

## Wick's theorem for charged spin systems

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We present a new Green's-function approach to charged spin systems which preserves the local constraints prohibiting double occupancy. It is a systematic fermionic expansion and yields  $1/(2z)$  as a control parameter for the Heisenberg model. For the  $t-J$  model the spin and hole Green's functions are treated on an equal footing. In the Ising limit, the Brinkman-Rice approximation and a bandwidth  $\sim J^2$  are recovered for, respectively, the incoherent and coherent hole motion. A new picture for the coherent hole propagation is obtained in the Heisenberg limit.

The subject of strongly correlated electrons on a lattice is one of the outstanding problems in condensed-matter physics. Such systems are characterized by an intrinsic strong coupling between charge and spin degrees of freedom, due to strong on-site Coulomb energies. These properties are thought to be exemplified by the  $t-J$  model [defined in Eq. (1)], an example of a charged spin system. When no holes (i.e., charges) are present, this model reduces to the antiferromagnetic Heisenberg model. The most widely used approximation in this context is the spin-wave approximation,<sup>1</sup> which can be regarded as the leading term in a  $1/S$  expansion.<sup>2</sup> On the other hand, the only simple treatment for the state with one hole is the Brinkman-Rice approximation<sup>3</sup> and its generalization to the Ising case.<sup>4</sup> In this approximation the spins are static and the hole excitation spectrum is completely incoherent; i.e., the hole cannot propagate coherently.

One might anticipate that a spin degree of freedom would permit coherent hole propagation, with spin processes cleaning up the string of flipped spins left behind by a moving hole. Kane, Lee, and Read<sup>5</sup> were the first to formulate an approach which takes both the spin and charge degrees of freedom into account by using the spin-wave approximation for the former and a slave boson formulation for the latter. They found that the hole can propagate coherently with a bandwidth  $\sim J^\perp$ , in the limit  $J^\perp \ll J^2 \ll t$ .

In this Rapid Communication we formulate a general method to apply standard Green's-function techniques to charged spin systems by introducing a fermion representation and perturbing around the mean-field Hamiltonian. The use of a fermion representation allows a unified treatment of the charge and spin degrees of freedom, without,

for example, expansion in  $1/S$ . Most importantly, the method satisfies order by order the local constraints which prevent double occupancy. These constraints prohibiting double occupancy are the essential characteristic of a strongly correlated system; this approach emphasizes the importance of satisfying them locally. We apply the method to the  $t-J$  model. At half-filling we obtain the spin-wave approximation in lowest order. Systematic higher-order corrections to the spin-wave velocity turn out to take the form of a  $1/(2z)$  expansion (where  $z$  is the number of nearest neighbors). Using these results, we find that the incoherent hole density of states is dominated by a pole at the lower band edge even in the Heisenberg limit, as well as near the Ising limit. With this we are able to discuss the nature of the coherent states in both limits.

A different Green's-function approach has been developed for the case  $J=0$  by Ruckenstein and Schmitt-Rink,<sup>6</sup> using the so-called Hubbard operators.<sup>7</sup> These operators do not obey simple commutation or anticommutation rules but form an algebra. This property, which is shared by spin operators, is one reason that Wick's theorem has up to now not been applicable to general spin systems (with the constraints locally satisfied), including the  $t-J$  model in its standard formulation. A second reason is the nontrivial time dependence of the spin operators (which do not correspond to free field operators) in an expansion around the Ising limit. We now reformulate exactly the  $t-J$  Hamiltonian and eliminate both difficulties.

Let us denote by  $c_{i,\sigma}^\dagger$  the creation operator for an electron with spin  $\sigma = \uparrow, \downarrow$  on the lattice site  $i$ . The  $t-J$  Hamiltonian is

$$H_{t-J} = -t \sum_{\langle i,j \rangle, \sigma} [(1 - c_{i,-\sigma}^\dagger c_{i,-\sigma}) c_{i,\sigma}^\dagger c_{j,\sigma} (1 - c_{j,-\sigma}^\dagger c_{j,-\sigma}) + \text{H.c.}] + \sum_{\langle i,j \rangle} [J^z S_i^z S_j^z + (J^\perp/2)(S_i^+ S_j^- + S_i^- S_j^+)]. \quad (1)$$

Here  $\langle i,j \rangle$  denotes pairs of nearest-neighbor (nn) sites.  $S_i^z = \frac{1}{2}(c_{i,\uparrow}^\dagger c_{i,\uparrow} - c_{i,\downarrow}^\dagger c_{i,\downarrow})$  is the Ising component of the antiferromagnetic ( $J^z, J^\perp \geq 0$ ) spin interaction.  $S_i^+ = c_{i,\uparrow}^\dagger c_{i,\downarrow}$  and  $S_i^- = c_{i,\downarrow}^\dagger c_{i,\uparrow}$  are the raising and lowering spin operators. The operators in parentheses in the first term in (1) (the kinetic energy, with  $t > 0$ ) are the constraints that enforce single occupancy. Doubly occupied

sites ( $c_{i,\uparrow}^\dagger c_{i,\uparrow}^\dagger$ ) are assumed to be so high in energy, due to a strong on-site Coulomb repulsion, that they are out of the Hilbert space.

In the following we will consider only bipartite lattices, although the method we will now describe could be implemented for a general kind of lattice. At half-filling (i.e., for one particle per site) and  $J^\perp = 0$ , the ground state is

the classical Néel state. We split the Ising part of the Hamiltonian into a mean-field and an interaction piece:

$$S_i^z S_j^z = \frac{1}{2} (-S_i^z + S_j^z) + (S_i^z - \frac{1}{2})(S_j^z + \frac{1}{2}) + \frac{1}{4}. \quad (2)$$

Here and in the following  $i$  and  $j$  denote sites on the  $A(\uparrow)$  and  $B(\downarrow)$  sublattices, respectively. The first part of (2), which is the mean-field part of the Ising interaction, has the Néel state,

$$\prod_{i \in A} c_{i,\uparrow}^\dagger \prod_{j \in B} c_{j,\downarrow}^\dagger |0\rangle,$$

as its ground state. We introduce this as the new vacuum at half-filling, and define  $a^\dagger, b^\dagger$  as creation operators of quasiparticles and holes with respect to the vacuum:  $a_i^\dagger = c_{i,\uparrow}^\dagger, b_i^\dagger = c_{i,\downarrow}^\dagger$  on the  $A$  sublattice and  $a_j^\dagger = c_{j,\uparrow}^\dagger, b_j^\dagger = c_{j,\downarrow}^\dagger$  on the  $B$  sublattice. We neglect the constant in (2) and obtain the following exact reformulation of  $H_{I-J}$  in terms of  $a, b$  operators:

$$\begin{aligned} H_{I-J} &= H_0 + H_1 + H_2 + T, \\ H_0 &= (\varepsilon_0/2) \sum_{i \in A,B} (a_i^\dagger a_i + b_i^\dagger b_i), \\ H_1 &= -(J^2/4) \sum_{\langle i,j \rangle} (a_i^\dagger a_i + b_i^\dagger b_i)(a_j^\dagger a_j + b_j^\dagger b_j), \\ H_2 &= (J^\pm/2) \sum_{\langle i,j \rangle} (a_i^\dagger b_i^\dagger a_j^\dagger b_j^\dagger + b_j a_j b_i a_i), \\ T &= -t \sum_{\langle i,j \rangle} [(a_i a_i^\dagger) b_i a_j (b_j^\dagger b_j) + (b_i^\dagger b_i) a_i^\dagger b_j^\dagger (a_j a_j^\dagger) + \text{H.c.}] \end{aligned} \quad (3)$$

Here  $\varepsilon_0 = zJ^2/2$ , where  $z$  is the number of nn's and the operators within parentheses in the expression for the kinetic energy are the constraints which enforce single occupancy.

By construction, the ground state of the unperturbed Hamiltonian  $H_0$  is the vacuum ( $\varepsilon_0 > 0$ ).  $H_0$  is quadratic, so that in the interaction representation  $a^\dagger(t) = \exp(i\varepsilon_0 t/2) a^\dagger$  and  $b^\dagger(t) = \exp(i\varepsilon_0 t/2) b^\dagger$ . This simple time dependence, and the fact that the  $a, b$  operators obey standard anticommutation rules, establishes Wick's theorem.<sup>8</sup>

Note that no unphysical configurations are created in any perturbation order, since the ground state has only singly occupied sites and the perturbations have only matrix elements within the allowed Hilbert space. Thus the unique feature of this formulation is that the constraints are satisfied locally, while a Wick's expansion is still possible. Diagrammatically, unphysical configurations are avoided as long as all diagrams contributing to a given order are taken into account. The perturbation in  $T$  is relatively simple, since  $T$  involves only the charge degrees of freedom and does not change the half-filled ground state.

Two kinds of graphical expansions are now possible: (i) a standard perturbation expansion in  $H_1, H_2$ ; and (ii) since  $H_0$  and  $H_1$  commute, an exact treatment of  $H_1$  is possible, summing up perturbations to all order in  $H_1$ . In this paper we will deal exclusively with the former kind of expansion; details of the latter will be presented elsewhere.

The zero-temperature time-ordered Green's functions are defined as

$$G_\Theta(t) = -i \langle T \Theta(t) \Theta^\dagger(0) \rangle.$$

In frequency space, the unperturbed single-particle ( $G_a$ )

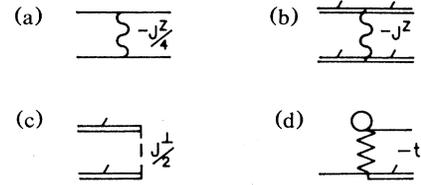


FIG. 1. Symbols for the graphical expansion. A single line represents the on-site  $G_b^{(0)}(\omega)$ , a hole line; with a tick mark  $G_a^{(0)}(\omega)$ , the propagator for a doubly occupied site. A double line represents a flipped spin  $G_{ab}^{(0)}(\omega)$ . (a)  $H_1$  has a vertex of  $-J^2/4$  between two nn single lines, and (b)  $-J^2$  between two nn double lines. (c)  $H_2$  destroys or creates pairs of nn flipped spins. (d) The kinetic-energy operator propagates a hole to a nn site, leaving a flipped spin behind. The loop in (d) is the constraint which enforces single occupancy.

and hole ( $G_b$ ) Green's functions are

$$G_a^{(0)}(\omega) = G_b^{(0)}(\omega) = 1/(\omega - \varepsilon_0/2 + i\delta)$$

and the Green's function for a particle-hole pair (a flipped spin) is  $G_{ab}^{(0)}(\omega) = 1/(\omega - \varepsilon_0 + i\delta)$ . Note that these are *site-diagonal* functions—the unperturbed intersite  $G$ 's vanish.

In Fig. 1 the graphical representation of the basic vertices is shown.  $H_1$  has a vertex of  $-J^2/4$  between two single lines and of  $-J^2$  between two double lines.  $H_2$  destroys or creates pairs of nn flipped spins. The kinetic energy  $T$  propagates a hole to a nn site, leaving a flipped spin behind. The additional equal-time loop  $\langle aa^\dagger \rangle$  enforces single occupancy and can be taken into account by retaining only the allowed hole propagation graphs. The evaluation of diagrams is particularly simple in coordinate space, since the unperturbed  $G$ 's are site diagonal. Not all higher-order graphs have a simple interpretation in terms of flipped spins.<sup>9</sup>

As a first example, we discuss the spin excitation spectrum at half-filling. For this we must consider the propagator for a local spin excitation (a flipped spin). In the lowest approximation, the flipped spin propagates within one sublattice by repetition of the basic step shown in Fig. 1(c). This basic step yields (in one dimension) a self-energy  $\Sigma_{i0} = (J^\pm/2)^2 G_{ab}^{(0)}(-\omega)(2\delta_{i0} + \delta_{i2} + \delta_{i,-2})$ , with a similar expression in two dimensions. If the flipped spin moves by repeating this step, then  $\Sigma_{i0}$  can be viewed as an effective hopping matrix element in a frequency-dependent tight-binding approximation, with hops to nearest-neighbor sites on the same sublattice. The Green's function for propagation from site 0 to site  $i$  becomes the random-phase-approximation- (RPA-) like sum

$$G_{i0}(\omega) = G_0 \delta_{i0} + G_0 \Sigma_{i0} G_0 + G_0 \Sigma_{ij} G_0 \Sigma_{j0} G_0 + \dots,$$

which when Fourier transformed becomes

$$[G_k(\omega)]^{-1} = (G_{ab}^{(0)})^{-1} - z^2 \gamma_k^2 (J^\pm/2)^2 G_{ab}^{(0)}(-\omega).$$

This yields the spin-wave spectrum  $\omega_k = \varepsilon_0 [1 - (J^\pm/J^2)^2 \gamma_k^2]^{1/2}$ , where  $\gamma_k = \cos(k)$  in one dimension and  $[\cos(k_x) + \cos(k_y)]/2$  in two dimensions. This is the usual spin-wave result.<sup>1</sup>

We have evaluated higher-order corrections to the

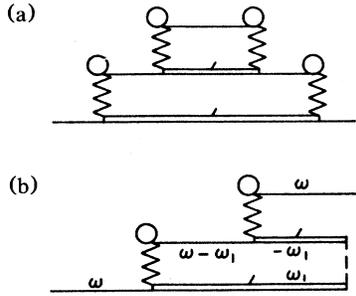


FIG. 2. (a) An order  $t^4$  example of the self-retracing paths which contribute to  $G_b^{\text{inc}}(\omega)$ . The hole hops away twice and follows the same path back. In the Heisenberg limit, this can be viewed as the emission and reabsorption of a spin wave. (b) The lowest-order graph giving coherent hole motion. The hole hops two times and the string of reversed spins left behind is swept up by a vacuum fluctuation. This can be treated as an effective hopping matrix element for motion within one sublattice. In our calculation, the single line  $G_b^{(0)}(\omega)$  is replaced by  $G_b^{\text{inc}}(\omega)$  so that the propagating object is the dressed Brinkman-Rice-type hole.

spin-wave velocity for  $J^\perp = J^z$ . These corrections appear to take the form of an expansion in  $1/(2z)$ ; the lowest-order correction gives  $\varepsilon_0 \rightarrow \varepsilon_0[1 + 1/(2z)]$  in the expression for  $\omega_k$ .<sup>9</sup> This interesting result may explain why the spin-wave approximation works so well in two dimensions even for  $s = \frac{1}{2}$ ; in our approach corrections are relatively small, going as  $1/(2z)$  rather than  $1/S$  as, for example, arises in the usual Holstein-Primakoff expansion.<sup>2</sup>

Next we consider the properties of a single hole. The graphs contributing to the hole propagation divide naturally into two distinct sets. The first set includes all self-retracing paths. These give rise to a localized dressed hole of the type first studied by Brinkman and Rice.<sup>3</sup> We will call this the incoherent part of the hole spectrum. Summing up the self-retracing graphs yields a self-energy correction  $\Sigma^{\text{inc}}(\omega)$  to the on-site hole Green's function. Physically this self-energy corresponds to the dressing of the localized hole by a cloud of reversed spins (more accu-

rately, strings of spins). We will calculate this self-energy in the Ising limit  $J^\perp \ll J^z$  and in the Heisenberg limit  $J^\perp = J^z$ .

The second set of graphs allows the dressed, localized hole to propagate coherently. In these graphs the off-diagonal term in the spin interaction erases the string dragged behind a moving hole, allowing it to move to other sites on the same sublattice, giving rise to a coherent contribution to the spectrum.

The incoherent part of the hole spectrum is given by the self-retracing paths;<sup>3</sup> e.g., the  $t^4$  graph shown in Fig. 2(a) is a two-step retracing path. In the limit  $J^z = J^\perp = 0$  our formulation becomes identical to that of Brinkman and Rice,<sup>3</sup> the sum of all self-retracing paths [of the form shown in Fig. 2(a)] then gives rise to a bandwidth of  $4(z-1)^{1/2}t$  for the incoherent hole motion. It is easy to generalize this result to  $J^z \neq 0$ . When the hole moves, it leaves a string of reversed spins behind. In the Ising case, the energy of this string increases linearly with length in two and three dimensions. Thus the hole is bound to the origin and the density of states becomes a series of discrete poles.<sup>4</sup> Near the Ising limit ( $J^\perp \ll J^z$ ) as well, the dominant contribution to the incoherent spectrum is given by self-retracing paths of the type shown in Fig. 2(a). One can thus describe the low-energy part of the hole Green's function accurately by the dominant pole approximation<sup>5</sup>  $G_b^{\text{inc}}(\omega) = a_0/(\omega - \omega_0) + C_0$ , with<sup>5</sup>  $a_0 \sim J^z/t$ .

A key question is whether this Ising result remains valid in the Heisenberg limit ( $J^\perp = J^z$ ), where conceivably the low-energy long-wavelength spin waves could effectively reduce the string energy to zero. To address this question, we replace the double lines in the self-retracing graphs [such as Fig. 2(a)] by the on-site spin-wave propagator  $\langle TS_i^+(t)S_i^-(t) \rangle$  ( $i \in A$ ). We expect this to incorporate the essential physics, the gaplessness of the spin excitation spectrum. In the Heisenberg limit, graphs of a second form also contribute; here the spin lines are the lowest contribution to  $\langle TS_i^-(t)S_i^+(t) \rangle$ , and we replace them by the spin-wave propagator as well. We can neglect  $H_1$ , which would merely renormalize the string energies. Summing up all self-retracing paths, we obtain the following self-consistency equation for the incoherent hole self-energy:<sup>9</sup>

$$\Sigma^{\text{inc}}(\omega) = \int \frac{d^d k}{\pi^d} \frac{a_k z t^2}{\omega - \varepsilon_0/2 - \omega_k + i\delta - [(z-1)/z]\Sigma^{\text{inc}}(\omega - \omega_k)}, \quad (4)$$

where  $\omega_k$  are the spin-wave energies and  $a_k = \varepsilon_0/\omega_k$ . We have only been able to solve (4) numerically. For  $d=2$ , we find that a single bound state persists, pushed slightly below a reduced Brinkman-Rice-type band edge, and so the low-energy hole is still bound to the origin. The dominant pole approximation is therefore also valid in the Heisenberg limit. Most interesting is that the spectral weight of the dominant pole turns out numerically to be linear in  $(J/t)$  only up to  $J/t \sim 0.01$ , beyond which a strong nonlinearity develops.<sup>10</sup> The self-consistency equation (4) has a qualitatively different form than that obtained by Kane, Lee, and Read.<sup>5,11</sup> We believe that this is because Kane *et al.* include additional graphs which in our approach are suppressed by the constraints prohibiting

both hole and spin excitations on the same site. The solution of (4) has no real pole for  $(z-1)/z \rightarrow 1$ , i.e., when paths are double counted in the self-retracing sum. The behavior of the spectral weight of the pole is therefore controlled by  $1/z$ .

Finally, we turn to the discussion of the coherent hole propagation. We are interested in the properties of the low-energy states which derive from the low-lying pole found in the incoherent spectrum in both the Ising and Heisenberg limits. The lowest-order (in  $J^\perp$ ) contribution to coherent motion is shown in Fig. 2(b): a hole hops twice and the string of reversed spins is swept up by a vacuum fluctuation. (An equivalent graph in which the reversed spin precedes the hop gives a factor of 2.) The

self-energy of this graph, which we denote by  $t_2$ , is given by

$$t_2 = t^2 \frac{J^\perp}{2} \int \frac{d\omega_1}{-2\pi i} G_b^{\text{inc}}(\omega - \omega_1) G_{ab}(\omega_1) G_{ab}(-\omega_1). \quad (5)$$

Near the Ising limit, (5) gives an effective hopping matrix element  $t_2$  for the hole. At the lower band edge,  $|\omega| \sim t \gg J \sim \omega_1$ , since  $G_{ab}(\pm \omega_1)$  is the propagator for a spin excitation. The frequency scales decouple and the remaining integral over  $\omega_1$  is just the lowest-order (in  $J^\perp$ ) contribution to  $\langle S_i^- S_j^+ \rangle$ . In the Heisenberg limit, therefore, making the same spin-wave replacement for the spin lines,  $t_2$  becomes  $t^2 \langle S_i^- S_j^+ \rangle G_b^{\text{inc}}(\omega)$ .

As in the spin-wave calculation above, in the lowest approximation the (dressed) hole propagates by repeating the step shown in Fig. 2(b) in an RPA-like sum. This leads to an effective kinetic energy  $t_2 \varepsilon_k$ , where  $\varepsilon_k = z^2 \gamma_k^2 - z$ . We obtain

$$G_b(k, \omega) = \frac{1}{[G_b^{\text{inc}}(\omega)]^{-1} - t^2 \varepsilon_k \langle S_i^- S_j^+ \rangle G_b^{\text{inc}}(\omega)}. \quad (6)$$

The poles of  $G_b(k, \omega)$  are real for  $\varepsilon_k < 0$ . For a quantitative solution, we use the dominant pole approximation for  $G_b^{\text{inc}}(\omega)$ . In the Ising limit, one obtains a bandwidth of order  $J^\perp$  due to the reduction of the spectral weight of the pole in  $G_b^{\text{inc}}(\omega)$  by  $J^2/t$ , in agreement with Ref. 5. In the Heisenberg limit, however, our numerical solution of (4) shows that the pole's spectral weight is nonlinear in  $J/t$  for

$J/t \sim 0.1$ .<sup>10</sup> Thus the coherent bandwidth ( $\sim a_0 t$ ) is linear in  $J/t$  for very small  $J/t$  but nonlinear in the region of interest. The minimum of the band lies at  $\pm k_x \pm k_y = \pi$ . The same degeneracy is found by exactly diagonalizing a 16-site lattice with one hole.<sup>12</sup> Physically, these propagating states develop from the localized states which form the lowest pole in the incoherent spectrum.

In conclusion, we have discussed a new way to apply Green's-function techniques to charged spin systems which satisfies the local constraints exactly, taking the  $t-J$  model on a bipartite lattice as an example. This approach is systematic and can be readily generalized to other lattices and charged spin systems. The approach treats spin and charge degrees of freedom on an equal footing and is therefore well suited to study the interplay between the two. We have used the formalism to treat the hole propagation, finding that holes can propagate coherently with a bandwidth  $\sim J^\perp$  in the Ising limit and by a nonlinear function of  $(J/t)$  in the Heisenberg limit, where the occurrence of coherent states is intrinsically related to the local constraints. The simple physical picture of these states is that of a dressed Brinkman-Rice-type hole which propagates coherently with the help to the transverse pieces of the spin-spin interaction.

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<sup>9</sup>Details will be presented elsewhere.

<sup>10</sup>For  $0.0002 \leq J/t \leq 0.2$ , the residue of the lowest peak [found by numerically solving (4) in a spherical approximation] is empirically fitted well by  $a_0 = 2.4(J/t) \exp[-2.0(J/t)^{1/3}]$ . The bandwidth of the coherent band derived from this peak  $\sim a_0 t$ . In the more limited range  $0.02 \leq J/t \leq 0.2$ , this empirical nonlinearity is also well described as  $\sim t(J/t)^{2/3}$ .

<sup>11</sup>We thank Charles L. Kane for having pointed this out to us and for having clarified the relation of this work to that of Ref. 5.

<sup>12</sup>J. Bonča, P. Prelovšek, and I. Sega (unpublished).