Brief Reports

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Ground-state quantum numbers of the half-filled Hubbard model

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Working on a square lattice with an even number of sites N^2 and assuming a smooth connection between strong and weak coupling, we show that the ground state of the two-dimensional half-filled Hubbard model has momentum $k_x = k_y = 0$, it is even under reflections, and transforms as an s wave under rotations when $N/2$ is even and as a d wave when $N/2$ is odd.

The discovery of high-T_c superconductivity[1] renewed interest in the study of the properties of the two-dimensional (2D) Hubbard model. Two of the important questions that an analysis of this model should answer is whether there is pair formation[2] and what is the symmetry under rotations of the operator that creates such a pair from the half-filled background. Numerical simulations seem to indicate[3] that the d-wave pairing susceptibility is enhanced at low temperatures suggesting that the ground state at half filling should have a different sign under rotations than the ground state with two holes. Exact diagonalization of a 2×2 lattice shows that the ground state at half-filling has d-wave symmetry while the two holes' lowest state has s-wave symmetry. On the other hand, the situation seems to be reversed on a 4×4 lattice.[4] This is a puzzling result if one notices that the strong-coupling limit of the half-filled Hubbard model corresponds to the Heisenberg model[5] where exact diagonalization of 2×2 and 4×4 lattices shows[6] that the ground state has s-wave symmetry in both cases.

In this Brief Report we clarify this paradox, confirming that the results reported for the 2D Hubbard model are correct and showing that the ground state for a half-filled Hubbard system on a $N\times N$ lattice is s (d) wave when $N/2$ is even (odd).

Our derivation is as follows. We know that for $U/t \gg 1$ the half-filled Hubbard Hamiltonian maps into a Heisenberg model[5] with $J = 4t^2/U$. For this model there is a theorem[7] that applies to lattices that can be divided into two equivalent sublattices A and B, such that A spins interact antiferromagnetically only with B spins and vice versa. This is the case for the Heisenberg model on a square lattice with an even number of sites, nearest-neighbors interactions, and periodic boundary conditions. The theorem states that any symmetry operator $\hat{O}$ that transforms the two sublattices into one another has eigenvalues $O = (-1)^{N^2 S}$ for the antiferromagnetic ground state. N^2 is the number of sites of the lattice and S is the spin of each site variable ($S = \frac{1}{2}$ in our case).

Consider the operators $\hat{T}_x$ and $\hat{T}_y$ that generate translations of the lattice by one lattice spacing in the direction x and y, respectively, and have eigenvalues $T_l = e^{ik_l} = e^{2\pi i n_l/N}$, where l is x or y, n_l ranges between 0 and $N-1$, and k_l is the momentum in the direction l. $\hat{T}_x$ and $\hat{T}_y$ satisfy the conditions of the theorem showing that $T_l = 1$ (or equivalently $k_x = k_y = 0$) for the ground state of the Heisenberg model on a square lattice with an even number of sites N^2. Another operator that fulfills the conditions of the theroem is $\hat{R}$, an operator that rotates the lattice by $\pi/2$ about an axis perpendicular to the lattice plane, passing through the center of any minimal square of four sites. For a square lattice, it has four possible eigenvalues: 1 (s wave), -1 (d wave), and $\pm i$. The theorem predicts $R = 1$ implying that the ground state of the Heisenberg model has s-wave symmetry. The theorem can also be applied to reflections in the x and y directions showing that under these operations the ground state is even. All these results have been checked by exact diagonalization studies on small lattices[6] so the situation in the Heisenberg model is very clear.

Now we analyze the Hubbard model. The first step is to consider our particles (spins in the Heisenberg framework, electrons within the Hubbard picture) as fermions instead of bosons. Thus, we need a convention to order the electrons of the lattice in a "one-dimensional" pattern. Our election for a square lattice is the following:

$$\begin{matrix} N^2-N+1 & N^2-N+2 & \cdots & N^2 \\ N^2-2N+1 & N^2-2N+2 & \cdots & N^2-N \\ \vdots & \vdots & & \vdots \\ N+1 & N+2 & \cdots & 2N \\ 1 & 2 & \cdots & N \end{matrix} \quad (1)$$

At every site we put first the spin down and then the spin up. For example, a Néel state that has particles with spin up (down) on even (odd) sites, is written as

$$c^\dagger_{1,\downarrow}c^\dagger_{2,\uparrow}c^\dagger_{3,\downarrow}\cdots c^\dagger_{N^2-2,\downarrow}c^\dagger_{N^2-1,\uparrow}c^\dagger_{N^2,\downarrow}|0\rangle \,. \quad (2)$$

The (arbitrary) way in which we order the fermions is very important to correctly keep track of the signs under permutations. The Hamiltonian eigenvalues and other physical quantities are, of course, independent of the convention. In the strong-coupling limit where there is one particle per site we have another possibility: We can treat the spins as bosons simply forgetting the signs under permutations (bosonic representation). Consider then the Heisenberg Hamiltonian defined as

$$H=J\sum_{\langle i,j\rangle}\mathbf{S}_i\cdot\mathbf{S}_j \,, \quad (3)$$

where $\langle i,j\rangle$ are neighboring sites and $S_i^k=c^\dagger_{i,\alpha}\sigma^k_{\alpha\beta}c_{i,\beta}$ are spin operators, $c^\dagger_{i,\alpha}$ creates a fermion with spin α ($\alpha=\uparrow,\downarrow$) at site i, and σ^k are Pauli matrices. With our particular choice and working in the basis defined by Eqs. (1) and (2), the matrix representation of H does not have any sign difference between the bosonic and fermionic conventions. This can be proved as follows: The nondiagonal part of the Hamiltonian can produce a change of sign if there is an odd number of permutations of fermionic operators over each other. However, with our convention this does not happen because the nondiagonal part is proportional to

$$S_i^+S_j^-=c^\dagger_{i,\uparrow}c_{i,\downarrow}c^\dagger_{j,\downarrow}c_{j,\uparrow} \,, \quad (4)$$

then the pair of operators at site j "jumps" over all the fermionic operators before site j without introducing a minus sign. The same happens with the pair of operators at site i. This means that the Hamiltonian matrix will be the same in the fermionic or bosonic base.

No signs appear either when we apply translations or reflections to any arbitrary state in the lattice Eq. (2). Then a state with $k_x=0$ will be given by a sum of N terms all with the same coefficient. Every term j is obtained by translating the original state j lattice spacings in the direction x. For example, on a 2×2 lattice a state with $k_x=0$ is

$$\begin{pmatrix}\uparrow & \downarrow\\ \uparrow & \downarrow\end{pmatrix}+\begin{pmatrix}\downarrow & \uparrow\\ \downarrow & \uparrow\end{pmatrix}, \quad (5)$$

and a state with $k_x=\pi$ is

$$\begin{pmatrix}\uparrow & \downarrow\\ \uparrow & \downarrow\end{pmatrix}-\begin{pmatrix}\downarrow & \uparrow\\ \downarrow & \uparrow\end{pmatrix}, \quad (6)$$

and these quantum numbers are the same in both the bosonic and fermionic convention.

However, minus signs appear under certain circumstances in the fermionic case when we rotate the lattice by $\pi/2$. The effect of applying $\hat{R}$ to the configuration Eq. (1) is

$$\begin{matrix} N^2 & N^2-N & \cdots & 2N & N \\ \vdots & \vdots & & \vdots & \vdots \\ N^2-N+2 & N^2-2N & \cdots & N+2 & 2 \\ N^2-N+1 & N^2-2N+1 & \cdots & N+1 & 1 \end{matrix} \quad (7)$$

When fermionic operators jump over each other minus signs appear. To go from Eq. (7) to Eq. (1) an overall $[(-1)^{N/2}]^{N-1}=(-1)^{N/2}$ will appear. To show that, we will try to reposition all the elements in Eq. (7). Element 1 will provide a factor $(-1)^{N-1}$ because it has to jump over $N-1$ fermions, element 2 will have to jump over $2(N-1)$ fermions providing a factor $(-1)^{2(N-1)}$, elements j with $j=3$ up to N will provide $(-1)^{j(N-1)}$ each. Then after rearranging an entire row we see that the number of minus signs is $N/2$. We will obtain $(-1)^{N/2}$ for all the rows that we will arrange except for the last one; this provides the factor $[(-1)^{N/2}]^{N-1}=(-1)^{N/2}$ that states that a minus sign will appear if $N/2$ is odd. This tells us that if the ground state in the bosonic convention transforms as an s wave under rotations, for $N/2$ odd it will transform as a d wave when we use a fermionic convention. As a simple example consider for a 2×2 lattice the following state

$$\begin{pmatrix}\uparrow & \downarrow\\ \uparrow & \downarrow\end{pmatrix}+\begin{pmatrix}\downarrow & \downarrow\\ \uparrow & \uparrow\end{pmatrix}+\begin{pmatrix}\downarrow & \uparrow\\ \downarrow & \uparrow\end{pmatrix}+\begin{pmatrix}\uparrow & \uparrow\\ \downarrow & \downarrow\end{pmatrix}, \quad (8)$$

which has s-wave symmetry for bosons but d-wave symmetry for fermions, while the state

$$\begin{pmatrix}\uparrow & \downarrow\\ \uparrow & \downarrow\end{pmatrix}-\begin{pmatrix}\downarrow & \downarrow\\ \uparrow & \uparrow\end{pmatrix}+\begin{pmatrix}\downarrow & \uparrow\\ \downarrow & \uparrow\end{pmatrix}-\begin{pmatrix}\uparrow & \uparrow\\ \downarrow & \downarrow\end{pmatrix} \quad (9)$$

has d-wave symmetry for bosons and s-wave symmetry for fermions. An interesting detail is that using a different convention to order fermions on the lattice, all spins down first for example, we would obtain a different Hamiltonian matrix and different eigenstates, but the conclusion about the quantum numbers would be the same.

Then we know that the ground state for the half-filled 2D Hubbard Hamiltonian with large U/t has momentum $k_x=k_y=0$, transforms evenly under reflections about the x and y axis, and have s-wave symmetry (even under rotations) if $N/2$ is even and d-wave symmetry (odd under rotations) if $N/2$ is odd. In principle, our results are valid in the Hubbard model for those values of U/t in a region analytically connected to the strong-coupling regime where the Heisenberg model is a good approximation to the problem. However, since numerical results based on quantum Monte Carlo techniques do not show any indication of a phase transition as a function of U/t for the 2D Hubbard model, we conclude that these results are in fact valid for all values of U/t.

Our prediction is in agreement with the exact results obtained for the 2×2 Hubbard model where the ground state has d-wave symmetry for all values of U and for the 4×4 lattice[4] with $U=4$ (not in the strong-coupling regime) where the ground state has s-wave symmetry.

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