ is not singular in the $J=0$ limit we know that it must depend only on t, (or the unrenormalized mass, m). Furthermore, if we are on shell, then we know that at the bottom of the band, $\nabla_{\mathbf{k}}\Sigma(\mathbf{k}^*,\Omega)|_{\Omega=\omega_{\mathbf{k}}}=0$, so that near the band minimum we may write $C(\omega=0, \Omega=\omega_{\mathbf{k}},\mathbf{k})=e/m(k-k^*)$. At higher frequencies we expect that $C(\omega,\Omega,\mathbf{k})$ should still be of order t, though we do not know its precise form.

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