Numerical results for generalized RVB wavefunctions.
Application to the Hubbard model

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Abstract :
Numerical results are presented for a generalized resonance valence bond state which includes both ionic and covalent contributions in each bond; non nearest-neighbor bonds are also considered. Variational calculations have been performed and the space group symmetry has been taken into account. The results for the Hubbard Hamiltonian are compared with the exact ones for the $2 \times 2$ and the $4 \times 4$ lattices. The agreement is quite satisfactory for large values of the interaction $U$ (for $U=40$ the overlap with the exact ground state wave function is 0.999). Several correlation functions are also compared.

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1. Introduction.

It is still under debate if the 2D one-band Hubbard model can provide the basic physics of high temperature superconductivity. Independently of this, and in spite of the obvious oversimplification introduced by the model in describing a strongly correlated electron system, the theoretical challenge offered by the 2D Hubbard model is certainly full of fascinating and unsolved problems. Only rough and tentative phase diagrams concerning antiferromagnetism, ferromagnetism and superconductivity have been produced, mainly in the large $U$ case, where the Hubbard model maps into the $t - J$ model.

It is interesting to compare the situation of our present knowledge of the Hubbard model and the theory of the fractional quantum Hall effect (FQHE). Both theories refer to strongly interacting two-dimensional electron systems; however the situation is much more satisfactory in the FQHE case, not only because of the simplicity of the experimental results, but for another fundamental reason: in the FQHE case we have at our disposal a valid theoretical tool, provided by the Laughlin's wave function [1]. All subsequent theories, like Jain's theory [2], make use of this beautiful form of the wave function.

In the case of the Hubbard model, we do not have a form of the wave function quite as satisfactory.

Many years ago, Gutzwiller [3] proposed a wave function obtained by applying a suitable operator to the Fermi sea wave function. The physical idea is simple: one tries to reproduce the main effect of the interaction, by weighting with a factor $\eta^D$ all the configurations containing $D$ doubly occupied sites; $\eta$ is a variational parameter. The interesting $\eta = 0$ case corresponds to a state with no doubly occupied sites (Gutzwiller projection).

The Gutzwiller wavefunction $\psi_G$ provides a noticeable insight into the physics of the Hubbard model. However, the expectation values with respect to $\psi_G$ cannot be computed without making some approximations. Furthermore the value of the ground state energy, tested in finite size cases, is not more accurate than the one given by the Hartree-Fock solution (spin density wave).

In 1987 Anderson [4] proposed that the electronic wave function of a high $T_c$ superconductor is a ”resonating valence-bond” (RVB) state. This state is obtained as the Gutzwiller projection of a BCS state with definite particle number. It can also be considered as a superposition of valence bond states, i.e. states describing pairs of electrons in different sites coupled to a spin singlet. A ”covering” of the lattice is a state in which all the electrons are coupled in pairs.

A number of calculations (see, e.g. [5] ) have been performed on the RVB state, especially in a simplified version in which only singlets formed by nearest-neighbor electrons are allowed (NNRVB). Almost all these works refer to the Heisenberg and $t$-$j$ two-dimensional models. Calculations involving NNRVB states are made possible by simple graphic rules [6],[7].
In this type of approach the Gutzwiller projection is not necessary, since the coverings of a lattice at half-filling are products of dimers created by operators like $C_{ij} = c_{i\uparrow} c_{j\downarrow} + c_{i\downarrow} c_{j\uparrow}$, where $i$ and $j$ are nearest-neighbor sites and $c_{i\uparrow}, c_{i\downarrow}$ denote the usual creation operators; therefore no doubly occupied site occurs.

It is interesting to notice that long before Anderson’s proposal of the RVB state for strongly interacting electrons, some theoretical chemists, Choi and Thorson [8] computed the one and two-particle density matrices for a generalized RVB state, both for a linear chain and a $4 \times 4$ lattice. By ”generalized RVB state” we mean an RVB state such that the operator $O_{ij}^+$ creating the valence bond between the sites $i$ and $j$ contains not only a covalent term $C_{ij}^+$, but also a ionic contribution $I_{ij}^+ = c_{i\uparrow} c_{i\downarrow} + c_{j\downarrow} c_{j\uparrow}$; therefore $O^+ = \lambda C_{ij}^+ + (1 - \lambda) I_{ij}^+$, where $\lambda$ is a variational parameter. These authors mentioned the Mott insulator and the Hubbard Hamiltonian as possible applications, but no explicit calculations of the ground state energy was presented.

This generalized RVB state has been proposed again for the Hubbard model, and independently, by Messager and Richard [9]; it was also studied for a strip of $2 \times N$ sites by Cicuta and Stramaglia [10]. To the best of our knowledge, there has been no further study on this proposal, despite the following arguments in favor of its consideration as a good variational state for the Hubbard model:

1) The state $O^+ |0 >$ is the exact ground state for a two electron system.

2) The state $(O_{12}^+ O_{34}^+ - O_{13}^+ O_{24}^+ ) |0 >$ is an extremely accurate approximation of the exact ground state of a $2 \times 2$ Hubbard model. ( We recall, that in the analogous case of the FQHE, the analytic part of the Laughlin’s wave function is a product of factors $(z_i - z_j)^m$, which correspond to the exact ground state for two particles; therefore the idea of building a many-particle wave function by combining some kind of product of two-particle wave functions deserves particular attention. Notice that the three particle Laughlin’s w.f. is exact on the sphere geometry.)

3) The introduction of a parameter $\lambda$ that controls the amount of double occupancy of the bond seems to be a natural way of constructing a wave function which covers both the large $U$ case ($\lambda \rightarrow 1$) and the small or medium $U$ case.

4) The ground state energy of the large $U$ limit of the Hubbard model at half filling (i.e. the Heisenberg model) can be reproduced with great accuracy by including in the RVB state also bonds connecting sites which are far apart. Indeed Liang, Doucot and Anderson [11] have studied this state on a bipartite lattice, by allowing bonds connecting only sites $i$ of the sublattice $A$ with sites $j$ of the sublattice $B$, and giving a weight factor $h(|i - j|)$ to each bond, where the factor $h$ decreases with a power law with the distance $|i - j|$; notice that the positivity of $h$ guarantees the important Marshall sign rule [12].

5) Even if we do not succeed in finding a form of the wave function as useful as Laughlin’s w.f., we believe that a good variational w.f. can be of use as an initial guess for modern numerical methods.

Numerical calculations on the Hubbard model can be performed either with great accuracy on small systems, or using Monte Carlo or other approximations on larger systems. Here we will be concerned with exact results on small systems ($2 \times 2 \times 2$ and $4 \times 4$). Full configuration interaction calculations at half filling on a $4 \times 4$ lattice are
greatly simplified by the consideration of the space symmetry group of the model. The best way of taking into account the space symmetry group is to replace the electron configurations by linear combinations of configurations contained in a group orbit (we recall that a group orbit is the set \( \{ g | c >, g \in G \} \) where \( | c > \) denotes a configuration); the coefficients of the linear combination are determined by the irreducible representations of the group, and are constant for the totally symmetric state. The orbits are of variable length; for instance the Néel configuration \( | n > \) gives rise to a small orbit, constituted by \( | n > \) itself and the ”anti-Néel” configuration \( | \pi > \) with reversed spins (indeed all rotations and translations of the lattice either send \( | n > \rightarrow | n > \) or \( | n > \rightarrow | \pi > \)). The dimension of the Hilbert space can be greatly reduced since the order \( | G | \) of the space group is large. For a square \( n \times n \) lattice with periodic boundary conditions the translation group in the two directions has \( n^2 \) elements, reflections in the direction of the main diagonals and one of the axis produce a further factor of 8; this gives \( | G | = 128 \) for \( n=4 \) (Actually the \( 4 \times 4 \) lattice is topologically equivalent to an ipercube in 4 dimensions, so a further symmetry arises and a larger group \( \hat{G} \) can be found such that \( | \hat{G} | = 384 \)). For a group-theretical analysis of the Hubbard model see ref.[13].

Besides space symmetry, the Hubbard Hamiltonian presents the usual spin symmetry. It is a very difficult task to use an orthogonal basis adapted to both symmetries. One of the advantages of the RVB approach, is that both space and spin symmetries are introduced in the wave function from the outset. Unfortunately, like in all valence bond methods, the wave functions to be used are not orthogonal.

In the present work we have considered \( 2 \times 2 \times 2 \) and \( 4 \times 4 \) systems with periodic boundary conditions and we have computed the expectation value of the energy and other observables (spin-spin and pairing correlation functions) for a generalized RVB state. Since on a bipartite lattice the next type of bond to be considered beside the nearest-neighbor case is provided by bonds between electrons at distance \( \sqrt{5} \) on the lattice (named KM or chess knight’s move bond [14]), we have taken into considerations wave functions admitting also one or more KM bonds.

All the numerical results presented here correspond to half-filling. However, the formalism can be easily extended in order to cover different fillings (see the end of Sec. 2).

2. Formalism. Let us consider an \( M \times N \) square lattice. A site \( i \) is determined by two integers \( (r, s) \). The sublattice \( A \) is formed by the sites such that \((-1)^{r+s} = 1\), and the sublattice \( B \) is formed by the sites such that \((-1)^{r+s} = -1\). Only bonds connecting the sublattices \( A \) and \( B \) will be allowed.

We define now the creation operator of a generalized valence bond between the sites \( i \) and \( j \):

\[
A_{ij}^+(x, y) = xI_{ij}^+ + yC_{ij}^+
\]

where \( x \) and \( y \) are variational parameters and \( I_{ij}^+, C_{ij}^+ \) are defined by:

\[
I_{ij}^+ = c_{i\uparrow}^+c_{j\downarrow}^+ + c_{i\downarrow}^+c_{j\uparrow}^+
\]
The operator $C_{ij}^+$ creates the usual covalent bond, while $I_{ij}^+$ creates an ionic bond. Normalization of the state vector $A_{ij}^+(x,y)|0>$ implies the condition:

\begin{equation}
2x^2 + 2y^2 = 1
\end{equation}

A covering of the lattice is obtained by considering the following product of operators applied to the vacuum:

\begin{equation}
|\phi_k> = A^+_{i_1j_1}(x_1,y_1)A^+_{i_2j_2}(x_2,y_2) \ldots A^+_{i_nj_n}(x_n,y_n) |0>
\end{equation}

where $i_1, i_2, \ldots, i_n$ belong to the sublattice $A$, $j_1, j_2, \ldots, j_n$ belong to the sublattice $B$, and the index $k$ runs over all possible coverings.

At half-filling the number of lattice sites is twice the number of dimers, i.e. $NM = 2n$. Because of condition (4), the states $|\phi_k>$ are normalized. However they are not orthogonal, and it is also possible that they are linearly dependent.

We assume that in each factor $A^+_{ij}(x,y)$ the variational parameter $x$ is a function of the distance $|i - j|$.

A generalized RVB state is a linear combination of coverings:

\begin{equation}
|\psi> = \sum_k c_k |\phi_k>
\end{equation}

Let $g$ denote an element of the space group. We assume that the coefficients $c_k$ are the same for all the coverings $g|\phi_k>$, $g \in G$. In this way $|\psi>$ becomes a totally symmetric state. It must be noticed that usually the ground state of a finite size Hubbard model is totally symmetric with respect to the space group; an exception is provided by the $2 \times 2$ Hubbard model.

In order to compute the matrix elements of the overlap matrix $S_{ij} = <\phi_i|\phi_j>$, Sutherland’s graphical rules [6] can be used. The scalar product $<\phi_i|\phi_j>$ can be written as $<\phi_i|\phi_j> = \prod_{k=1}^m l_k$, where $l_k$ denotes the contribution of a loop with an even number of bonds. In order to compute the factors $l_k$, the following simple algebraic rules can be employed. From the commutator:

\begin{equation}
[A_{ij}(x_2,y_2), A^+_{ij}(x_1,y_1)] = 2(\overline{x_2}x_1 + \overline{y_2}y_1) \\
- (\overline{x_2}x_1 + \overline{y_2}y_1)(c^+_{i\uparrow}c_{i\uparrow} + c^+_{i\downarrow}c_{i\downarrow} + c^+_{j\uparrow}c_{j\uparrow} + c^+_{j\downarrow}c_{j\downarrow}) \\
- (\overline{x_2}y_1 + \overline{y_2}x_1)(c^+_{i\uparrow}c_{j\uparrow} + c^+_{i\downarrow}c_{j\downarrow} + c^+_{j\uparrow}c_{i\uparrow} + c^+_{j\downarrow}c_{i\downarrow})
\end{equation}

we can deduce the formula:

\begin{equation}
<X|A_{ij}(x_2,y_2)A^+_{ij}(x_1,y_1)|Y> = 2(\overline{x_2}x_1 + \overline{y_2}y_1) <X|Y>
\end{equation}

for any partial coverings $|X>$, $|Y>$ such that the sites $i, j$ are not occupied (i.e. coverings of the lattice without the sites $i$ and $j$).
Analogously, from the commutator \((k \neq j)\): \( [A_{ik}(x_2, y_2), A_{ij}^+(x_1, y_1)] = \overline{x}_2 x_1 - \overline{x}_2 x_1 (c_{i\uparrow}^+ c_{i\uparrow} + c_{i\downarrow}^+ c_{i\downarrow} - \overline{x}_2 y_1 (c_{j\uparrow}^+ c_{i\uparrow} + c_{j\downarrow}^+ c_{i\downarrow}) - \overline{y}_2 x_1 (c_{i\uparrow}^+ c_{k\uparrow} + c_{i\downarrow}^+ c_{k\downarrow} - \overline{y}_2 y_1 (c_{j\uparrow}^+ c_{k\uparrow} + c_{j\downarrow}^+ c_{k\downarrow}) \)

we obtain:

\( <X|A_{jl}(x_3, y_3)A_{ik}(x_2, y_2)A_{ij}^+(x_1, y_1)|Y> = <X|A_{ik}(\overline{x}_1 x_2 x_3, -\overline{y}_1 y_2 y_3)|Y> \)

where in the partial coverings \(|X>, |Y>\) the sites \(i, j, k, l\) are empty.

In Fig. 1 it is shown how formulas (8), (10), can be used to simplify a Sutherland’s graph.

From relations (8), (9), it follows that the contribution of a loop with \(m\) nearest-neighbor bonds is given by (we assume \(x, y\) real):

\[
 l = 2x^m + (-1)^{1 + \frac{m}{2}} y^m
\]

in agreement with previous results [10], [11].

Let us now denote by \(A_{ij}^+(\tilde{x}, \tilde{y})\) the operator creating a ”knight’s move bond” (KM bond) between the sites \(i\) and \(j\) whose relative distance is \(\sqrt{5} (1^2 + 2^2 = 5)!\). The introduction of a KM bond simply modifies the parameters \(x, y\) into \(\tilde{x}, \tilde{y}\); therefore the contribution of a loop containing \(r\) KM bonds and \(m - r\) nearest-neighbor bonds is given by:

\[
 l = 2x^{m-r} \tilde{x}^r + (-1)^{1 + \frac{m}{2}} 2y^{m-r} \tilde{y}^r
\]

Formulas (11), (12) allow us to compute the overlap matrix \(<\phi_i|\phi_j>\).

Let us now compute the matrix elements \(<\phi_r|H\phi_s>\) of the Hubbard Hamiltonian. Denoting by \(T_{ij}\) the operator:

\[
 T_{ij} = c_{i\uparrow}^+ c_{j\downarrow} + c_{i\downarrow}^+ c_{j\uparrow} + c_{j\uparrow}^+ c_{i\downarrow} + c_{j\downarrow}^+ c_{i\uparrow}
\]

the Hubbard Hamiltonian can be written as:

\[
 H = - \sum_{<ij>} T_{ij} + U \sum_i n_{i\uparrow} n_{i\downarrow}
\]

where \(\sum_{<ij>}\) denotes the sum over all nearest-neighbor pairs.

As for the matrix elements of the operator \(T_{ij}\), we must distinguish three cases:

i) The operator \(T_{ij}\) acts on a pair of sites \(i, j\) belonging to two different closed loops. Since the total particle number must be conserved inside a loop, the contribution vanishes. The corresponding graph is shown in Fig.2.

ii) The operator \(T_{ij}\) acts on a pair of sites connected by a bond. For any partial coverings \(|X>, |Y>\) such that the sites \(i, j\) are empty, we have:

\[
 <X|T_{ij} A_{ij}^+(x, y)|Y> = 2 <X|A_{ij}^+(y, x)|Y>
\]
Hence the hopping operator exchanges the covalent and ionic bonds.

iii) The operator $T_{ij}$ divides a loop into two parts of lengths $m, n$; if $m$ and $n$ are odd, by repeated application of Eq. (10) we reduce ourselves to the preceding case, and Eq.(15) still holds; if $m$ and $n$ are even we can repeat the same procedure. In this way we arrive to an expression of the form:

$$<0|A_{il}(x_1, y_1)A_{jm}(x_2, y_2)T_{ij}A_{ij}^+(x_3, y_3)A_{im}^+(x_4, y_4)|0>$$

whose contribution vanishes. The corresponding graph is shown in Fig. 3.

Let us denote by $V_{ij} = U(n_i\uparrow n_i\downarrow + n_j\uparrow n_j\downarrow)$ the contribution to the potential energy of the sites $i$ and $j$. Since $V_{ij}$ counts the double occupations, the action of $V_{ij}$ on $A_{ij}^+(x, y)$ is simply to annihilate the covalent part of the bond. Hence:

$$<X|V_{ij}A_{ij}^+(x, y)|Y> = U<X|A_{ij}^+(x, 0)|Y>$$

Let us add a few words on the modifications of the formalism that are necessary to cover cases different from half-filling. In general, the scalar product of two coverings can still be easily computed. However, the formula $<\phi_i|\phi_j> = \prod_{k=1}^n l_k$ does not hold any more. The Sutherland’s graph corresponding to $<\phi_i|\phi_j>$ contains in general not only closed loops, but also open paths. These paths can be easily simplified by using repeatedly formula (10). If the number of bonds of a given open path is odd, the final result vanishes, since $<A_{i,j}(x, y)> = 0$; if it is even, the final contribution is of the type:

$$<A_{i,j}(x_1, y_1)A_{j,k}^+(x_2, y_2)> = \overline{x_1}x_2.$$ 

Notice that only the ionic coefficients $x_1, x_2$, enter in the last formula.

The generalization of the rules to be used in order to compute $<\phi_i|H|\phi_j>$ is straightforward.

**Numerical results and conclusions.**

In order to obtain a first insight about the values of the variational parameters, the scalar product with the exact ground state, etc., we have first considered a toy model, i.e. the $2 \times 2 \times 2$ cube, which is topologically equivalent to the $4 \times 2$ lattice (see e.g. ref. [14] for the case of the Heisenberg model).

Denoting the vertices of the cube by the numbers 1, 2, ..., 8, we can choose five coverings that give rise to five different orbits of the space group; in Fig.4 the coverings that generate these five orbits are shown: there are two coverings without KM bonds, and three coverings with 1, 2 and 3 KM bonds respectively.

Since we are interested in the totally symmetric state, all the covering structures of an orbit are taken with equal weight.

Notice that the KM correspond to bonds between opposite vertices of the cube. The matrix elements $S_{rs}, T_{rs}, V_{rs}(r, s = 1, 2, ...5)$ of the overlap, hopping and interaction matrices can be easily computed (see Appendix), where the indexes $r, s$ run over the five orbits of Fig.4.
In Table I we give, for the $2 \times 2 \times 2$ case, the value of the energies of the knight’s move resonating valence bond state $|\text{KM}>$ and the nearest neighbor resonating valence bond state $|\text{NN}>$, compared with the exact energy $E$ and the best Hartree-Fock energy $E_{HF}$; we denote by $|E>$ the exact ground state and we give the values of the overlaps $<E|\text{NN}>, <E|\text{KM}>$.

Even in this toy model we can learn something: the RVB variational states (nearest-neighbor and knight’s move) are worse than the Hartree-Fock state for small $U$, but are superior (especially the KMRVB state) for $U > 8$.

We have repeated the same calculation for the more interesting case of the $4 \times 4$ lattice. For this model there are 272 NNRVB coverings; this number increases to 40320 if we include also KMRVB coverings. In Fig. 5 an exemple of covering of the lattice containing 3 KM bonds is shown.

We know from previous works (see, e.g. ref.[13]) that the ground state is totally symmetric with respect to the space group $G$. Averaging over $G$, we can reduce the dimension of the secular problem to 13 in the nearest-neighbor case, and to 458 if KM bonds are present. For comparison, the dimension of the whole Hilbert space is $\binom{16}{8}^2 \approx 1.6 \times 10^8$, and the dimension of the totally symmetric subspace is $\approx 1.3 \times 10^6$.

In Table II the values of the ground state energies and the overlaps with the ground state are given for the $4 \times 4$ case. The notations are the same as those used in Table I.

From Table II we see that for large $U$ (e.g. for $U=40$) the KMRVB state has an energy value (-1.8973 compared to -1.9084) and an overlap with the exact ground state of 0.999. Both are very satisfactory values.

It is also interesting to remark that considering the projection of the exact ground state wave function $|E>$ in the subspace generated by the coverings $|\phi_k>$, the absolute values of the coefficients $c_k = <\phi_k|E>$ varies very little (typical values are 0.025, 0.0248, 0.0253, 0.0269); furthermore their sign agrees with the Marshall-Peierls rule; this kind of behaviour is well known for the Heisenberg model (see ref. [14]). The variational state considered in refs.[10],[11] consists in taking all the $|c_k|$ equal; this approximation is very good in the restricted class of the NNRVB states.

In Table XXXX the variations of the ionicity parameters $r = \hat{x} y, \tilde{r} = \hat{\tilde{x}} y$ with $U$ are exibited for the models $2 \times 2 \times 2$ and $4 \times 4$.

From the Table we see that the values of the variational parameters are not exactly the same for a given $U$, but their order of magnitude is the same. Hence we can speak of an ” approximate transferability ” from one model to another.

In table III we show the results for the spin-spin correlation function $<S_z(0)S_z(\vec{r})>$ for $\vec{r} = (0,0), (1,0), (2,0), (2,1), (2,2)$; (in order to save space, in the table only the value of $|r| = \sqrt{r_x^2 + r_y^2}$ is indicated).

As is well known the antiferromagnetic order of the Hartree-Fock state is too strong compared with the exact ground state values, since the best mean field solution is a spin-density wave; the antiferromagnetic order of the NNRVB state is reasonable but decays too fast as expected (see also ref [8]). The spin-spin correlation function derived from the KMRVB state is almost exact for $U=40$, but even for $U=4$ it reproduces the correct behaviour, while this is not the case for the Hartree-Fock solution.

In table IV we have examined the d-wave pair correlation function in order to see...
the effect of the approximation on a physical quantity which is probably crucial in high

\(T_c\) superconductivity. This correlation function is defined as

\[ \langle \Delta^+ (0) \Delta (\vec{r}) \rangle \]

where:

\[ \Delta (i) = \sum_{u=\pm x, \pm y} f(u)(c_{i\uparrow} c_{i+u\downarrow} + c_{i+u\uparrow} c_{i\downarrow}), \]

and denoting by \(x\) and \(y\) unit vectors in the two lattice directions, \(f(\pm x) = 1\) and \(f(\pm y) = -1\). Both correlation functions, derived from the NNRVB and KMRVB wave functions, show a quite reasonable behaviour for the rate of decay at increasing values of \(|r|\). We have also computed the s-wave pair correlation function which shows a similar behaviour. This kind of agreement for the s and d-wave pair correlation functions is present only for large values of \(U\). No indications of ODLRO appears.

Concluding, the type of variational wave functions studied in this work certainly captures a good part of the physics of the Hubbard model, especially for large values of \(U\). Hence, it would be of interest to study the excited states, obtained by substituting one triplet bond for a singlet, or to introduce holes in the system. A strong limitation of the formalism is constituted by the non orthogonality of the coverings.
Appendix

In the following, the matrix elements $S_{rs}, T_{rs}, V_{rs}$ ($r, s = 1, 2, .., 5$) of the overlap, hopping and interaction matrices for the 2x2x2 cube are given. $(\tilde{x}, \tilde{y})$ are the parameters of KM bonds, $(x, y)$ are the parameters of NN bonds.

OVERLAP MATRIX

\[
\begin{align*}
S_{11} &= \frac{1}{3}[1 + 2(x^2 - y^2)^2] \\
S_{12} &= \frac{1}{3}(x^2 - y^2)[x^4 + y^4 + 2] \\
S_{13} &= \frac{1}{3}[6(x^5 \tilde{x} + y^5 \tilde{y})] \\
S_{14} &= \frac{1}{3}[2(x^2 \tilde{x}^2 - y^2 \tilde{y}^2) + 4(x^6 \tilde{x}^2 - y^6 \tilde{y}^2)] \\
S_{15} &= [2(x^2 \tilde{x}^2 - y^2 \tilde{y}^2)]^2 \\
S_{22} &= \frac{1}{6}[1 + (x^2 - y^2)^2 + (x^6 + y^6)] \\
S_{23} &= \frac{1}{6}[6(x^3 \tilde{x} - y^3 \tilde{y}) + 6(x^7 \tilde{x} - y^7 \tilde{y})] \\
S_{24} &= \frac{1}{6}[8(x^4 \tilde{x}^2 + y^4 \tilde{y}^2) + 8(x^3 \tilde{x} - y^3 \tilde{y})^2] \\
S_{25} &= 2(x^4 \tilde{x}^4 - y^4 \tilde{y}^4) \\
S_{33} &= \frac{1}{8}[1 + 6(x^4 \tilde{x}^2 + y^4 \tilde{y}^2) + 2(x^6 + y^6) + 12(x^3 \tilde{x} - y^3 \tilde{y})^2] \\
S_{34} &= (x^3 \tilde{x} - y^3 \tilde{y}) + (x^5 \tilde{x}^3 - y^5 \tilde{y}^3) \\
S_{35} &= 2(x^3 \tilde{x}^3 + y^3 \tilde{y}^3) \\
S_{44} &= \frac{1}{6}[1 + [2(x^2 \tilde{x}^2 - y^2 \tilde{y}^2)]^2 + 8(x^4 \tilde{x}^2 + y^4 \tilde{y}^2)] \\
S_{45} &= 2(x^2 \tilde{x}^2 - y^2 \tilde{y}^2)
\end{align*}
\]
\[ S_{55} = 1 \]

**HOPPING MATRIX**

\[ T_{11} = \frac{32}{3} xy(1 + 2(x^2 - y^2)^2) \]

\[ T_{12} = \frac{16}{3} xy[2(x^6 - y^6) + (xy)^2(y^2 - x^2) + 4(x^2 - y^2)] \]

\[ T_{13} = \frac{1}{3}[16xy(x^5\tilde{x} + y^5\tilde{y}) + 20xy(x^3\tilde{x} + y^3\tilde{y}) - 8x^2y^2(y\tilde{x} + x\tilde{y})] \]

\[ T_{14} = \frac{1}{3}\{2[24xy(x^4\tilde{x}^2 - y^4\tilde{y})^2] + 16\tilde{y}x^2y^2(y^2 - x^2) + 8x^3y^3(\tilde{y}^2 - tx^2)] + \\
+ 32xy(x^2\tilde{x}^2 - y^2\tilde{y}^2) + 8xy(\tilde{x}^2 - \tilde{y}^2)\} \]

\[ T_{15} = 32[xy(\tilde{x}^2 - \tilde{y}^2)(x^2\tilde{x}^2 - y^2\tilde{y}^2)] \]

\[ T_{22} = \frac{16}{3}[1 + 4(x^4 + y^4) - 3(xy)^2 + 2(x^6 + y^6)] \]

\[ T_{23} = \frac{1}{2}\{32xy(x^3\tilde{x} - y^3\tilde{y}) + 12xy(x\tilde{x} - y\tilde{y}) + \\
+ 28xy(x^5\tilde{x} - y^5\tilde{y}) + 12x^2y^2(-x^3\tilde{y} + y^3\tilde{x}) + 8x^3y^3(-x\tilde{x} + y\tilde{y})\} \]

\[ T_{24} = \frac{1}{3}\{2[16xy(x^4\tilde{x}^2 - y^4\tilde{y})^2] + 16xy(x^2\tilde{x}^2 + y^2\tilde{y}^2) - 16x^2y^2\tilde{x}\tilde{y} + \\
+ xy(x^2\tilde{x}^2 + y^2\tilde{y}^2)] + 48xy(x\tilde{x} - y\tilde{y})(x^3\tilde{x} - y^3\tilde{y})\} \]

\[ T_{25} = 16[xy(x^2\tilde{x}^4 - y^2\tilde{y}^4) + xy\tilde{x}^2\tilde{y}^2(y^2 - x^2) + x^2y^2\tilde{x}\tilde{y}(\tilde{y}^2 - \tilde{x}^2)] \]

\[ T_{33} = \frac{1}{8}[24xy + 24xy(x^4 + y^4) + 3[16xy(x^4\tilde{x}^2 + y^4\tilde{y}^2) + 16xy(x^2\tilde{x}^2 + y^2\tilde{y}^2) + \\
+ 4x^2y^2\tilde{x}\tilde{y}] + 3 \cdot 48xy(x\tilde{x} - y\tilde{y})(x^3\tilde{x} - y^3\tilde{y})\} \]

\[ T_{34} = \frac{1}{2}[12xy(x\tilde{x} - y\tilde{y}) + 16xy(x^3\tilde{x} - y^3\tilde{y}) + 20xy(x^3\tilde{x}^3 - y^3\tilde{y}^3) + \\
+ 4xy\tilde{x}\tilde{y}(-x^3\tilde{y} - y^3\tilde{x}) + 24x^2y^2\tilde{x}\tilde{y}(-x\tilde{x} + y\tilde{y})\] + \]

\[ T_{35} = 12[xy(x\tilde{x}^3 + -y\tilde{y}^3) - x\tilde{x}y\tilde{y}(x\tilde{y} + y\tilde{x})] \]
\[ T_{44} = \frac{1}{6}[16xy + 4(16xy(x^2\tilde{x}^2 + y^2\tilde{y}^2) - 16x^2y^2\tilde{x}\tilde{y}) + 32xy(x^2\tilde{x}^2 - y^2\tilde{y}^2)(\tilde{x}^2 - \tilde{y}^2)] \]

\[ T_{45} = 8xy(\tilde{x}^2 - \tilde{y}^2) \]

\[ T_{55} = 0 \]

**INTERACTION MATRIX**

\[ V_{11} = \frac{8}{3}[1 + 2x^2(x^2 - y^2)] \]

\[ V_{12} = \frac{8}{3}x^4(1 + 5x^4) \]

\[ V_{13} = 4x^2(x^5\tilde{x} + y^5\tilde{y}) + 6x^5\tilde{x} \]

\[ V_{14} = \frac{1}{3}[16x^6\tilde{x}^2 + 8x^2(x^2\tilde{x}^2 - y^2\tilde{y}^2) + 4x^2\tilde{x}^2] \]

\[ V_{15} = 16x^2\tilde{x}^2(x^2\tilde{x}^2 - y^2\tilde{y}^2) \]

\[ V_{22} = \frac{4}{3}[1 + 2(x^6 + y^6) + 6x^4 + x^2(x^2 - y^2)] \]

\[ V_{23} = \frac{1}{2}[8x^2(x^2\tilde{x}^2 - y^2\tilde{y}^2) + 4x^2\tilde{x}^2 + 8x^7\tilde{x}] \]

\[ V_{24} = \frac{1}{3}[12x^4\tilde{x}^2 + 8x^2(x^4\tilde{x}^2 + y^4\tilde{y}^2) + 16x^3\tilde{x}(x^3\tilde{x} - y^3\tilde{y})] \]

\[ V_{25} = 16x^4\tilde{x}^4 \]

\[ V_{33} = \frac{1}{8}[12x^2(x^4\tilde{x}^2 + y^4\tilde{y}^2) + 9x^4\tilde{x}^2 + 48x^3\tilde{x}(x^3\tilde{x} - y^3\tilde{y}) + 6x^6 + 4\tilde{x}^2(x^6 + y^6) + 6x^2 + 2\tilde{x}^2] \]

\[ V_{34} = 2x^3\tilde{x} + 2(\tilde{x}^2 + x^2)(x^3\tilde{x} - y^3\tilde{y}) + 8x^5\tilde{x}^3 \]

\[ V_{35} = 4\tilde{x}^2(x^3\tilde{x}^3 + y^3\tilde{y}^3) + 6x^3\tilde{x}^3 \]

\[ V_{44} = \frac{1}{3}[x^2 + 2\tilde{x}^2 + 12x^4\tilde{x}^2 + 8\tilde{x}^2(x^4\tilde{x}^2 + y^4\tilde{y}^2) + 8x^2\tilde{x}^2(x^2\tilde{x}^2 - y^2\tilde{y}^2)] \]
\[ V_{45} = 8\bar{x}^2 (x^2 x^2 - y^2 y^2) + 4x^2 x^2 \]

\[ V_{55} = 8\bar{x}^2 \]
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Table I. Energy values of the ground state, Hartree-Fock and RVB states for the $2 \times 2 \times 2$ lattice.

| $U$ | $E$  | $E_{HF}$ | $E_{NN}$ | $E_{KM}$ | $\langle E|NN\rangle$ | $\langle E|KM\rangle$ |
|-----|------|----------|----------|----------|----------------------|----------------------|
| 0   | -12.0000 | -12.0000 | -8.8000  | -9.3463  | 0.5477               | 0.6941               |
| 1   | -10.1187 | -10.0000 | -7.2887  | -7.7171  | 0.5097               | 0.6765               |
| 4   | -5.9542  | -5.0274  | -4.8152  | -5.0079  | 0.6887               | 0.8101               |
| 8   | -3.4671  | -2.8341  | -3.1667  | -3.2697  | 0.9218               | 0.9763               |
| 16  | -1.8772  | -1.4772  | -1.8002  | -1.8464  | 0.9760               | 0.9986               |
| 40  | -0.7763  | -0.5985  | -0.7553  | -0.7728  | 0.9850               | 0.9993               |

Table II. Energy values of the ground state, Hartree-Fock and RVB states for the $4 \times 4$ lattice.

| $U$ | $E$  | $E_{HF}$ | $E_{NN}$ | $E_{KM}$ | $\langle E|NN\rangle$ | $\langle E|KM\rangle$ |
|-----|------|----------|----------|----------|----------------------|----------------------|
| 1   | -20.7936 | -20.6542 | -15.5266 | -16.9183 | 0.44317              | 0.64978              |
| 4   | -13.6218 | -12.5665 | -10.7020 | -11.5642 | 0.58962              | 0.79090              |
| 8   | -8.4689  | -7.3896  | -7.2782  | -7.7707  | 0.78905              | 0.94436              |
| 16  | -4.6119  | -3.9116  | -4.2421  | -4.4830  | 0.89713              | 0.99489              |
| 40  | -1.9084  | -1.5941  | -1.8051  | -1.8973  | 0.92734              | 0.99904              |
Table III. Values of the spin-spin correlation function for the exact ground state, the Hartree-Fock and the RVB states.

| $|r|$ | $\langle S_z(0)S_z(r)\rangle$ | $HF$ | $N N R V B$ | $K M R V B$ | $G R O U N D$ |
|-----|-----------------|-----|------------|------------|-----------|
| 0   | 0.18704         | 0.21316 | 0.20883 | 0.19244 |
| 1   | −0.13706        | −0.08782 | −0.08841 | −0.06879 |
| 2   | 0.12321         | 0.03401 | 0.05120 | 0.03750 |
| $\sqrt{5}$ | −0.12501 | −0.02010 | −0.05170 | −0.04520 |
| $2\sqrt{2}$ | 0.12201 | 0.01447 | 0.04442 | 0.03851 |

$U = 4$

| $|r|$ | $\langle S_z(0)S_z(r)\rangle$ | $HF$ | $N N R V B$ | $K M R V B$ | $G R O U N D$ |
|-----|-----------------|-----|------------|------------|-----------|
| 0   | 0.24876         | 0.24863 | 0.24855 | 0.24853 |
| 1   | −0.24784        | −0.11094 | −0.11579 | −0.11590 |
| 2   | 0.24753         | 0.05014 | 0.07110 | 0.07085 |
| $\sqrt{5}$ | −0.24753 | −0.03262 | −0.06811 | −0.06750 |
| $2\sqrt{2}$ | 0.24753 | 0.02476 | 0.06048 | 0.05997 |

Table IV. Values of the pair correlation function for the exact ground state, and the RVB states.

| $|r|$ | $\langle \Delta \dagger(0)\Delta(r)\rangle$ | $d$-wave, $U = 40$ |
|-----|-----------------|--------|
| 0   | 2.33389         | 2.39191 | 2.38947 |
| 1   | 0.59034         | 0.60339 | 0.60118 |
| 2   | 0.00199         | 0.00114 | 0.00252 |
| $\sqrt{5}$ | 0.00002 | 0.00003 | 0.00005 |
| $2\sqrt{2}$ | 0.00000 | 0.00000 | 0.00000 |
| $\sqrt{2}$ | 0.00589 | 0.00487 | 0.00261 |
FIGURE CAPTIONS

Fig. 1 The operators $A_{ij}$ (dotted line) and $A_{ij}^+$ (full line) are represented by a bond connecting the points i and j.

Fig. 2 Graph representing the operator $T_{ij}$ acting on a pair of sites $i, j$ belonging to two different closed loops. The corresponding contribution vanishes.

Fig. 3 Graph corresponding to the expectation value:

$$<0|A_{il}(x_1, y_1)A_{jm}(x_2, y_2)T_{ij}A_{ij}^+(x_3, y_3)A_{im}^+(x_4, y_4)|0>$$

whose contribution vanishes.

Fig. 4 Representative coverings of the $2 \times 2 \times 2$ lattice which generate different orbits of the space group.

Fig. 5 An example of covering of the $4 \times 4$ lattice containing 3 KM bonds; point 13 and point 16 are connected by a bond because of periodicity.
$$1 \ 2 = 2(x_1 x_2 + \overline{y}_1 y_2) \quad \Downarrow \quad 1 \ 3 \ 1 \quad \Downarrow \quad (x_1 x_2 x_3, -\overline{y}_1 y_2 y_3)$$

Fig. 1
Fig. 2

$$T_{ij} = 0$$
Fig. 3
Fig. 4
