CANONICAL TRANSFORMATION OF THE HUBBARD
MODEL AND W=0 PAIRING: COMPARISON WITH EXACT
DIAGONALIZATION RESULTS

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Received (2000)

We have recently developed a canonical transformation of the Hubbard and related models, valid for systems of arbitrary size and for the full plane; this is particularly suited to study hole pairing. In this work we show that exact diagonalization results of the one band Hubbard model for small clusters with periodic boundary conditions agree well with the analytical ones obtained by means of our canonical transformation. In the presence of a pairing instability, the analytic approach allows us to identify the Cooper pairs. They are W=0 pairs, that is, singlet two-hole eigenstates of the Hubbard Hamiltonian with vanishing on-site repulsion. Indeed, we find that the Coulomb interaction effects on W=0 pairs are dynamically small, and repulsive or attractive, depending on the filling.

1 Introduction: the Hubbard model

Let us consider the Hubbard model on a square lattice of $N \times N$ sites, with Hamiltonian

$$H = H_0 + W,$$

where

$$H_0 = t \sum_{\sigma} \sum_{(r,r')} c^\dagger_{r\sigma} c_{r'\sigma}$$

(1)
with \( r, r' \) nearest neighbours and

\[
W = U \sum_r \Delta n_{\sigma r} n_{\bar{\sigma} r}.
\]  

(3)

We use periodic boundary conditions and the one-body wave vectors are \( k = (k_x, k_y) = \frac{2\pi}{N} (p, q) \) with \( p \) and \( q \) integers.

\section{W=0 pairs}

The strong on-site repulsion between two opposite spin fermions normally prevents the formation of singlet bound states. However, the planar square symmetry of the Hubbard and related models allows singlet two body eigenstates of \( H_0 \) belonging to the zero eigenvalue of \( W \). We will refer to these states as W=0 pairs. This means that the two fermions of a W=0 pair do not interact directly, but only by means of virtual electron-hole excitations. The background particles play a crucial role in determining the structure of the effective interaction which can be, in principle, attractive or repulsive.

In previous works\textsuperscript{1,2} we have shown how to build W=0 pairs with zero total momentum. There the idea was to project the determinantal state

\[
|d(k)\rangle = c_k^\dagger c_{-k}^\dagger |\text{vac}\rangle
\]

(4)
on the Irreducible Representations (irreps) of the point symmetry group \( C_{4v} \). Remarkably, by projecting on the irreps \( A_2 \), \( B_1 \) and \( B_2 \) one obtains exclusively W=0 pairs. Here we want to point out a new and more general criterion to get W=0 pairs. Let \( G \) a symmetry group of the non interacting Hubbard Hamiltonian \( H_0 \), big enough to justify the degeneracy of the single particle energy levels. Let us consider a two body state of opposite spins transforming as the \( i \)-th component of the irrep \( \Gamma \) of \( G \):

\[
|\Psi^{(\Gamma)}_i(r, r)\rangle = \sum_{r_1, r_2} \Psi^{(\Gamma)}_i(r_1, r_2) c_{r_1, \uparrow}^\dagger c_{r_2, \downarrow}^\dagger |\text{vac}\rangle
\]

(5)

Then we have

\[
n_{\uparrow r} n_{\downarrow r} |\Psi^{(\Gamma)}_i\rangle = \Psi^{(\Gamma)}_i(r, r) c_{r, \uparrow}^\dagger c_{r, \downarrow}^\dagger |\text{vac}\rangle \equiv \Psi^{(\Gamma)}_i(r, r) |r, \uparrow, \downarrow\rangle.
\]

(6)

Let \( P^{(\Gamma)}_i \) be the projection operator on the \( i \)-th component of the irrep \( \Gamma \). Since

\[
P^{(\Gamma)}_i \sum_r \Psi^{(\Gamma)}_i(r, r) |r, \uparrow, \downarrow\rangle = \sum_r \Psi^{(\Gamma)}_i(r, r) |r, \uparrow, \downarrow\rangle
\]

(7)

if

\[
P^{(\Gamma)}_i |r, \uparrow, \downarrow\rangle = 0 \quad \forall r
\]

(8)

then

\[
\Psi^{(\Gamma)}_i(r, r) = 0 \quad \forall r.
\]

(9)
Clearly eq. (8) is true if and only if
\[ P^{(r)}_{i} |r\sigma\rangle = 0 \quad \forall r \]
where \(|r\sigma\rangle = c^\dagger_{r\sigma} |\text{vac}\rangle\).

It is always possible to write \(|r\sigma\rangle\) as
\[ |r\sigma\rangle = \sum_{\Gamma \in E} \sum_{i} c_{i}^{(\Gamma)}(r) |\varphi^{(\Gamma)}_{i,\sigma}\rangle \]  
(10)
where \(E\) is the set of the irreps of the one-body spectrum of \(H_{0}\) and \(|\varphi^{(\Gamma)}_{i,\sigma}\rangle\) the corresponding eigenstate with spin \(\sigma\). From (10) it follows directly that if \(\Gamma'\) does not belong to \(E\)
\[ P^{(\Gamma')} |r\sigma\rangle = 0 \]
and so
\[ P^{(\Gamma')} |\uparrow, \downarrow\rangle = 0. \]

We have proven the following

**THEOREM:** Let \(|\Psi\rangle\) be a two-body eigenstate of the kinetic energy \(H_{0}\) with spin \(S_{z} = 0\). Projecting \(|\Psi\rangle\) on an irrep not contained in \(E\), we get either zero or an eigenstate of \(H_{0}\) with no double occupancy.

The singlet component of this state is a \(W=0\) pair, and its momentum does not generally vanish.

### 3 Binding energy: analytic approach

From now on we call hole the fermion created by \(c^\dagger\) and electron its antifermion.

The Schrödinger equation for the ground state of our \(N \times N\) square lattice with \(n_{h}\) holes is
\[ H |\Psi_{0}\rangle = E_{h}(n_{h}) |\Psi_{0}\rangle. \]  
(11)
If the non interacting ground state with \(n_{h} - 2\) holes can be written in terms of a single determinantal state, the exact \(|\Psi_{0}\rangle\) can always be expanded in terms of excitations over it:
\[ |\Psi_{0}\rangle = \sum_{m} a_{m} |m\rangle + \sum_{\alpha} b_{\alpha} |\alpha\rangle + \sum_{\beta} c_{\beta} |\beta\rangle + \ldots \]  
(12)

here \(m\) runs over pair states, \(\alpha\) over 4-body states (2 holes and 1 electron-hole pair), \(\beta\) over 6-body ones (2 holes and 2 electron-hole pairs) and so on. Eq. (12) is an expansion in the number of virtual excitations.

In the following we set up a procedure which 1) carries out the “Configuration Interaction” calculation in a compact and efficient way 2) separates neatly the effective interaction from the self-energy contributions to the ground state energy. To understand how this mechanism works, for the moment we truncate the expansion to the \(\beta\) states. Then equation (11) yields
\[ (E_{m} - E_{h}(n_{h})) a_{m} + \sum_{m'} a_{m'} W_{m,m'} + \sum_{\alpha} b_{\alpha} W_{m,\alpha} + \sum_{\beta} c_{\beta} W_{m,\beta} = 0 \]  
(13)
Choosing the $\beta$ states in such a way that
\[(H_0 + W)_{\beta\beta'} = E'_\beta \delta_{\beta\beta'}\]
we exactly decouple the 6-body states getting
\[(E_m - E_h(n_h)) a_m + \sum_{m'} a_{m'} W_{m,m'} + \sum_{\alpha} b_{\alpha} W_{m,\alpha} = 0\]
\[(E_\alpha - E_h(n_h)) b_\alpha + \sum_{m'} a_{m'} W_{\alpha,m'} + \sum_{\alpha'} b_{\alpha'} W_{\alpha,\alpha'} = 0\]
where $W'$s are the renormalized interaction coefficients. It is clear that if we had truncated the expansion to an arbitrary number $n$ of electron-hole virtual excitations, we should have obtained the same results but with further renormalizations. This is a recursion method to perform the full canonical transformation; it applies to all the higher order interactions, and we can recast our problem as if only 2 and 4-body states existed. Now we choose the $\alpha$ states in such a way that
\[(H_0 + W')_{\alpha,\alpha'} = E'_\alpha \delta_{\alpha,\alpha'}\]
getting the following eigenvalue problem
\[(E_h(n_h) - E_m) a_m = \sum_{m'} a_{m'} \langle m | F[E_h(n_h)] + W_{eff}[E_h(n_h)] | m' \rangle,\]
where
\[\langle m | F[E_h(n_h)] + W_{eff}[E_h(n_h)] | m' \rangle = W'_{m,m'} + \sum_{\alpha} \frac{\langle m | W' | \alpha \rangle \langle \alpha | W' | m' \rangle}{E_h(n_h) - E'_\alpha}.\]
Equation (16) determines the amplitudes $a_m$ of the $m$ states in the $n_h$ hole ground state and the corresponding eigenvalue $E_h(n_h)$ relative to the hole vacuum. Here $F$ is the forward scattering operator and $W_{eff}$ the **effective interaction**. After the shift
\[H_0 \to H_0 - E_h(n_h - 2),\]
it is perfectly consistent to interpret $a_m$ as the wave function of the **dressed pair**. It is worth to underline that this canonical transformation enables us to identify the effective interaction between two holes in a $n_h - 2$ holes background self-consistently. In principle we can work it out analytically and the expansion is neither in $U$ nor in $t$ but in the number of virtual excitations. It permits us to identify the binding energy $|\Delta(n_h)|$ too. After the shift (18) we write the ground state energy $E_h(n_h)$ of the Hubbard Hamiltonian as
\[E_h(n_h) = 2E_F + \Delta(n_h)\]
where $E_F$ is the renormalized Fermi energy and $\Delta(n_h)$ the two holes energy gain of the interacting system with respect to the non interacting one. If the effective interaction $W_{\text{eff}}$ is attractive and $\Delta(n_h) < 0$ we can speak of hole pairing.

4 Pairing in the 4×4 lattice Hubbard model

In this section we want to compare the results for the binding energy $|\Delta(n_h)|$ obtained 1) from eq.(19) by truncating the canonical transformation to the $\alpha$ states and 2) from the definition

$$\Delta(n_h) = E_h(n_h) + E_h(n_h - 2) - 2E_h(n_h - 1) \quad (20)$$

by computing exactly the three ground state energies involved in eq.(20). The equivalence of the two definitions of the binding energy was shown in Refs[2],[6].

We consider a 4×4 lattice Hubbard model with $t = -1$ and periodic boundary conditions; we investigate the possibility of pairing when two holes are added to a two hole background. The one particle energy spectrum of $H_0$ has 5 equally spaced levels having degeneracy 1,4,6,4,1 respectively.

Our first task is to determine of the symmetry group $G$. The Space Group containing the translations and the 8 $C_4v$ operations is not enough to explain the degeneracy 6. Indeed the largest dimension of the irreps of the Space Group for this 4×4 lattice is 4. The Space Group has 128 elements and 20 classes.

As observed by previous authors3,4 there must be additional space symmetries. We have found how to obtain them. Label the sites from 1 to 16 in the natural way; then rotate the plaquettes 1,2,5,6 and 11,12,15,16 clockwise and the other two counterclockwise by 90 degrees. This is one of the missing space symmetries, as one can see that each site preserves its first neighbours. It is not an isometry. The other missing symmetries are generated by adding this one to the Space Group. In this way we obtain the Symmetry Group $G$ of 384 elements, which is large enough to justify the degeneracy of each one particle energy level. It still has 20 classes; the dimensions of the irreps are 1,1,1,1,2,2,3,3,3,3,4,4,4,4,4,4,6,6,6,6,8,8.

The exact interacting ground state of the system with 4 holes is threefold degenerate and belongs to an irrep of $G$ that contains the irreps $A_1$ and $B_1$ of $C_4v$ once and two times respectively. This irrep is not contained in the one particle spectrum of $H_0$, which does not admit degeneracy 3. By the above theorem, pairs belonging to it must be $W=0$ pairs. These $W=0$ pairs arise from the single-particle states of $H_0$ with eigenvalue -2, and their irrep is contained in the square of the irrep of the single-particle level.

The $m$ states of the expansion (12) are all the $W=0$ pairs belonging to the ground state irrep. We have computed the binding energy $|\Delta(4)|$ analitically from eq.(19) by truncating the expansion (12) to the $\alpha$ states and also by means of exact diagonalization from eq.(20). The results are listed below for different values of the on-site interaction $U$ (energies are in eV):
As expected, with increasing $U$ the difference $|\Delta(4)_{\text{exact}} - \Delta(4)_{\text{analytic}}|$ increases because the renormalization induced by virtual electron-hole excitations becomes important and it is no longer a good approximation to consider the $\alpha$ states only. Nevertheless the canonical transformation still predicts the right sign of $\Delta$.

The above canonical transformation applies when two holes are added to a determinantal vacuum. To study the system at and close to half filling, we have extended the above canonical transformation to the case when the vacuum is degenerate. We are able to demonstrate analytically that holes pair and to explain the ground state symmetries that were found numerically in Ref.\cite{3},\cite{5}. Thus, $W=0$ pairs are responsible for pairing and for the symmetry of the interacting ground state. This is also confirmed by the superconducting quantization of magnetic flux; in previous works\cite{2,6} we show that the $C_{4v}$ symmetry is restored exactly at half fluxon $\phi_0/2 = hc/2e$ allowing the existence of $W=0$ pairs. The symmetry of the interacting ground state is still the same of the possible $W=0$ pairs and the corresponding energy versus flux has there a second minimum. A full account of the theory will be submitted elsewhere\cite{7}. It is clear by now, however, that the existence of bound pairs of nonvanishing momentum opens up the possibility of a Jahn-Teller distortion and the present approach is likely to predict charge inhomogeneities.

**Acknowledgements**

This work has been supported by the Istituto Nazionale di Fisica della Materia.

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