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2002 J. Phys.: Condens. Matter 14 L19

(http://iopscience.iop.org/0953-8984/14/1/103)

J. Phys.: Condens. Matter **14** (2002) L19–L28 PII: S0953-8984(02)30566-6

LETTER TO THE EDITOR

A Jordan–Wigner transformation for the t–J and Hubbard models with holes

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Received 7 November 2001
Published 7 December 2001
Online at stacks.iop.org/JPhysCM/14/L19

Abstract

A Jordan–Wigner (JW) transformation for the t–J and Hubbard models is described. Holon and doublon particles for hole and double occupied sites are introduced. There is only a single spin sector particle. Flux tubes occur in a natural fashion, within a specific gauge, when the method is adapted to two dimensions. In order to accommodate three dimensions 'JW sheets' are defined. The adaptation of the method to the t–J model in the context of high T_c is described.

(Some figures in this article are in colour only in the electronic version)

While the Jordan–Wigner transformation [1] is well known in the context of spin only models such as the Heisenberg or X–Y model it does not seem to be widely known that a similar approach can be used for doped systems such as the t–J or Hubbard models and that this provides a useful alternative formulation of such models in two dimensions in the context of high-T_c superconductors. The purpose of this Letter is to describe such a formalism along with some elementary conclusions which are evident on the basis of this formalism.

Recall first the basic JW transformation in one dimension. It is trivial for $S = 1/2$ that σ_n^+ obey on-site Fermi commutation rules and that

$$f_n^\dagger = \exp\left(\mathrm{i}\pi \sum_{m=1}^{n-1} \hat{Q}_m\right)\sigma_n^+ \tag{1}$$

obeys such rules even when the site indices are different. Here $\hat{Q}_n = f_n^\dagger f_n$, i.e. is the number of particles at site n. It is then straightforward to show [1] that, for example, the one-dimensional Heisenberg Hamiltonian $\mathcal{H} = J\sum_n \vec{S}_n \cdot \vec{S}_{n+1}$ becomes

$$\mathcal{H} = \frac{J}{2}\sum_n (f_n^\dagger f_{n+1} + \mathrm{H.c.}) + J\sum_n f_n^\dagger f_n f_{n+1}^\dagger f_{n+1} - J\hat{N}_\uparrow \tag{2}$$

where, with $\hat{N}_\uparrow = \sum_n f_n^\dagger f_n$, the last term reflects an effective chemical potential $\mu = J$.

This can, in fact, be generalized to include charge. Since σ_n^+ is considered to be a creation operator it is implicit that the vacuum is the down spin ferromagnetic state. Creating an $f_n^\dagger$-fermion implies an up spin at the site n. In the usual way a $b_n^\dagger$-boson corresponds to a true vacuum state $|0\rangle$ without any particle, i.e. to the presence of a hole, while a $d_n^\dagger$-boson implies that the site n is in the state $c_{\uparrow n}^\dagger c_{\downarrow n}^\dagger |0\rangle$, which is doubly occupied. The physical operators are given by

$$\sigma_n^+ = \exp\left(-\mathrm{i}\pi \sum_{m=1}^{n-1} \hat{Q}_m f_n^\dagger\right) \tag{3a}$$

$$c_{\uparrow n}^\dagger = \left(f_n^\dagger b_n + d_n^\dagger \exp\left(-\mathrm{i}\pi \sum_{m=1}^{n-1} \hat{Q}_m\right)\right) \exp(\mathrm{i}\pi \hat{N}_\uparrow) \tag{3b}$$

$$c_{\downarrow n}^\dagger = \left(b_n \exp\left(-\mathrm{i}\pi \sum_{m=1}^{n-1} \hat{Q}_m - d_n^\dagger f_n\right)\right) \exp(\mathrm{i}\pi \hat{N}_\uparrow) \tag{3c}$$

where now $\hat{Q}_n = f_n^\dagger f_n + b_n^\dagger b_n + d_n^\dagger d_n$ counts all particles and where there is a *constraint* that $Q_n \leqslant 1$, i.e. the particles have a hard core. It is straightforward to check that these obey the appropriate commutation rules when the site indices are different.

When the the site indices are the same it is *not* the case that $\{c_{\uparrow n}, c_{\uparrow n}^\dagger\} = 1$ if the algebra of the auxiliary particles is applied without strictly applying the constraint. What *is* easily verified is that the matrix elements of say $c_{\uparrow n}^\dagger$ *on the physical sub-space* are correctly given; however, it is implied that in the product, for example $c_{\uparrow n}^\dagger c_{\uparrow n}$, it is necessary to include a physical complete set of states between the two operators. In this regard the present scheme differs from the traditional auxiliary particle scheme [2], for which this is not necessary. It is implied that care must be exercised when constructing, in particular, the auxiliary particle version of the Hamiltonian. Every physical operator, for the site n, can be written in terms of the product of one or two of the new auxiliary particles since any operator can be written in terms of

$$\begin{array}{lll}
|\downarrow\rangle\langle\downarrow| = 1 - (f_n^\dagger f_n + b_n^\dagger b_n + d_n^\dagger d_n) & |\uparrow\rangle\langle\uparrow| = f_n^\dagger f_n & \\
|0\rangle\langle 0| = b_n^\dagger b_n & |\uparrow\downarrow\rangle\langle\uparrow\downarrow| = d_n^\dagger d_n & \\
|0\rangle\langle\uparrow| = b_n^\dagger f_n & |\uparrow\downarrow\rangle\langle\uparrow| = d_n^\dagger f_n & |\uparrow\downarrow\rangle\langle 0| = d_n^\dagger b_n \\
|\uparrow\rangle\langle\downarrow| = \exp\left(-\mathrm{i}\pi \sum_{m=1}^{n-1} \hat{Q}_m\right) f_n^\dagger & & \\
|0\rangle\langle\downarrow| = \exp\left(-\mathrm{i}\pi \sum_{m=1}^{n-1} \hat{Q}_m\right) \exp(\mathrm{i}\pi \hat{N}_\uparrow) b_n^\dagger & & \\
|\uparrow\downarrow\rangle\langle\downarrow| = \exp\left(-\mathrm{i}\pi \sum_{m=1}^{n-1} \hat{Q}_m\right) \exp(\mathrm{i}\pi \hat{N}_\uparrow) d_n^\dagger & &
\end{array} \tag{4}$$

and their Hermitian conjugates.

For the one-dimensional t–J model the phase operators, $\exp(\mathrm{i}\pi \hat{N}_\uparrow)$ and $\exp(-\mathrm{i}\pi \sum_{m=1}^{n-1} \hat{Q}_m)$, cancel and the result is

$$\begin{aligned}
\mathcal{H} = -t \sum_n (f_n^\dagger b_n b_{n+1}^\dagger f_{n+1} + b_n^\dagger b_{n+1} + \text{H.c.}) + \frac{J}{2} \sum_n (f_n^\dagger f_{n+1} + \text{H.c.}) \\
+ \frac{J}{4} \sum_n (2 f_n^\dagger f_n + b_n^\dagger b_n)(2 f_{n+1}^\dagger f_{n+1} + b_{n+1}^\dagger b_{n+1}) - J \hat{N}_\uparrow.
\end{aligned} \tag{5}$$

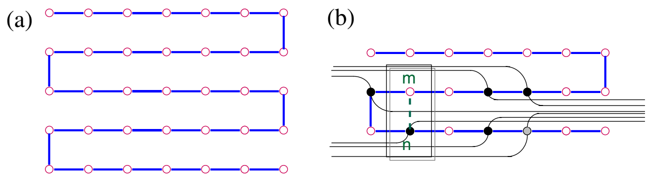

Figure 1. (a) The zig-zag path used for the Jordan–Wigner transformation. (b) The 'string' flux lines used to evaluate the sign changes due to the Jordan–Wigner transformation.

The Hubbard model becomes

$$\mathcal{H} = -t \sum_n (f_n^\dagger b_n b_{n+1}^\dagger f_{n+1} + d_n^\dagger f_n f_{n+1}^\dagger d_{n+1} + b_n^\dagger b_{n+1} + d_n^\dagger d_{n+1} + \mathrm{H.c.}) + U d_n^\dagger d_n$$
$$-t \sum_n \left(f_n^\dagger b_n d_{n+1} \exp\left(-\mathrm{i}\pi \sum_{m=1}^{n} \hat{Q}_m\right) + d_n f_{n+1}^\dagger b_{n+1} \exp\left(-\mathrm{i}\pi \sum_{m=1}^{n-1} \hat{Q}_m\right)\right.$$
$$\left. + d_n^\dagger f_n b_{n+1}^\dagger \exp\left(-\mathrm{i}\pi \sum_{m=1}^{n} \hat{Q}_m\right) + b_n^\dagger d_{n+1}^\dagger f_{n+1} \exp\left(-\mathrm{i}\pi \sum_{m=1}^{n-1} \hat{Q}_m\right) + \mathrm{H.c.}\right). \quad (6)$$

Even in one dimension, for the Hubbard model, the JW formulation leads to non-cancelling factors of $\exp\left(-\mathrm{i}\pi \sum_{m=1}^{n-1} \hat{Q}_m\right)$ while in two dimensions the occurrance of these factors is quite general. The challenge is therefore to develop a formalism in which these factors can be systematically accounted for. The transformation can be used for a two-dimensional system once a mapping to one dimension is defined. One possible map, shown in figure 1(a), is to use a zig-zag path whence even for the t–J model the factors of $\exp\left(-\mathrm{i}\pi \sum_{m=1}^{n-1} \hat{Q}_m\right)$ appear. Each site is ordered by a single site label and the sum in this factor simply counts the number of particles with smaller such labels. It is well known that, for example, the up spins of the problem, which are equivalent to hard-core bosons, might be converted to fermions by attaching a unit flux tube. The awkward factors of $\exp\left(-\mathrm{i}\pi \sum_{m=1}^{n-1} \hat{Q}_m\right)$ in fact represent such flux tubes in a certain 'string' gauge.

Consider the appropriate such phase factor for vertical exchange J-coupling, between sites n and m, as shown in figure 1(b). The appropriate term in the Hamiltonian is easily seen to be

$$\exp\left(-\mathrm{i}\pi \sum_{q=n+1}^{m-1} \hat{Q}_q\right) J(f_m^\dagger f_n + \mathrm{H.c.}) \qquad n < m \quad (7)$$

where the sum $\sum_{q=n+1}^{m-1} \hat{Q}_m$ counts the number of particle between the two sites following the prescribed path. The resulting phase factor $\exp\left(-\mathrm{i}\pi \sum_{q=n+1}^{m-1} \hat{Q}_q\right)$ can be evaluated using the diagram method illustrated in this figure. To each particle are attached two lines or 'strings', as shown, which leave the system without crossing the zig-zag path, i.e. leave by the open ends. It follows that

$$\exp\left(-\mathrm{i}\pi \sum_{q=n+1}^{m-1} \hat{Q}_q\right) = (-1)^L \quad (8)$$

where L is the number of lines which cross a straight line joining the sites n and n'. Put differently, L is the number of lines cut when the particle hops from site n to site m. In a fermion plus flux tube formulation the same phase factor would be $\exp[-\mathrm{i} \int_n^m \vec{a} \cdot \mathrm{d}\vec{r}]$, where $\vec{a}$ is an appropriately defined vector potential. The identification is therefore

$$\int \vec{a} \cdot \mathrm{d}\vec{r} = \pi L. \quad (9)$$

Any path which encloses a single particle cuts two lines and has

$$\int \vec{a} \cdot \mathrm{d}\vec{r} = 2\pi \tag{10}$$

corresponding to a single flux quantum. Evidently different mappings from one to two dimensions correspond to a different version of this JW string gauge. The phase factors appropriate to the correlation function are also determined, for example

$$\langle [S_n^+(t), S_m^-(0)] \rangle = (-1)^{L_{nm}} \langle [f_n^\dagger(t), f_m(0)] \rangle \tag{11}$$

where L_{nm} is the number of lines crossed for any path joining the sites n and m which does not pass through any particle. (It need not necessarily follow bonds.)

With this method, for example, the full t–J model for a two-dimensional square lattice is

$$\begin{aligned}\mathcal{H} = &- \sum_{\langle ij \rangle} (t f_i^\dagger b_i b_j^\dagger f_j + t_{ij} b_i^\dagger b_j + \mathrm{H.c.}) + \sum_{\langle ij \rangle} \frac{J_{ij}}{2} (f_i^\dagger f_j + \mathrm{H.c.}) \\ &+ \frac{J}{4} \sum_{\langle ij \rangle} (2 f_i^\dagger f_i + b_i^\dagger b_i)(2 f_j^\dagger f_j + b_j^\dagger b_j) - J(2\hat{N}_\uparrow + \hat{N}_0)\end{aligned} \tag{12}$$

where $t_{ij} = (-1)^{L_{ij}} t$ and $J_{ij} = (-1)^{L_{ij}} J$ and where L_{ij} is the number of strings crossed in going for the site i to j as described above. Here $\hat{N}_0 = \sum_i b_i^\dagger b_i$. There is no factor $(-1)^{L_{ij}}$ in the $f_i^\dagger b_i b_j^\dagger f_j$ term since the factors $\exp\left(-\mathrm{i}\pi \sum_{m=n+1}^{n'-1} \hat{Q}_m\right)$ cancel. (The term involves the exchange of particles and hence each crosses the same number of strings and the total number is necessarily even.) These factors also cancel in the static interaction term with the prefactor $\frac{J}{4}$. (Here there is no movement of particles and hence no strings are crossed.)

It is rather obvious, for the, $x = 0$, undoped case, that for the physical correlation function $\langle [S_n^+(t), S_m^-(0)] \rangle = (-1)^{L_{nm}} \langle [f_n^\dagger(t), f_m(0)] \rangle$ the string prefactor $(-1)^{L_{nm}}$ cancels against the similar factors in J_{ij} contained in the propagator and that hence this quantity is gauge invariant. In the doped case the same result is less obvious since the spin particle can propagate by an exchange with a holon (or doublon) and such a hopping process does not 'see' the flux. *However*, the holon (or doublon) must move on a closed path and in the end the $(-1)^{L_{nm}}$ factors involved in closing the path compensate. Similarly for charge propagators, for example, within the t–J model $\langle T_\tau c_{n\downarrow}^\dagger(\tau) c_{m\downarrow}(0) \rangle = (-1)^{L_{nm}} \langle T_\tau b_n(\tau) b_m^\dagger(0) \rangle$ and similar statements can be made. Thus in general, for example,

$$\langle [S_n^+(t), S_m^-(0)] \rangle = \exp\left[-\mathrm{i} \int_n^m \vec{a} \cdot \mathrm{d}\vec{r} \right] \langle [f_n^\dagger(t), f_m(0)] \rangle. \tag{13}$$

When making potential gauge transformations it is worth noting that the sense of a unit flux tube is immaterial. In particular, for a bipartite lattice, alternating the sense of the flux according to the sub-lattice is an easy way to avoid making gauge transformations which create (unphysical) currents at the boundaries.

Important also is the observation that, with the JW gauges, all matrix elements of $\mathcal{H}$ are real. For such a Hamiltonian matrix it is a trivial fact that either the ground state vector (i) is real (or can be made real with a simple change of phase) and therefore carries not currents or (ii) is degenerate. In case (ii) the real and imaginary parts of the ground state vector correspond to degenerate states which also carry no current. Case (ii) does *not* exclude the possibility of broken symmetry ground states which carry currents. If the degeneracy of the ground state is associated with the spin part of the wavefunction then there must be a finite value of $S(S+1) = \hat{S}^2$; i.e., such degenerate ground states must have a net ferromagnetic moment, albeit as small as $S = 1/2$.

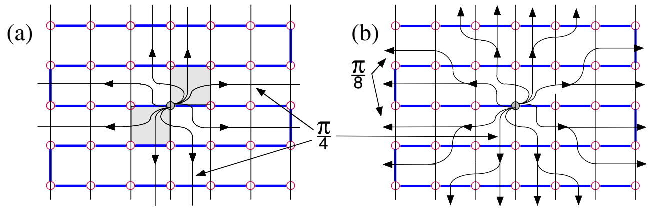

Figure 2. (a) The $\pi/4$ string gauge transformation. There is an effective half flux quantum in the shaded squares. (b) The equivalent with $\pi/8$ strings.

Up to this point the flux tubes have been attached to the particles. It is equally possible to attach the flux tubes, and the false charge which sees them, to the 'empty', i.e. down spin sites. This scheme will be assumed in what follows.

It is clearly possible to associate an operator with a flux tube at a given site. In the operator $u_n(\{\hat{Q}_i\}) = \exp[-\mathrm{i}\int_0^{n-1} \vec{a}\cdot \mathrm{d}\vec{r}]$ the integral from the origin to site n passes by any path which does not include particles and specifically along some path which does not pass through any sites. The argument $\{\hat{Q}_i\}$ indicates that u_n is a function of the position of all of the particles, or more precisely reflects the position of all of the down spin sites since it is these which determine $\vec{a}$. Clearly this is a unitary operator such that $u_n^\dagger u_n = u_n u_n^\dagger = 1$. For a JW gauge $u_n^\dagger = u_n$. Trivially these $u_n^\dagger$ operators commute with each other but anti-commute with the particle operators. This formal development permits the, for example, $t_{ij} b_i^\dagger b_j$ term to be written as

$$-t b_i^\dagger u_i u_j^\dagger b_j \tag{14}$$

and, for example, $c_{i\downarrow}^\dagger = u_i^\dagger b_i$. It should be noted that these unitary operators always appear in such a fashion that $u_i^\dagger$ is associated with the creation of a down spin site *along with a flux tube* while u_i only occurs when such a tube is destroyed. Using these operators the t–J model,

$$\begin{aligned}\mathcal{H} = -t \sum_{\langle ij\rangle} (f_i^\dagger b_i b_j^\dagger f_j + b_i^\dagger u_i u_j^\dagger b_j + \text{H.c.}) + \sum_{\langle ij\rangle} \frac{J}{2}(f_i^\dagger u_i u_j^\dagger f_j + \text{H.c.}) \\ + \frac{J}{4}\sum_{\langle ij\rangle}(2f_i^\dagger f_i + b_i^\dagger b_i)(2f_j^\dagger f_j + b_j^\dagger b_j) - J(2\hat{N}_\uparrow + \hat{N}_0).\end{aligned} \tag{15}$$

The present JW gauge does not reflect the symmetries of the lattice and in addition the interaction between fermions which is induced by the π-flux strings is of infinite range. The usual gauge with $\vec{a} = (1/r)\vec{\phi}$ is an evident alternative but is not particularly adapted to lattice problems. It is simpler to adapt a different string gauge. Each π string can be thought of as made of four $\pm\pi/4$ strings, where the sign is arbitrary. Separating one such string and moving it so it cuts different bonds, see figure 2(a), amounts to some gauge transformation. (The flux pattern is such that there is an effective half flux tube in each of the two shaded plaquettes.) If instead $\pi/8$ strings are used it is possible to have the gauge convention shown in figure 2(b). Continuing this bifurcation process will lead to interactions which $\sim(1/r)$. The arrow indicates the sign of the phase change. As in electrostatics, a positive magnetic flux tube with arrows heading away from the tube will have positive sign changes when a particle crosses a line heading in a clockwise direction.

It is of interest to generalize the present approach to bi-layers and three dimensions in general. While the fermion-plus-flux-tube type of aynon does not generalize to three dimensions there is no real problem with applying the JW transformation. A bi-layer can

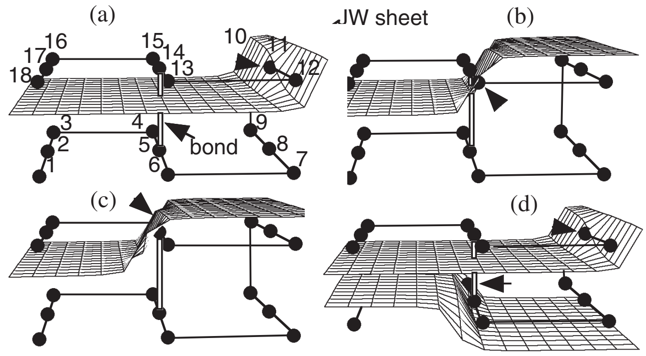

Figure 3. (a) An 18-site bi-layer is viewed as being a single folded plane and the zig-zag path $1, 2, \ldots, 17, 18$ is designated on that plane. (Site 10 is hidden behind the sheet but can be seen in (b) and (c).) The JW sheet is attached to site 11, which lies on the path between the illustrated bond between sites 5 and 14. That the sheet cuts this bond implies that the sign of the bond changes. (b) A similar JW sheet attached to site 13 also lies on the path between these sites and the sheet cuts the bond, indicating again that such a particle causes a change of sign. However in (c) the sheet attached to site 15 is not on the path between 5 and 14 and indeed the sheet does not cut the bond indicating that there is no change in sign. In general there are many sheets as in (d). The sheet attached to site 4 in the lower plane does not cut the bond and there is therefore only a single change of sign associated with the particle at site 11. Explicitly the sheet which passes through site 11, coordinates $x = -1$, $y = 0$ and $z = 1$, was generated by $z = 1 - 0.4\tan^{-1}[3(y + 4\tan^{-1}\{3(x+1)\})]$.

be considered as a single sheet which is folded over and the single sheet is then reduced to one dimension using again, for example, the zig-zag path of figure 1(a). A fully three-dimensional system can similarly be mapped to a corrugated sheet and then the sheet reduced to one dimension. On two dimensions the JW transformation is effected by attaching π flux strings to the particles. The generalization to three dimensions is to attach sheets to each particle. Consider, by way of illustration, the 18-site bi-layer shown in figure 3. By design, if a sheet is cut at the level of a given plane then the resulting line has the same topology as the flux strings of figure 1 and the sign of a intra-plane bond (not shown) is given, as before, by $(-1)^L$ where L is the number of such lines, or now sheets, which cross a bond. Each site on the zig-zag path, indicated by the black lines, has been labelled and advances in the sense $1, 2, \ldots, 17, 18$ as shown in figure 3(a). Focus attention on the white bond which connects sites 5 and 14. Within the JW transformation the sign associated with this bond is $(-1)^S$ where S is the number of particles on the sites $6, 7, \ldots, 12, 13$ which lie between the ends of the bond on the prescribed path. The number S is counted using the JW sheets. In figure 3(a) the sheet is attached to a particle at site 11, identified by an arrow. This sheet cuts the bond indicating, correctly, that this site must be included in S. Similarly, figure 3(b), the sheet attached to site 13 cuts the bond and is to be reflected in S. However site 15 which lies on the same row as this latter site should not have an effect on S and indeed, figure 3(c), the sheet attached to this site does not cut the bond. Of course, in general there are many particles and many sheets which potentially are reflected in the factor $(-1)^S$. In figure 3(d) are shown two sheets, the one attached to site 4 is not in the sequence $6, 7, \ldots, 12, 13$ and the sheet does not cut the bond between 5 and 14, while, as described above that attached to the site at 11 does, and should, cut the bond. Notice the sheets never cross the zig-zag path.

When two particles are interchanged it is necessarily the case that one particle hops through the JW sheet of the other particle an odd number of times thereby converting the fermions to hard-core bosons. Once defined with a specific zig-zag path, deforming the sheets amounts to a gauge transformation, and a π sheet can be separated into n, π/n sheets which can be deformed almost at will. In this way the interactions between particles, reflected by the sheets, can be made short ranged.

(At a technical level it is to be noted that the generalization of two-dimensional flux strings as three-dimensional JW sheets is a special case corresponding to hard-core bosons. In two dimensions anyons are realized when the π-strings are replaced by $\alpha_s\pi$-strings where α_s is the usual statistical parameter defined relative to fermions. Now the sense of the string phase shift matters. In order to have a finite attached flux the string phase shift must change sign upon passing through a particle. Since it is possible to pass from one side of a particle to the other on the JW sheet this method cannot be used to directly generalize anyons to three dimensions. *However* $\alpha_s\pi$ JW sheets *do* represent a possible extrapolation between fermions and bosons in three dimensions which reduces to flux strings in two dimensions *but* without the sign change. In is easy to appreciate that in any dimension the corresponding $\vec{a} = \nabla\phi(\vec{r})$ with a suitable $\phi(\vec{r})$; i.e., the flux is strictly zero.)

Whatever the dimension, the *bare* vacuum $|\rangle_{-N/2}$ reflects the absence of particles and comprises the spin state with $S_z = -N/2$. It is important that the bare ferromagnetic vacuum state is highly degenerate. A new vacuum $|\rangle_{-N/2+1} = (S_0^+/M_{-N/2}^{-N/2+1})|\rangle_{-N/2}$ is obtained by acting with the total spin raising operator S_0^+ where $M_n^m = \sqrt{S(S+1)-nm}$. The *physical* spin vacuum $|S\rangle$ comprises the Fermi spin sea. To be specific define this as

$$|S\rangle = \prod_{\epsilon_{\vec{k}}\leqslant 0} f_{\vec{k}}^\dagger |\rangle_{-N/2} \tag{16}$$

where $\epsilon_{\vec{k}} \propto -\gamma_{\vec{k}}$; $\gamma_{\vec{k}} = \cos k_x + \cos k_y$. Given that there are $N/2$, f-particles (and that this is an integer) this is a spin *singlet*. Although this description of $|S\rangle$ is appealing, it is sometimes more appropriate to imagine $|S\rangle$ as derived from the $S_z = 0$ bare vacuum $|\rangle_0$. In the wavefunction $f_{\vec{k}}^\dagger$ is replaced by $p_\uparrow = \sqrt{2}(\frac{1}{2}+S_{n\,z})$ and the empty (down) sites are projected out using $p_\downarrow = \sqrt{2}(\frac{1}{2} - S_{n\,z})$. With this $|S\rangle = F(\{S_{n\,z}\})|\rangle_0$, where $\{S_{n\,z}\}$ is the collection of local z-component spin operators.

The states $f_{\vec{k}}^\dagger|S\rangle$ and $f_{-\vec{k}}|S\rangle$ are momentum $\vec{k}$ excitations with $S_z = \pm 1$ respectively and are related by a particle–hole symmetry at half-filling. In addition to these f-particle excitations are similar states generated by the flux tube operators u_i. A arbitrary state with a given vacuum $S_z = n$ is of the form $F_1(\{S_{n\,z}\})|\rangle_n$ and an typical matrix element of u_i is

$$\begin{aligned}
{}_m\langle|F_2^* u_i F_1|\rangle_n &= {}_m\langle|F_2^* u_i (f_i^\dagger f_i + f_i f_i^\dagger) F_1|\rangle_n \\
&= \big[{}_n\langle|F_2^* f_i F_1|\rangle_{n+1}\delta_{m,n} + {}_n\langle|F_2^* f_i^\dagger F_1|\rangle_{n-1}\delta_{m,n} \\
&\quad + {}_{n+1}\langle|F_2^* f_i^\dagger F_1|\rangle_n \delta_{m,n+1} + {}_{n-1}\langle|F_2^* f_i F_1|\rangle_n \delta_{m,n+1}\big] + \cdots
\end{aligned} \tag{17}$$

where the ellipsis reflects terms which are vacuum on-diagonal. Use is made of the fact that both u_i and the projectors $p_\uparrow = f_i^\dagger f_i$ and $p_\downarrow = f_i f_i^\dagger$ commute with the $F_n(\{S_{n\,z}\})$ and each other, and that for example, $u_i f_i^\dagger f_i = N^{-3/2}\sum_{\vec{k}\vec{k}'\vec{k}''}\exp(\mathrm{i}\vec{k}\cdot\vec{r}_n)\exp(\mathrm{i}\vec{k}'\cdot\vec{r}_n)\exp(\mathrm{i}\vec{k}''\cdot\vec{r}_n) u_{\vec{k}} f_{\vec{k}'}^\dagger f_{\vec{k}''}$. The vacuum off-diagonal part corresponds to contracting out a factor of $S^\pm/N$. This occurs in two ways for each term to give (17). The two vacuum diagonal terms have a different number of particles in the final state, corresponding to (spin) particle–hole excitations. The result can be written symbolically as

$$u_i = \tfrac{1}{2}[f_i S^+ + f_i^\dagger S^- + S^+ f_i + S^- f_i^\dagger] + \cdots \tag{18}$$

with the understanding that for, for example, in $S^+ f_i$ the S^+ acts only on the $|\rangle_0$ vacuum to the left. The ellipsis represents terms which are necessarily diagonal in the bare vacuum state. Since u_n is unitary $u_n|S\rangle$ is a normalized state vector and it is to be noted that the four vacuum off-diagonal terms displayed above exhausted exactly one half of this normalization. The on-diagonal ellipsis, evidently, has equal weight.

That, when it acts on the physical vacuum, the flux tube operator u_n can create excitations (with a cancelling change in the total S_z) is also evident from a comparison between $S_{zn} + 1/2 = f_n^\dagger f_n$ and $S_n^+ = f_n^\dagger u_n$. The effect of these two operators acting upon the singlet physical vacuum must be essentially the same; i.e., the effect of u_n is the same as f_n *but* without a change in S_z. Multiplying (18) by f_n^+ gives $S_n^+ = f_n^\dagger f_n (S^+/N) + (S^+/N) f_n f_n^\dagger$. (There is no commutator with S^+ in the last term because of the understanding that this acts on the vacuum to the left.)

Upon examining the ensemble of physical operators it should be observed that these can be consistently interpreted in terms of f-particles which are $S = 1/2$ *spinons* with $S_z = +1/2$ while the flux-tube particles are the equivalent with $S_z = -1/2$.

For the t–J model, in the absence of doping, the spin sector kinetic energy is generated by the vacuum diagonal part of the transverse exchange, i.e.

$$+\frac{J}{2} f_i^\dagger u_i u_j^\dagger f_j. \tag{19}$$

For a near uniform state this must have an expansion $+\frac{J}{2} f_i^\dagger u_i u_j^\dagger f_j = a^1 f_i^\dagger f_j + f_i^\dagger f_j \sum a_m^2 \delta n_m$ where the δn_m are deviations from the uniform state. Since, by definition $a^1 = \langle u_i u_j^\dagger \rangle$ does not depend upon the uniform state involved, it can be evaluated, with a suitable gauge, for a state vector which is an equal weight of the two Néel states. Both states have a uniform field with one half a flux quantum per plaquette and in a (non-JW) gauge which reflects the symmetry of the lattice this implies that the change of phase introduced by the $u_i u_j^\dagger \to \exp(\pm \mathrm{i}\pi/4)$. There are no direct matrix elements between these two states and so a^1 is given by a simple average of these two phases; i.e., the leading term site diagonal part of (19) is

$$+\frac{J}{2} \cos\frac{\pi}{4} f_i^\dagger f_j \equiv \frac{J'}{2} f_i^\dagger f_j \tag{20}$$

with $J' = J/\sqrt{2}$. Thus, for example, for two dimensions the bare energy of an excitation of momentum $\vec{k}$ is $\epsilon_{\vec{k}} = 2J'\gamma_{\vec{k}}$.

The next term in the expansion of (19), written as $+\frac{J}{2} S_i^+ S_j^-$, is obtained using the vacuum off-diagonal part of S_n^+ deduced above. There are four equivalent contributions to give the result,

$$+Jf_i^\dagger f_i f_j f_j^\dagger + \mathrm{H.c.} \Rightarrow +Jf_i^\dagger f_j^\dagger \langle f_j f_i \rangle + \mathrm{H.c.} \equiv \pm\Delta_0 f_i^\dagger f_j^\dagger + \mathrm{H.c.} \tag{21}$$

which admits a pair amplitude. With suitable signs, the Fourier transform corresponds to d-wave pairing, i.e. a term

$$\frac{1}{N} \sum_{\vec{k}} \Delta_{\vec{k}} f_{\vec{k}}^\dagger f_{-\vec{k}}^\dagger + \mathrm{H.c.} \tag{22}$$

where $\Delta_{\vec{k}} = \Delta_0(\cos k_x - \cos k_y)$. Clearly, the original exchange term does not change the value of S_z and the pairing in (22) is to be interpreted in terms of $\vec{k}$, $S_z = 1/2$ and $-\vec{k}$, $S_z = -1/2$ spinon pairs.

The final version (15) of the JW formalism would appear very similar to the usual auxiliary (slave boson) particle scheme. The down spin fermion has been replaced by a flux tube operator $u_i^\dagger$. However this parallel is *very* misleading. In terms of up and down fermions the transverse exchange is $+\frac{J}{2} \sum_{\langle ij \rangle} (f_{\uparrow i}^\dagger f_{\downarrow i} f_{\downarrow j}^\dagger f_{\uparrow j} + \mathrm{H.c.})$. Invariably in the 'slave boson' approach this interaction is subjected to a mean field factorization:

$$-\sum_{\langle ij \rangle} \frac{J}{2} \langle f_{\downarrow j}^\dagger f_{\downarrow i} \rangle f_{\uparrow i}^\dagger f_{\uparrow j} + \mathrm{H.c.} \tag{23}$$

which changes the sign and reduces the magnitude of the matrix elements for the hopping of the spin particles. This latter philosophy is very attractive since it separates the up and down degrees of freedom and leads to an identification of the $f^\dagger_{\sigma i}$ as spinons, i.e. spin 1/2 particles. The cost is that the constraint is all but sacrificed. The point of the present formalism is precisely to maintain this constraint exactly and yet to show that the excitations are indeed spinons.

The present formalism has its own natural approximations. If $t \gg J$, the motion of the holes is certainly rapid compared to the dynamics of the lowest-lying spin levels. If the concentration of holes is sufficient there will occur a motional averaging of the spin wave function. The co-movement of the spins, as the holes hop, will cause the spinon–spinon interactions to be averaged and suppress the associated correlations (and ordering). Given their rapid motion, the holons can be added by perturbation theory. On the charge timescale the spins can be considered as frozen. Consider a given up spin at site n, it sees itself in a virtual crystal in which there is a certain density of holes at near neighbour sites. This up spin then admixes with the holes on the neighbour sites and this implies a probability $\sim xt/|\mu| \to x$ of observing a hole at n. Whatever the details, it is implied that the state which was $f^\dagger_n|\rangle$ now becomes

$$(\alpha f^\dagger_n + \beta b^\dagger_n u^\dagger_n)|\rangle \equiv \tilde{f}^\dagger_n|\rangle \tag{24}$$

where $|\alpha|^2 + |\beta|^2 = 1$ with the concentration of holes $x = |\beta|^2$ and where the flux tube $u^\dagger_n$ is needed in order that $\tilde{f}^\dagger_n$ have fermion commutation rules. A Fermi sea is now constructed from the Fourier transform of the $\tilde{f}^\dagger_n$. The combination found in $\tilde{f}^\dagger_n$ implies a pairing between the $b^\dagger_n$ *holons* and f_n. This can be associated with Kondo physics since with a small β the excitations are relatively heavy. Likewise, by spin symmetry, the state for a down spin site,

$$u^\dagger_n|\rangle \to (\alpha u^\dagger_n + \beta b^\dagger_n u^\dagger_n)|\rangle. \tag{25}$$

With $S_z = 0$, the presence of a $\tilde{f}^\dagger_n$ particle implies a probability of $1-x$ of finding an up spin at site n, and there are $N/2$ such particles independent of x. In total, there are $(N/2)(1+x)$ degrees of freedom for such a system and the present 'Kondo' approximation implies that there are only $N/2$ low-energy excitations and that these are predominantly 'spinon-like' with a small admixture of holon character. For low enough energies, the remaining holes are reflected (25) as a renormalization of the vacuum. The site independence of β implies a holon *condensate* with $\vec{q} = 0$. The admixture of holon character into the f-particles implies that the term, for example $-tb^\dagger_i u_i u^\dagger_j b_j$ contributes to the hopping matrix elements for these renormalization particles. As a result $J' \to J_e = (1-x)J' - 2xt$. With this approximation, the effective Hamiltonian is

$$\mathcal{H}_s = J_e \sum_{\vec{k}} \gamma_{\vec{k}} \big(\tilde{f}^\dagger_{\vec{k}} \tilde{f}_{\vec{k}} + \text{H.c.}\big) + (1-x)^2 \sum_{\vec{k}} \big[\Delta_{\vec{k}} \tilde{f}^\dagger_{\vec{k}} \tilde{f}^\dagger_{-\vec{k}} + \text{H.c.}\big]. \tag{26}$$

All interactions between spinons and holons which appeared in (15) have been dropped since these will be averaged towards constants by the rapid hole motion. The physical conduction electron propagators $\langle T_\tau c^\dagger_{n\uparrow}(\tau) c_{m\uparrow}(0)\rangle = c\langle T_\tau f_n(\tau) f^\dagger_m(0)\rangle$, i.e. are c, the fraction of sites with a *condensed* holon, times the spinon propagators.

Of considerable importance is the fact that the kinetic energy is proportional to $J_e = \big(J' - 2xt\big)$. Nagaoka's theorem [3] implies that a small hole doping favours ferromagnetism. The ferromagnetic, i.e. negative sign of the $2xt$ reflects this fact. (This is the itinerant hole version of ring exchange.) Clearly the anti-ferromagnetic J'-term must have the opposite sign. As a consequence, *in the absence of pairing*, this Hamiltonian would exhibit a quantum critical point (QCP) at $x_c = (J'/2t)$ at which the spinon band collapses. Clearly the specific heat and magnetic susceptibility diverge at such a point. Since superconductivity is favoured by such a large density of states, T_c will be a maximum near x_c and superconductivity will 'hide' this QCP. This might be described as a pseudo-QCP with the real QCP being shifted to smaller concentrations at which the holons condensate and superconductivity first appears.

This work was supported by a Grant-in-Aid for Scientific Research on Priority Areas from the Ministry of Education, Science, Culture and Technology of Japan, CREST. SEB is on sabbatical leave from the Physics Department, University of Miami, FL, USA and wishes to thank the members of IMR for their kind hospitality. SM acknowledges support of the Humboldt Foundation.

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