Structure of Single-Particle States in Spherical Nuclei within the Framework of the Multistep Shell-Model Method

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The structure of single-particle states in spherical nuclei is analyzed within the shell model by use of a representation which consists of a correlated basis.

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We recently proposed to solve the many-body shell-model equations by means of a representation consisting of many-particle correlated states.[1] In general, a system with a number of particles p can be evaluated in terms of systems with q and r particles, respectively, such that $p=q+r$. One proceeds in several steps. First the one-particle states that span the shell-model space are chosen. In the second step one calculates the two-particle states which define the interaction matrix elements. Then one proceeds by adding particles in successive steps. To evaluate the p-particle system mentioned above, one assumes that the q- and r-particle systems have been solved so that the basis set of elements is given by

$$\{P^\dagger(\alpha_q)P^\dagger(\alpha_r)|0\rangle\}, \qquad (1)$$

where $P^\dagger(\alpha_n)$ creates the n-particle state α_n (but, as an exception, the one-particle states are labeled with Latin letters and the corresponding creation operator is $c_i^\dagger$, as usual) and $|0\rangle$ is

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the core ground state.

If only the few lowest states of the q- and r-particle systems are enough to describe the lowest states of the p-particle system (as is usually the case with the one-particle states in the standard shell-model representation[2]), one may be able to use this multistep shell-model method (MSM) to calculate the states of medium and heavy nuclei with many nucleons outside closed-shell cores. Such calculations would require the diagonalization of very large matrices (with dimensions of the order of hundreds of millions) within the standard shell-model representation.

In each step of the MSM one calculates the energies and wave functions of a given system. These calculated quantities are like building blocks that are used as a whole in later steps. Since the algebraic complexities inherent in each step are not passed to later steps the formalism turns out to be rather simple.[1]

The idea behind the MSM is not new. More than twenty years ago de-Shalit proposed to use correlated states to describe nuclear spectra[3] and since then many models and methods that include correlated states in the basis set of elements have been introduced.[4-10] What is new in the MSM is that it provides a general and systematic procedure to solve exactly the many-body shell-model equations within such a correlated basis. Moreover, the number of particles of the subsystems used to construct the MSM basis is arbitrary. Thus, a $2n$-particle system can be solved by use of n two-particle states (as the interacting-boson model[10] or nuclear field theory[9] would do) or any other partition of that system.

A problem faced by the MSM (and all methods which use correlated bases) is that the basis elements may violate the Pauli principle. As a result, the MSM basis is not orthogonal and its dimension is larger than the physical (shell-model) dimension. To get around this problem one must also evaluate the overlap matrix among the basis elements (the so-called metric matrix). By means of the metric matrix one restores the Pauli principle and, eventually, the MSM matrices have the right dimensions. Therefore no spurious states appear in the calculation.[7]

The evaluation of the metric matrix is also carried out within the MSM in terms of quantities related to the systems that constitute the correlated basis.[1]

The analysis of nuclear spectra in terms of the MSM basis (1) allows one to gain physical insight into the structure of those spectra if a very small basis can be used. Yet the necessity of considering simultaneously both the dynamical and the metric matrices may blunt the relative importance of the states α_q and α_r [Eq. (1)] in the building up of the states α_p. For instance, if only one kind of particles is considered in the calculation, some MSM basis vectors may rapidly become blocked by the Pauli principle when the number of particles is increased. As a result, the norm of those vectors soon becomes very small and thereby it may not be clear which other states become important, unless a full calculation is performed. To avoid this inconvenience we analyze here "quasiparticle" states of a given kind of particles (neutrons or protons) as a function of the number of the other kind of particles. To facilitate the presentation we will speak of a proton and many (an even number) neutron particles but the inverse situation is obviously included.

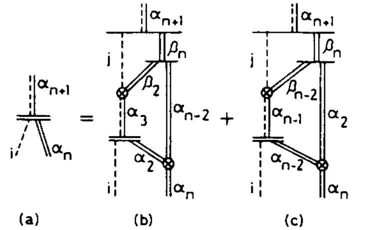

FIG. 1. Dashed and solid lines represent proton and neutron states, respectively. Coupled dashed-solid lines represent one-proton–many-neutron states. (a) Double-bar vertex. The expression of this vertex is given by the left-hand side of Eq. (3). This vertex was also called "coupling constant" in Ref. 1. (b) The nucleus α_n, with n (an even number) neutrons outside the core, is described in terms of the two- and $(n-2)$-neutron nuclei. In this graph the proton interacts with the two-neutron nucleus. The crossed vertices represent the MSM wave function amplitudes [as the quantities X in Eq. (2)]. (c) The proton interacts with the $(n-2)$-neutron nucleus.

The one-proton, n-neutron physical state can be written as

$$|\alpha_{n+1}\rangle = \sum_{i,\alpha_n} X(i,\alpha_n;\alpha_{n+1})[c_i^\dagger P^\dagger(\alpha_n)]_{\alpha_{n+1}}|0\rangle. \quad (2)$$

The corresponding metric matrix is diagonal, i.e.,

$$\langle 0|[c_i^\dagger P^\dagger(\alpha_m)]^\dagger [c_i^\dagger P^\dagger(\alpha_n)]|0\rangle = \delta(i,j)\,\delta(\alpha_m,\alpha_n).$$

Therefore, the MSM dynamical matrix which provides the energies of the system $\{\alpha_{n+1}\}$ is already Hermitian. This matrix can be calculated directly from Fig. 1 (for details see Ref. 1) to obtain

$$
\begin{aligned}
&[W(\alpha_{n+1})-\epsilon_i-W(\alpha_n)]F(i,\alpha_n;\alpha_{n+1})\\
&=\sum_{j\beta_n}\Big[\sum_{\alpha_2\beta_2\alpha_3\alpha_{n-2}}Y(\alpha_2,\alpha_{n-2};\alpha_n)F(\beta_2,\alpha_{n-2};\beta_n)[W(\alpha_3)-\epsilon_i-W(\alpha_2)]\\
&\qquad\times F(i,\alpha_2;\alpha_3)X(j,\beta_2;\alpha_3)\hat\beta_n\hat\alpha_n(\hat\alpha_3)^2\begin{Bmatrix}\alpha_{n-2}&\alpha_2&\alpha_n\\ i&\alpha_{n+1}&\alpha_3\end{Bmatrix}\begin{Bmatrix}\alpha_{n-2}&\beta_2&\beta_n\\ j&\alpha_{n+1}&\alpha_3\end{Bmatrix}\\
&+[1-\delta(n,4)]\sum_{\alpha_2\alpha_{n-2}\beta_{n-2}\alpha_{n-1}}Y(\alpha_{n-2},\alpha_2;\alpha_n)F(\beta_{n-2},\alpha_2;\beta_n)[W(\alpha_{n-1})-\epsilon_i-W(\alpha_{n-2})]\\
&\qquad\times F(i,\alpha_{n-2};\alpha_{n-1})X(j,\beta_{n-2};\alpha_{n-1})\hat\beta_n\hat\alpha_n(\hat\alpha_{n-1})^2\begin{Bmatrix}\alpha_2&\alpha_{n-2}&\alpha_n\\ i&\alpha_{n+1}&\alpha_{n-1}\end{Bmatrix}\begin{Bmatrix}\alpha_2&\beta_{n-2}&\beta_n\\ j&\alpha_{n+1}&\alpha_{n-1}\end{Bmatrix}\Big]F(j,\beta_n;\alpha_{n+1}),\qquad(3)
\end{aligned}
$$

where ϵ is a single-particle energy and W is energy referred to the core, while

$$F(\alpha_q,\alpha_r;\alpha_p)=\langle\alpha_p\|[P^\dagger(\alpha_q)P^\dagger(\alpha_r)]_p\|0\rangle \qquad (4)$$

and

$$Y(\alpha_q,\alpha_r;\alpha_p)=[1+\delta(\alpha_q,\alpha_r)]X(\alpha_q,\alpha_r;\alpha_p),$$

with X the amplitude corresponding to the wave function $|\alpha_p\rangle$, as in Eq. (2). We use the same symbols to denote states as well as the corresponding angular momentum, as seen in the 6-j symbols of Eq. (3) or Eq. (2).

The quantities F and X in Eq. (3) are the building blocks calculated in previous steps of the present calculation. Taking into account the generality of Eq. (3), one can say that it is a simple equation. The diagonalization of the matrix (3) provides the shell-model energies and wave functions. But the dimension of this matrix can be very large. Yet one may hope to be able to truncate this dimension drastically, as was the case for ground states in spherical nuclei.[1] This would also be the case for quasiparticle states k for which α_n [Eq. (2)] is the ground state of the n-neutron system (γ_n). In this case Eq. (2) becomes

$$|\alpha_{n+1}\rangle=[c_k^\dagger P^\dagger(\gamma_n)]_k|0\rangle. \qquad (5)$$

Since the ground state γ_n can be written as[1]

$$|\gamma_n\rangle=N[P^\dagger(\gamma_2)P^\dagger(\gamma_{n-2})]_0|0\rangle, \qquad (6)$$

where N is a normalization constant, one obtains from Eq. (3) (note that in the 6-j symbols $\alpha_n=\gamma_n=0$ if n is even)

$$W(\alpha_{n+1})=W(\alpha_{n-1})+W(\alpha_3)-\epsilon_k+W(\gamma_n)-W(\gamma_{n-2})-W(\gamma_2). \qquad (7)$$

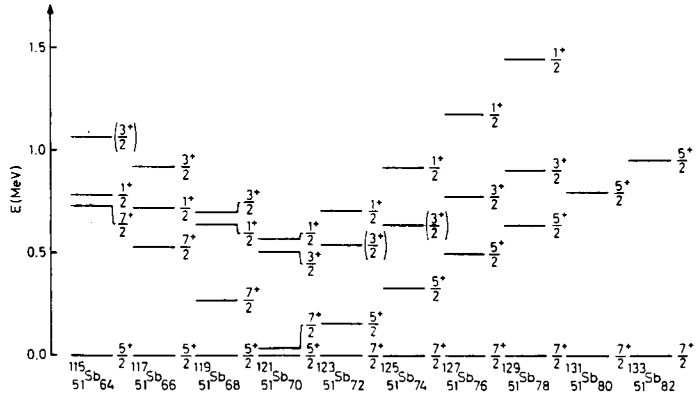

FIG. 2. Experimental (Ref. 11) quasiparticle states in Sb isotopes. The neutrons run from the major shells filling $N_0=64$ [for protons this may be considered a "magic number (Ref. 12)] to $N_0=82$.

To obtain Eq. (7), we used the fact that $1=\langle\alpha_{n+1}\|[c_k^\dagger P^\dagger(\gamma_n)]_k\|0\rangle$ and $1=N\langle\gamma_n\|[P^\dagger(\gamma_2)P^\dagger(\gamma_{n-2})]_0\|0\rangle$, which stem from Eqs. (5) and (6), respectively. Equation (7) gives the quasiparticle energies of the $(n+1)$ nucleus, with Z_0+1 protons and N_0+n neutrons, where n is even and (Z_0, N_0) is the core. Since for different states of the $(n+1)$ nucleus $W(\gamma_m)$ is the same, one has

$$W(\alpha_{n+1}) - W(\beta_{n+1}) = W(\alpha_{n-1}) - W(\beta_{n-1}) + W(\alpha_3) - W(\beta_3) - (\epsilon_k - \epsilon_j), \tag{8}$$

where the state α_{n+1} (β_{n+1}) carries angular momentum k (j). Equation (8) indicates that the energy difference between two quasiparticle states would decrease (increase) montonically as a function of the number of neutrons n if the energies decrease (increase) in the beginning of the major shell. Assume now that β labels the ground states of odd nuclei in Eq. (8). If there is a state α for which the energy difference (8) decreases in the beginning of the major shell, there might be a value of n for which the roles of the states α and β would change (i.e., α becomes the ground state). But the monotonic variation of that energy difference would not be affected by this switch of ground states. This is indeed what happens in spherical nuclei. In Fig. 2 we show, as an example, the Sb odd isotopes. As we go from ^{121}Sb to ^{123}Sb the ground states have changed, but the tendency given by Eq. (8) is followed throughout the figure by any given pair of quasiparticle states. In particular, the distance between the states $\frac{3}{2}^+$ and $\frac{1}{2}^+$ first decreases and these states are interchanged in ^{121}Sb. Afterwards that distance becomes more and more negative, in agreement with Eq. (8).

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