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On the bound state of holes for the square-lattice Hubbard model with resonating valence bonds

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Abstract. The Hubbard model for the square planar lattice in the limit $t/U \ll 1$ is discussed. The ground state is chosen to be the product of the Hubbard model's exact solutions for four-site blocks. One-particle excitations appear to be Fermi particles with spin $\frac{1}{2}$. Their effective mass near the bottom of the band coincides with the effective mass of excitations in the paramagnetic state in the 'Hubbard-I' approximation. However, minima of the spectrum are situated at other points in the Brillouin zone. The possibility of the binding of two excitations into singlet pair with charge $2e$ is demonstrated. Cohesive energy is calculated to be equal to $0.1t$. The superfluid state of the Bose gas of such pairs is assumed to be connected with high-T_c superconductivity.

1. Introduction

The Hubbard model [1] for the square planar lattice with resonating valence bonds (RVBS) [2] has been recently treated in connection with the high-T_c superconductivity problem. In particular, the possibility of hole pairing has been discussed. For this purpose it is important to construct the RVB ground state Ψ_{gr} as well as to determine the elementary excitation spectrum.

The RVB state Ψ_{gr} is usually constructed on the basis of the two-electron nearest-neighbour singlet Φ_0 [3–6]:

$$\Phi_0 = \tfrac{1}{2}[(a_1^+ b_2^+ - b_1^+ a_2^+) - 2(t/U)(a_1^+ b_1^+ - b_2^+ a_2^+)] \tag{1}$$

where t and U are standard model parameters, and a_i^+ and b_i^+ create an electron on the ith site with $+\frac{1}{2}$ and $-\frac{1}{2}$ spin projections, respectively. We shall construct Ψ_{gr} originating from the singlet ground state $|4^0\rangle$ of a square four-site block with four electrons. In comparison with Φ_0 (equation (1)) the singlet state $|4^0\rangle$ is more appropriate for square symmetry of the problem and from the very beginning takes better account of short-range order. In the following, we determine the variational energy value for the ground RVB-like state on the two-dimensional square lattice with one electron per site: $\alpha = t/U \ll 1$. We also calculate the elementary one-particle excitation spectrum. In our block approach, excitations are naturally described as small magnetic polarons—the lowest-energy states of the block with three electrons. We demonstrate that it may be energetically favourable for two such excitations to be bound into a localised pair, i.e. a

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bipolaron. It should be emphasised that our results have a variational character; the approximations involved are discussed at the end of each section. We shall also discuss the special case of the RVB state for a square ladder, which was recently considered in [7].

2. Variational ground-state function

The Hubbard Hamiltonian has the form

$$\hat{H} = t\sum_{\langle ij\rangle}(a_i^+ a_j + b_i^+ b_j) + U\sum_i a_i^+ a_i b_i^+ b_i. \tag{2}$$

As usual, t and U are the hopping integral and the on-site Coulomb repulsion, and $\langle ij\rangle$ denote nearest neighbours. For construction of the ground state let us now divide the plane into square four-site blocks and rewrite the Hamiltonian in block form:

$$\begin{aligned} &\hat{H} = \sum_n \hat{h}_n + \sum_{\langle nm\rangle}\hat{t}_{nm} \qquad \hat{h}_n = \sum_{S,i}\hat{X}_n^{S^iS^i}\varepsilon_S^i \\ &\hat{t}_{nm} = \sum_{\substack{Sij\\ Pkl}}(\hat{t}_{nm,SP}^{ij,kl}\hat{X}_n^{(S-1)^iS^j}\hat{X}_m^{(P+1)^kP^l} + \mathrm{HC}) \end{aligned} \tag{3}$$

where $\hat{h}_n$ is the Hamiltonian of the block $\boldsymbol{n}$, $\hat{t}_{nm}$ is the inter-block hopping operator. $\langle \boldsymbol{nm}\rangle$ are the nearest-neighbour blocks, $\hat{X}_n^{\lambda\mu}$ is Hubbard's operator [1] transferring the block n from state μ to state λ, $|S\rangle$ is the eigenstate of the four-site block with S electrons (s = 0–8) and energy ε_S^i, i is the set of quantum numbers and $t_{nm,SP}^{ij,kl}$ are the corresponding hopping matrix elements. Transformation from (2) to (3) is exact because (3) is simply the representation of Hamiltonian (2) in the basis of the block operators $\hat{X}_n^{\lambda\mu}$.

It is at first necessary to find eigenstates $|S\rangle$ of a block containing S electrons. It is appropriate to choose indexes i to be the eigenvalues q, v of the block's Hamiltonian symmetry operators: $\hat{C}_4$ indicates rotation by $\pi/2$, and $\hat{\sigma}_y$ reflection by the Oy axis. The ground state $|4^0\rangle$ for the block with four electrons (one electron per site) appears to be a singlet. It has $q = -1$, $v = +1$ and energy $\varepsilon_4^0 = -12\alpha t[1 + \mathrm{O}(\alpha^2)]$. The expression for its wavefunction is presented in the Appendix. Let us note that the first excited state $|4^1\rangle$ has spin equal to unity and $\varepsilon_4^1 = -8\alpha t$.

We now introduce a variational wavefunction of the ground state of the system with $4N$ electrons (N is the number of blocks). It is constructed on the base of $|4^0\rangle$ and all states $|3^i\rangle$, $|5^j\rangle$ with three and five electrons in a block:

$$\Psi_{\mathrm{gr}} = \sum_n\Big(1 + \sum_{g,i,j}\beta_g^{ij}\hat{X}_n^{3^i4^0}\hat{X}_{n+g}^{5^j4^0}\Big)\Psi_0 \qquad \Psi_0 = \prod_n|4_n^0\rangle \tag{4}$$

where β_g^{ij} are variational parameters, and $\boldsymbol{g}$ is the nearest-neighbour vector for the block lattice. The zero approximation Ψ_0 is built from independent blocks with four electrons in the singlet state $|4^0\rangle$ with lowest energy ε_4^0. Straightforward calculations of $\langle\Psi|H|\Psi\rangle/\langle\Psi|\Psi\rangle$ with the trial function (4) involving all states $|3^i\rangle$, $|5^j\rangle$ lead to a variational value of energy per block, i.e. $\varepsilon^0 = \varepsilon_4^0 + \tilde{\varepsilon}_4$, $\tilde{\varepsilon}_4 = -4\alpha t$, $\varepsilon^0 = -16\alpha t + \mathrm{O}(\alpha^3 t)$; this is the same value of energy per site, i.e. $e_0 = \varepsilon_0/4 = -4\alpha t = -4t^2/U$, as for the classical Néel state (e_{N}). However, the state (4) has the following typical RVB properties: magnetic sublattices are absent, the mean spin projection on each site is zero, while the antiferromagnetic correlators are non-zero.

For a quasi-one-dimensional square ladder the same calculation yields $e^0 = -3.5\alpha t$ for the energy per site, in contrast with $e_N^0 = -3\alpha t$. For a one-dimensional chain (two-site block), $e^0 = -2.5\alpha t$ [8] and lies much closer to exact solution $e_{exact} = -2.77\alpha t$ [9] than to $e_N = -2\alpha t$.

The function Ψ_{gr} (4) accounts for correlation mainly inside the 2×2 block. If Ψ_{gr} has the form (4), the energy e_0 in the linear approximation in α is not lowered because of the complicated nature of state $|4\rangle$, i.e. by admixing other states $|4^i\rangle$. In order to account for long-range correlation, one must enlarge the block size in (4), dividing the plane into blocks of 16 sites (compare [8]). It is difficult to diagonalise the Hamiltonian of such a block, but we may construct its states approximately. The states of the 4×4 block may be considered as non-factorisable combinations which include products of the states of four 2×2 blocks. Taking into consideration hops between them (states $|15\rangle^i$ and $|17^j\rangle$), we obtain in the simplest case $e = -4.06\alpha t$ for the energy per site. An analogous complication for the quasi-one-dimensional square ladder leads to an energy $e = -3.56\alpha t$.

Note that the variational estimate of energy $e = -3.73\alpha t$ for a square ladder obtained in [7] is lower. The trial function in [7] is a superposition of different bonds (1) connecting pairs of nearest-neighbour sites and it accounts for correlation on the scale of several blocks better than function (4) does. Nevertheless, the trial function in [7] is essentially quasi-one-dimensional and is difficult to generalise for the plane case; this function should also not be used in considering one-particle excitation.

The block structure of trial function (4) allows us to take better account of correlation, but at the same time the block structure is the drawback of function (4), because it leads to an artificial change in the lattice period (which doubles in the present case).

3. One-particle excitations

Let us consider one-particle hole-type excitations above ground state (4). One must use block states $|3^i\rangle$ with three electrons in a block to construct wavefunctions of such an excitation (we shall classify these states, as all other block states, by the block's Hamiltonian symmetry group representation). Every state $|3^i\rangle$ is characterised, besides the symmetry indexes q, v, by the value of energy ε_3^i and spin of the block in this state. The ground state $|3^0\rangle$ has a spin $\frac{3}{2}$ (i.e. it is a quartet) and energy $\varepsilon_3^0 = -2t + O(\alpha t)$; its value of $q = v = -1$. The next four states $|3^{v,\sigma}\rangle$ are transformed by the two-dimensional representation $\hat{C}_4|3^{v,\sigma}\rangle = -v|3^{-v,\sigma}\rangle$, $v = \pm 1$. The spin is $\frac{1}{2}$ (two degenerate doublets), and the energy $\varepsilon_3^v = -\sqrt{3}t + O(\alpha t)$. The wavefunctions of these states are presented in the Appendix.

The state $|3^i\rangle$ is in fact an immovable magnetic polaron, restricted by the block sizes. Let us take into consideration possible motion of polaron, which may lead to energy lowering. Then, in the framework of the ground state involved, the trial function of hole-type excitation is as follows:

$$\Psi_p^j = \sum_n \exp(i\boldsymbol{p} \cdot \boldsymbol{n})\, \hat{X}_n^{3/4^0} \Psi_{gr} \tag{5}$$

where $\boldsymbol{n}$ is the block's vector, and the quasi-momentum $\boldsymbol{p}$ lies in the reduced Brillouin zone.

The spectrum of states (5) is defined by the matrix elements $\langle 4_{n+g}^0 3_n^i | \hat{H} | 4_n^0 3_{n+g}^j \rangle$. It is easy to show that these matrix elements containing states $|3^0\rangle$ are equal to zero,

because the state $|3^0\rangle$ has spin, equal to $\frac{3}{2}$. That is why the energy of the state ψ_p^0 is independent of the momentum and is equal to $-2t + O(\alpha t)$. The spectrum corresponding to states built from $|3^{v,\sigma}\rangle$ is equal to

$$\varepsilon_v(\boldsymbol{p}) = \varepsilon_3^v + \tilde{\varepsilon}_3 \qquad \tilde{\varepsilon}_3 = -2\gamma v[\cos(P_x 2a) - \cos(p_y 2a)] - \tilde{\varepsilon}_4$$
$$\gamma = |\langle 4^0_{n+g} 3^{v,\sigma}_n | \hat{H} | 4^0_n 3^{v,\sigma}_{n+g}\rangle = 0.125t[1 + 2\sqrt{6}\alpha + O(\alpha^2)] \tag{6}$$

where a is the lattice constant. Thus the hole in the state with the lowest self-energy $|3^0\rangle$ is immovable, and the energy of the state $|3^{v,\sigma}\rangle$ is lower than the energy value of $|3^0\rangle$, because of motion through the crystal. The hole in the state $|3^{v,\sigma}\rangle$ has the lowest energy $\varepsilon_3^v = -(\sqrt{3}t + 4\gamma) + O(\alpha t) = -2.23t$ and band width $8\gamma = t$. Note that, unlike the case of RVB, motion of the holes in the Néel state is difficult [10]. The effective mass of the hole $|3^{v,\sigma}\rangle$ near the bottom of the band is $1/8\gamma a^2$. It coincides with the 'Hubbard-I' approximation. The hole band (6) is degenerate in v, because the representation of the $|3^{v,\sigma}\rangle$ transformation is two-dimensional. In the following this feature appears to be essential when considering the bound states of two holes.

The spectrum of electron excitations (five electrons in a block) can be found in a similar way. This calculation is simplified by the electron–hole symmetry of the problem and leads to the following expression for the gap in the one-particle excitation spectrum: $\Delta = U - 4.46t$. It should be noted that Hubbard's scheme for Green function decoupling in the paramagnetic ground state yields $\Delta = U - 4t$, and for the Néel state $\Delta \simeq U - t^2/U$. The corresponding gap values in the one-dimensional case are $U - 3.27t$ (present approach), $U - 2t$ (decoupling) and approximately $U - t^2/U$ (the Néel state). Rigorous solution, which is known in one dimension only, gives $\Delta = U - 4t$ [9].

Note the following restrictions of the variational deduction of spectrum (6).

(i) The magnetic polaron size is restricted by the 2×2 block.

(ii) The wavefunction (5) does not account for the hybridisation of state $|3^{v,\sigma}\rangle$ with higher states $|3^i\rangle$. Such hybridisation could take place because of the inter-block hopping part of the Hamiltonian.

(iii) Spectrum (6) is sensitive to the specific form of the ground state Ψ_{gr}. It can be seen from (6) that the kinetic energy γ directly contains block states from Ψ_{gr}.

Nevertheless, we consider, that the spectrum of excitations above the RVB-like ground state near the bottom of the zone is described sufficiently well by equation (6), and this expression is dramatically different from the spectrum in the tight-binding or 'Hubbard-I' approximation.

4. Two-particle excitation spectrum

Let us now consider the case of two holes in the system. We shall describe the holes localised in different blocks by the states $|3^{v,\sigma}\rangle$, which were found earlier. One must also consider the situation of two holes in one block, involving block states $|2\rangle$ with two electrons, i.e. with two holes.

State $|2^0\rangle$ with the lowest energy $\varepsilon_2^0 = -2\sqrt{2}t$ is a singlet; is has $q = v = +1$. It is discussed in the Appendix. In fact, state $|2\rangle$ is a bipolaron, in the same sense as $|3\rangle$ is a polaron. It is noteworthy that the first excited state $|2^1\rangle$ has the energy $\varepsilon_2^1 = -2t$.

The effective interaction of two neighbouring holes is determined by their hopping into one block $|3_n\rangle|3_{n+g}\rangle \rightarrow |4_n\rangle|2_{n+g}\rangle$ and by the inverse process. $2\varepsilon_3^v < \varepsilon_2^0 + \varepsilon_4^0$ and so,

from the viewpoint of the block's self-energies, the interaction of holes has a repulsive character. However, it will be seen in the following that consideration of the dynamical processes, i.e. the matrix elements $\langle 2_{n+g}4_n|\hat{H}|3_n3_{n+g}\rangle$, may lead to the attraction of two holes. The symmetry of states $|2^0\rangle$, $|4^0\rangle$ is such that this matrix element is non-zero only in the case when states $|3_n\rangle$ and $|3_{n+g}\rangle$ have opposite spin projections σ and equal parities v. Simple but cumbrous calculation yields $\tau = \langle 2^0_{n+g}4^0_n|\hat{H}|3^{v,\sigma}_n 3^{v,-\sigma}_{n+g}\rangle = 0.197t$.

We shall consider the problem of two holes in the system against a background of Ψ_{gr} (equation (4)). When describing holes, we shall restrict ourselves to the states with lowest energy, i.e. $|2^0\rangle$, $|3^j\rangle$ $(j = v, \sigma)$. Then the Hamiltonian in block projection Hubbard operators is rewritten in the form

$$\hat{H} = \sum_n (\varepsilon_2 \hat{X}^{22}_n + \sum_j \varepsilon_3 \hat{X}^{jj}_n) + \gamma \sum_{n,g,j} v S_g \hat{X}^{j4}_n \hat{X}^{4j}_{n+g} + \tau \sum_{n,g,j} S_g \sigma (\hat{X}^{2\bar{j}}_n \hat{X}^{4j}_{n+g} + \hat{X}^{j4}_{n+g} \hat{X}^{2\bar{j}}_n) \tag{7}$$

$$j = (v, \sigma) \qquad \bar{j} = (v, -\sigma) \qquad v, \sigma = \pm 1 \qquad S_g = (|g_x| - |g_y|)/|g| = \pm 1$$

$$\varepsilon_2 = -2\sqrt{2}t \qquad \varepsilon_3 = -\sqrt{3}t.$$

S_g accounts for the fact that matrix elements with hops τ along the Ox and Oy axes have different signs.

The Hamiltonian (7) describes the self-energies of polarons and the bipolaron, free motion of polarons (partly by the matrix element γ from (6)) and the formation of the bipolaron. The Hubbard operators on each block are connected by the constraint $\hat{X}^{44}_n + \Sigma_j \hat{X}^{jj}_n + \hat{X}^{22}_n = 1$.

The spectrum of the system is determined by the poles of the retarded Green functions

$$F_n = \langle\langle \hat{X}^{42}_n | \hat{X}^{24}_n \rangle\rangle \qquad G^v_{n,n+m} = \sigma \langle\langle \hat{X}^{4j}_n \hat{X}^{4j}_{n+m} | \hat{X}^{24}_n \rangle\rangle \qquad j = (v, \sigma). \tag{8}$$

In the equations of motion for these Green functions we shall omit commutators in the right-hand side, which are unimportant for spectrum determination:

$$(z - \varepsilon_2)F_n = \tau \sum_{g,v} (G^v_{n,n+g} + G^v_{n+g,n})$$

$$(z - 2\varepsilon_3)G^v_{n,n+m} = \tau \sum_g \delta_{m,g} S_g (F_n + F_{n+g}) + (1 - \delta_{m,0})\gamma \sum_{g,v} v S_g (G^v_{n,n+m+g} + G^v_{n+g,n+m}) \tag{9}$$

$$z = \omega + i\delta.$$

These equations are deduced as a result of the simplest decoupling of 'Hubbard-I' type. We ignored states with more than two holes in the system and assumed that $\langle X^{44}_n \rangle = 1$. The first of equations (9) describes the break-up of the bipolaron into two polarons in neighbouring blocks. The second equation corresponds to the inverse process and to the free motion of polarons. System (9) is analogous to the system of equations

appearing in the problem of the bound state of two spin waves. It can be solved exactly if one makes a Fourier transformation:

$$F^q = N^{-1} \sum_n \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{n})\, F_n$$

$$G_k^{qv} = N^{-2} \sum_{n,m} \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{n} + \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{m})\, G_{n,n+m}^{v}$$

$$(z - \varepsilon_2)F^q = \tau \sum_{k,v} P_k^q G_k^{qv} \tag{10}$$

$$(z - 2\varepsilon_3)G_k^{qv} = \tau P_k^q F^q + \gamma v G_k^{qv} - \gamma v \sum_{k_1} P_{k_1}^q G_{k_1}^{qv}$$

$$P_k^q = \sum_g [1 + \exp(\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{g})] \exp(-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{g}).$$

$\boldsymbol{q}$ is the total momentum of two polarons. The solution of system (10) leads to the following equation, which determines the spectrum $z = \omega(q)$:

$$\Theta\tilde{U} + (1 - \Theta)\omega = w_q^{-1}$$

$$\Theta = \tfrac{1}{2}(\gamma/\tau)^2 \qquad \tilde{U} = \varepsilon_2 - 2\varepsilon_3$$

$$w_q = \sum_k \left[\omega + \mathrm{i}0 - \varepsilon\left(\frac{\boldsymbol{q}}{2} + \boldsymbol{k}\right) - \varepsilon\left(\frac{\boldsymbol{q}}{2} - \boldsymbol{k}\right)\right]^{-1} \tag{11}$$

$$\varepsilon(\boldsymbol{k}) = 2\gamma[\cos(k_x 2a) - \cos(k_y 2a)].$$

Here the spectrum (11) is measured from the centre of the zone of the two holes of energy $2\varepsilon_3$.

One type of solution of equation (11) describes the free motion of two particles with total momentum $\boldsymbol{q}$ and the lowest energy -8γ. However, we are interested in the solution corresponding to the stable bound state of two holes ($\omega_q < -8\gamma$). Analysis of equation (11) shows that such solutions appear when the following inequality between the energy parameters of the Hamiltonian is fulfilled:

$$8\gamma(\Theta^{-1} - 1) > \tilde{U}. \tag{12}$$

(8γ in the left-hand side is replaced by 4γ in the case of a square ladder.)

This condition is true for the parameters $\gamma = 0.125t$, $\Theta = 0.26$ and $\tilde{U} = 0.64$ of the problem obtained earlier. The bottom of the zone of bound states is at $\boldsymbol{q} = 0$. Equation (11) with these parameters yields for the gap $\Delta = -8\gamma - \omega_{q=0}$ the value $\Delta \approx 0.1t$. It is close to the gap obtained in [11] by means of a variational treatment. When $\Delta \ll 8\tau$, the effective mass m is $2m_0$, where m_0 is the mass of one hole. An analogous consideration for one chain based on two-site blocks does not lead to the bound state because condition (12) is violated.

Thus, in the framework of the approximations involved, we are led to the conclusion that two independent holes on a plane are energetically favoured to be bound into a singlet pair with charge $2e$. This pair is the state $|2^0\rangle$ with a coherent admixture of two states $|3^{\nu,\sigma}\rangle$.

The results of this section are obtained with the following approximations:

(i) the approximations noted at the end of § 4;

(ii) on the assumption that it is enough to consider only the ground state $|2^0\rangle$ to describe the bipolaron;

(iii) by considering only two holes, which corresponds to the case of a low hole concentration.

5. Conclusion

To summarise, we have constructed a simple RVB-like state on the base of square blocks, found the one-particle elementary excitation spectrum and shown the possibility of binding for two holes in the framework of the planar Hubbard model. We should emphasise that our RVB approach contains reformulation of the one-site Hamiltonian (2) to the block form (3). In such an approach a hole is considered as a magnetic polaron of size equal to the block size. Two holes in the system may correspond either to two polarons (holes in different blocks) or to a bipolaron (holes in one block). In this case the block Hamiltonian is equivalent to the Hubbard Hamiltonian with on-site (where the new 'site' is the block) repulsion, i.e. $\tilde{U} = \varepsilon_2 - 2\varepsilon_3 > 0$, which is of the order of hopping t. Another difference from the usual Hubbard Hamiltonian is that the matrix element τ of hole hopping to the block containing another hole appears to be larger than the matrix element γ of hopping to the block without holes. This dynamical mechanism may be responsible for pair formation.

Our method has a variational character. Only the lowest-energy states of polarons and the bipolaron were considered when calculating the excitation spectrum. So the conclusion that it is energetically favourable for two holes to be bound into a pair in the limit $t \ll U$ is obviously inconclusive.

At low temperatures, the Bose gas of such pairs undergoes superfluid transmission, which corresponds to the possibility of superconductivity in the model discussed.

Let us evaluate the lowest value of the parameter $\alpha = t/U$ when one can neglect the formation of a 'ferromagnetic bag' [12, 13]. For this purpose we compare at fixed α the energy of a RVB state with one hole (the minimal value $-(\sqrt{3} + 0.5)t$ was formerly obtained for this energy) and the energy $\varepsilon_F(N)$ of the hole localised in the ferromagnetic region containing N sites. The energies $\varepsilon_F(N)$ for $N = 1.4$, 8 and ∞ are equal to 0, $-2t$, $-2.62t$ and $-4t$, respectively. If we take into account that for each site in the ferromagnetic region one has energy deficit $4\alpha t$ relative to the RVB state, we easily conclude that the RVB state is stable at least when $\alpha > 0.025$. Thus, there is a sufficiently large α range where the involved approximation $\alpha \ll 1$ holds.

Appendix

In the following, some states of the four-site block discussed in the text are presented.

a_i^+ and b_i^+ create an electron on the ith site ($i = 1, 2, 3, 4$, clockwise from the higher left site) with $\frac{1}{2}$ and $-\frac{1}{2}$ spin projections. $\hat{C}_4$ is a rotation by $\pi/2$ (change in indexes $1 \to 2$, $2 \to 3$, $3 \to 4$, $4 \to 1$). $\hat{\sigma}_y$ is a reflection by the Oy axis ($1 \rightleftarrows 2$, $3 \rightleftarrows 4$). $|0\rangle$ is the vacuum state.

The lowest energy four-electron state $|4^0\rangle$ is

$$|4^0\rangle = w\sum_{k=1}^{4}\nu_k|X_k\rangle$$

$$|X_1\rangle = \frac{1}{\sqrt{2}}(1-\hat{C}_4)a_1^+b_2^+a_3^+b_4^+|0\rangle$$

$$|X_2\rangle = \tfrac{1}{2}\hat{\Theta}_-a_1^+a_2^+b_1^+b_2^+|0\rangle$$

$$|X_3\rangle = (1/2\sqrt{2})\hat{\Theta}_-(1-\hat{C}_4^{-1}\hat{\sigma}_y)a_1^+b_1^+a_2^+b_2^+|0\rangle$$

$$\hat{\Theta}_q = \sum_{m=0}^{3}q^m\hat{C}_4^m \qquad q=\pm1 \qquad w=\left(\sum_{i=1}^{4}\nu_i^2\right)^{-1/2}$$

$$\nu_1=-\sqrt{2} \qquad \nu_2=1 \qquad \nu_3=-6\alpha+O(\alpha^3) \qquad \nu_4=6\alpha^2+O(\alpha^3).$$

The three-electron ground state $|3^0\rangle$ is a quartet. The next four states $|3^{v,\sigma}\rangle$ are two degenerate doublets. In the following, only states with spin projection $-\frac{1}{2}$ are given.

$$|3^0\rangle = w_\xi(\xi_1|h^1_{--}\rangle+\xi_2|h^2_-\rangle+\xi_3|h^3_{--}\rangle+\xi_4|h^4_-\rangle)$$

$$w_\xi=\left(\sum_{i=1}^{4}\xi_i^2\right)^{-1/2} \qquad \xi_1=\sqrt{2} \qquad \xi_2=-1 \qquad \xi_3,\xi_4\sim\alpha$$

$$|3^{v,-}\rangle = (1/\sqrt{2})(|K^-\rangle+v|L^-\rangle)$$

$$|K^-\rangle = w_\mu(-\mu_1|h^1_{4-}\rangle+\mu_2|h^1_{3-}\rangle+\mu_3|h^2_3\rangle-\mu_4|h^3_{4-}\rangle+\mu_5|h^3_{3-}\rangle-\mu_6|h^4_4\rangle)$$

$$|L^-\rangle = w_\mu(\mu_1|h^1_{3+}\rangle+\mu_2|h^1_{4+}\rangle+\mu_3|h^2_4\rangle+\mu_4|h^3_{3+}\rangle+\mu_5|h^3_{4+}\rangle+\mu_6|h^4_3\rangle)$$

$$w_\mu=\left(\sum_{i=1}^{6}\mu_i^2\right)^{-1/2} \qquad \mu_1=\frac{1}{\sqrt{6}} \qquad \mu_2=\frac{1}{\sqrt{2}} \qquad \mu_3=\frac{1}{\sqrt{3}} \qquad \mu_4,\mu_5,\mu_6\sim\alpha$$

$$|h^{1(3)}_{qs}\rangle = (1/2\sqrt{2})\hat{\Theta}_q\hat{T}_s|h^{1(3)}\rangle \qquad |h^{1(3)}_{3s}\rangle = \tfrac{1}{4}\hat{\Theta}_3\hat{T}_{-s}|h^{1(3)}\rangle$$

$$|h^{1(3)}_{4s}\rangle = \tfrac{1}{4}\hat{\Theta}_4\hat{T}_s|h^{1(3)}\rangle$$

$$|h^{2(4)}_q\rangle = \tfrac{1}{2}\hat{\Theta}_q|h^{2(4)}\rangle \qquad |h^{2(4)}_3\rangle = (1/2\sqrt{2})\hat{\Theta}_3|h^{2(4)}\rangle$$

$$|h^{2(4)}_4\rangle = (1/2\sqrt{2})\hat{\Theta}_4|h^{2(4)}\rangle$$

$$\hat{\Theta}_3=2(\hat{C}_4-\hat{C}_4^3) \qquad \hat{\Theta}_4=2(1-\hat{C}_4^2) \qquad \hat{T}_s=1+s\hat{C}_4^{-1}\hat{\sigma}_y \qquad q,s=\pm1$$

$$|h^1\rangle = b_2^+b_3^+a_4^+|0\rangle \qquad |h^2\rangle = b_1^+a_2^+b_3^+|0\rangle$$

$$|h^3\rangle = a_2^+b_2^+b_3^+|0\rangle \qquad |h^4\rangle = a_2^+b_2^+b_4^+|0\rangle.$$

The singlet two-electron ground state $|2^0\rangle$ is

$$|2^0\rangle = w(|d^1_+\rangle-|d^2_{++}\rangle+\eta|d^3_+\rangle)$$

$$|d^1_+\rangle = \tfrac{1}{2}\hat{\Theta}_+a_2^+b_4^+|0\rangle \qquad |d^2_{++}\rangle = (1/2\sqrt{2})\hat{\Theta}_+\hat{T}_+a_2^+b_3^+|0\rangle$$

$$|d^3_+\rangle = \tfrac{1}{2}\Theta_+a_2^+b_2^+|0\rangle \qquad \eta\sim\alpha \qquad w=(2+\eta^2)^{-1/2}.$$

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