Internal structure of hole quasiparticles in antiferromagnets

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Holes in an Ising antiferromagnet give rise to quasiparticles with an internal structure associated with the distortion of the spin ordering. We show that the spectrum of excited states (of this internal structure) commences at a lower energy than previously thought, at an energy of the order of the exchange constant. The character of the corresponding states differ from those previously discussed in that the phases associated with the various spin configurations with the same number of spin flips differ. Moreover, these excited states dominate the optical absorption and may explain the experimental results of Thomas *et al.* [Phys. Rev. Lett. **61**, 1313 (1988)].

I. INTRODUCTION

Experiments, particularly neutron (Birgeneau and coworkers[1,2]) and Raman (Lyons *et al.*[3]) scattering, show that any theory of high-temperature superconductors must consider charge carriers (usually holes) moving through spins with short-range antiferromagnetic order. How the holes drive the system paramagnetic and whether the superconducting order is caused by the paramagnetic state are subtle questions. In this paper we focus on the more restricted issue of how a single hole in an antiferromagnetic affects, and is affected by, the spin system. The antiferromagnetic might be a high-T_c material, or a more conventional Mott insulator.

Since the materials are driven paramagnetic by a sufficient concentration of holes (e.g., Kitazawa *et al.*[4]), we deduce that the holes and spins are coupled to some degree. In this paper we are concerned with the effect of strong coupling between the holes and spins. (We have discussed the case of weak coupling in another paper[5]). Of course there are many ways to couple the holes to the spins. Initially we will be motivated by simplicity in deciding which model to pick and will return at a later stage to argue its applicability to the high-T_c materials.

One expects that the "bare" (i.e., before coupling to the spins) bandwidth of the holes is larger than the superexchange constant (approximately 0.1 eV), which characterizes the energy scale of the spin system alone. Thus for energy scales of greater than 0.1 eV the dynamics of the hole (and its interaction with the spin system) will predominate. The coupling of the spins among themselves is of secondary importance.

The simplest model, which includes the effect of spins on hole motion, is one hole in an infinite-U Hubbard model. (Two-band models including both Cu and O sites explicitly will be discussed later.) In that case all spin configurations are degenerate until the hole is added, whereupon the system (on a square lattice) is driven ferromagnetic (see Nagaoka[6]). Excitations in that limit have been considered by Brinkman and Rice,[7] whose results we will return to.

Experimentally we know that there is exchange coupling of the Cu spins; the simplest way to include this is by adding an Ising coupling to the infinite-U Hubbard model (e.g., Bulaevskii, Nagaev, and Khomskiĭ.[9]) The rest of this paper will be concerned with the analysis of this model. As already stressed, the virtue of the model is its simplicity; the implications for the real case of the Heisenberg coupling will be discussed later—as will an application of the Ising coupled model to the $BaBiO_3$ family of superconductors. In the discussion section we will consider the issue of one- versus two-band models.

Qualitatively (see Bulaevskii, Nagaev, and Khomskiĭ,[8] and for a review see Nagaev,[9]) it is easy to see what hole motion does in such a model, starting with a hole in an otherwise perfect Néel state. It will leave a trail of displaced spins as it moves, giving rise to a potential depending linearly on the arc length of the trail (due to the increase in exchange energy of the displaced spins). This potential confines the hole to the neighborhood of its "original state."

There is one important proviso to this description (less important qualifications are raised in the next section). There is a special class of trajectories, "Trugman cycles," where the hole may end up displaced from its original site but with no displaced spins (Trugman[10]). The simplest example of such a trajectory is where the hole moves around a plaquette one and half times, ending on the other site on the same sublattice.

We will argue that the "polaronic" distortion of the spin system and the net motion (due to the Trugman cycles) can be separated, and we will focus on the former. We will show that there are "internal" excited states of the polaronic distortions. Some of these have been discussed before (e.g., Nagaev[9]), where the different states have different probabilities of given arc lengths of distortion, but give the same amplitude to all trajectories with the same arc length. We will also construct other states that have the same *probabilities* for all configurations with given arc length, but different *phases* are associated

with the different configurations. As we will show, it is the latter excited states that determine the optical absorption, which is the main potential probe of such states.

Where is Nagaoka's ferromagnetism in this picture? It is concealed: Clearly the state with maximal $S^z=N/2$ is not coupled to the states that we consider, as only states having total $S^z=0$ are connected to the original Néel state. However, the set that we do consider, all of the $S^z=0$ states, contains one that corresponds to $S=N/2$, the magnetization being in the XY plane. As long as all $S^z=0$ are accessible, the Hilbert space contains the necessary states. Thus one might expect the ferromagnetism to occur in the limit of the Ising exchange, J, tending to zero, yielding a ferromagnetic spin polaron of diverging size (de Gennes[11]). We will show that there are such ferromagnetic tendencies in our treatment. However, for values of J that are not too small, the ferromagnetic tendencies are very weak (this is indicated by the variational results of Shraiman and Siggia[12]).

The plan of the paper is as follows: In Sec. II we construct the configuration space of the model; in Sec. III we introduce the Hamiltonian; in Sec. IV we solve the Schrödinger equation; in Sec. V we calculate the optical absorption; and in Sec. VI we discuss the results and conclude the paper.

II. CONFIGURATION SPACE: THE BETHE LATTICE

How do we describe the set of all configurations of one hole and the $(N-1)$ spins on a N-site lattice? First, one must specify the total S^z of the spins, which is a constant of the motion for the Hamiltonians that will interest us here. We will assume that we have $S^z=\pm\frac{1}{2}$, having in mind a Néel state to which a hole has been added to the down-spin–up-spin sublattice, respectively. Second, one must label those configurations; we will take a constructive approach, in that we start from a hole added to a Néel state and consider those states (or configurations) that are "accessible" from that starting point.

To be more precise, consider the model introduced in the Introduction: a hole moving in an Ising antiferromagnet with initial Néel order. Since, as the hole moves through the lattice, it disturbs only the spins on sites that it has visited, each trajectory creates a particular spin configuration. It seems natural to use the trajectories to label the spin configurations; however, there are some difficulties.

For instance, does every spin configuration (subject to the constraint on total S^z) correspond to a *particular* trajectory? It is easy to see that the trajectory may not be unique: Consider the example of a "Trugman cycle" (TC) (see Trugman[10]). Here the hole moves around a plaquette one and a half times to move to the other site on the same sublattice. However, it can do this in either a clockwise or anticlockwise TC. Thus there are two trajectories corresponding to the same spin configuration. In practice this redundancy is not a problem as the set of trajectories with a significant TC component is small, roughly 1% for the walls of length 6 in two dimensions. We will return at the end of the paper to the more accurate treatment of this aspect. So much for uniqueness. What of existence: Does every spin configuration *have* a corresponding trajectory? Nagaoka[6] in an appendix demonstrated that an arbitrary spin configurations with the same total S^z are always accessible from each other.

We may, therefore, assume that the space of accessible spin-hole configurations can be represented by the space of all trajectories of the hole. In fact we may restrict the space to those that do not have side branches that *only* consist of backtracks. (Any spin configuration associated with a backtracked trajectory is clearly identical to that with the hole on the same final state without the backtrack.) The trajectories may, however, self-intersect. Thus the "configuration space" may be deduced recursively: Starting with the hole on its "initial" site there are Z possible configurations after one step of the trajectory and $Z-1$ for each subsequent step. This defines a Bethe lattice with the same coordination as the underlying lattice, say for the square lattice in two dimensions $Z=4$.

Let us now define some terminology for the Bethe lattice. First there is the "generation number" n associated with the number of times the preceding construction has been performed. This runs up from -1 for the initial site. Then we have a set of "sibling numbers,"

$$\{i_{-1},i_0,\ldots,i_m,\ldots,i_n\}\equiv n;\{\mathbf{i}\}\ ,$$

that denote a particular site by the sequence of sites on the Bethe lattice visited to arrive at that site from the central site. The actual assignation of the sibling numbers to the sites of one generation connected to a give site of the previous generation is arbitrary, and it is not necessary to make a particular choice. The sibling numbers take on the following values $0\le i_n\le\xi_n^2-1$, where

$$\xi_n^2=\begin{cases}(Z-1) & n>0\\ Z & n=0\\ 1 & n=-1\ .\end{cases} \tag{2.1}$$

We will find in the next section that not only is the Bethe lattice the configuration space of the problem, but that its geometric structure enables a rather natural representation of *both* the hopping and (more suprisingly) the "potential" parts of the Hamiltonian of the problem.

III. THE HAMILTONIAN

There has been much work previously on the Bethe-lattice tight-binding model, in terms of deriving the local density of states from the Green function; however, there is none that are aware of that discusses the nature of the eigenstates (in particular the "noninvariant" states that we discuss here). It turns out that the nature of the eigenstates is crucial to the determination of the optical absorption, so we will discuss this point at some length. The Hamiltonian has both a kinetic (hopping) part, $\mathcal{H}_h$, associated with the thole motion, and a potential part, $\mathcal{H}_s$, due to the Ising exchange between the spins. Let us consider the hopping part first:

$$\mathcal{H}_h=-t\sum_{n\langle|i\}\{j|\rangle}\{|n;\{\mathbf{i}\}\rangle\langle n+1;\{\mathbf{j}\}|+\text{H.c.}\}\ , \tag{3.1}$$

where $\langle\{\mathbf{i}\},\{\mathbf{j}\}\rangle$ indicate paths which up to n are equivalent. Here the states $|n;\{\mathbf{i}\}\rangle$ are naturally associated with the Bethe lattice sites, $n;\{\mathbf{i}\}$. We will assume that the hopping parameter, t, is positive.

The potential part of the Hamiltonian is due to the hole scrambling the spin configuration from the Néel state. We will approximate the change in the exchange energy of the spins due to the hole motion as being proportional to the arc length of the trajectory, measured from the site that the hole started from in the perfect Néel state. The interpretation of this is that the hole leaves a "string" of flipped spins behind it, each of which is parallel to all but two of its neighbors (or all but one in the case of the first site of the trajectory). Thus for each unit of arc length the hole increases its energy by an amount proportional to the exchange constant, J. Since the arc length is the same as the generation number (remember that backtracks do not exist), we see that the $\mathcal{H}_s$ may be expressed as

$$\mathcal{H}_s=\sum_{n\{\mathbf{i}\}} V_n|n;\{\mathbf{i}\}\rangle\langle n;\{\mathbf{i}\}|\ , \tag{3.2}$$

where

$$V_n=\begin{cases}(Z-2)J/2n+(Z-1)J/2 & n\geq 0\\ 0 & n=-1.\end{cases} \tag{3.3}$$

Let us discuss the validity of the assumption of the potential being proportional to the generation number. There are, in fact, no devitations from linearity unless the trajectory encounters itself, or a site neighboring itself (in the future we will call both possibilities "encounters"). So in high dimensions the potential becomes linear. Since we are in two dimensions, we must, however, consider this point more carefully, first in the specific context of the Trugman cycle. In that case the potential initially grows linearly, but then returns to zero, as the spin system is returned to the Néel state on completion of the TC. Thus the TC's gives rise to "pits" in the linear potential, which however are rather dilute, as will be estimated in the last section of the paper.

In the more general case, it is clear that the potential is at best when large and typically decreased by the encounter. Let us estimate, roughly, the diminution of the potential at large generation numbers. We will use the faact that "typical" trajectories will be random walks and so, in two dimensions, be area filling. "Typical" means that we select a site on the Bethe lattice at random that corresponds to picking a random trajectory in real space. (We do not expect the exclusion of trajectories with backtracks to be important asymptotically.) The area filling implies that the hole will scramble an area of spins, meaning on average that the potential should still be linear with the generation number [since in a two-dimensional (2D) random walk the arc length is proportional to area covered], but with a coefficient corresponding to half the neighbors of a given spin being ferromagnetically aligned (i.e., approximately $ZJ/4$). Thus one expects that the potential will still be asymptotically linear *on average,* although the coefficient will be diminished by a factor of around 2.

IV. SOLUTION

Given that the the potential only depends on the generation number, it is not suprising that the dependence of the eigenstates on the generation number "separates" from the dependence on the sibling numbers. As a consequence we will see that the equation for the general dependence of the eigenstate includes a term depending on the quantum numbers associated with the variation with sibling number. This has some parallel with the separation of the radial and angular dependence in a central potential and the presence of a centrifugal potential, respectively. Mathematically the origin of the separation is the symmetry of the Hamiltonian under permutations of the sibling numbers.

Were the generational dependence to be considered alone, the problem becomes that of a single particle in a one-dimensoinal linear potential; the role of the spin configuration, or string, is merely to produce the potential. The relative phases of the string configurations are obtained from the sibling dependence. The latter is the novel part of this treatment, and will lead to some surprising results such as states where the hole is *never* found with an arc length less than a given amount.

We will initially illustrate this distinction by considering the simple case where the hole is confined to within one lattice site of its initial position. (We will call this problem the "tight-binding star" for future reference.) The "star" is a central site connected to, say, four neighbors, the "arms." Assume that the site energy of the cogenerational sites are the same. There are two "invariant" states with no phase differences between the amplitudes on the arms. Then there are the three noninvariant states, with phase variation between the arms, necessitating a zero on the central site. A useful way of describing these states is by assigning the corresponding phases on each arm as powers of the four roots of unity, the invariant states being labeled by the power zero and the three noninvariant states by the next three powers.

This mode of description may be applied to all the nodes of the Bethe lattice in the following way. First let us define ω_{i_n} to be the appropriate roots of unity that will play a similar role to those used in the tight-binding star:

$$\omega_{i_n}=\exp(2\pi i/\xi_n^2)\ , \tag{4.1}$$

Then let us transform the states of daughter sites, associated with a given parent site, weighting this with the different powers of the appropriate roots of unity. The utility of the transformation is then made clear by reexpressing the Hamiltonian in the new basis. Let us define the unitary transformation:

$$|n;\{\alpha\}\rangle=\frac{1}{\sqrt{S_n}}\sum_{\{\mathbf{i}\}}\cdots\omega_{i_n}^{\alpha_m}\cdots|n;\{\mathbf{i}\}\rangle\ . \tag{4.2}$$

Here we have defined the normalization, $S_n=Z(Z-1)^n$ for $n\geq 0$ and $S_{-1}=1$. The Greek indices, $\{\alpha\}$ denote the conjugate entities to $\{i\}$ and we will be labeled the "sibling momenta," in analogy with the conjugate coordinates and momenta. For convenience let us associate the sibling numbers with "real" space and the sibling mo-

menta with "momentum" space. Notice that these definitions are specific to the Bethe lattice. The number of basis states in momentum space scale with generation in the same way as the states in real space and may be thought of as defining a conjugate Bethe lattice. However, by examining the Hamiltonian in the transformed basis, the connectivity of the states is shown to be different:

$$\mathcal{H}=-t\sum_{n\langle\{\alpha\}\{\beta\}\rangle}\xi_{n+1}\{|n;\{\alpha\}\rangle\langle n+1;\{\beta,\beta_{n+1}=0\}|+\text{H.c.}\}+\sum_{n\{\alpha\}}V_n|n;\{\alpha\}\rangle\langle n;\{\alpha\}| \ . \tag{4.3}$$

Again, the notation $\langle\{\alpha\}\{\beta\}\rangle$ is used to indicate that a parent state is connected to a daughter state. However, in contrast to the real-space representation, a parent state is connected to only one daughter state. This is understood by realizing that in real space, the state that is coupled describes an invariant combination of daughter states. Conversely, the states that are decoupled describe a noninvariant combination of real daughters states that force the amplitude at their parent site to be zero. We will now see how this is manifested in the Schrödinger equation. Here $\psi_{\{\alpha\};\mathbf{n}}$ is the amplitude of the state $|n;\{\alpha\}\rangle$:

$$(E-V_n)\psi_{\{\alpha\};\mathbf{n}}=-t(\xi_{n+1}\psi_{\{\alpha,0\};n+1}+\xi_n\delta_{\alpha_n,0}\psi_{\{\alpha\};\mathbf{n}-1}) \ . \tag{4.4}$$

Let us consider a state that has an amplitude at some generation, m, and in particular, has an invariant sibling momentum of $\alpha_m=0$ at that generation. Firstly use the Schrödinger equation (4.4) to determine the amplitudes at higher generations, n, only sibling momenta, $\alpha_{n>m}=0$, have a nonzero amplitude. This may be interpreted in real space by the following: An eigenstate that has a nonzero amplitude at a given site forces the daughter sites to have the same amplitude and phase as each other. This implies the definition that states with sibling momenta, $\alpha=0$, are invariant. Secondly, we may deduce the eigenstate amplitudes at *lower* generations. Providing the momenta, $\alpha_n=0$ the amplitudes remain nonzero as we progress inward. However, suppose we assign an amplitude to a noninvariant momenta $\alpha_n>0$. Then we are forced to terminate the series: The amplitudes at generations $n-1$ through to the central site are forced to be zero. Effectively, we have disconnected a one-dimensional branch of the lattice in momentum space.

The quantum numbers that emerge from the separation of the variables are the following: m is the first generation where the wave function has a nonzero amplitude, η labels the choice of the noninvariant momenta α_m, and μ labels the set $\{\alpha\}$ for $n<m$. The wave function separates into a product form [cf. $R_{n,l}(r)Y_m^l(\theta,\phi)$]:

$$\psi_{\{\alpha\};\mathbf{n}}=\mathcal{G}_{n,m}\mathcal{S}_{\eta,\nu} \ , \tag{4.5}$$

and substitution of (4.5) into (4.4) yields

$$(E-V_n)\mathcal{G}_{n,m}=-t[\xi_{n+1}\mathcal{G}_{n+1,m}+\xi_n(1-\delta_{n,m})\mathcal{G}_{n-1,m}], \quad n\geq m \ . \tag{4.6}$$

We see that each of the eigenvalues of (4.6) has a degeneracy, of order $(\xi_m^2-1)S_{m-1}$, associated with the freedom in $\mathcal{S}_{\eta,\mu}$. To illustrate the form of the eigenstates, the wave functions for states where $m=-1$ (where all the hole trajectories of a given length enter with the same amplitude *and phase*), and states where $m=0$ (where a noninvariant collection of phases at generation $n=0$ force a node at the central site) are shown schematically in Fig. 1.

Let us return to consider the rather surprising feature that the wave functions describing the noninvariant states have areas of zeros about the central site. The physical

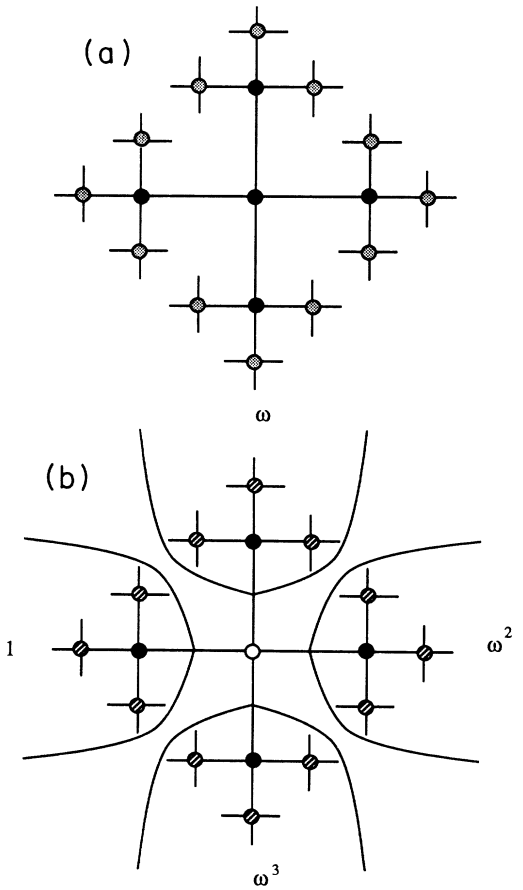

FIG. 1. Schematic diagram of the amplitudes of the hole trajectories up to two lattice parameters entering: (a) the purely invariant wave function where $m=-1$, and (b) a noninvariant wave function where $m=0$. Circles with similar shading have the same amplitude, but in the case of the noninvariant wave function the phase of each site on the four branches is denoted by the appropriate factor in the diagram. The central site of the noninvariant state has zero amplitude.

significance of the zeros is that these states have lower limits to the lengths of trajectories that the hole may explore. There is a certain parallel with the centrifugal barrier encountered in the central potential problem, but this contrasts with the evanescent decay of the wave function in that instance. The reason for this is that in the central potential problem the phase variation only enforces a node at the origin. However in the Bethe-lattice problem the wave function is continually forces to have nodes as the generation number is increased, due to phase variation round each parent site.

In fact we may further simplify (4.6), as the generation number enters only as an offset to the potential. Since the potential is linear, the difference equation relating near-neighbor generations may be written in a general form where the quantum number, m, is absorbed into a redefinition of the potential. By defining the dimensionless ratio $z=8\sqrt{(Z-1)^t}/ZJ$ and $E=J(m+\frac{3}{2}-\nu)$ the Schrödinger equation may be rewritten as

$$\frac{2(n+\nu)}{z}\mathcal{G}_n(z)=\mathcal{G}_{n-1}(z)+\mathcal{G}_{n+1}(z)\ . \tag{4.7}$$

The difference equation is satisfied by the Bessel functions of both the first, $J_{n+\nu}(z)$, and the second kind, $Y_{n+\nu}(z)$, in the semi-infinite limit pertinent to the Bethe lattice. (Note that the energy of the state enters only in the *order* of the Bessel function.) Since Bessel functions of the second kind diverge as $n\to\infty$, we may discard them as we are seeking finite energy, i.e., localized, states.

The eigenvalues are determined from the boundary condition imposed at the origin or termination of the tree: This is the requirement that the amplitude of the wave function vanish at generation, $m-1$. The order of the Bessel function is determined by this, leading to the final "generational" quantum number s. Generally, the eigenvalues are determined by $J_{-1+\nu}(z)=0$. However, the eigenvalues of the *purely* invariant states ($m=-1$) are complicated by the coordination of the origin. In this case we need to use the first two difference equations, which relate the wave-function amplitudes on the first three generations [here $\zeta=\sqrt{Z}/(Z-1)$]:

$$\begin{aligned}\frac{2\nu}{z}\mathcal{G}_0&=\zeta\mathcal{G}_1\ ,\\ \frac{2(\nu+1)}{z}\mathcal{G}_1&=\zeta\mathcal{G}_0+\mathcal{G}_2\ .\end{aligned} \tag{4.8}$$

For a given value quantum number, m, there will be an infinite set of states that are denoted by the quantum number s. For weak string tension ($t\gg J$) then $\nu\sim(t/J)-(t/J)^{2/3}f(s)$ (the Nagaev[13]), which may be obtained by scaling, with $f(s)$ being estimated to be $s^{2/3}$ by Wentzel, Kramers, and Brillouin. So the gap between the states for a given m scales like $(t/J)^{2/3}J$, whereas the gap between successive m scales like J. This implies that the first excited state is the first noninvariant state and not a higher invariant state. In fact for a large range of t/J, the second excited state is also a noninvariant state.

We may now comment on the relation between our results and Nagaoka's[6] theorem by determining the spin order induced by the hole. The spin order is changed by the hole by its motion, in particular, leading to a superposition of states with different spin configurations, with the hole on the same site. The simplest example of this is the superposition of spin configurations induced by the amplitudes for the hole to be on its initial site and the same site after a cycle (*not* a TC, but two steps short of it) around a plaquette. In that case there is a superposition of states for the two spins on the sites that would be visited to complete a TC. In the second state, they are reversed and, in the ground state for hole-spin system, superposed with the same phase. Thus by comparison with the Néel state where the two spins are in an equal mixture of singlet and triplet states, one now has a predominantly triplet configuration. (If the sign of the superposition had been negative, then the state would have been mainly singlet.) As the string tension tends to zero, these two configurations tend to have the same amplitude, and hence one gets a pure triplet state. This is the sign of Nagaoka ferromagnetism, occurring in the XY plane (as one is always dealing with total $S^z=0$). [Equivalently one may examine the "transverse" part of the spin-spin correlation function (i.e., in the XY plane) to note that there are "ferromagnetic" correlations.]

The tendency towards Nagaoka ferromagnetism may be deduced for the case of several spins being on the wrong sublattice by noting that the expression for the operator for the total spin may be rewritten as follows:

$$\begin{aligned}\mathbf{S}_{\rm tot}^2&=2\sum_{n=1}^{N}\mathbf{S}_n^2+2\sum_{n\neq n'}\mathbf{S}_n\cdot\mathbf{S}_{n'}\\ &=2\sum_{n=1}^{N}\mathbf{S}_n^2+2\sum_{n\neq n'}[S_n^zS_{n'}^z+\tfrac{1}{2}(S_n^+S_{n'}^-+S_{n'}^+S_n^-)]\ .\end{aligned} \tag{4.9}$$

In evaluating the expectation values of this, the only part that has off-diagonal contributions from the superposition of different spin configurations is the sum over the spin raising and lowering operators. To make this contribution maximal (ferromagnetic) the different spin configurations must have the same phase. Since the ground state *does* have the same phase for all spin configurations (with the hole at the same site), the hole, within its confined region, tends to create ferromagnetic (Nagaoka) order.

The situation with excited states, both invariant and noninvariant, is more complicated—some pairs of spins are in relative triplets and some are in relative singlets, depending on the sign of the superposition of the two components. Thus there is at least a tendency for Nagaoka ferromagnetism in the ground state, growing as the string tension tends to zero. More cannot be said without the consideration of TC's, as the nature of the real lattice enters into statements about which an eigenvalue of *total* S^2 is the ground state (e.g., whether the lattice is frustrated or not and the sign of the hopping term).

We have seen that the momentum space representation provides a simple way of understanding the separation of the variables. However, since we imagine the Bethe lattice embedded on the square lattice, let us reexpress the wave functions in the real-space representation. Since all

the wave functions with a common value of m are degenerate, instead of labeling the eigenstates by a sequence of momenta we may specify a path in real space, redefining the quantum number μ. That is, μ describes a path on the real-space Bethe lattice and not the momentum space version. Incorporating the normalization, the wave functions are described by

$$|m,\mu,\eta,s\rangle = \sum_{n\{\mathbf{i}\}} \tilde{\mathcal{G}}^{m\mu\eta s}_{n\{\mathbf{i}\}} |n;\{\mathbf{i}\}\rangle \ , \tag{4.10}$$

where

$$\tilde{\mathcal{G}}^{m\mu\eta s}_{n\{\mathbf{i}\}} = \begin{cases} g^{m,n,s}\omega_{\eta}^{i_m}\delta_{\mu,\{\mathbf{i}\}_{m-1}} & n \geq m \\ 0 & n < m \end{cases} \tag{4.11}$$

and

$$g^{m,n,s} = \frac{J_{n-m-1+\nu_s}(z)}{(\mathcal{N}_{ms}S_{n-m-1})^{1/2}} \ . \tag{4.12}$$

Finally, the normalization is given by

$$\mathcal{N}_{ms} = \sum_{p\geq 0}[J_{p+\nu_s}(z)]^2 \begin{cases} \dfrac{(Z-1)^2}{Z} & m>0 \\ (Z-1) & m=0 \\ 1 & m=-1 \ . \end{cases} \tag{4.13}$$

V. OPTICAL ABSORPTION

How many the internal excited states of the quasiparticle be experimentally detected? The change in the nature of the spin distortion between the states might imply that neutron scattering would allow transitions between the states to be observed. However, neutrons, when scattered, flip only one spin in the system, and none of the states mixed by the hole motion contains a single spin flip. Optical absorption only couples to the hole motion (to a good approximation), and hence transitions between the "internal" states are not ruled out by any such selection rule. In this setion we will calculate the optical absorption noting that only transitions between the invariant and noninvariant states are allowed.

The inclusion of a vector potential for a single band was first discussed by Peierls[14] (see also Harper[15]). Here we adopt a more direct approach of constructing the simplest gauge invariant tight-binding model—in the same spirit as the introduction of a gauge field on a lattice in particle physics. The treatment agrees with Peierls' for long-wavelength small-amplitude disturbances. The electromagnetic field is conveniently represented by a vector potential, $A(\mathbf{n},\hat{\mathbf{e}})$, associated with each link, $\hat{\mathbf{e}}$ between lattice sites $\mathbf{n}$ and $\mathbf{n}+\hat{\mathbf{e}}$. One makes connection with the continuum case by equating (assuming slow variation of the continuum vector potential):

$$A(\mathbf{n},\hat{\mathbf{e}}) = \int_{\mathbf{n}}^{\mathbf{n}+\hat{\mathbf{e}}} A(\mathbf{x})\cdot d\mathbf{l} \ . \tag{5.1}$$

To couple the hole motion to the electromagnetic field, while maintaining gauge invariance, we form the modified hopping term, $\mathcal{H}_{\rm hem}$:

$$\mathcal{H}_{\rm hem} = -t\sum_{\mathbf{n},\hat{\mathbf{e}}} \{ |\mathbf{n}\rangle e^{iA(\mathbf{n},\hat{\mathbf{e}})} \times \langle \mathbf{n}+\hat{\mathbf{e}}| + |\mathbf{n}+\hat{\mathbf{e}}\rangle e^{-iA(\mathbf{n},\hat{\mathbf{e}})}\langle \mathbf{n}| \} \ . \tag{5.2}$$

For linear-response theory, we will make the gauge noninvariant expansion of the exponential factors and moreover assume that we may approximate the vector potential to be independent of the position of the link (long-wavelength limit) and to be nonzero only for links in the $\hat{\mathbf{x}}$ direction (of course this constitutes a limitation of gauge freedom):

$$A(\mathbf{n},\hat{\mathbf{e}}) \simeq A_0\delta(\hat{\mathbf{e}},\hat{\mathbf{x}}) \ . \tag{5.3}$$

When substituted into (5.2) and the ordinary hopping term is neglected, we find

$$\mathcal{H}_{\rm em} \simeq -it\sum_{\mathbf{n},\hat{e}} A_0\delta(\hat{\mathbf{e}},\hat{\mathbf{x}})\{|\mathbf{n}\rangle\langle\mathbf{n}+\hat{\mathbf{e}}| - |\mathbf{n}-\hat{\mathbf{e}}\rangle\langle\mathbf{n}|\}$$
$$= -(\hbar)A_0\sum_{n,\hat{\mathbf{e}}}\delta(\hat{\mathbf{e}},\hat{\mathbf{x}})\mathcal{J}(n,\hat{\mathbf{e}}) \ , \tag{5.4}$$

where we have implicity defined the non-gauge-invariant current operator, $\mathcal{J}(\mathbf{n},\hat{\mathbf{e}})$, associated with link $\hat{\mathbf{e}}$ emanating from site $\mathbf{n}$.

We immediately see a difficulty in coupling the hole and its spin distortion to the electromagnetic field: The perturbation is naturally discussed in terms of the underlying square lattice, however the hole dynamics are most easily described on the Bethe lattice. The relationship between the two lattices (i.e., which links on the Bethe lattice are in the $\hat{\mathbf{x}}$ direction) is not simple. Fortunately we will see that we do not need to know the precise relationship between links on the Bethe lattice an in real space. The method that we employ is similar to that of Brinkman and Rice,[7] with some modification: We have a finite string tension, which they did not; and we will construct our arguments around the consideration of matrix elements directly, rather than in the Kubo formula itself. Our approach makes it clear which states contribute to the absorption.

The tight-binding star again provides intuition for the more general problem. Matrix elements of the current operator between the invariant states are zero, due to the states being of even parity while the operator is odd parity. However, the electromagnetic field is able to excite transitions from the invariant to the noninvariant states, exploiting the mixed-parity nature of those states. The foundation of the discussion of the general case will be similar parity considerations.

In practice we need only consider excitations from the ground state, which is the lowest invariant state. As in the case of the tight-binding star, the lack of phase variation forbids transitions between invariant states, although the argument is a little more subtle (due to the relation between the underlying lattice and the Bethe lattice being less simple than in the tight-binding star). Every trajectory with a component parallel to the vector potential (i.e., parallel to $\hat{\mathbf{x}}$) has an "image" trajectory formed by

reflection perpendicular to the $\hat{\mathbf{x}}$. As a consequence of the invariance of the wave function, the contribution to the matrix element from a hole moving along $\hat{\mathbf{x}}$ is canceled by the contribution from the image trajectory, where the hole moves in the negative $\hat{\mathbf{x}}$ direction. This notion is contained in Brinkman and Rice.[7]

Matrix elements to the noninvariant states fall into two classes. The first noninvariant set of states with $m=0$ is particularly simple, and we will consider it first. (We will see that this is due to the coordination of the origin being four.) Transitions between the ground state and the first noninvariant states closely resemble the tight-binding star. As in the case of the invariant states most of the contributions to the matrix elements vanish pairwise (Fig. 2). The only contribution that survives comes from hole motion purely parallel and antiparallel to the $\hat{\mathbf{x}}$ direction where the noninvariance of the states provides the required phase to prevent cancellation. Specifically, for the first noninvariant states we have seen that there are three possible wave functions described by η. The amplitudes of the wave function along each branch from the origin are the same but their phases are prescribed by the direction of the link to the first generation (cf. the tight-binding star). For two of the three excited states, denoted by $\tilde{\eta}$, the phase along $+\hat{\mathbf{x}}$ is of opposite sign to the phase along $-\hat{\mathbf{x}}$. However, in the third case they are the same. This sign change is exploited by the current operator to yield the following:

$$\langle 0,0,\tilde{\eta},s|\mathcal{J}(\hat{\mathbf{n}},\hat{\mathbf{x}})|0\rangle = 2\chi^{+}(1,s) , \tag{5.5}$$

where the function χ is purely a function of the radial variation of the wave function defined more generally for arbitrary m and is given by

$$\chi^{\pm}(m,s) = \sum_{n \geq m} g^{n,-1,0} g^{n+1,m,s} \pm \sum_{n>m} g^{n,m,s} g^{n+1,-1,0} . \tag{5.6}$$

Notice that since the only terms that contribute enter from at most two paths emanating from the origin of a Bethe lattice, the contribution from higher-order terms in (5.6) decay exponentially due to the normalization associated with the density of possible paths. Thus, the leading order terms represent a good approximation to the sum.

The higher noninvariant states ($m>0$) are also able to couple to the ground state by exploiting the phase variation at their "terminating" generation (the lowest generation with a nonzero amplitude). However there are now two distinct possibilities, this complication arising from the presence of only three links from one site to the next generation whereas there are *four* directions: when looking for an image path, we will see that it may not exist. Consider a site in the terminating generation. Nonexistent image paths occur when the link (from the previous generation) to the site has a nonzero vector potential (i.e., corresponds to a link in the real lattice in the $\pm\hat{\mathbf{x}}$ direction). In that case, the image path does not exist, as there is no link in the next generation of the appropriate type. So in this case, there is no constructive interference (Fig. 3).

Matrix elements to the higher noninvariant states, $m>0$, dependent on the link, $\hat{\mathbf{e}}$, to the branch node as already explained, are given by

$$\langle m,\mu,\eta,s|\mathcal{J}(\mathbf{n},\hat{\mathbf{x}})|0\rangle = \begin{cases} \frac{1}{2}[\chi^{+}(m,s) - i\chi^{-}(m,s)] & \mu:\hat{\mathbf{e}}\perp\mathbf{A} \\ \chi^{+}(m,s) & \mu:\hat{\mathbf{e}}\parallel\pm\mathbf{A} . \end{cases} \tag{5.7}$$

Let us concentrate on the limit of interest where the string tension is relatively high. For $t \geq J$ the spacing of the zeros of the Bessel function show that the first two excited states have $m=0,1$ and $s=0$. In this limit (5.6) may be convienently approximated by

$$\chi^{\pm}(m,0) = g^{m,-1,0} g^{m+1,m,0} . \tag{5.8}$$

This is clearly very small in the limit of weak string tension, due to the small amplitude on the initial sites. Amplitudes for transitions to particular higher states are strongly suppressed by normalization factors. We will comment on the relation to experiment in the discussion section.

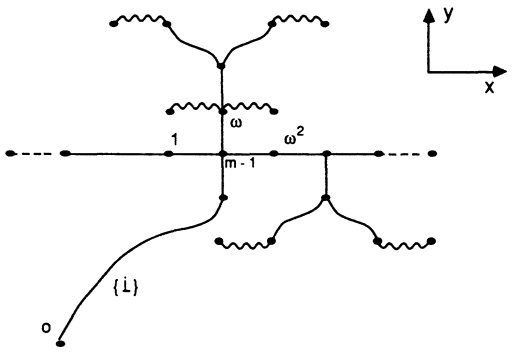

FIG. 2. Contributions to the matrix elements of the current operator taken between the ground state and the first noninvariant state: "vanishing pairs" are shown wavy, "contributing pairs" are shown dashed.

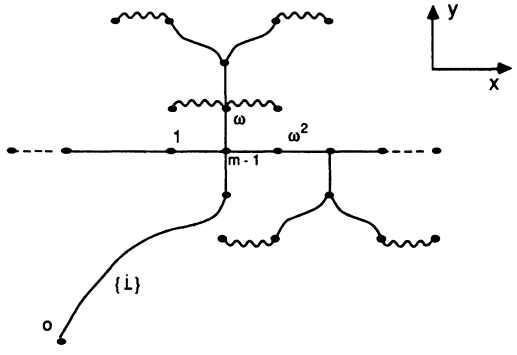

FIG. 3. Contributions to the matrix elements of the current operator taken between the ground state and a higher noninvariant state for the different directions of link: (a) $\hat{\mathbf{e}}\perp\mathbf{A}$, (b) $\hat{\mathbf{e}}\parallel\pm\mathbf{A}$.

VI. DISCUSSION

We will now review the approximations that we made, comment on the differences caused by the introduction of Heisenberg coupling between the spins, consider the changes required to discuss "Cu-O" planes and conclude.

The most important approximation that we made was the neglect of Trugman cycles. We argued that in sufficiently high dimensions this approximation becomes exact, since trajectories intersect themseleves very infrequently and the proportion of TC's is even smaller—varying as d^{-4} for the shortest examples (not the even in 2D this is rather small). The main effect of the TC's is to delocalize the quasiparticle and the scale of this effect may be estimated by considering the Bethe lattice. Given that a TC is performed by looping around a plaquette, this suggestion may appear strange, as the Bethe lattice has no loops. However, it must be remembered that the Bethe lattice is the configuration space of the *trajectories*, not merely the position of the hole—so that a loop in real space need not be a loop in configuration space, as the spin configuration will not be returned to the starting point in general.

We may qualitatively consider the resulting "band structure" for the hole, by using a "tight-binding" picture. Initially consider the *nonorthogonal* set of lowest invariant states that are centered on the sites ["Trugman sites" (TS)] on the Bethe lattice associated with Trugman cycles from the original site. These states will broaden into bands under the combined influence of the nonorthogonality and the difference between the assumed and real potentials on the lattice—the potential not actually increasing with the generation number as a TS is approached, but diminishing. Due to the dilute nature of the TS's in large dimensions, the wave function based on a particular TS has a small amplitude at neighboring TS's. Thus we expect that the band width to tend to zero as $d \to \infty$.

We may also include higher states based on each TS in the same manner, each generating a corresponding band. However the band widths will decrease as the generational quantum number becomes large, since the amplitude at the low order TS's (which are the least dilute) will diminish. Similarly for the noninvariant states. (In all of these considerations, we are neglecting the weaker—in the sense of an even more dilute set of sites—effect of returning both hole and spin systems to their original configuration after performing the same TC twice.)

Surprisingly, the Ising model that we have discussed is most appropriately applied to the $Ba_{1-x}K_xBiO_3$ materials. Varma[16] has shown that the formal charge ordering of Bi^{3+} and Bi^{5+} may be regarded as analogous to antiferromagnetic order, with the two charge states being two pseudospin states. The nearest-neighbor electrostatic repulsion plays the role of the (dominant) Ising coupling, and the XY coupling is related to the kinetic energy. In that case the motion of a hole is analogous to that of the motion of a hole in an antiferromagnetic (d'Ambrumenil[17]), with a "string" of displaced charge order behind it.

Let us now examine whether the Ising limit provides insight into the case with finite X-Y coupling. First the X-Y coupling provides an additional means for the hole to delocalize, as has been discussed by Shraiman and Siggia.[12] S^+S^- may operate on the two spin flips at the end of the string annihilating them. The string then appears to start at one magnetic lattice parameter removed from the initial site, hence allowing the quasiparticle to move. Of course this is the simplest possibility; in general the tendency of spin dynamics is to cause the destruction of the strings—the set of spin flips that constitute the strings evaporating into individual spin waves. The question as to whether so remnant of the string picture remains has been considered by Kane, Lee, and Reed[18] for the case of *invariant* states. They find, using a Green function approach, that peaks in the spectral weight at the energies estimated by a string approach should still be visible. More detailed calculations by Gros and Johnson[19] show that some string features remain in their calculations, namely a discrete quasiparticle pole at low energies. They do not comment on the distribution of spectral weight at higher energies.

Providing some remnant of the Ising string remains in the presence of Heisenberg exchange, the following prescription provides a useful way of deducing its immediate effect on the hole quasiparticle. In the absence of TC's, a hole becomes localized in a quasiparticle centered on the sublattice state at which it was notionally introduced. In this case, each lattice site may be associated with a Bethe lattice of spin configurations associated with hole trajectories from that site. We have seen how TC's provide weak links between Bethe lattices on sublattice sites. The spin dynamics provide further connections at an order as low as two generations. The action of the spin dynamics on the displaced spins of a string of length two creates a new string this time of zero length but attached to a neighboring sublattice site. The hole acquires a bandwidth which, when the string tension is high is expected to scale with the exchange constant. Furthermore, it becomes energetically favorable for a hole quasiparticle to acquire a component of a noninvariant state to enhance the "effective hopping integral" along the direction of motion. We are currently making an extensive study of the leading order effects on the XY exchange.

It is interesting to note that the original data of Thomas *et al.*[20] are not inconsistent with absorption associated with transition to the lowest noninvariant states. Note that the transition will occur at an energy of order J, which does not depend on the hopping parameter, t, which is very hard to estimate. The peak visible at low temperatures at approximately 0.5 eV is consistent with a high string tension, with $J \sim 0.1$ eV, which may derived from the neutron-scattering results (Birgeneau and coworkers[1]).

Finally we should discuss the relation of our results to two-band models (e.g., Emergy[21] and Varma and coworkers[2]), where the O sites are included explicitly. Zhang and Rice[23] have argued that an effective one-band model may be constructed by forming singlets from a Cu-spin and a hole on neighboring O sites. However the form of the resulting Hamiltonian is still controversial (see, for instance, Emery and Reiter[24] and Long[25]).

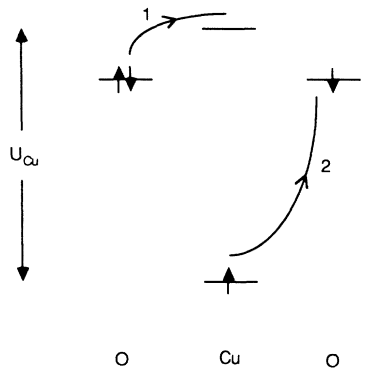

FIG. 4. Assumed relative position of the Cu^{1+} and Cu^{3+} configurations, with respect to the O p states and illustration of a hopping process via the Cu^{1+} configuration.

Let us consider the two-band case where hopping is *via* the Cu^{+} configuration (see Fig. 4), that is the Cu^{3+} configuration is inaccessible. We may then consider, as before, "trajectories" that are now defined on both the Cu and O sites. When the holes "cross" a Cu site, they may flip the spin and hence as they move leave a wake of flipped spins, as in the one-band case. The complication is that there is also a matrix element for non-spin-flip hopping. This is an alternative avenue for delocalization to the XY coupling. However in the limit that we have chosen, the spin-flip amplitude is larger. Thus there is a considerable parallel with the one-band case, and our results should have some applicability in that case as well.

To conclude, we have examined a model consisting of a hole moving in an Ising Néel background. We argued that to a good approximation, the configuration space is a Bethe lattice. The eigenstates were found and it was pointed out that some of these had not previously been considered. They consisted of weighting different configurations with the same arc length of trajectory with different phases. These were shown to determine the optical absorption. We pointed out that the feature observed in the optical absorption at approximately 0.5 eV may be a remnant, in a Heisenberg system, of the Ising string. Work by Kane, Lee, and Read[18] and a Gros and Johnson[19] was mentioned in support of this.

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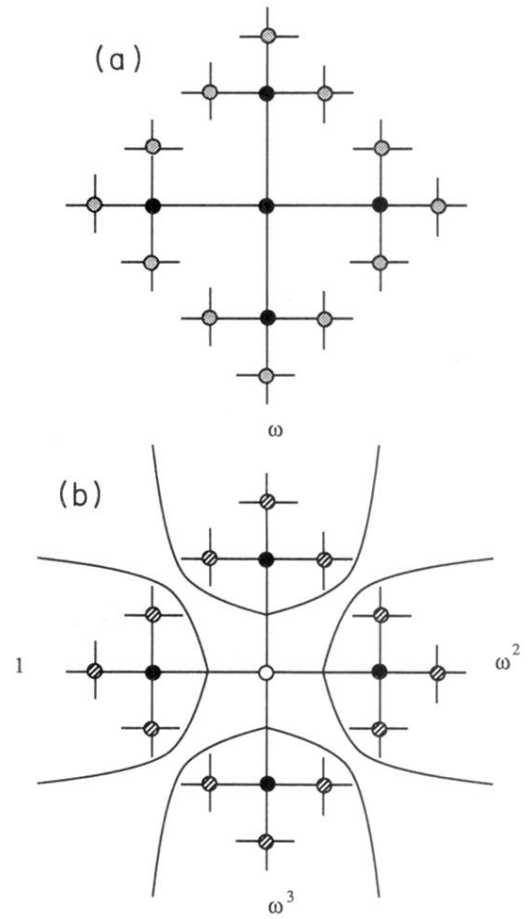

FIG. 1. Schematic diagram of the amplitudes of the hole trajectories up to two lattice parameters entering: (a) the purely invariant wave function where $m=-1$, and (b) a noninvariant wave function where $m=0$. Circles with similar shading have the same amplitude, but in the case of the noninvariant wave function the phase of each site on the four branches is denoted by the appropriate factor in the diagram. The central site of the noninvariant state has zero amplitude.