Exact Ground State of the 2D Hubbard Model at Half Filling for $U = 0^+$

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We solve analytically the $N \times N$ square lattice Hubbard model for even $N$ at half filling and weak coupling by a new approach. The exact ground state wave function provides an intriguing and appealing picture of the antiferromagnetic order. Like at strong coupling, the ground state has total momentum $K_{\text{tot}} = (0, 0)$ and transforms as an $s$ wave for even $N/2$ and as a $d$ wave otherwise.

The 2D Hubbard model is one of the simplest descriptions of itinerant interacting electrons on a lattice. The Lieb theorem [1] states that at half filling the ground state for a bipartite lattice is unique and has spin $\frac{N}{2}$, where $|S_1|$ ($|S_2|$) is the number of sites in the $S_1$ ($S_2$) sublattice; here and in the following, $|S|$ will be the number of elements in the set $S$. For a $N \times N$ (with even $N$) square lattice, the ground state is a singlet. In Ref. [2] it was shown that in the strong coupling limit the ground state has total momentum $K_{\text{tot}} = (0, 0)$ and has $s$-wave or $d$-wave symmetry for even or odd $N/2$, respectively.

In this paper we build the exact ground state of the Hubbard model at half filling in the weak coupling limit. We find the same quantum numbers as predicted by Refs. [1] [2], and this result strongly supports the conjecture that no phase transition takes place for finite values of the Coulomb interaction parameter $U$.

Let us consider the Hubbard model with hamiltonian

$$H = H_0 + W = \sum_{r} \sum_{\sigma} \epsilon_r c_{r\sigma}^\dagger c_{r\sigma} + \sum_{r} U \hat{n}_r \hat{n}_{\bar{r}}, \quad U > 0$$

on a square lattice of $N \times N$ sites with periodic boundary conditions and even $N$. Here $\sigma = \uparrow, \downarrow$ is the spin and $r$, $r'$ the spatial degrees of freedom of the creation and annihilation operators $c_r^\dagger$ and $c_r$ respectively. We represent sites by $r = (i_x, i_y)$ with $i_x, i_y = 0, \ldots, N - 1$. The sum on $(r, r')$ is over the pairs of nearest neighbor sites and $\hat{n}_{r\sigma}$ is the number operator on the site $r$ of spin $\sigma$. The point symmetry is $C_{4v}$, the Group of a square [3]. We Fourier expand the fermion operators: $c_{k\sigma} = \frac{1}{\sqrt{N}} \sum_r e^{ikr} c_r^\sigma$, where $k = (k_x, k_y) = 2\pi (i_x, i_y)$; then, $H_0 = \sum_k \epsilon(k) c_{k\sigma}^\dagger c_{k\sigma}$ where $\epsilon(k) = 2t(\cos k_x + \cos k_y)$. The starting point is the following property of the number operator $\hat{n}_r = c_r^\dagger c_r$ (for the moment we omit the spin index).

Theorem: Let $S$ be an arbitrary set of plane-wave eigenstates $\{|k_i\rangle\}$ of $H_0$ and $\langle n_r | i_j = \langle k_i | \hat{n}_r | k_j \rangle = \frac{1}{N} \sum_{r} e^{i(k_i - k_j)r} \text{ the matrix of } \hat{n}_r \text{ in } S$. This matrix has eigenvalues $\lambda_1 = \frac{|S|}{N}$ and $\lambda_2 = \ldots = \lambda_{|S|} = 0$.

Note that $|S| \leq N^2$: if $|S| = N^2$ the set is complete, like the set of all orbitals, and the theorem is trivial (a particle on site $r$ is the $\hat{n}_r$ eigenstate with eigenvalue 1). Otherwise, if $|S| < N^2$, the theorem is an immediate consequence of the fact [3] that

$$\det(\langle n_r | i_j - \lambda \delta_{ij} |) = (-\lambda)^{|S|-1}\left(\frac{|S|}{N^2} - \lambda\right), \quad \forall r.$$  

Let $S_{hf}$ denote the set (or shell) of the $k$ wave vectors such that $\epsilon(k) = 0$. These $k$ vectors lie on the square having vertices $(\pm \pi, 0)$ and $(0, \pm \pi)$; one can show that the number of solutions, that is, the dimension of the set $S_{hf}$, is $|S_{hf}| = 2N - 2$. At half filling ($N^2$ holes) for $U = 0$, $S_{hf}$ is half occupied.

In the $S_z = 0$ sector there are $\left(\frac{2N - 2}{N - 1}\right)^2$ degenerate unperturbed ground state configurations for $N^2$ holes, where all $|k|$ orbitals such that $\epsilon(k) < 0$ are occupied. The first-order splitting of the degeneracy is obtained by diagonalizing the $W$ matrix over the unperturbed basis; like in elementary atomic physics, the filled shells just produce a constant shift of all the eigenvalues and for the rest may be ignored in first-order calculations. In other terms, we consider the truncated Hilbert space $\mathcal{H}$ spanned by the states of $N - 1$ holes of each spin in $S_{hf}$, and we want the exact ground state(s) of
W in \( \mathcal{H} \): by construction \( \mathcal{H} \) is the kernel of \( H_0 \), so the ground state of \( W \) is the ground state of \( H \) as well. We call \( W = 0 \) state any vector in \( \mathcal{H} \) which also belongs to the kernel of \( W \). Since the lowest eigenvalue of \( W \) is zero, it is evident that any \( W = 0 \) state is a ground state of \( H \). We want to calculate the unique ground state of the Hubbard Hamiltonian for \( \ell = 0^+ \) at half filling which is a \( W = 0 \) singlet with \( 2N - 2 \) holes in \( \mathcal{H}_{4f} \) (filled shells are understood).

To diagonalize the local operator \( W \) in closed form we need to set up a local basis set of one-body states. If \( \mathcal{H}_{4f} \) were the complete set of plane-wave states \( |k \rangle \), the new basis would be trivially obtained by a Fourier transformation, but this is not the case. The question is: how can we define for each site \( r \) the local counterparts of \( k \) states using only those that belong to a degenerate level? The answer is: build a set \( \{ |\varphi^{(0)}_\alpha \rangle \} \) of orbitals such that the number operator \( \hat{n}_r \) and the Dirac characters of the point symmetry Group \( C_{4v} \) are diagonal. Using such a basis set for the half-filled shell the unique properties of the antiferromagnetic ground state become simple and transparent. The eigenvectors \( |\varphi^{(0)}_\alpha \rangle \) of \( n_r = 0 \) and those \( |\varphi^{(r)}_\alpha \rangle \) of other sites \( r \) are connected by translation and also by a unitary transformation, or change of basis set. Picking \( r = \hat{e}_i \), \( l = x \) means \( \hat{e}_i = (1, 0) \) or transfer by one step towards the right and \( l = y \) means \( \hat{e}_i = (0, 1) \) or transfer by one step upwards. The unitary transformation reads:

\[
|\varphi^{(r)}_\alpha \rangle = \sum_{\beta=1}^{2N-2} |\varphi^{(0)}_\beta \rangle \langle \varphi^{(0)}_\beta | \varphi^{(r)}_\alpha \rangle \equiv \sum_{\beta=1}^{2N-2} |\varphi^{(0)}_\beta \rangle T_{\alpha \beta}.
\]

(3)

The transfer matrix \( T_\alpha \) knows all the translational and point symmetry of the system, and will turn out to be very special.

For large \( N \), to find \( \{ |\varphi^{(r)}_\alpha \rangle \} \) it is convenient to separate the \( k \)'s of \( \mathcal{H}_{4f} \) in irreducible representations (irreps) of the space Group \( \mathbf{G} = C_{4v} \otimes T \); here \( T \) is the Abelian Group of the translations and \( \otimes \) means the semidirect product. Choosing an arbitrary \( k \in \mathcal{H}_{4f} \) with \( k_x \geq k_y \geq 0 \), the set of vectors \( R_{ik}k \), where \( R_i \in C_{4v} \), is a (translationally invariant) basis for an irrep of \( \mathbf{G} \): the accidental degeneracy of several irreps is due to the presence of extra symmetry, i.e. \( \mathbf{G} \) is a subgroup of the Optimal Group defined in [3]. The high symmetry vectors \( (0, \pi) \) and \( (\pi, 0) \) always transform among themselves and are the basis of the only two-dimensional irrep of \( \mathbf{G} \), which exists for any \( N \). If \( N/2 \) is even, one also finds the high symmetry wavevectors \( k = (\pm \pi/2, \pm \pi/2) \) which mix among themselves and yield a four-dimensional irrep. In general, the vectors \( R_{ik} \) are all different, so all the other irreps of \( \mathbf{G} \) have dimension 8, and the number of operations of the point Group \( C_{4v} \).

Next, we show how to build our local basis set and derive \( W = 0 \) states for each kind of irreps of \( \mathbf{G} \). For illustration, we will consider the case \( N = 4 \); then \( \mathcal{H}_{4f} \) contains the bases of two irreps of \( \mathbf{G} \), of dimensions 2 and 4. The one with basis \( k_A = (\pi, 0) \), \( k_B = (0, \pi) \) breaks into \( A_1 \oplus B_1 \) in \( C_{4v} \).

The eigenstates of \( (\nu=0) \) of (3) one finds that \( |\psi^{(0)}_{A_1} \rangle \leftrightarrow |\psi^{(0)}_{B_1} \rangle \) with \( \lambda_1 = 1/8 \) and \( |\psi^{(0)}_{B_1} \rangle = \frac{\sqrt{2}}{2} (|k_A \rangle + |k_B \rangle) \) with \( \lambda_0 = 1 \). Since under translation by a lattice step \( T_{1} \) along the \( l = k \) direction \( |k \rangle \rightarrow e^{i k j} |k \rangle \), using Equation (3) one finds that \( |\psi^{(0)}_{A_1} \rangle \leftrightarrow (-1)^{\theta^x} |\psi^{(0)}_{B_1} \rangle \), with \( \theta^x = 1 \), \( \theta^y = 0 \); so \( |\psi^{(r)}_{A_1} \rangle \) has vanishing amplitude on a sublattice and \( |\psi^{(r)}_{B_1} \rangle \) on the other. The two-body state \( |\psi^{(r)}_{A_1} \rangle |\psi^{(r)}_{B_1} \rangle \) has occupation for spin \( \sigma \) but not for spin \( -\sigma \) on the site \( r = 0 \); under a lattice step translation it flips the spin and picks up a \((-1)\theta^x\) phase factor: \( |\psi^{(r)}_{A_1} \rangle |\psi^{(r)}_{B_1} \rangle \rightarrow (-1)^{\theta^x} |\psi^{(r)}_{B_1} \rangle |\psi^{(r)}_{A_1} \rangle \); therefore it has double occupation nowhere and is a \( W = 0 \) state \( (W = 0 \) pair \( \boxtimes \) \( \boxtimes \)).

The 4-dimensional irrep with basis \( k_1 = (\pi/2, \pi/2) \), \( k_2 = (-\pi/2, \pi/2) \), \( k_3 = (\pi/2, -\pi/2) \) \( k_4 = (-\pi/2, -\pi/2) \) breaks into \( A_1 \oplus B_2 \oplus E \) in \( C_{4v} \); letting \( I = 1, 2, 3, 4 \) for the irreps \( A_1, B_2, E_x, E_y \) respectively, we can write down all the eigenvectors of \( (\nu=0) \) of \( C_{4v} \): with \( i, j = 1, \ldots, 4 \), as \( |\psi^{(i)}_j \rangle = \sum_{i=1}^4 O'_{ij} |k_i \rangle \), where \( O' \) is the following 4×4 orthogonal matrix:

\[
O' = \frac{1}{2} \begin{bmatrix}
1 & 1 & 1 & 1 \\
1 & -1 & -1 & 1 \\
1 & -1 & 1 & -1 \\
-1 & -1 & 1 & 1
\end{bmatrix}.
\]

(4)

The state with non-vanishing eigenvalue is again the \( A_1 \) eigensate. After a little bit of algebra we have shown [4] that under \( T_1 \) the subspace of \( A_1 \) and \( B_2 \) symmetry is exchanged with the one of \( E_x \) and \( E_y \) symmetry. Thus we can build a 4-body eigenstate of \( W \) with vanishing eigenvalue: \( |\psi^{(0)}_{A_1} \psi^{(0)}_{B_2} \rangle |\psi^{(r)}_{E_x} \psi^{(r)}_{E_y} \rangle \). As before under a lattice step translation this state does not change its spatial distribution but \( \sigma \rightarrow -\sigma \) without any phase factor: \( |\psi^{(0)}_{A_1} \psi^{(0)}_{B_2} \rangle \psi^{(r)}_{E_x} \psi^{(r)}_{E_y} \rangle \rightarrow \psi^{(r)}_{E_x} \psi^{(r)}_{E_y} \rangle \sigma |\psi^{(0)}_{A_1} \psi^{(0)}_{B_2} \rangle \sigma \).
Now we use these results to diagonalize $n_{r=0}$ on the whole set $S_{hf}$ (we could have done that directly by diagonalizing $6 \times 6$ matrices but we wanted to show the general method). The eigenstate of $n_{r=0}$ with nonvanishing eigenvalue always belongs to $A_1$. The matrix $n_r$ has eigenvalues $3/8$ and $(5$ times $)0$, as predicted by eq. (3). For $r = 0$ the eigenvector of occupation $3/8$ is $|\phi_1(0)\rangle \equiv |\phi_{1,A_1}\rangle = \frac{1}{\sqrt{3}}|\psi''_1\rangle + \sqrt{\frac{2}{3}}|\psi'_1\rangle$. The other $A_1$ eigenstate of $n_{r=0}$ has 0 eigenvalue and reads: $|\phi_2(0)\rangle \equiv |\phi_{2,A_1}\rangle = \sqrt{\frac{2}{3}}|\psi'_1\rangle - \frac{1}{\sqrt{3}}|\psi''_1\rangle$.

The other eigenvectors, whose symmetry differs from $A_1$, are $|\phi_3(0)\rangle \equiv |\phi_{B_2}\rangle = |\psi'_B\rangle$, $|\phi_5(0)\rangle \equiv |\phi_{E_2}\rangle = |\psi'_E\rangle$ and $|\phi_6(0)\rangle \equiv |\phi_{E_4}\rangle = |\psi''_E\rangle$. One finds that the transfer matrices $T_i$ of Equation (3) such that $|\phi'_{i,j}\rangle \equiv \sum_j |\phi_{i,j}\rangle T_{ij}$, are:

$$T_x = \begin{pmatrix} 0 & 0 & 0 & -\frac{1}{\sqrt{2}} & i\sqrt{\frac{2}{3}} & 0 \\ 0 & 0 & 0 & -\frac{2}{\sqrt{3}} & -\frac{i}{\sqrt{3}} & 0 \\ 0 & 0 & 0 & 0 & 0 & -i \\ -\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ i\sqrt{\frac{2}{3}} & i\sqrt{\frac{2}{3}} & 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 & 0 & 0 \end{pmatrix} , \quad T_y = \begin{pmatrix} 0 & 0 & 0 & \frac{1}{\sqrt{2}} & 0 & -i\sqrt{\frac{2}{3}} \\ 0 & 0 & 0 & \frac{2}{\sqrt{3}} & 0 & \frac{1}{\sqrt{3}} \\ 0 & 0 & 0 & 0 & i & 0 \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 \\ 0 & 0 & i & 0 & 0 & 0 \end{pmatrix} . \quad (5)$$

The reason why this choice of the basis set is clever is now apparent. The local basis at any site $r$ splits into the subsets $S_a = \{|\phi_{1,A_1}(r)\rangle, |\phi_{2,A_1}(r)\rangle, |\phi_{B_2}(r)\rangle\}$, and $S_b = \{|\phi_{E_2}(r)\rangle, |\phi_{E_4}(r)\rangle\}$; a shift by a lattice step sends members of $S_a$ into linear combinations of the members of $S_b$, and conversely.

Consider the 6-body eigenstate of $H_0$

$$|\Phi_{AF}(\sigma)\rangle = |\phi_{1,A_1}^{(0)}\phi_{2,A_1}^{(0)}\phi_{B_2}^{(0)}\phi_{E_2}^{(0)}\phi_{E_4}^{(0)}\rangle_\sigma |\phi_{2,A_1}^{(0)}\phi_{B_2}^{(0)}\phi_{E_2}^{(0)}\phi_{E_4}^{(0)}\rangle_{-\sigma} . \quad (6)$$

In this state there is partial occupation of site $r = 0$ with spin $\sigma$, but no double occupation. It turns out that a shift by a lattice step produces the transformation

$$|\Phi_{AF}(\sigma)\rangle \longleftrightarrow -|\Phi_{AF}(-\sigma)\rangle \quad (7)$$

that is, a lattice step is equivalent to a spin flip, a feature that we call antiferromagnetic property. Since the spin-flipped state is also free of double occupation, $|\Phi_{AF}(\sigma)\rangle$ is a $W = 0$ eigenstate. A ground state which is a single determinant is a quite unusual property for an interacting model like this.

Note that $|\phi_{1,A_1}^{(0)}\phi_{2,A_1}^{(0)}\rangle$ is equivalent to $|\psi''_1,\psi'_1\rangle$, because this is just a unitary transformation of the $A_1$ wave functions; so $|\Phi_{AF}(\sigma)\rangle$ can also be written in terms of the old local orbitals (without any mix of the local states of different irreps of $G$):

$$|\Phi_{AF}(\sigma)\rangle = |\psi''_1,\psi'_1\rangle |\psi''_1,\psi''_2\rangle \sigma |\psi''_1,\psi'_E\rangle |\psi''_E,\psi'_E\rangle_{-\sigma} . \quad (8)$$

This form of the ground state lends itself to be generalised (see below). For $N > 4$, $k$ vectors arise that do not possess any special symmetry, the vectors $R_1k$ are all different for all $R_i \in C_{4v}$, and we get eight-dimensional irreps of $G$. Recalling that $|S_{hf}| = 2N - 2$, one finds that $S_{hf}$ contains $N_\sigma = \frac{1}{2}(N - 2)$ irreps of dimension 8, one of dimension 4 and one of dimension 2 if $N/2$ is even and $N_\sigma = \frac{1}{2}(N - 1)$ irreps of dimension 8 and one of dimension 2 if $N/2$ is odd.

To extend the theory to general $N$, we note that these $k$ vectors, since $R_1k$ are all different, are a basis of the regular representation of $C_{4v}$. Thus, by the Burnside theorem, each of them breaks into $A_1 \oplus A_2 \oplus B_1 \oplus B_2 \oplus E \oplus E$; diagonalizing $n_{r=0}$ and the point Group characters on the basis of the $m$-th eight-dimensional irrep of $G$ one gets one-body states $|\psi_{m}\rangle$, where $I$ stands for the $C_{4v}$ irrep label, $I=A_1, A_2, B_1, B_2, E_x, E_y, E'_x, E'_y$; here we denote by $E'$ the second occurrence of the irrep $E$. The ground state wave function in $H$ for the half filled case is a generalized version of Equation (8). For even $N/2$, we have

$$|\Phi_{AF}(\sigma)\rangle = \prod_{m=1}^{N_\sigma} |\psi_{A_1}\rangle |\psi_{B_2}\rangle |\psi_{E_2}\rangle |\psi_{E_4}\rangle |\psi_{A_1}\rangle |\psi_{B_2}\rangle |\psi_{E_2}\rangle |\psi_{E_4}\rangle_{-\sigma} \prod_{m=1}^{N_\sigma} |\psi_{A_2}\rangle |\psi_{B_1}\rangle |\psi_{E_x}\rangle |\psi_{E_y}\rangle |\psi_{E_x}\rangle |\psi_{E_y}\rangle_{-\sigma} . \quad (9)$$
with $\sigma = \uparrow, \downarrow$. For odd $N/2$, $|\Phi_{AF}\rangle_\sigma$ is similar but the maximum $m$ is $N_\sigma$ and the $|\psi\rangle$ states do not occur. $|\Phi_{AF}\rangle_\sigma$ is a $W = 0$ state, transforms into $-|\Phi_{AF}\rangle_-\sigma$ for each lattice step translation and manifestly shows an antiferromagnetic order (antiferromagnetic property). Since $W$ is a positive semidefinite operator $|\Phi_{AF}\rangle_\sigma$ is actually a ground state. In the basis of local states these are the only two determinantal states ($\sigma = \uparrow, \downarrow$) with the above properties.

A few further remarks about $|\Phi_{AF}\rangle_\sigma$ are in order. 1) Introducing the projection operator $P_S$ on the spin $S$ subspace, one finds that $P_S|\Phi_{AF}\rangle_\sigma \equiv |\Phi_{AF}^S\rangle_\sigma \neq 0$, $\forall S = 0, \ldots, N - 1$. Then, $\sigma \langle \Phi_{AF}|W|\Phi_{AF}\rangle_\sigma = \sum_{S=1}^{N-1} \sigma \langle \Phi_{AF}^S|W|\Phi_{AF}^S\rangle_\sigma = 0$, and this implies that there is at least one ground state of $W$ in $\mathcal{H}$ for each $S$. The actual ground state of $H$ at weak coupling is the singlet $|\Phi^0_{AF}\rangle_\sigma$.

2) The existence of this singlet $W = 0$ ground state is a direct consequence of the Lieb theorem [1]. Indeed the maximum spin state $|\Phi^{N-1}_{AF}\rangle_\sigma$ is trivially in the kernel of $W$; since the ground state must be a singlet it should be an eigenvector of $W$ with vanishing eigenvalue. 3) The above results and Lieb’s theorem imply that higher order effects split the ground state multiplet of $H$ and the singlet is lowest. 4) The Lieb theorem makes no assumptions concerning the lattice structure; adding the ingredient of the $G$ symmetry we are able to explicitly display the wave function at weak coupling.

Using the explicit form of $P_{S=0}$ one finds that $P_{S=0}|\Phi_{AF}\rangle_\sigma = -P_{S=0}|\Phi_{AF}\rangle_-\sigma$. This identity allows us to study how the singlet component transforms under translations, reflections and rotations. We have found [2] that the total momentum is $K_{tot} = (0, 0)$. To make contact with Ref. [2] we have also determined how it transforms under the $C_{4\pi}$ operations with respect to the center of an arbitrary plaquette. It turns out that it is even under reflections and transforms as an $s$ wave if $N/2$ is even and as a $d$ wave if $N/2$ is odd. The present approach lends itself to obtain exact results for other fillings as well, but this will be shown elsewhere [11].

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[1] E. H. Lieb, Phys. Rev. Lett. 62 1201 (1989).
[2] A. Moreo and E. Dagotto, Phys. Rev. B 41, 9488 (1990).
[3] $C_{4\pi}$ is the symmetry Group of a square. It is a finite Group of order 8 and it contains 4 one dimensional irreps, $A_1$, $A_2$, $B_1$, $B_2$, and 1 two-dimensional one called $E$. The table of characters is

| $C_{4\pi}$ | $C_2$ | $C_2^{(+)}$, $C_2^{(-)}$ | $\sigma_x$, $\sigma_y$, $\sigma_x'$, $\sigma_y'$ |
|-----------|-------|-----------------|-----------------|
| $A_1$     | 1     | 1               | 1               |
| $A_2$     | 1     | -1              | -1              |
| $B_1$     | 1     | -1              | 1               |
| $B_2$     | 1     | -1              | -1              |
| $E$       | 2     | -2              | 0               |

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