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A new auxiliary particle method for the Hubbard, t–J and Heisenberg models

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Abstract. A new bond auxiliary particle method for the Hubbard, t–J and Heisenberg Hamiltonians is presented. First, the one-dimensional (1D) Heisenberg Hamiltonian is studied as a test case. The exact ground state is approached rapidly via perturbation theory. At the level of second-order perturbation theory, the ground state energy is accurate within a few per cent, while in the 15th order it is accurate to five figures. Without any renormalization, the spin velocity is given with 10% accuracy, and the spectrum is correctly gapless. The degeneracy is also correct, giving a Wilson ratio $R = 2$. The method is used to calculate analytically the full Green's function for a single hole in a half-filled (one electron per site) t–J model.

The principal problem with the usual 'slave boson' auxiliary particle method, devised by one of the present authors [1], is that as a practical matter it is impossible to describe accurately the RVB-type spin ground state [2], appropriate to the 1D Hubbard, t–J and Heisenberg Hamiltonians *and* maintain the constraint, $Q_i = 1$, that the number of auxiliary particles at a site is always exactly unity. This is unfortunate since it is an exact result, that for $U \gg t$, $(t \gg J)$, this type of spin ground state is the spin 'vacuum' for the 1D Hubbard and t–J Hamiltonians with a thermodynamic density of holes. It is also widely speculated that a similar RVB state is relevant, at finite doping, for the two-dimensional problem of interest in the high-T_c context. What is proposed here is a new bond-orientated auxiliary particle method which can accurately describe this spin vacuum state.

The usual slave boson method [1] has auxiliary particles assigned to each site. With the new approach, similar particles are assigned to each possible state of a bond, i.e. two sites i and j. There is now a constraint that $Q_{ij} = 1$ for each bond. As explained above, the difficult problem in connection with the Hubbard and t–J model, is the accurate description of the spin vacuum near half filling, i.e. a relevant test case is the one-dimensional Heisenberg Hamiltonian. This motivates us to demonstrate that the present new bond approach accurately describes the ground state and certain key excited states of this simpler Hamiltonian. It is shown here that a second-order perturbation theory for which $Q_{ij} = 1$ is maintained *exactly* yields results for the ground state energy accurate to $\sim 1\%$. In 15th order, this perturbation theory converges to the exact ground state energy to five figures and with a similar precision it can be asserted that the perturbation series does in fact converge [3].

While it is impressive to recover known results with great accuracy, what is needed in the present context is a mathematically tractable quantum field theory for the excitations and in the presence of holes. Still, for the 1D Heisenberg Hamiltonian, the lowest-lying 'spinwave' excitations with a given wavevector have been calculated long ago [4]. In a more modern language these are a set of gapless fermionic excitations which are characterized

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by a spin velocity v_s. (For the Hubbard, or t–J Hamiltonians there is a second charge velocity v_c.) Without any renormalization, the present approach yields the correct gapless excitations with a v_s which is good to better than 10%. However, in the authors' opinion, the most impressive part of this development is its simplicity. At the present level of renormalization this 'spinwave' problem is no more difficult than, see equation (9), and probably as accurate as, the Holstein–Primakoff theory for true spinwaves for the symmetry broken antiferromagnetic ground state. (The theories, while similar mathematically, *are* different: it is an important point that the present 'spinwaves' are three times degenerate while true antiferromagnetic spinwaves are only doubly degenerate. The velocities also differ.)

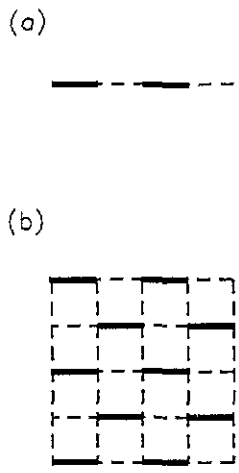

Figure 1. (a) The 1D and (b) 2D bond scheme. The solid bonds are taken to have parameters t and J, while the other, dashed bonds, have different, smaller values $t' < t$ and $J' < J$. The *limit $t' \to t$ and $J' \to J$ is taken at the end of the calculation.*

Since the results described above are well known, and since these calculations do not test the utility of the approach in connection with the kinetic energy terms, the method has also been used to calculate the Green's function $\mathcal{G}_{k\sigma}$ of a single hole for the t–J model. To the authors' knowledge, results for this quantity are not known, at least analytically and in the thermodynamic limit. It is shown that, if k is the physical momentum of the hole, and if k' is the momentum of the spinless fermions, with $\epsilon_{k'} = -2t\cos k'$, which describe the charge sector of this model, then $\mathcal{G}_{\sigma k}$ has poles at energies corresponding to $k' = k \pm \pi/2$. It is implied that the Fermi surface opens at $\pm\pi/2$, as is known. It is possible to calculate the Green's function for a thermodynamic density of holes; however, this corresponds to the Luttinger liquid behaviour, is much more complicated, and involves a number of simple, but involved, steps. These developments will be reported elsewhere.

Consider the t–J model

$$\mathcal{H} = -t\sum_{\langle ij\rangle}(c^{\dagger}_{i\sigma}c_{j\sigma} + \text{HC}) + J\sum_{\langle ij\rangle} \boldsymbol{S}_i \cdot \boldsymbol{S}_j.$$

This Hamiltonian includes both magnetic interactions and hole motion and serves to illustrate well the formalism in its generality. This is first generalized as illustrated in figure 1. The

solid bonds are taken to have parameters t and J, while the other, dashed bonds, have different, smaller, values $t' < t$ and $J' < J$. The limit $t' \to t$ and $J' \to J$ is to be taken at the end of the calculation. Within this more general t–J model and when $t' = J' = 0$, the eigenstates of a bond with one or two, and trivially, zero electrons are determined exactly. For $J > 0$, the ground state of a doubly occupied bond is a spin singlet with an energy of $-J$ relative to a triplet. The auxiliary Bose particles $s_i^\dagger$ and $t_{i\sigma}^\dagger$, with $\sigma = -1, 0, +1$, are associated with these states and this configuration. For a singly occupied bond there is no exchange energy. The exact eigenstates are bonding and anti-bonding orbitals at $-t$ and $+t$ respectively. The associated Fermi particles are $b_{i\sigma}^\dagger$ and $a_{i\sigma}^\dagger$, $\sigma = \pm 1$ corresponding to spin $\pm 1/2$. Clearly the empty bond has no energy. The associated (Bose) particle is $e_i^\dagger$. In this new scheme the physical conduction electron field is

$$c_{i\pm 1/2,j\sigma}^\dagger = \frac{1}{\sqrt{2}}(b_{ij\sigma}^\dagger \mp a_{ij\sigma}^\dagger)e_{ij} \mp \frac{1}{\sqrt{2}}t_{ij\sigma}^\dagger(b_{ij\sigma} \pm a_{ij\sigma}) \mp \frac{1}{2}(t_{ij,0}^\dagger \mp \sigma s_{ij}^\dagger)(b_{ij-\sigma} \pm a_{ij,-\sigma}) \quad (1)$$

where the sign depends on whether the $c^\dagger$ corresponds to the right or left hand side of a bond, $\sigma = \pm 1$ as the spin is up or down, and where i is an even integer which labels a bond on a row with integer label j. There is, as usual with auxiliary particle methods, a constraint that the bond charge

$$Q_{ij} = s_{ij}^\dagger s_{ij} + e_{ij}^\dagger e_{ij} + \sum_{\sigma=\pm 1}(b_{ij\sigma}^\dagger b_{ij\sigma} + a_{ij\sigma}^\dagger a_{ij\sigma}) + \sum_{\sigma=\pm 1,0} t_{ij\sigma}^\dagger t_{ij\sigma} = 1.$$

The unperturbed part, $\mathcal{H}_0$, of the Hamiltonian accounts for the t and J bonds and is explicitly

$$\mathcal{H}_0 = -t \sum_{\langle ij\rangle\sigma=\pm 1}(b_{ij\sigma}^\dagger b_{ij\sigma} - a_{ij\sigma}^\dagger a_{ij\sigma}) + J \sum_{ij\langle\sigma\rangle=\pm 1,0} t_{ij\sigma}^\dagger t_{ij\sigma} \quad (2)$$

where the singlet has been re-assigned a zero energy and the energy associated with the empty bond has been dropped. Here the sum on $\langle ij\rangle$ implies solid bonds.

The last step in the formalism is to include the t' and J' bonds as coupling terms. The J' terms are

$$\mathcal{H}_{J'} = -\frac{J'}{4} \sum_{\langle ij,i'j'\rangle\sigma=\pm 1,0}(d_{\sigma ij}^\dagger d_{\sigma i'j'} + (-1)^\sigma d_{\sigma ij}^\dagger d_{-\sigma i'j'}^\dagger + \text{HC}) + \frac{J'}{4} \sum_{\langle ij,i'j'\rangle} \boldsymbol{S}_{ij} \cdot \boldsymbol{S}_{i'j'} + \frac{J'}{4} \sum_{\langle ij,i'j'\rangle} (\boldsymbol{S}_{ij} \cdot \boldsymbol{s}_{i'j'} - \boldsymbol{s}_{ij} \cdot \boldsymbol{S}_{i'j'}) \quad (3)$$

which is written in terms of the operators

$$\begin{aligned} d_{\sigma ij}^\dagger &= t_{\sigma ij}^\dagger s_{ij} \qquad (\sigma = 0, \pm 1) \\ S_{ij} &= \sum_{\sigma,\sigma'=0\pm 1} t_{\sigma ij}^\dagger S_{\sigma,\sigma'} t_{\sigma' ij} = \sum_{\sigma,\sigma'=0\pm 1} d_{\sigma ij}^\dagger S_{\sigma,\sigma'} d_{\sigma' ij} \\ s_{ij}^z &= d_{0,ij}^\dagger + d_{0,ij} \qquad s_{ij}^+ = -\sqrt{2}\left(d_{1,ij}^\dagger - d_{-1,ij}\right) \end{aligned} \quad (4)$$

where $S_{\sigma,\sigma'}$ is set of $S = 1$ spin matrices and where it is understood that here the sums $\langle ij, i'j'\rangle$ are over all dashed bonds where the bond $i'j'$ is to the right of that with the labels ij. In terms of the same operators, the last term in $\mathcal{H}_0$ is

$$+J \sum_{\langle ij\rangle\sigma=\pm 1,0} t_{ij\sigma}^\dagger t_{ij\sigma} = +J \sum_{\langle ij\rangle\sigma=\pm 1,0} d_{ij\sigma}^\dagger d_{ij\sigma}.$$

The $d^{\dagger}_{ij\sigma}$ have on-site fermion, and off-site boson, commutation rules, i.e. are hard core bosons. In one dimension this, via a Jordan–Wigner transformation, is equivalent to fermions. (These fermions are hard core with respect to the equivalent particle but with a different σ.)

In their full generality, the t' terms cannot be very usefully abbreviated. They are

$$-t' \sum_{\langle ij,i'j'\rangle\sigma} \left(c^{\dagger}_{i+\frac{1}{2},j\sigma} c_{i'-\frac{1}{2},j'\sigma} + \text{HC} \right) \tag{5}$$

were the $c^{\dagger}_{i\pm\frac{1}{2},j\sigma}$ are defined by (1).

Consider, first, the Heisenberg model where the t and t' terms are not relevant. Fortunately for both the one- and two-dimensional (2D) cases the convergence problem of the present perturbation approach to the spin vacuum is well understood. Singh *et al* [3], have developed a systematic scheme for the perturbative diagonalization of the present generalized model using the same basis set as is implicit here. They show, based on 15th-order perturbation theory for the 1D case, there is extremely strong evidence that the perturbation theory converges even when $J = J'$, in the present notation. For two dimensions the series expansion is not absolutely convergent under the same circumstances. However, the good convergence properties in low order leads us to speculate that the series is asymptotic and that in low order it converges reasonably well to a *local* minimum which lacks the broken symmetry of the true ground state but which is very close in energy.

In fact, it is an old observation that $\mathcal{H}_0$ reflects a large part of the ground state energy in both one and two dimensions. In one dimension, this corresponds to $\langle \boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle = -(3/8)J = -0.37J$ while the exact result is $\simeq -0.44J$. In two dimensions the corresponding figures are $-0.19J$ and $-0.33J$, where this latter corresponds to an estimate [5] for the ground state energy for the true broken symmetry antiferromagnetic state. The state vector corresponding to this singlet bond ground state is $|\frac{1}{2}\rangle_0 = \prod_{ij} s^{\dagger}_{ij} |\,\rangle$ where $|\,\rangle$ is the vacuum with no auxiliary particles. The state $|\frac{1}{2}\rangle_0$ can be thought of as the vacuum for perturbation theory.

The only terms which couple $|\frac{1}{2}\rangle_0$ to excited states are $(J'/4)d^{\dagger}_{\sigma ij} d^{\dagger}_{-\sigma i'j'}$ and, at the level of second-order perturbation theory the renormalized wavefunction is

$$\begin{aligned} |\tfrac{1}{2}\rangle &= \prod_{\langle ij,i'j'\rangle} \left(1 + \alpha \sum_{\sigma} (-1)^{\sigma} t^{\dagger}_{ij\sigma} t^{\dagger}_{i'j'-\sigma} s_{ij} s_{i'j'} \right) |\tfrac{1}{2}\rangle_0 \\ &= \prod_{\langle ij,i'j'\rangle} \left(1 + \alpha \sum_{\sigma} (-1)^{\sigma} d^{\dagger}_{ij\sigma} d^{\dagger}_{i'j'-\sigma} \right) |\tfrac{1}{2}\rangle_0 \end{aligned} \tag{6}$$

which is of a BCS form. The parameter α can be determined by perturbation theory or can be used as a variation parameter. Determining α by the variational principle leads to a strict bound for the energy.

Consider one dimension and second-order perturbation theory. The matrix element is $J'/4$ to each of three possible excited states. This excited state would be at an energy of $2J$ if it were not for the interaction between the adjacent triplets and which lowers the energy to $3J/2$ when $J' = J$. Since there are three possible triplet excitations, the energy correction is $3 \times (J/4)^2/(3J/2) = (J/8)$ per dashed bond. Since there are half dashed and half solid bonds the net energy per bond is

$$-\frac{1}{2}\frac{3J}{4} - \frac{1}{2}\frac{J}{8} = -0.438J \tag{7}$$

which is within about 1% of the exact result $\langle -J\boldsymbol{S}_i \cdot \boldsymbol{S}_j \rangle = -0.443147J$. Singh *et al* [3], obtain -0.44314 ± 0.00001 with 15th-order perturbation theory. It is impressive that the result is already very good at the level of the second-order theory and lends support the idea that the theory at that level will yield reliable results. The variational estimate gives an upper bound of $-0.427J$, which remains impressively close to the exact value.

It is to be recognized that rather bad wavefunctions can give rather good energies. Clearly a good theory must give a good energy, however that the energy is good within the second order theory can only be interpreted as lending support for our approach. In effect, when $J = J'$, the 'smallness parameter' is $1/2(\sqrt{3}) = 0.289$ which is encouraging, especially in view of the fact that the first correction is only $1/8$. It is implied that second-order perturbation omits only a correction of roughly $0.037J$ and which, consistently, represents a little more than 2% of the ground state energy.

For two dimensions, in the equivalent perturbation calculation, there is an extra correction to the excited state energy due to a resonance between six different configurations of excited triplet configurations. This lowers the excited state configuration by an extra $J/2$. The energy per bond is now

$$-\frac{1}{4}\frac{3J}{4} - \frac{3}{4}\frac{3J}{16} = -0.328J. \tag{8}$$

Here the exact result is not known; in fact, the calculations of Singh *et al* [3], indicate that when $J'/J > 0.39$ the perturbation theory diverges. As stated above, we speculate that there exists a locally stable ground state, i.e., that the series is only asymptotically divergent. The energy of the *absolute*, antiferromagnetic, ground state is estimated [5] to be $\simeq -\frac{1}{3}J$ per bond, and again our perturbation result is impressively close. However, here the lower bound given by the variation wavefunction is $-0.27J$, indicating higher-order terms are required in order to obtain a reliable result.

It is to be emphasized in the context of the 2D calculations that the present perturbative vacuum can only become the true vacuum at finite doping.

While the calculations of Singh *et al* provide more precise results, they do not provide a theory for the excitation spectrum. These aspects of the problem are dealt with next. Of course, the reliability of such an approach is predicated upon that for the vacuum, i.e. ground state.

The Bethe approach [4,6] shows that the lowest-lying spin excitations, with a given wavevector, are triply degenerate corresponding to $S = 1$. These 'spinwaves' correspond to spin-flip excitations relative to the ground state. If we consider only a single such excitation, the relevant Hamiltonian is

$$\mathcal{H}_{\rm sw} = J \sum_{\langle ij\rangle\sigma=\pm1,0} d^\dagger_{ij\sigma} d_{ij\sigma} - \frac{J'}{4} \sum_{\langle ij,i'j'\rangle\sigma=0\pm1} (d^\dagger_{\sigma ij} d_{\sigma i'j'} + (-1)^\sigma d^\dagger_{\sigma ij} d^\dagger_{-\sigma i'j'} + \text{HC}). \tag{9}$$

This is easily diagonalized by a Bogoliubov transformation, to yield for $J = J'$ the gapless dispersion relationship

$$\epsilon_q = \sqrt{2}J \sin q. \tag{10}$$

The Bethe method yields [4] a dispersion relationship $\epsilon_q = \frac{\pi}{2} J \sin q$, i.e. implies that the spin velocity $v_s = \frac{\pi}{2}J$. In (10) the coefficient $\sqrt{2} = 1.414$ has replaced the exact $\pi/2 = 1.570$. More important than the relatively good result for the spin velocity, is

the fact that the degeneracy is correct *and* that the spectrum is gapless. The latter is a delicate result. For all values of $J' < J$ there *is* a spin gap. It should be noted that (i) the spinwave theory for the antiferromagnet ground state is similar, with a coefficient $1.0J$, but has the wrong degeneracy. (ii) In two dimensions, the spinwave energy is imaginary for small q when $J' = J$, indicating the global instability of the ground state towards the antiferromagnetic possibility. In fact the imaginary roots appear when $J'/J = 1/3$, in relatively good agreement with the 'critical' value 0.39 obtained by Singh *et al* [3], using sixth-order perturbation theory.

Of course, using the Bogoliubov transformation to solve the spin excitation problem is inconsistent with the assumption that there is only a single excitation present. In fact the approach leads to a new ground state wavefunction which we have not yet fully investigated. However, due to restrictions implied by the value of the ground state energy, the total number n_t of triplet excitations must be such that $n_t < 0.3$ in one dimension and implies that the terms omitted in the present approach are not too important. However, in reality there are renormalization effects and presumably including such corrections will improve the value for v_s. It is perhaps worth pointing out that an exactly similar approximation of ignoring interactions is made in the Holstein–Primakoff theory [7] of antiferromagnetic spinwaves.

It should be that, for a Heisenberg chain, the spin susceptibility $\chi = \mu^2/2\pi v_s$ where the Zeeman energy is $-|\mu|HS_z$. In the present development the change in S_z produced by the presence of the field implies a finite number of free $\sigma = +1$ triplet excitations which leads directly to the quoted result for the susceptibility and implies the same level of error in χ as there is in v_s. Within the Bethe method [4, 6] the specific heat is calculated with a fixed number of overturned spins, i.e. for a fixed value of S_z. In the absence of a field it is implied that the equivalent of particle–hole excitations correspond to either the excitation of two t_0 excitations or a t_1, t_{-1} pair, i.e. there are only two sets of thermodynamic excitations for fixed S_z rather than the three that might be first expected for $S = 1$. It follows from an elementary calculation that the Wilson ratio is $R = 2$ as for the exact solution.

The last problem to be treated here is that of the propagation of single hole. It is now necessary to consider the spin ground state problem when there are an odd number of spins. Evidently if one begins with an even number of spins and creates a hole, as the first step in calculating a Green's function, then one inevitably encounters the odd spin problem. Technically it is better to begin with an even number of spins but with a single hole in the system and then create an electron at this position thereby adding an extra spin. This procedure is better since the odd spin can be though of as an isolated spinon which is destroyed when the hole is created. The alternative creates a hole and a spinon 'hole' in the same process and leads to a technically more involved two-particle problem.

If there is a hole and an even number of spins there must be an odd number of sites, and therefore there is a single site which cannot be covered by a bond. The convention is chosen that this be site zero. At this site there is either a fermion $f_\sigma^\dagger$ or a boson $b_0^\dagger$ corresponding to the two singly occupied and unoccupied sites, respectively. Sites 1, 2; 3, 4; and 5, 6 etc, correspond to bonds and have associated bond particles. The bond spin vacuum has this same site occupied by an electron and corresponds to

$$|\sigma, 0\rangle = f_\sigma^\dagger s_{1,2}^\dagger s_{3,4}^\dagger \ldots s_{N-1,N}^\dagger |\,\rangle. \tag{11}$$

It is doubly degenerate, corresponding to $\sigma = \pm 1/2$. If there is a hole at site 0 the state vector is

$$|0\rangle = b_0^\dagger s_{1,2}^\dagger s_{3,4}^\dagger \ldots s_{N-1,N}^\dagger |\,\rangle. \tag{12}$$

Creating an electron via $c^{\dagger}_{i=0,\sigma} = f^{\dagger}_{\sigma} b_0$ at this site relates the two vectors, i.e.

$$|\sigma, 0\rangle = c^{\dagger}_{i=0,\sigma}|0\rangle \tag{13}$$

and implies the matrix element

$$\langle \sigma, 0|c^{\dagger}_{i=0,\sigma}|0\rangle = 1. \tag{14}$$

There is an essentially equivalent state, with the hole at site 2, generated by the action of the transfer terms $p_{12}p_{01}$ where $p_{i,j} = \sum_{\sigma} c^{\dagger}_{i,\sigma} c_{j,\sigma}$. Explicitly this state is

$$|2\rangle = p_{12}p_{01}|0\rangle = \frac{1}{\sqrt{2}} \sum_{\sigma} f^{\dagger}_{\sigma}(b^{\dagger}_{1,2;-\sigma} + a^{\dagger}_{1,2;-\sigma}) s^{\dagger}_{3,4} \ldots s^{\dagger}_{N-1,N}|\,\rangle. \tag{15}$$

The first two sites are now occupied by a singlet and there is the hole at site 2. If the singlets are assigned zero energy, and if the perturbative corrections to the energy are ignored, then the exchange energy of the state $|0\rangle$ is evidently zero. The $|2\rangle$ has the same energy at the same level of renormalization, if $J' = J$. Since it might be unclear what is and what is not a perturbation, this unperturbed energy is defined as that obtained by taking the expectation value of the Hamiltonian. On this basis, the state

$$|1\rangle = p_{01}|0\rangle \tag{16}$$

which has the hole in the middle of a singlet has a different, higher, energy. This lacks the exchange energy $-3J/4$ associated with this latter singlet. In general, the odd site states, $|2n+1\rangle$, have an exchange energy $3J/4$ larger than the even site equivalents, i.e. $|2n\rangle$. The set of, e.g., even site states are degenerate. It follows that, in the ground state, these states can differ at the most by a phase factor. Also, since these same states only differ from each other by translations, this phase factor must define a momentum, i.e. be of the form $e^{ik(2n)}$. The matrix elements of the kinetic energy connect the even to the odd site states but there are no matrix elements of this term with any other states. It follows that, at the present level of approximation for the exchange interaction, the ground state is of the form

$$|k\rangle = A \sum_{n=0}^{N} e^{ik(2n)}|2n\rangle + B \sum_{n=0}^{N} e^{ik(2n+1)}|2n+1\rangle. \tag{17}$$

For reasons which will become evident below, it is important to reflect upon the nature of the boundary conditions for the above wavefunction. If the conditions to be used are periodic, then there are two distinct states with a hole at a given site. There is a state obtained by translating, towards increasing site numbers, the hole the minimum number of times to arrive at a given site. In addition, there is a different state obtained by a translation which is longer by N, the total number of sites. At least in the thermodynamic limit, the corresponding two spin states are independent and orthogonal, to a very good approximation. These two spin configurations have been implicitly included, using an evident definition, by extending the upper limit of the sums from $N/2$ to N.

Assuming $t \gg J$, then the secular equation for the coefficients A and B simplifies to the dispersion relationship

$$\epsilon_k = \frac{3J}{8} + 2t\cos k \tag{18}$$

i.e. except for the unimportant shift $3J/8$, the result expected for a free hole (holon).

Turning to the single spinon problem, it is tempting to define exactly equivalent states obtained by filling the hole with an electron of a given spin direction. However, this strategy is flawed since the resulting spin states are not linearly independent. It is simple to define a state, evolved from

$$|\sigma, 0\rangle \tag{19}$$

by the spin permutation operator,

$$P_{ij} = \left(2\boldsymbol{S}_i \cdot \boldsymbol{S}_j + \frac{1}{2}\right). \tag{20}$$

Consider the three states, $|\uparrow, 0\rangle$, $P_{01}|\uparrow, 0\rangle$and $P_{12}P_{01}|\uparrow, 0\rangle$. These are not independent since, $|\uparrow, 0\rangle + P_{12}P_{01}|\uparrow, 0\rangle = P_{01}|\uparrow, 0\rangle$. It suffices to define the $|\sigma, 2n\rangle$ in order to have a linearly independent set. However, it remains the case that this set are not orthogonal. It is observed that the interaction between adjacent spins can be written either as $J\boldsymbol{S}_i \cdot \boldsymbol{S}_j$ or $\frac{J}{2}P_{ij}$, since the two definitions differ only by an unimportant additive constant. Clearly the effect of the interaction is, e.g.

$$\frac{J}{2}P_{01}|\sigma, 0\rangle = \frac{J}{2}\left[|\sigma, 2\rangle + |\sigma, 0\rangle\right]. \tag{21}$$

Again ignoring the perturbative corrections to the spin wavefunction, the spin ground state must be a linear combination of the form

$$|\sigma, k\rangle = \mathcal{A}\sum_{n=0}^{N/2} \mathrm{e}^{\mathrm{i}k(2n)}|\sigma, 2n\rangle$$

involving only even sites. However, again care must be exercised with the periodic boundary conditions.

There is a second possibility for the spinon to occupy an odd-numbered site. This new possibility is obtained from the reference state by more than N permutations. Again, for a thermodynamic system, this second state is independent. With this the single spinon ground state is now

$$|\sigma, k\rangle = \mathcal{A}\sum_{n=0}^{N} \mathrm{e}^{\mathrm{i}k(2n)}|\sigma, 2n\rangle, \tag{22}$$

using a similar convention for an index greater than $N/2$. Despite the fact that this involves non-orthogonal states, it is easy to show, ignoring perturbative corrections, that this is a good approximative eigenstate with an energy

$$E_k = J + J\cos 2k \tag{23}$$

and therefore that the ground state corresponds to $k = \pi/2$. It is implied that the wavefunction changes sign each time the spinon hops the mandatory minimum of two sites.

Since there is not a direct correspondence between the spinon basis states and the hole basis, and because the spinon basis are not orthogonal, the calculation of the relevant matrix

elements necessary in the determination of the Green's function for a single hole is a little involved. As already noted, in the spin wavefunction, there are not the equivalent states generated by filling the hole in the 'odd' site terms with the coefficient B. However, this term can be eliminated by taking the combination

$$|k\rangle + |k+\pi\rangle. \tag{24}$$

The effect of $c^{\dagger}_{k'\sigma} = \frac{1}{\sqrt{N}} \sum_n e^{ik'n} c^{\dagger}_{n\sigma}$ on this combination is, to within a normalization constant, $|\sigma, k+k'\rangle$. If this is to be the spinon ground state, then it must be that $k+k' = \pi/2$ or that,

$$k = -k' + \frac{\pi}{2}. \tag{25}$$

The minus sign reflects the fact that one of the momenta corresponds to an electron coordinate while the other reflects that of a hole. The shift by $\frac{\pi}{2}$ reflects the momentum of the spinon in the spin ground state. It is implied that

$$\tfrac{1}{2}\big[|-k-\pi/2\rangle + |-k+\pi/2\rangle\big] = c_{k\sigma}|\sigma, \pi/2\rangle \tag{26}$$

where it is intended that all the vectors are normalized. The coefficients in this expression follow from sum rule considerations, a requirement of a gauge symmetry reflected by the existence of zero energy ($\pi/2\uparrow, -\pi/2\downarrow$) spinons, and the fact that there is one electron per site in the spin ground state (see below).

Since, at the present level of approximation, the $|-k\pm\frac{\pi}{2}\rangle$ are single-hole eigenvectors of the energy, it is simple to write down the Green's function in momentum–frequency space, i.e.

$$\mathcal{G}_{k\sigma} = \frac{1}{4}\left[\frac{1}{\epsilon + is - \epsilon_{k-\frac{\pi}{2}}} + \frac{1}{\epsilon + is - \epsilon_{k+\frac{\pi}{2}}}\right] \tag{27}$$

where, since $t \gg J$, some energies $\sim J$ have been ignored. The hole states have no spin label, hence each value $k'' = k \pm \frac{\pi}{2} = (2\pi/N)n$, with n an integer, occurs once with k lying in the range $-\pi$ to π. All the available levels are filled and hence each of the two poles in the Green's function contributes $1/4$ to n_k and the net value is $n_k = 1/2$. This flat distribution in momentum space is trivially correct for half filling and the value of $1/2$ correctly obeys the relevant sum rule confirming the normalization shown in (26).

Clearly if there are a small number of holes, it is those hole states with the smallest energy near $k'' = \pm\pi$ which are filled first. Because of the translations by $\pm\pi/2$, it is the n_k values near $\pm\pi/2$ which change first. It follows, $n_k = 1/4$ in a symmetric region about $\pm\pi/2$, however more extensive calculations not reported here, show the presence of a thermodynamic density of holes (i) changes the spin wavefunction so that $\pm\pi/2 \to \pm k_F$ where k_F is the Luttinger value of the Fermi momentum, i.e. one half of the spinless fermion value, so that the Fermi 'breaks' occur at k_F and $3k_F$. (ii) There are new contributions to the Green's function, and (iii) there is a phase shift of $\pi/2$ for each site occupied by a hole which lies between the beginning and end site of the real space Green's function. It is (iii) which leads to the famous power-law behaviour at the Fermi breaks.

It should be noted that (26), and the totally coherent result (27), are equivalent to an assumption of a limiting maximum thermodynamic density of ($\pi/2\uparrow, -\pi/2\downarrow$) spinon pairs in the ground state. This needs more detailed investigation.

In summary, we have developed a bond auxiliary particle formalism which at the level of second-order perturbation theory reproduces the ground state energy for the Heisenberg chain with an accuracy at the per cent level and yields, without renormalization, the key parameter, the spin velocity v_s, with an accuracy of better than ten per cent. The degeneracy of the excitations is correct leading to the value $R = 2$ for the Wilson ratio. It has been shown how the method may be used to calculate the single-hole Green's function in the thermodynamic limit of the t–J model for $t \gg J$. It will be shown elsewhere that with a thermodynamic density of holes the same methods lead to Luttinger liquid behaviour.

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