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Cluster states of fermions in the single l-shell model

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Abstract. The paper deals with the ground state structure of the partly filled l-shell of a fermionic gas of atoms of spin s in a spherically symmetric spin independent trap potential. At particle numbers $N = n(2s+1)$, $n = 1, 2, \ldots, 2l+1$ the basic building blocks are clusters consisting of $(2s+1)$ atoms, whose wave functions are completely symmetric and antisymmetric in space and spin variables, respectively. The creation operator of a cluster is constructed and applied also to create multi cluster states. Ground state energy expressions are derived for the n-cluster states at different l, s values and interpreted in simple terms.

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1 Introduction

The many body problem as applied to finite systems has a long history in atomic and nuclear physics [1–4]. One of the central problems has been the nature of the ground state in case of a partially filled shell.

When we consider atoms (a Bose or Fermi gas at zero temperature) in an external potential the possible behaviors are quite rich. One can assume that the collision between atoms does not excite internal degrees of freedom and the atoms can be regarded as structureless objects (particles in the following) whose spins are fixed being in a definite hyperfine state. The external potential can be supplied by a magnetic or optical trap [5]. In the past few years a very intensive research has been done in case of Bose-particles both theoretically and experimentally in a variety of such systems. Fermion systems along these lines have been less studied until recently, but important results are already available and one can be sure that rapid development will continue in the future. In particular the achievement and study of the superfluid state has become one of the frontiers in physics (see for reviews [6–9], which contain references to earlier works).

In this paper we treat the open shells of trapped fermionic systems. The external potential which includes the trap potential and the average field of the closed shells will be assumed to be spherically symmetric and the interaction between atoms in the partly filled shell will be described by a spin independent δ function like attractive pseudopotential widely used for trapped gases. We focus on effects coming from the fact that the spin of the trapped atoms can be larger than 1/2. Note that the atoms are in a definite hyperfine state, whose total angular momentum is often denoted by F. For the sake of simplicity we shall speak about the spin of the particle and use the symbol s. First examples when the degeneracy temperature has been achieved are isotopes ^{6}Li and ^{40}K whose spins can be as high as $s = 3/2$ and $s = 9/2$, respectively [10,11].

Attractive interaction prefers a state as symmetric as possible in the spatial coordinates. This leads to cluster structure of the ground state, since $(2s+1)$ particles can have a completely antisymmetric spin function and consequently, the ground state is completely symmetric in spatial variables.

We concentrate on multi cluster states containing particles of numbers $N_n = n(2s+1)$ in the open shell, where $n = 1, 2, \ldots, 2l+1$ (It is similar to considering even particle numbers in case of spin 1/2). The importance of clusters consisting of $2s+1$ particles has been pointed out by us previously [12]. It has been shown that the binding energy per particle has a local maximum at multi cluster states. The cluster state is completely antisymmetric

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in spin variables and the cluster can be considered as a generalization of the singlet Cooper pair for $s > 1/2$, in other words clusters take over the role of Cooper pairs. In the present paper we extend our previous investigations to several directions and provide the proofs of some results used already in [12]. It is shown that to a good approximation the open shell Hamiltonian $\hat{H}$ can be replaced by a simplified one $\hat{H}_0$ built of the the operator of the particle number, of the quadratic Casimir operators of the groups $SU(2l+1)$ and $SO(2l+1)$. It is pointed out that the clusters can be conceived as interacting (Cooper) pairs if $s > 1/2$, the interaction being of statistical origin. The Hamiltonian $\hat{H}_0$ coincides with $\hat{H}$ for $l = 1, 2$ (These are the special cases mainly investigated in [12]).

For the Hamiltonian $\hat{H}_0$ the multi cluster states are explicitly given and the energy of the n-cluster state is written as the sum of energies of the clusters proportional to n and an "interaction term" term between the clusters proportional to $n(n-1)/2$, again of statistical origin. It is found that the second term disappears when $s = 1/2$. (For $s = 1/2$ it was shown already by Racah and Talmi in 1952 [13] that the ground state consists of independent pairs). It is proven that the mean values of the Hamiltonian $\hat{H}$ agrees with the eigenvalues of $\hat{H}_0$ in multi cluster states.

Investigations of particles in an open shell has been an important area in atomic and nuclear physics. As discussed above in the trapped gas of Fermi atoms new features appear due to the fact that the spin of the particles can be higher than $1/2$. Comparing with the situation in the electron shell of atoms a further important difference is that instead of the long ranged Coulomb force between the electrons the atom-atom interaction which has to be considered here is short ranged, while comparing the situation with that of an open neutron shell in a nucleus an important difference is that in our case the open shell is an l-one (since no spin-orbit interaction is present) as contrasted to the j-one in the nucleus. Note, however, that the interaction between the neutrons is often modelled by a δ function potential.

As mentioned it is assumed that the external potential contains besides the confining potential (which is typically of a harmonic oscillator type) the mean field of the atoms building the closed shells. There are two conditions then to be fulfilled in order that the single-l shell model apply. Firstly, the mean field due to the closed shells should be strong enough that the possible degeneracy of the levels of different l values be lifted considerably. Secondly, the characteristic interaction energy of the atoms in the partly occupied shell should be smaller than the relevant level distance in the external potential and that the polarization of the completed shells be negligible (frozen or inert core approximation, often applied in the theory of the electron shell of atoms and in the nuclear shell model to treat the dynamics of particles in the partially filled shell [3,4,14]). Both requirements can be satisfied simultaneously if the strength of the interaction between the atoms is weak and the number of the atoms in the trapped gas is sufficiently large [15,16]. We restrict ourselves to the situation when these conditions are met. This makes possible to exhibit clearly and explicitly the new qualitative features showing up when the spin of the Fermi particles is bigger than $1/2$.

Though our main purpose in this paper is to enlarge the picture we have about the dynamics of fermionic particles in a partly filled shell, a few words about the relevance of the model for physically realizable situations in case of trapped gases are in order. Obviously optical traps are the suitable ones which allow the free rotation of the spins. One can hope, for instance, that the procedure of all-optical production [17] of the spin 1/2 states of ^{6}Li atoms can be applied to keep the spin 3/2 states of these atoms.

The paper is organized as follows. In Section 2 the Hamiltonian $\hat{H}$ is written in terms of irreducible tensor operators and a simplified Hamiltonian $\hat{H}_0$ is introduced built from the operator of particle number and from the quadratic Casimir operators of the groups $SU(2l+1)$ and $SO(2l+1)$. Section 3 is devoted to the extensive investigation of the one-cluster state. Energy eigenvalues of the Hamiltonian $\hat{H}_0$ for cluster states generated by the cluster creation operator are calculated in Section 4. In Section 5 it is proven that $\hat{H}_0$ and $\hat{H}$ have the same ground states and the same ground state energies for particles of spin 1/2. In the general case $s \geq 1/2$ it is shown in Section 6 that the expectation value of the Hamiltonian agrees with the eigenvalue of $\hat{H}_0$ for cluster states. Section 7 contains the summary and a discussion of the results. Appendix A derives the properties of the symmetrizing operator. Appendices B and C present certain steps of proofs outlined in the main text. Appendix D is devoted to properties of the spectra of $\hat{H}$ which can be obtained by particle-hole transformation.

2 Formulation

The Hamiltonian of the particles in the open shell can be cast in the form

$$\mathcal{H} = \sum_{i=1}^{N} \mathcal{H}^{(1)}(\mathbf{r}_i) + H_{int} \tag{1}$$

$$\mathcal{H}^{(1)}(\mathbf{r}) = -\frac{\hbar^2 \Delta}{2M} + U(r), \tag{2}$$

where $\mathcal{H}^{(1)}$ represents the kinetic energy of a particle and the one-particle potential, which includes the external potential and the average field of the closed shells. It is assumed that U is spherically symmetric and the solutions of the eigenvalue problem

$$\mathcal{H}^{(1)} \Psi_{n_r,l,m,s,\nu} = \mathcal{E}^{(1)}(n_r, l) \Psi_{n_r,l,m,s,\nu} \tag{3}$$

are known. The one particle normalized wavefunctions have the usual form

$$\Psi_{n_r,l,m,s,\nu}(r, \vartheta, \varphi, \varsigma) = R_{n_r,l}(r) Y_m^l(\vartheta, \varphi) \chi_\nu^s(\varsigma). \tag{4}$$

Here ς is the discrete spin variable and $\chi_\nu^s(\varsigma)$ is the normalized spin eigenfunction. In the model the quantum numbers (n_r, l, s) are fixed, m and ν can take the values $m = -l, -l+1, \ldots, l$ and $\nu = -s, -s+1, \ldots, s$ and the particle number N can vary between 0 and $(2l+1)(2s+1)$. The interaction between the particles in the partially filled shell is given by

$$H_{int} = -\frac{\lambda}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{N} \delta(\mathbf{r}_i - \mathbf{r}_j), \quad \lambda > 0 \tag{5}$$

corresponding to a spin independent s-wave scattering with negative scattering length. Our aim is to diagonalize (5) on the fixed basis (4).

Let us denote the operator which annihilates a particle with quantum numbers (n_r, l, m, s, ν) by $a_{m,\nu}$. The Hamiltonian (5) in second quantization reads as

$$\hat{H}_{int} \equiv g\hat{H} = -\frac{g\pi}{2} \sum_{\substack{m_1,m_2 \\ m_3,m_4}} \sum_{\nu_1,\nu_2} f_{m_1,m_2;m_3,m_4} \times a^{+}_{m_1,\nu_1} a^{+}_{m_2,\nu_2} a_{m_4,\nu_2} a_{m_3,\nu_1}, \tag{6}$$

where g is the characteristic energy

$$g = \frac{\lambda}{\pi} \int_0^\infty |R_{n_r,l}(r)|^4 r^2 \, dr, \tag{7}$$

and f is

$$f_{m_1,m_2;m_3,m_4} = \int d\Omega \, Y^{l*}_{m_1}(\Omega) Y^{l*}_{m_2}(\Omega) Y^{l}_{m_3}(\Omega) Y^{l}_{m_4}(\Omega). \tag{8}$$

f can be expressed in terms of the Wigner-3j symbols [18]

$$f_{m_1,m_2;m_3,m_4} = \frac{[l]^2}{4\pi} \sum_{L=0}^{2l} [L] \begin{pmatrix} L & l & l \\ 0 & 0 & 0 \end{pmatrix}^2 (-1)^{(m_2+m_3)} \times \sum_{M=-L}^{L} \begin{pmatrix} l & l & L \\ m_1 & -m_3 & -M \end{pmatrix} \begin{pmatrix} l & l & L \\ m_4 & -m_2 & -M \end{pmatrix}. \tag{9}$$

For notational simplicity we introduced the symbol $[\ldots]$ defined by

$$[p] \equiv (2p+1).$$

The dimensionless Hamiltonian $\hat{H}$ (see Eq. (6)) can be written as

$$\hat{H} = \frac{[l]}{8} \hat{N} - \frac{[l]^2}{8} \sum_{L=0}^{2l} \begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix}^2 \hat{B}^2_L, \tag{10}$$

where

$$\hat{B}^2_L = \sum_{M=-L}^{L} (-1)^{L-M} \hat{B}_{L,M} \hat{B}_{L,-M}. \tag{11}$$

In fact, the Wigner-3j symbol in equation (10) vanishes for L odd, thus the sum over L runs over even values of L. The operators $\hat{B}_{L,M}$ defined as

$$\hat{B}_{L,M} = \sum_{m=-l}^{l} \sum_{\nu=-s}^{s} (-1)^{l-m} \sqrt{[L]} \times \begin{pmatrix} l & l & L \\ m & M-m & -M \end{pmatrix} a^{+}_{m,\nu} a_{m-M,\nu} \tag{12}$$

are spin scalars and irreducible tensor-operators with respect to angular momentum [1]. They take the form for $L = 0$ and $L = 1$

$$\hat{B}_{0,0} = \frac{\hat{N}}{\sqrt{[l]}} = \frac{1}{\sqrt{[l]}} \sum_{m=-l}^{l} \sum_{\nu=-s}^{s} a^{+}_{m,\nu} a_{m,\nu} \tag{13}$$

and

$$\hat{B}_{1,0} = \frac{\sqrt{3}}{\sqrt{l(l+1)[l]}} \hat{L}_z, \qquad \hat{B}_{1,\pm 1} = \mp \frac{\sqrt{3}}{\sqrt{2l(l+1)[l]}} \hat{L}_{\pm}, \tag{14}$$

respectively. The operator $\hat{B}_{0,0}$ commutes with all the other $\hat{B}_{L,M}$ operators. The operators $\hat{B}_{L,M}$ for $L \geq 1$ form a Lie-group, which is isomorphic to $SU(2l+1)$. The commutators are

$$\left[\hat{B}_{L,M}, \hat{B}_{L',M'}\right] = -\sum_{L'',M''} \sqrt{[L][L'][L'']} \times \left[1 - (-1)^{L+L'+L''}\right] (-1)^{M''} \begin{pmatrix} L & L' & L'' \\ M & M' & -M'' \end{pmatrix} \times \begin{Bmatrix} L & L' & L'' \\ l & l & l \end{Bmatrix} \hat{B}_{L'',M''}, \tag{15}$$

where $\{\ldots\}$ denotes the Wigner-6j symbol. Due to the special form of the structure coefficients the operators $\hat{B}_{L,M}$ for odd L form a subgroup, which is isomorphic to $SO(2l+1)$. This latter also has a subgroup $SO(3)$ [19] spanned by $\hat{B}_{1,M}$, $M = 0, \pm 1$. The Casimir-operator of $SU(2l+1)$ is

$$\hat{C}_u = \sum_{L=1}^{2l} (-1)^L \hat{B}^2_L \tag{16}$$

and that of $SO(2l+1)$

$$\hat{C}_o = -\sum_{\substack{L=1 \\ L:\mathrm{odd}}}^{2l-1} \hat{B}^2_L. \tag{17}$$

The Hamiltonian $\hat{H}$ defined in equation (10) commutes with $\hat{L}^2$, $\hat{L}_z$, $\hat{S}^2$, $\hat{S}_z$ and with the Casimir operator $\hat{C}_u$. In the special case $l = 1$, because the operator $\hat{B}^2_2 = \hat{C}_u - \hat{C}_o$, and in case $l = 2$, because of the accidental coincidence

$$\begin{pmatrix} 2 & 2 & 2 \\ 0 & 0 & 0 \end{pmatrix}^2 = \begin{pmatrix} 2 & 2 & 4 \\ 0 & 0 & 0 \end{pmatrix}^2 = \frac{2}{35},$$

$\hat{H}$ can be expressed entirely in terms of $\hat{N}$, $\hat{C}_u$ and $\hat{C}_o$. For $l > 2$ this is not true anymore, and furthermore $\hat{C}_o$ does not commute with $\hat{H}$.

It is useful to introduce a splitting of the Hamiltonian as follows

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \tag{18}$$

where

$$\hat{H}_0 = \frac{[l]}{8}\hat{N} - \frac{\hat{N}^2}{8} - \frac{[l]}{4(2l+3)}\left(\hat{C}_u - \hat{C}_o\right), \tag{19}$$

and

$$\hat{H}_1 = \hat{H} - \hat{H}_0 = -\frac{[l]^2}{8}\sum_{\substack{L=2\\L:even}}^{2l}\left(\begin{pmatrix} l & l & L\\ 0 & 0 & 0\end{pmatrix}^2 - \frac{2}{(2l+3)[l]}\right)\hat{B}_L^2. \tag{20}$$

Furthermore we will use the notations

$$\hat{H}_0|\Psi\rangle_0 = \epsilon|\Psi\rangle_0, \tag{21}$$

$$\hat{H}|\Psi\rangle = E|\Psi\rangle, \tag{22}$$

$$\hat{\mathcal{H}}|\Psi\rangle = \mathcal{E}|\Psi\rangle. \tag{23}$$

$E(\gamma, N)$ is the intrashell energy (in units of g). The total energy of the particles in the open shell is

$$\mathcal{E}(n_r, \gamma, N) = E(\gamma, N)g + \mathcal{E}^{(1)}(n_r, l)N \tag{24}$$

according to (3), where γ is the necessary set of quantum numbers to characterize uniquely an eigenstate of $\hat{H}$. The parameters in $\hat{H}_0$ have been chosen so that $\hat{H}_1 = 0$ for p and d shells and in general the average ${}_0\langle ncl|\hat{H}_1|ncl\rangle_0 = 0$ as will be shown in Section 6. Here $|ncl\rangle_0$ refers to the n-cluster state, i.e., to the ground state of $\hat{H}_0$ for particle number

$$N_n = n(2s+1), \quad n = 0, 1, \ldots, (2l+1). \tag{25}$$

We calculate in the next section the exact ground state eigenvalues of $\hat{H}$ for different l, s values ($l > 2$, $s > 1/2$) to demonstrate that the effect of $\hat{H}_1$ is small. Later we will also show that $\hat{H}$ and $\hat{H}_0$ share the same ground states for even particle numbers if $s = 1/2$.

3 Cluster states

Making a full numerical diagonalization of the Hamiltonian (10) is not easy. Fock-vectors have $(2l+1)(2s+1)$ slots, and in each slot there is a zero or 1 due to the fermionic character of the problem. The dimension of the full Hilbert-space is $2^{(2l+1)(2s+1)}$. The spectra do not depend on L_z and S_z, thus we can restrict ourselves to the fermionic sectors $L_z = 0$, $S_z = 0$ (even particle numbers) or $L_z = 0$, $S_z = 1/2$ (odd particle numbers). Conserved operators such as $\hat{S}^2$, $\hat{L}^2$, $\hat{N}$ and $\hat{C}_u$ make the numerical problem block-diagonal, but still the computer time and storage required grows exponentially fast as soon as we increase the open shell quantum numbers s or l. This motivates our analytical approach besides the numerical efforts.

In this section we give an overview of main features of clusters. In the special case spin of 1/2 the cluster is the well-known singlet pair which is created by

$$\hat{Q}^+_{0,0} = \sqrt{\frac{2}{[l]}}\sum_{m=-l}^{l}(-1)^{l-m}a^+_{m,\uparrow}a^+_{-m,\downarrow}, \quad s = 1/2 \tag{26}$$

from the vacuum: $\hat{Q}^+_{0,0}|0\rangle$. It will be shown that this state is an eigenstate not only of $\hat{H}_0$, but also of $\hat{H}$ with the same eigenvalue.

In [12] we have investigated the ground state wave function at the particle number $N_1 = 2s+1$ in first quantization. In second quantization we seek the corresponding wave function in the form of

$$|1cl\rangle = \sum_k c_k S_m\left(\prod_{i=1}^{(2s+1)} a^+_{m_i, s+1-i}\right)|0\rangle,$$

$$k \equiv (m_1, \ldots, m_{2s+1}), \tag{27}$$

with some coefficients c_k to be determined from equation (22). Here the symbol S_m is an operator which symmetrizes the product of creation operators with respect to the indices $m_1, \ldots, m_{2s+1}$ (see Appendix A for the properties of this operator). The state (27) is antisymmetric in the spin variables.

For notational simplicity let us introduce the integer σ by

$$\sigma = \frac{(2s+1)}{2}. \tag{28}$$

In case of $\hat{H}_0$ the ground state (27) takes the form

$$|1cl\rangle_0 = S_m(\hat{Q}^{+\sigma}_{0,0})|0\rangle \tag{29}$$

(for the proof see Sect. 4). The operator $\hat{Q}^+_{0,0}$ in (29) shall play a central role in the following analysis. It creates a pair state from the vacuum with quantum numbers $L = S = 0$ and with fixed open shell quantum numbers (l, s):

$$\hat{Q}^+_{0,0} = \frac{1}{\sqrt{[l][s]}}\sum_{m,\nu}(-1)^{s-\nu+l-m}a^+_{m,\nu}a^+_{-m,-\nu}. \tag{30}$$

$\hat{Q}^+_{0,0}$ is an example for a pair creation operator when the two particles occupy time reversed states and is a generalization of (26) for $s \geq 1/2$. Obviously

$$S_m(\hat{Q}^+_{0,0}) = \hat{Q}^+_{0,0}. \tag{31}$$

Since $\hat{H}$ and $\hat{H}_0$ coincide for $l = 1, 2$ the first example when (29) is not an eigenstate of $\hat{H}$ occurs for $l = 3$, $s = 3/2$. $N = N_1 = 4$ is then the corresponding first cluster particle number. The ground state is in the $L = L_z = S = S_z = 0$ fermionic sector. In this sector there are five orthonormal basis vectors. The matrix elements of $\hat{H}$ on this basis are the following

$$H_{i,j} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0\\ 0 & -\frac{14}{11} & 0 & 0 & 0\\ 0 & 0 & -\frac{7}{2} & 0 & 0\\ 0 & 0 & 0 & -\frac{4886}{2145} & -\frac{14}{3}\sqrt{\frac{2}{715}}\\ 0 & 0 & 0 & -\frac{14}{3}\sqrt{\frac{2}{715}} & -\frac{35}{6}\end{pmatrix}.$$

The true ground state energy for $N = 4$ comes from the lowest 2×2 block-diagonal and has the value for the

Table 1. Ground state energies of $\hat{H}$ (upper part) and $\hat{H}_0$ (lower part) up to two decimal digits precision at the one-cluster particle numbers $N_1 = (2s+1)$.

	$s = 1/2$	$s = 3/2$	$s = 5/2$	$s = 7/2$
$l = 1$	–0.75	–3.30	–7.65	–13.80
$l = 2$	–1.25	–4.64	–10.18	–17.86
$l = 3$	–1.75	–5.85	–12.32	–21.17
$l = 4$	–2.25	–6.99	–14.26	–24.12
$l = 5$	–2.75	–8.09	–16.09	—
$l = 6$	–3.25	–9.17	–17.83	—
$l = 1$	–0.75	–3.30	–7.65	–13.80
$l = 2$	–1.25	–4.64	–10.18	–17.86
$l = 3$	–1.75	–5.83	–12.25	–21.00
$l = 4$	–2.25	–6.95	–14.11	–23.72
$l = 5$	–2.75	–8.04	–15.86	—
$l = 6$	–3.25	–9.10	–17.55	—

ground state

$$E_0 = -\frac{7(1657 + \sqrt{537729})}{2860} \approx -5.85038,$$

which is quite close to $h_{5,5} = -35/6 \approx -5.83333$. Numerically $H_{i,j}$ in the same 2×2 block is

$$H_{i,j} \approx \begin{pmatrix} -2.27786 & -0.246813 \\ -0.246813 & -5.83333 \end{pmatrix},$$

and the lowest energy state belongs to the eigenvector

$$v_g \approx \begin{pmatrix} 0.0690865 \\ 1 \end{pmatrix}. \tag{32}$$

It is interesting to present the matrix elements of $\hat{C}_u$

$$C(SU(7))_{i,j} = \begin{pmatrix} \frac{264}{7} & 0 \\ 0 & \frac{264}{7} \end{pmatrix}$$

and that of $\hat{C}_o$

$$C(SO(7))_{i,j} = \begin{pmatrix} 18 & 0 \\ 0 & 0 \end{pmatrix}.$$

In (32) there is a small admixture of two vectors belonging to different eigenvalues of $\hat{C}_o$ and the dominant part is provided by the eigenvector of $\hat{C}_o$ with eigenvalue zero. Analyzing further this fifth vector it turns out that it is still given by (29) with $l = 3, s = 3/2$. The average value of $\hat{H}$ by this vector is equal to that of $\hat{H}_0$. Similar property will be proven in Section 6 also for multi cluster states. It is important to stress that the fourth vector and the true ground state v_g (32) are also symmetrized states (27).

In Table 1 we show the numerically calculated ground state energies of $\hat{H}$ (10) and $\hat{H}_0$ (19). From the data it is clearly seen that for $l = 1, 2$ or for $s = 1/2$ the expression given in (29) is the exact ground state and for all the other cases $|1cl\rangle \approx |1cl\rangle_0$ is quite a good approximation. This shows the importance of the simplified Hamiltonian $\hat{H}_0$. The dominating contribution to the energy (lower part of Tab. 1) can be written in the form

$$\epsilon_1 = -\sigma\epsilon^{(2)} - \frac{\sigma(\sigma-1)}{2}\delta,$$

where $\epsilon^{(2)}$ and δ are independent of the spin. Their explicit expressions will be derived in Section 4. The first term gives the energy of σ independent pairs while the second term lowers this energy, indicating clearly that the cluster wave function gives lower energy than the wave function of independent pairs. Note that an eigenfunction of $\hat{H}_0$ exists with the eigenvalue $-\sigma\epsilon^{(2)}$ if the inequality $\sigma \leq 2l+1$ is fulfilled. For spin one half particles one has only the first term, the energy of a single pair.

4 Cluster states and ground state energies of $\hat{\mathbf{H}}_0$

Let us consider the states

$$|ncl\rangle_0 = \hat{Q}^{+n}|0\rangle, \quad n = 0, \dots, (2l+1), \tag{33}$$

where the operator $\hat{Q}^+$ is given in terms of the operator (30) by

$$\hat{Q}^+ = S_m(\hat{Q}^{+\sigma}_{0,0}). \tag{34}$$

$\hat{Q}^+$ creates a $(2s+1)$ particle state. In the following we shall prove that $|ncl\rangle_0$ is an eigenstate of the Hamiltonian $\hat{H}_0$ (19).

We deal first with the special case $s = 1/2$ ($\sigma = 1$). According to (31), (34)

$$\hat{Q}^+ = \hat{Q}^+_{0,0}, \quad s = 1/2. \tag{35}$$

and $\hat{Q}^+_{0,0}$ is given by equation (26). The procedure is that the $\hat{B}_{L,M}$ operators are moved to the vacuum when $\hat{C}_u$ or $\hat{C}_o$ is applied to the state $|ncl\rangle_0 = \hat{Q}^{+n}_{0,0}|0\rangle$. One can see using the fact $[\hat{Q}^+_{0,0}, \hat{Q}^+_{L,M}] = 0$ that

$$\left[\hat{B}_{L,M}, \hat{Q}^{+n}_{0,0}\right] = \frac{2n}{\sqrt{[l]}}\hat{Q}^{+(n-1)}_{0,0}\hat{Q}^+_{L,M}, \tag{36}$$

where

$$\hat{Q}^+_{L,M} = \sqrt{\frac{[L]}{2}}(-1)^M\left[1 + (-1)^L\right] \times \sum_{m=-l}^{l}\begin{pmatrix} l & l & L \\ m & M-m & -M \end{pmatrix} a^+_{m,\uparrow}a^+_{M-m,\downarrow}. \tag{37}$$

Note that $\hat{Q}^+_{L,M} = 0$ for L odd. Consequently, $\hat{C}_o|ncl\rangle_0 = 0$. Next step is to calculate

$$\hat{B}_{L,-M}\hat{B}_{L,M}\hat{Q}^{+n}_{0,0}|0\rangle = \left(\frac{4n(n-1)}{[l]}\hat{Q}^{+(n-2)}_{0,0}\hat{Q}^+_{L,M}\hat{Q}^+_{L,-M} + \frac{2n}{\sqrt{[l]}}\hat{Q}^{+(n-1)}_{0,0}[\hat{B}_{L,-M}, \hat{Q}^+_{L,M}]\right)|0\rangle. \tag{38}$$

Summation over L and M according to (16) and (11) can be performed using the two identities

$$\sum_{M=-L}^{L}(-1)^M\left[\hat{B}_{L,-M},\hat{Q}^+_{L,M}\right]=\frac{2[L]}{\sqrt{[l]}}\hat{Q}^+_{0,0},\quad L:\text{even},\tag{39}$$

$$\sum_{L=0}^{2l}\sum_{M=-L}^{L}(-1)^{L-M}\hat{Q}^+_{L,M}\hat{Q}^+_{L,-M}=-\frac{[l]}{2}\hat{Q}^{+2}_{0,0},\quad s=1/2.\tag{40}$$

One arrives at the result that $|ncl\rangle_0$ is an eigenvector of $\hat{C}_u$ and that

$$\hat{H}_0|ncl\rangle_0=-\frac{n(2l+1)}{4}|ncl\rangle_0,\quad s=1/2,\tag{41}$$

where we used (19) and that $\hat{N}|ncl\rangle_0=2n|ncl\rangle_0$.

We turn now to the general case $s>1/2$. Using the identity (80) of Appendix A one gets

$$\left[\hat{B}_{L,M},S_m(\hat{Q}^{+\sigma}_{0,0})\right]=\frac{2\sigma}{\sqrt{[l]}}S_m(\hat{Q}^+_{L,M}\hat{Q}^{+\sigma-1}_{0,0}),\tag{42}$$

where

$$\hat{Q}^+_{L,M}=\sqrt{\frac{[L]}{[s]}}\sum_{m=-l}^{l}\sum_{\nu=-s}^{s}(-1)^{s-\nu+M}\times\begin{pmatrix}l & l & L\\ m & M-m & -M\end{pmatrix}a^+_{m,\nu}a^+_{M-m,-\nu}.\tag{43}$$

$\hat{Q}^+_{L,M}=0$ for L odd as can be easily seen. For $L=M=0$ this expression agrees with (30) and for $s=1/2$ goes over to (37). Furthermore

$$S_m(\hat{Q}^+_{L,M})=\hat{Q}^+_{L,M}.\tag{44}$$

$\hat{C}_o$ is built up from operators $\hat{B}_{L,M}$ with L odd (see Eq. (17)), but the right hand side of (42) in that case is zero. As a result $\hat{C}_o$ when applied to the state given in (33) can be moved to the vacuum, which is annihilated by $\hat{C}_o$

$$\hat{C}_o|ncl\rangle_0=0.\tag{45}$$

As a byproduct we have the property

$$\left[\hat{C}_o,\hat{Q}^+\right]=0,\tag{46}$$

i.e., the operator $\hat{Q}^+$ commutes with $\hat{C}_o$.

To show that $|ncl\rangle_0$ is an eigenvector of $\hat{C}_u$ in case $s>1/2$ requires more elaborate calculations. In moving the operators $\hat{B}_{L,M}$ towards the vacuum one encounters several new objects from the commutators as anticipated from equation (42). In deriving them one needs the property that S_m and the operator of commutation commutes for the operators occurring as shown in the Appendix A.

For the new objects one can use the identities (see Appendix B)

$$\sum_{L=0}^{2l}\sum_{M=-L}^{L}(-1)^M S_m(\hat{Q}^+_{L,M}\hat{Q}^+_{L,-M}\hat{Q}^{+\sigma-2}_{0,0})=[l]S_m(\hat{Q}^{+\sigma}_{0,0}),\tag{47}$$

which is valid for $\sigma\geq 2$ and

$$\sum_{L=0}^{2l}\sum_{M=-L}^{L}(-1)^M S_m(\hat{Q}^+_{L,M}\hat{Q}^{+\sigma-1}_{0,0})S_m(\hat{Q}^+_{L,-M}\hat{Q}^{+\sigma-1}_{0,0})=-\frac{[l]}{[s]}S_m(\hat{Q}^{+\sigma}_{0,0})^2.\tag{48}$$

As a result one has

$$\hat{C}_u|ncl\rangle_0=\frac{n([l]-n)}{[l]}[s]([l]+[s])|ncl\rangle_0,\tag{49}$$

i.e., $|ncl\rangle_0$ as given by (33) is really an eigenvector of $\hat{C}_u$. Correspondingly for $\hat{H}_0$ (19) using (45) one obtains:

$$\hat{H}_0|ncl\rangle_0=\epsilon_n|ncl\rangle_0,\tag{50}$$

with

$$\epsilon_n=-\frac{n(2l+1)(2s+1)}{8(2l+3)}\left[n(2s-1)+2l+1+4s\right].\tag{51}$$

This expression can be cast into the form

$$\epsilon_n=n\epsilon_1+\frac{n(n-1)}{2}\gamma,\tag{52}$$

where

$$\epsilon_1=-\frac{(2l+1)(2s+1)}{4(2l+3)}(3s+l)\tag{53}$$

and

$$\gamma=-\frac{(2l+1)(2s+1)}{4(2l+3)}(2s-1).\tag{54}$$

The first term on the right hand side of equation (52) can be interpreted as the energy of n independent one-clusters and the second term as a kind of cluster-cluster interaction energy. Furthermore the energy ϵ_1 can be rewritten as

$$\epsilon_1=-\sigma\epsilon^{(2)}-\frac{\sigma(\sigma-1)}{2}\delta,\tag{55}$$

where

$$\epsilon^{(2)}=\frac{2l+1}{4},\quad\delta=\frac{12}{2l+3}\epsilon^{(2)}.\tag{56}$$

They are independent of the spin. For spin one-half particles $\gamma=0$ and the prefactor of δ in (55) is zero, which means that the clusters consist of pairs which are independent, as already stated.

One can raise the question what is the ratio of the interaction energies in average of two pairs within the same cluster and when they belong to two different clusters. This ratio is equal to

$$\frac{\delta}{\gamma/\sigma^2}=\frac{3(2s+1)}{2s-1},\quad s>1.\tag{57}$$

It is remarkable that this expression is l-independent. This ratio is always bigger than one, monotonically decreasing with increasing s.

5 Ground state energies of spin 1/2 particles

In (41) we have shown that for $s = 1/2$ the state $|ncl\rangle_0$ is an eigenvector of $\hat{H}_0$. Let us consider now first how $\hat{H}_1$ acts to a one cluster state. Direct calculation gives

$$\hat{B}_L^2|1cl\rangle_0 = \frac{4n[L]}{[l]}|1cl\rangle_0, \quad s = 1/2, \quad L : \text{even}. \tag{58}$$

Substituting this into equation (20) and performing the sum over L in (20) results in

$$\hat{H}_1\hat{Q}^+_{0,0}|0\rangle = 0. \tag{59}$$

For multi cluster states we proceed as follows. Carrying out the summation over L in (20) leads after some rearrangements to

$$\hat{H}_1|ncl\rangle = -\frac{[l]}{2}n(n-1)\sum_{L=0}^{2l}\begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix}^2|\mu_L\rangle, \tag{60}$$

where

$$|\mu_L\rangle = \hat{Q}^{+(n-2)}_{0,0}\sum_{M=-L}^{L}(-1)^M\hat{Q}^+_{L,M}\hat{Q}^+_{L,-M}|0\rangle. \tag{61}$$

Using (26) and (37) and the identity

$$0 = \sum_{L=0}^{2l}[L]\begin{pmatrix} L & l & l \\ 0 & 0 & 0 \end{pmatrix}^2 \times \sum_{M=-L}^{L}\left[\begin{pmatrix} l & l & L \\ m_1 & m_2 & -M \end{pmatrix}\begin{pmatrix} l & l & L \\ m_3 & m_4 & -M \end{pmatrix} -(-1)^{(m_2+m_3)}\begin{pmatrix} l & l & L \\ m_1 & -m_3 & -M \end{pmatrix}\begin{pmatrix} l & l & L \\ m_4 & -m_2 & -M \end{pmatrix}\right] \tag{62}$$

we arrive at the rather long form

$$\sum_{L=0}^{2l}\begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix}^2|\mu_L\rangle = 2\hat{Q}^{+(n-2)}_{0,0}\sum_{\substack{m_1,m_2\\ m_3,m_4}}(-1)^{m_1+m_3} \times \sum_{\substack{L=0\\ L:\text{even}}}^{2l}[L]\begin{pmatrix} l & l & L \\ 0 & 0 & 0 \end{pmatrix}^2\sum_{M=-L}^{L}\begin{pmatrix} l & l & L \\ m_1 & m_3 & -M \end{pmatrix} \times \begin{pmatrix} l & l & L \\ -m_4 & -m_2 & -M \end{pmatrix}a^+_{m_1,\uparrow}a^+_{m_2,\downarrow}a^+_{m_3,\uparrow}a^+_{m_4,\downarrow}|0\rangle \tag{63}$$

for the expression occurring on the right hand side of equation (60). The operator $a^+_{m_1,\uparrow}a^+_{m_2,\downarrow}a^+_{m_3,\uparrow}a^+_{m_4,\downarrow}$ is antisymmetric in m_1, m_3, while its coefficient is symmetric in the same indices, thus the right hand side must be zero. This completes the proof that

$$\hat{H}_1|ncl\rangle_0 = 0, \quad s = 1/2, \tag{64}$$

i.e., the state $|ncl\rangle_0$ is an eigenstate of both $\hat{H}_0$ and $\hat{H}$ for $s = 1/2$ with the same eigenvalue as given in (41). This provides an alternative proof of the result of Racah and Talmi [13] within our framework that the ground state of spin 1/2 particles interacting by an attractive δ-function potential consists of independent pairs.

6 Average energies in cluster states

In this section it will be proven that the expectation values of $\hat{H}$ (Eq. (10)) by the cluster states (33) are always the same as the corresponding eigenvalues (52) of $\hat{H}_0$. Acting with the operators $\hat{B}_L^2$ (see Eqs. (10), (11)) on the cluster states of $\hat{H}_0$ using the rules (91), (80) one gets three terms (see Appendix C and A):

$$\hat{B}_L^2|ncl\rangle_0 = \frac{4n\sigma[L]}{[l]}|ncl\rangle_0 + \frac{4n\sigma(\sigma-1)}{[l]}|\alpha_L\rangle + \frac{4n(n-1)\sigma^2}{[l]}|\beta_L\rangle, \quad L : \text{even}, \tag{65}$$

and zero for L odd. The vectors $|\alpha_L\rangle$ and $|\beta_L\rangle$ are defined as follows:

$$|\alpha_L\rangle = \hat{Q}^{+(n-1)}\sum_{M=-L}^{L}(-1)^M S_m(\hat{Q}^+_{L,M}\hat{Q}^+_{L,-M}\hat{Q}^{+\sigma-2}_{0,0})|0\rangle \tag{66}$$

and

$$|\beta_L\rangle = \hat{Q}^{+(n-2)}\sum_{M=-L}^{L}(-1)^M \times S_m(\hat{Q}^+_{L,M}\hat{Q}^{+\sigma-1}_{0,0})S_m(\hat{Q}^+_{L,-M}\hat{Q}^{+\sigma-1}_{0,0})|0\rangle. \tag{67}$$

In the special case $L = 0$ the two vectors agree with $|ncl\rangle_0$, and for $L = 2, 4, \ldots, 2l$ it can be shown that $|\alpha_L\rangle$ and $|\beta_L\rangle$ can be decomposed as

$$|\alpha_L\rangle = \frac{4[L]}{2l+3}|ncl\rangle_0 + |\alpha_L^\perp\rangle, \quad L = 2, 4, \ldots, 2l \tag{68}$$

and

$$|\beta_L\rangle = -\frac{[L]([l]+[s])}{l[s](2l+3)}|ncl\rangle_0 + |\beta_L^\perp\rangle, \quad L = 2, 4, \ldots, 2l \tag{69}$$

(see Appendix C), where $|\alpha_L^\perp\rangle$ and $|\beta_L^\perp\rangle$ are possibly zero vectors, but if not, they are eigenvectors of $\hat{C}_o$ with positive eigenvalues, and are automatically orthogonal to $|ncl\rangle_0$ (which is also an eigenvector of $\hat{C}_o$ but with zero eigenvalue).

Using the above results the energy of the system described by $\hat{H}$ averaged with $|ncl\rangle_0$ is

$$\frac{\langle ncl|\hat{H}|ncl\rangle_0}{\langle ncl|ncl\rangle_0} = \frac{\langle ncl|\hat{H}_0|ncl\rangle_0}{\langle ncl|ncl\rangle_0} = \epsilon_n, \tag{70}$$

where ϵ_n is given by (51) according to (50) . Furthermore, we remind the reader that for $l = 1, 2$ the operators $\hat{H}$ and $\hat{H}_0$ coincide.

Equation (70) shows that in the general case $|ncl\rangle_0$ can be regarded as a trial wave function, i.e., the ground state energy of the n-cluster state lies below ϵ_n given by (51). Furthermore, if we make the decomposition, according to (18), as $\hat{H} = \hat{H}_0 + \hat{H}_1$ and if we consider $\hat{H}_0$ as an unperturbed Hamiltonian with unperturbed ground state $|ncl\rangle_0$ then equation (70) shows that we do not obtain correction to the unperturbed energy ϵ_n to first order, corrections are at least of second order, which can be small because the off-diagonal matrix elements can be small. This explains the numerical finding for $l = 3$, $s = 3/2$ and $N = 4$ that the deviation of ϵ_n from the true ground state energy is of the order 0.3% (see Sect. 3). The true ground state, in general, is not a state, which is annihilated by the Casimir operator of $SO(2l + 1)$, even in the case $n = 1$, but it has a small admixture of some other eigenstates of $\hat{C}_o$ with positive eigenvalues.

7 Discussion

In preceding sections we have analyzed in detail the cluster formation for $s > 1/2$ as a generalization for pairing for $s = 1/2$ in the open shell model with attractive δ interaction between the particles. We have constructed the states $|ncl\rangle_0 = \hat{Q}^{+n}|0\rangle$ and showed that in a certain subset of shell parameters l, s these states are exact and in other cases they are fairly good approximate ground states. We expressed the cluster creation operator $\hat{Q}^+$ in terms of the symmetrized product of the pair creation operator $\hat{Q}^+_{0,0}$ as $\hat{Q}^+ = S_m(\hat{Q}^{+\sigma}_{0,0})$. It is interesting to note that the operator S_m itself, which by definition symmetrizes with respect to the angular momentum indices, can be interpreted as an antisymmetrizer, which acts on spin indices. The introduction of the symmetrizing operator is basic for $s > 1/2$ since this operator ensures that the spin function of the cluster, written in terms of spatial and spin variables of the particles, is the Slater determinant of $(2s + 1)$ linearly independent one particle spin functions [12].

Let us assume that an optical trap producing a harmonic oscillator potential is filled gradually with atoms of spin s. Though it can be only of academic interest we find it enlightening to look at the situation for small particle numbers. The first shell (specified by the harmonic oscillator quantum number $n_{ho} = 0$) is completed when the particle number is $2s + 1$, i.e., one cluster is created ($l = 0$, of course). The shells $l = 1, 2, 3$ appear first in the harmonic oscillator shells $n_{ho} = 1, 2, 3$, respectively. Concerning the spectrum there is a qualitative difference between the cases $l \leq 2$ and $l > 2$ since for the latter l values $\hat{H}$ is no more equal to $\hat{H}_0$. This is demonstrated in Figures 1 and 2. The regularity in the spectrum for $l = 2$, $s = 3/2$ (Fig. 2) is obviously lost for $l = 3$, $s = 1/2$ (Fig. 1). Note that in the Figures 1 and 2 the shifted eigenvalues

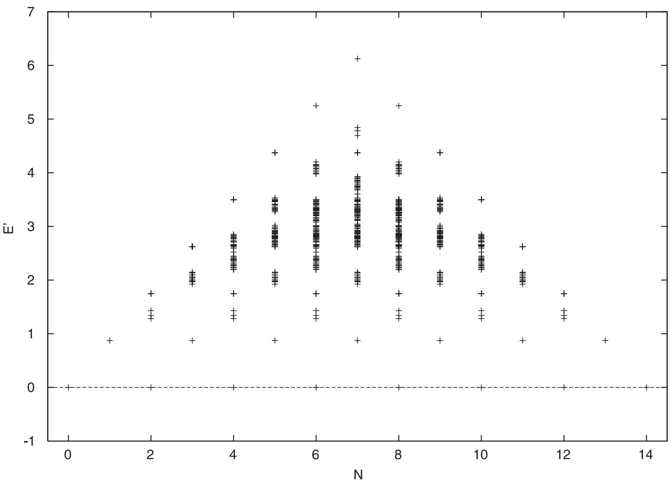

Fig. 1. The shifted energy levels E' of the dimensionless Hamilton operator as a function of the particle number N for $l = 3$, $s = 1/2$. Individual energy levels are denoted by crosses (+). The dashed line is the function (72).

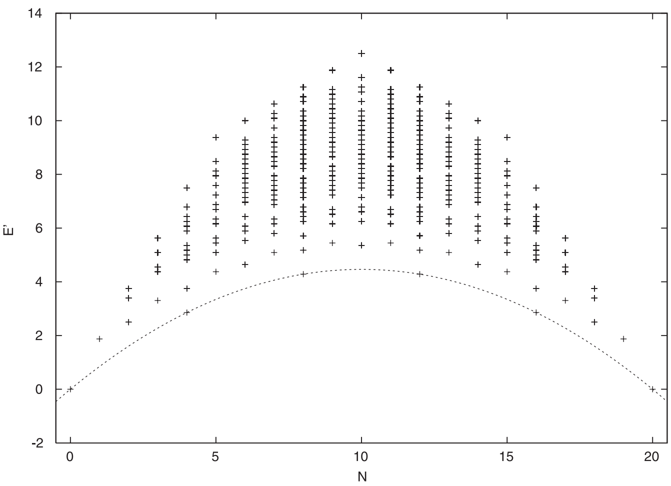

Fig. 2. The shifted energy levels E' of the dimensionless Hamilton operator as a function of the particle number N for $l = 2$, $s = 3/2$. Individual energy levels are denoted by crosses (+). The dashed line is the function (72).

defined by

$$E' = E + \frac{Ns(2l+1)}{4} \tag{71}$$

are depicted. This leads to the symmetry with respect to the half filled shell as explained in Appendix D.

Shifting the energies of the ground and excited states of $\hat{H}_0$ according to (71) the lowest shifted energies of $\hat{H}_0$ are on the curve

$$E'(N) = \frac{N(2l+1)(2s-1)}{8(2l+3)(2s+1)}\left[(2s+1)(2l+1) - N\right] \tag{72}$$

at the nth cluster particle number, i.e., if $N = N_n$, $n = 0, 1, \ldots, 2l + 1$. The energy of the particles in the open shell can be obtained from equations (24) and (71) as

$$\mathcal{E} = E'g + \left(\mathcal{E}^{(1)} - g\frac{s(2l+1)}{4}\right)N. \tag{73}$$

For large l values the ground state energy can be estimated by equation (70) which we consider one of our main results. The values $l \gg 1$ can occur when also $n_{ho} \gg 1$. It has been shown by Bruun and Heiselberg [15] (using semiclassical method valid in the case of large systems) that the condition for the applicability of the single l-shell model is satisfied when $n_{ho} > 200$ and $l \approx n_{ho}$. For large l values ϵ_n (see Eq. (51)) simplifies as

$$\frac{\epsilon_n}{l} = -n\frac{2s+1}{4}\left(1 + \frac{n(2s-1)}{2l} + \frac{4s-1}{2l} + O(1/l)\right). \tag{74}$$

Note that $n(2s+1)$ is just the particle number N_n in the open shell. As long as $N_n \ll l$ the energy per particle in the multi cluster state is practically the same as for $s = 1/2$ particles at even particle numbers calculated first by Racah and Talmi [13]. The spectrum is expected to be similar qualitatively to that appearing in Figure 1. When the open shell is half filled, however, then $n = l + O(1)$ and the ground state energy gets a factor of $(2s+1)/2 \geq 1$ according to equation (74). It is expected that the critical temperature is increased by a similar factor. (At finite temperature the gap becomes temperature dependent, of course, and the details of the spectrum are smeared.)

The main technical problem in deriving values for the approximate (or exact) cluster energies ϵ_n was relegated to Appendix C. Here we applied a powerful projection technique in a non-orthonormal and linearly non-independent basis. During this procedure it has turned out that the ground state eigenvalue of $\hat{H}_0$ is non-degenerate.

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Appendix A: The properties of the symmetrizer S_m

Let us introduce the symmetrizer symbol S_m by the following properties: (i) S_m is linear for its argument, (ii) S_m symmetrizes an operator-product $a^+_{m_1,\nu_1} \dots a^+_{m_p,\nu_p}$ of creation operators $a^+_{m_i,\nu_i}$, $i = 1, \dots, p$ with respect to *all* m_i without changing the order of spin projections $(\nu_1, \dots, \nu_p)$ including the combinatorical normalization. As an example:

$$S_m(a^+_{0,3/2}a^+_{1,1/2}a^+_{0,-1/2}) = \frac{1}{3}\big(a^+_{0,3/2}a^+_{1,1/2}a^+_{0,-1/2} + a^+_{1,3/2}a^+_{0,1/2}a^+_{0,-1/2} + a^+_{0,3/2}a^+_{0,1/2}a^+_{1,-1/2}\big).$$

Very important special case is $p = 2s+1$. Writing down all the terms in $S_m(a^+_{m_1,\nu_1} \dots a^+_{m_{2s+1},\nu_{2s+1}})$ it turns out that it must be antisymmetric in all spin indices $(\nu_1, \dots, \nu_{2s+1})$. Therefore, by inspection we have

$$S_m(a^+_{m_1,\nu_1} \dots a^+_{m_{2s+1},\nu_{2s+1}}) = \epsilon_{\nu_1,\dots,\nu_{2s+1}} \times S_m(a^+_{m_1,s} \dots a^+_{m_{2s+1},-s}), \tag{75}$$

where $\epsilon_{\nu_1,\dots,\nu_{2s+1}}$ is the antisymmetric tensor with the convention $\epsilon_{s,s-1,\dots,-s} = 1$. Further expansion is possible for the combination

$$S_m(a^+_{m_1,s} \dots a^+_{m_{2s+1},-s}) = \frac{1}{(2s+1)!} \times \sum_{\nu_1} \dots \sum_{\nu_{2s+1}} \epsilon_{\nu_1,\dots,\nu_{2s+1}} a^+_{m_1,\nu_1} \dots a^+_{m_{2s+1},\nu_{2s+1}}. \tag{76}$$

Next, we enumerate some properties of S_m useful in the following. If

$$\hat{B} = \sum_{m,n,\nu} f_{m,n} a^+_{m,\nu} a_{n,\nu}$$
$$\hat{A}_\alpha = \sum_{m,n,\nu} (-1)^{s-\nu} g^{(\alpha)}_{m,n} a^+_{m,\nu} a^+_{n,-\nu}, \quad \alpha = 1, \dots, \sigma,$$
$$g^{(\alpha)}_{m,n} = g^{(\alpha)}_{n,m} \tag{77}$$

where $f_{m,n}$ and $g^{(\alpha)}_{m,n}$ are numbers, then

$$S_m(\hat{A}_1 \dots \hat{A}_\sigma) = \frac{2^\sigma \sigma! (-1)^{\frac{\sigma(\sigma-1)}{2}}}{(2\sigma)!} \sum_{\substack{m_1,\dots,m_{2\sigma} \\ \nu_1,\dots,\nu_{2\sigma}}} \epsilon_{\nu_1,\dots,\nu_{2\sigma}} \times g^{(1)}_{m_1,m_2} \dots g^{(\sigma)}_{m_{2\sigma-1},m_{2\sigma}} a^+_{m_1,\nu_1} a^+_{m_2,\nu_2} \dots a^+_{m_{2\sigma},\nu_{2\sigma}}. \tag{78}$$

This identity can be proven using equations (75)–(78) and

$$\sum_{\nu_1} \dots \sum_{\nu_\sigma} (-1)^{s-\nu_1} \dots (-1)^{s-\nu_\sigma} \epsilon_{\nu_1,-\nu_1,\dots,\nu_\sigma,-\nu_\sigma} = 2^\sigma \sigma! (-1)^{\frac{\sigma(\sigma-1)}{2}}. \tag{79}$$

If conditions (77) hold then again from equations (75)–(78) one can derive the identity

$$\left[\hat{B}, S_m(\hat{A}_1 \dots \hat{A}_\sigma)\right] = S_m([\hat{B}, \hat{A}_1 \dots \hat{A}_\sigma]), \tag{80}$$

where $[\dots]$ denotes a commutator.

Appendix B: Proof of the identities (47) and (48)

Let us introduce the spin dependent antisymmetric matrix $\hat{G}_{\nu,z}$ by

$$\hat{G}_{\nu,z} = \sum_m (-1)^{l-m} a^+_{m,\nu} a^+_{-m,z}. \tag{81}$$

If we use (78) with $\hat{A}_1 = \dots = \hat{A}_\sigma = \hat{Q}^+_{0,0}$ we have

$$S_m(\hat{Q}^{+\sigma}_{0,0}) = \frac{2^\sigma \sigma! (-1)^{\frac{\sigma(\sigma-1)}{2}}}{(2\sigma)! \; ([l][s])^{\frac{\sigma}{2}}} \sum_{\nu_1,\dots,\nu_{2\sigma}} \epsilon_{\nu_1,\dots,\nu_{2\sigma}} \times \hat{G}_{\nu_1,\nu_2} \hat{G}_{\nu_3,\nu_4} \dots \hat{G}_{\nu_{2\sigma-1},\nu_{2\sigma}}. \tag{82}$$

If, for the expression on the left hand side of equation (47) we use once again (78) with $\hat{A}_1 = \hat{Q}^+_{L,M}$, $\hat{A}_2 = \hat{Q}^+_{L,-M}$ and with $\hat{A}_3 = \ldots = \hat{A}_\sigma = \hat{Q}^+_{0,0}$ and perform the standard sum over L and M we arrive to

$$\sum_{L=0}^{2l}\sum_{M=-L}^{L}(-1)^M S_m(\hat{Q}^+_{L,M}\hat{Q}^+_{L,-M}\hat{Q}^{+\sigma-2}_{0,0})$$
$$= \frac{2^\sigma\sigma!(-1)^{\frac{\sigma(\sigma-1)}{2}}[l]}{(2\sigma)!\ ([l][s])^{\frac{\sigma}{2}}}\sum_{m_1,n_1}(-1)^{l-m_1}(-1)^{l-n_1}$$
$$\times\sum_{\nu_1,\ldots,\nu_{2\sigma}}\epsilon_{\nu_1,\ldots,\nu_{2\sigma}}a^+_{m_1,\nu_1}a^+_{n_1,\nu_2}a^+_{-m_1,\nu_3}a^+_{-n_1,\nu_4}$$
$$\times\hat{G}_{\nu_3,\nu_4}\hat{G}_{\nu_5,\nu_6}\ldots\hat{G}_{\nu_{2\sigma-1},\nu_{2\sigma}}. \quad (83)$$

If now we change the order of $a^+_{n_1,\nu_2}\ a^+_{-m_1,\nu_3}$ using anti-commutativity we can get two more $\hat{G}$ factors. In the next step if we change the second and third indices of the ϵ tensor after comparison with (82) we arrive at the operator identity equation (47).

In order to prove equation (48) we proceed as above. Changing the order of two creation operator (and dividing both sides with a common factor) it is left to prove that

$$\frac{1}{[s]}\sum_{\substack{\nu_1,\ldots,\nu_{2\sigma}\\ z_1,\ldots,z_{2\sigma}}}\epsilon_{\nu_1,\ldots,\nu_{2\sigma}}\hat{G}_{\nu_1,\nu_2}\hat{G}_{\nu_3,\nu_4}\ldots\hat{G}_{\nu_{2\sigma-1},\nu_{2\sigma}}$$
$$\times\epsilon_{z_1,\ldots,z_{2\sigma}}\hat{G}_{z_1,z_2}\hat{G}_{z_3,z_4}\ldots\hat{G}_{z_{2\sigma-1},z_{2\sigma}}$$
$$=\sum_{\substack{\nu_1,\ldots,\nu_{2\sigma}\\ z_1,\ldots,z_{2\sigma}}}\epsilon_{\nu_1,\ldots,\nu_{2\sigma}}\hat{G}_{\nu_1,z_1}\hat{G}_{\nu_3,\nu_4}\ldots\hat{G}_{\nu_{2\sigma-1},\nu_{2\sigma}}$$
$$\times\epsilon_{z_1,\ldots,z_{2\sigma}}\hat{G}_{\nu_2,z_2}\hat{G}_{z_3,z_4}\ldots\hat{G}_{z_{2\sigma-1},z_{2\sigma}}. \quad (84)$$

By introducing the spin dependent matrix operator

$$\hat{F}_{\nu,z}=\sum_{\nu_2,\ldots,\nu_{2\sigma}}\epsilon_{\nu,\nu_2\ldots,\nu_{2\sigma}}\hat{G}_{z,\nu_2}\hat{G}_{\nu_3,\nu_4}\ldots\hat{G}_{\nu_{2\sigma-1},\nu_{2\sigma}} \quad (85)$$

and the spin-scalar operator

$$\hat{F}=\sum_{\nu_1,\ldots,\nu_{2\sigma}}\epsilon_{\nu_1,\ldots,\nu_{2\sigma}}\hat{G}_{\nu_1,\nu_2}\hat{G}_{\nu_3,\nu_4}\ldots\hat{G}_{\nu_{2\sigma-1},\nu_{2\sigma}} \quad (86)$$

from (84) it is left to be proven that

$$\frac{1}{2s+1}\hat{F}^2=\sum_{\nu,z=-s}^{s}\hat{F}_{\nu,z}\hat{F}_{z,\nu}. \quad (87)$$

Next, we show that

$$\hat{F}_{\nu,z}=\frac{\delta_{\nu,z}}{2s+1}\hat{F}. \quad (88)$$

If this is true then equations (87), (84) and correspondingly (48) are also true.

Let us study first the $\nu\neq z$ case in equation (85). In that case among the indices $(\nu_2,\ldots,\nu_{2\sigma})$ of the antisymmetric tensor ϵ the index z should occur. Let it be the index $\nu_i = z$. This cannot be ν_2, because $\hat{G}_{z,z} = 0$. It means that two *different* $\hat{G}$ has the same index z. However, in the indices ν_2 and ν_{i+1} (if the index z occur in the first index of the second $\hat{G}_{z,\nu_{i-1}}$) or ν_{i-1} (if the index z occur in the second index of the second $\hat{G}_{\nu_{i-1},z}$ factor) the product of two G factor is symmetric, while the antisymmetric tensor ϵ in the same indices is antisymmetric. Summing over ν_2 and ν_{i+1} or ν_{i-1} we get zero. It means, that

$$\hat{F}_{\nu,z}=0,\quad \text{if } \nu\neq z. \quad (89)$$

Next, let us consider $\hat{F}_{\nu,\nu}$ with ν fixed. Changing the order of indices on the right hand side of (86) such that ν be the first in the ϵ tensor and in the first $\hat{G}$ factor (using antisymmetry of the $\hat{G}$-s and ϵ) one gets

$$\hat{F}=(2s+1)\sum_{\nu_2,\ldots,\nu_{2\sigma}}\epsilon_{\nu,\nu_2\ldots,\nu_{2\sigma}}\hat{G}_{\nu,\nu_2}\hat{G}_{\nu_3,\nu_4}\ldots\hat{G}_{\nu_{2\sigma-1},\nu_{2\sigma}}$$
$$=(2s+1)\hat{F}_{\nu,\nu}, \quad (90)$$

where we have used (85). Equations (89) and (90) together give the operator identity (88), which completes the proof of equation (48).

Appendix C: Decomposition of $|\alpha_L\rangle$ and $|\beta_L\rangle$

Let us consider how $|\alpha_L\rangle$ or $|\beta_L\rangle$ behaves on applying $\hat{C}_o$ to these vectors (see Eqs. (66), (67)). Here we treat the calculation for $|\beta_L\rangle$. Exactly the same method can be applied for $|\alpha_L\rangle$ with one minor difference, which will be shown below.

It is easy to show that

$$\left[\hat{B}_{L_1,M_1},\hat{Q}^+_{L_2,M_2}\right]=2\sqrt{[L_1][L_2]}(-1)^{M_1}$$
$$\times\sum_{\substack{L=0\\ L:even}}^{2l}\sum_{M=-L}^{M}\sqrt{[L]}(-1)^M\begin{pmatrix}L_1 & L_2 & L\\ M_1 & M_2 & -M\end{pmatrix}$$
$$\times\begin{Bmatrix}L_1 & L_2 & L\\ l & l & l\end{Bmatrix}Q^+_{L,M} \quad (91)$$

with L_2 even. In using equations (80) and (91) one obtains

$$\hat{C}_o|\beta_L\rangle=2[l](1-\delta_{L,0})|\beta_L\rangle-4[L]$$
$$\times\sum_{\substack{L_1=0\\ L_1:even}}^{2l}\left(\frac{1}{[l]}-\begin{Bmatrix}L & l & l\\ L_1 & l & l\end{Bmatrix}\right)|\beta_{L_1}\rangle \quad (92)$$

with L even. In other words, the vector space V spanned by the vectors $\{|\beta_L\rangle|L=0,2,\ldots,2l\}$ is invariant under $\hat{C}_o$. If we define matrix elements in V for an operator $\hat{O}$, for which V is an invariant vector space by

$$\hat{O}|\beta_L\rangle=\sum_{L'}{}'O_{L',L}|\beta_{L'}\rangle, \quad (93)$$

where $\sum'_{L'}$ stands for $\sum_{L'=0,L':even}^{2l}$, the matrix elements of $\hat{C}_o$ obtained from (92):

$$\hat{C}_o|\beta_L\rangle\equiv\sum_{L'}{}'C_{L',L}|\beta_{L'}\rangle, \quad (94)$$

$$C_{L',L} = 2[l](1-\delta_{L,0})\delta_{L',L} - 4[L]\left(\frac{1}{[l]} - \begin{Bmatrix} L & l & l \\ L' & l & l \end{Bmatrix}\right)$$
$$= (1-\delta_{L,0})(1-\delta_{L',0}) \times \left(2[l]\delta_{L',L} - 4[L]\left(\frac{1}{[l]} - \begin{Bmatrix} L & l & l \\ L' & l & l \end{Bmatrix}\right)\right) \quad (95)$$

for L, L' even. The second equality follows from

$$\begin{Bmatrix} L & l & l \\ 0 & l & l \end{Bmatrix} = \begin{Bmatrix} 0 & l & l \\ L & l & l \end{Bmatrix} = \frac{1}{[l]} \quad (96)$$

for L even. Actually the same matrix elements occur in vector space $V' = \{|\alpha_L\rangle | L = 0, 2, \ldots, 2l\}$:

$$\hat{C}_o|\alpha_L\rangle \equiv {\sum_{L'}}' C_{L',L}|\alpha_{L'}\rangle. \quad (97)$$

Unfortunately, neither the vectors $|\alpha_L\rangle$, nor the vectors $|\beta_L\rangle$ for $L = 0, 2, \ldots, 2l$ are linearly independent. This clearly follows from equations (47) and (48) if we apply both sides to the vacuum and multiply from the left by an appropriate power of $\hat{Q}^+$. However, even in the linearly not independent (and correspondingly not orthonormal) basis one can still calculate matrix elements of operator products such as

$$\left(\hat{O}^{(1)}\hat{O}^{(2)}\right)_{L',L} = {\sum_{L''}}' O^{(1)}_{L',L''} O^{(2)}_{L'',L} \quad (98)$$

provided V is an invariant vector space of $\hat{O}^{(1)}$ and $\hat{O}^{(2)}$, and furthermore, the matrix elements for $\hat{O}^{(1)}$ and $\hat{O}^{(2)}$ are fixed (This statement follows from (93) if $\hat{O} \equiv \hat{O}^{(2)}$ and we act on both sides with $\hat{O}^{(1)}$ from the left). If one calculates matrix elements of the operator $\hat{R}$

$$\hat{R} = \hat{C}_o^3 - (8l+6)\hat{C}_o^2 + 8l(2l+3)\hat{C}_o \quad (99)$$

by the well-known properties [18] of the Wigner $6j$-symbols it turns out that

$$\hat{R}_{L',L} = 0. \quad (100)$$

It also means that the operator $\hat{C}_o$ on V or V' fulfills

$$\hat{C}_o\left(\hat{C}_o - 4l\hat{I}\right)\left(\hat{C}_o - (4l+6)\hat{I}\right) = 0, \quad (101)$$

where $\hat{I}$ is the identity operator.

If an operator $\hat{O}$ has the the minimal polynomial

$$0 = \left(\hat{O} - \lambda_1\hat{I}\right)\ldots\left(\hat{O} - \lambda_d\hat{I}\right) \quad (102)$$

with finite d then $\hat{O}$ admits the decomposition

$$\hat{O} = \sum_{i=1}^{d} \lambda_i \hat{P}_i, \quad (103)$$

where $\hat{P}_i$ is a projector, i.e., $\hat{P}_i\hat{P}_j = \hat{P}_i\delta_{i,j}$ and

$$\hat{P}_i = \prod_{\substack{j=1 \\ j\neq i}}^{d} \frac{\hat{O} - \lambda_j\hat{I}}{\lambda_i - \lambda_j}. \quad (104)$$

From equation (101) it is clear that on V at most we have $d = 3$, and the three eigenvalues of $\hat{C}_o$ are $\lambda_1 = 0$, $\lambda_2 = 4l$ and $\lambda_3 = (4l+6)$ respectively. Our main purpose is to calculate the orthogonal projection of $|\beta_L\rangle$ to $\hat{Q}^{+n}|0\rangle = |\beta_0\rangle$. This latter vector is an eigenvector of $\hat{C}_o$ with eigenvalue 0, thus let us consider the projector of $\hat{P}_1$:

$$\hat{P}_1 = \frac{\left(\hat{C}_o - 4l\hat{I}\right)\left(\hat{C}_o - (4l+6)\hat{I}\right)}{4l(4l+6)}. \quad (105)$$

Taking matrix elements on both sides is easy. Straightforward calculation leads to

$$\left(\hat{P}_1\right)_{L',L} = \delta_{L,0}\delta_{L',0} + \frac{[L]}{l(2l+3)}(1-\delta_{L,0})(1-\delta_{L',0}). \quad (106)$$

If we consider the decomposition

$$|\beta_L\rangle = \hat{P}_1|\beta_L\rangle + (\hat{I} - \hat{P}_1)|\beta_L\rangle \quad (107)$$

the first term $\hat{P}_1|\beta_L\rangle$ is an eigenvector of $\hat{C}_o$ with eigenvalue zero, the second term, if it is nonzero, belongs to the subspace in which $\hat{C}_o$ has positive eigenvalues. Thus, the two vectors on the right hand side of (107) are orthogonal to each other. Most important is the first term. Knowing the matrix elements of $\hat{P}_1$ it reads as

$$\hat{P}_1|\beta_L\rangle = \delta_{L,0}|\beta_0\rangle + \frac{[L](1-\delta_{L,0})}{l(2l+3)} \sum_{\substack{L'=2 \\ L':even}}^{2l} |\beta_{L'}\rangle. \quad (108)$$

Equation (48) implies (by applying both sides to the vacuum and multiplying by $\hat{Q}^{+(n-2)}$ from the left)

$$\sum_{\substack{L'=2 \\ L':even}}^{2l} |\beta_{L'}\rangle = -\frac{[l]+[s]}{[s]}|\beta_0\rangle. \quad (109)$$

Putting equations (107)–(109) together we obtain the result (69).

To prove the corresponding result (68) for the decomposition of $|\alpha_L\rangle$ we can proceed as above, but instead of (109) we should use

$$\sum_{\substack{L'=2 \\ L':even}}^{2l} |\alpha_{L'}\rangle = 2l|\alpha_0\rangle, \quad (110)$$

which follows from the operator identity (47) if we apply both sides to the vacuum and multiply by $\hat{Q}^{+(n-1)}$ from the left.

Appendix D: Particle-hole transformation

Let us consider the operator $\hat{C}$ (see Ref. [2]), which acts as

$$\hat{C}a^+_{m,\nu}\hat{C}^{-1} = (-1)^{l-m+s-\nu}a_{-m,-\nu},$$
$$\hat{C}a_{m,\nu}\hat{C}^{-1} = -(-1)^{-l-m-s-\nu}a^+_{-m,-\nu}. \quad (111)$$

These transformations preserve the anticommutation relations between the a^+-s and a-s. The operator $\hat{C}$ connects a state to an other one where particles (holes) are replaced by holes (particles). By simple calculation one obtains

$$\hat{C}\hat{B}_{L,M}\hat{C}^{-1} = (-1)^{L+1}\hat{B}_{L,M} + [s]\sqrt{[l]}\delta_{L,0}\delta_{M,0}$$
$$\hat{C}\hat{B}_L^2\hat{C}^{-1} = \hat{B}_L^2 - (2[s]\sqrt{[l]}\hat{B}_{0,0} - [s]^2[l])\delta_{L,0}. \quad (112)$$

If the single-shell Hamiltonian has the multipol expansion form

$$\hat{H} = t\hat{N} + \sum_{L=0}^{2l} p_L \hat{B}_L^2 \quad (113)$$

where t and the p_L-s are some numbers, then

$$\hat{C}\hat{H}\hat{C}^{-1} = \hat{H} - (t + p_0[s])(2\hat{N} - N_t). \quad (114)$$

Here N_t is

$$N_t = [l][s] = (2l+1)(2s+1). \quad (115)$$

The Hamiltonian (10) belongs to the family (113). Now, let us given an eigenstate of (113) with definite particle number N: $\hat{H}|\gamma, N\rangle = E(\gamma, N)|\gamma, N\rangle$ (γ denotes here the other quantum numbers). Then, there exists an other state $|\gamma, N_t - N\rangle$ with particle number $N_t - N$ connected by $\hat{C}$ as

$$|\gamma, N_t - N\rangle = \hat{C}^{-1}|\gamma, N\rangle \quad (116)$$

which is also an eigenstate of (113) by equation (114) with eigenvalue

$$E(\gamma, N_t - N) = E(\gamma, N) + (t + p_0[s])(N_t - 2N). \quad (117)$$

This property is quite general, does not depend on the form of spin independent, rotational invariant interaction and reflects the particle-hole symmetry. For instance in case of equivalent electrons in atoms t and p_0 can be expressed by the well-known radial integrals. By introducing

$$E'(\gamma, N) = E(\gamma, N) - (t + p_0[s])N \quad (118)$$

one obtains using (117)

$$E'(\gamma, N_t - N) = E'(\gamma, N). \quad (119)$$

Note that by putting $N = 0$ one gets that the energy of the completed shell is $E(\gamma, N_t) = (t+p_0[s])(2l+1)(2s+1)$. In the special case (10) $t = [l]/8$ and $p_0 = -[l]/8$ and (118) leads to equation (72) and (119) explains the symmetry of the shifted spectrum in Figures 1 and 2. One can easily convince oneself that the eigenstates and the eigenvalues of $\hat{H}$ and $\hat{H}_0$ coincide when $N = N_t$. Finally, we note that an expression similar to (117) exists in the single j-shell model (relevant in the nucleus), namely $(t + p_0[s])$ is to be replaced by p_0 to get formally the relationship valid there [20].

If the Hamiltonian $\mathcal{H}$ is considered (117) and (118) need an obvious modification. Namely,

$$\mathcal{E}(n_r, \gamma, N_t - N) = \mathcal{E}(n_r, \gamma, N) + \left(gt + \mathcal{E}^{(1)}(n_r, l) + gp_0[s]\right)(N_t - 2N). \quad (120)$$

Furthermore, defining $\mathcal{E}'(\gamma, N)$ by

$$\mathcal{E}'(\gamma, N) = \mathcal{E}(n_r, \gamma, N) - \left(gt + \mathcal{E}^{(1)}(n_r, l) + gp_0[s]\right) N, \quad (121)$$

it follows that

$$\mathcal{E}'(\gamma, N_t - N) = \mathcal{E}'(\gamma, N). \quad (122)$$

Note that using equation (24) one gets $gE' = \mathcal{E}'$, i.e., the one-particle energies are canceled from the shifted spectrum of $\mathcal{H}$. This shows the usefulness of dealing with the shifted spectrum.

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