Generalized approximation to seniority shell model

Y. K. Gambhir, S. Haq, and J. K. Suri

Indian Institute of Technology, Bombay-400 076, India

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A generalized approximation to seniority shell model, based on the number conserving quasiparticle theory, is presented which includes the cases where both neutrons and protons are present in the valence shells. The numerical calculations are carried out for even Zr isotopes. The results obtained compare well with the corresponding exact shell model results, demonstrating thereby the validity of the present approximation for this nuclear region.

[NUCLEAR STRUCTURE Shell Model, Seniority Shell Model, Broken-Pair Approximation (BPA), Generalized BPA, Zr-isotopes]

It is well known that the shell model or even the seniority ($\nu \leq 4$) shell model calculations with configuration mixing are permanently limited to the cases where only a few valence particles are present in a few valence levels. This is because with the increase in the number of valence particles (levels), the dimension of the Hamiltonian matrix increases tremendously which is formidable in practice. However, in such practical calculations, the dimensions of the Hamiltonian matrices can be reduced if the problem is reviewed with some approximation based on phenomenology derived from the effective nucleon-nucleon interactions. One such practical approximation is the quasiparticle model based on the strong pairing correlations among nucleons. Unfortunately, the results of the quasiparticle calculation do not correspond to the specific nuclear model due to the noncommutability of the actual number operator with the quasiparticle Hamiltonian. This number nonconservation also introduces spurious states. To remove these drawbacks and to retain the basic advantages of the model, various methods have been proposed. One such method is the broken-pair approximation (BPA), the validity of which has been demonstrated in the 2p-1f region as well as for $N=50$, even A nuclei. So far these projection methods have been applied only for the identical particles (neutrons or protons) in the valence shells. In this report we generalize the broken-pair approximation (referred to as GBPA) to include the cases where both the neutrons and the protons are active in the valence shells.

Approaching the problem in the same manner as in the identical nucleon case, we write the approximate ground state for even-even nuclei as a product of a proton paired ($p$ pairs) state $\tau^+_p(0)$, and a neutron paired ($n$ pairs) state $\tau^+_n(0)$, i.e.,

$$[\tau^+_p \otimes \tau^+_n]|0\rangle,$$

where the operator $\tau^+_p$ is given by

$$\tau^+_p = \sum_{a} \varphi^*_a \frac{\hat{a}}{2} A^{p}_{aa}(aa)$$

with

$$\varphi^*_a = v_p / u_p, \quad u_p^2 + u_a^2 = 1,$$

$$\hat{a} = (2j_n + 1)^{1/2},$$

and $A^p_{a}(ab)$ is a two-particle creation operator with total angular momentum $J$ and projection $M$. The structure of $\tau^+_p(0)$ state is similar to the projected BCS (with $p$ pairs of identical particles) state. In fact $\tau^+_p(0)$ becomes identical to the projected BCS state if one replaces the ground state parameters by the occupation ($v_p$), nonoccupation ($u_p$) probabilities of the pairing model. This approximate ground state wave function (1) is valid specially for the cases where neutrons and protons fill different major shells.

In the next approximation (one GBPA) the basis space is constructed as in the identical nucleon case by coupling the wave functions obtained by replacing one proton distributed pair $S_p$ by an arbitrary two proton configurations $A^p_{s}(p_1p_2)$ and a similar replacement for neutrons. Explicitly the basis states are written as

$$\{[\tau^+_p \otimes A^p_{s}(p_1p_2)] \otimes [\tau^+_n \otimes A^n_{s}(n_1n_2)]\}|0\rangle.$$  (3)

For seniority ($\nu$) zero the state (1) is the linear combination of states (3). Moreover, for $J_p=0$ (or $J_n=0$) the states (3) are not orthogonal. Therefore, it suffices to work with an orthonormal set constructed from the states (3). Clearly, the states (3) contain all the low seniorities ($\nu=0, 2, 4$) components of the shell model wave functions except $\nu=4$ proton components and $\nu=4$ neutron components. For the case of four valence particles (two protons and two neutrons) the states (3) exactly coincide with the exact shell model states.
Therefore, the GBPA results for this case will be identical to the exact shell model results. It further implies that whatever be the number of valence particles (even-even) the basis constructed from (3) gives the number of states equal to the shell model basis corresponding to two neutrons and two protons. This shows a great reduction in the dimensionality of the GBPA Hamiltonian matrices, thereby enabling one to perform GBPA calculations where exact shell model calculations are not feasible. It is to be noted that when more and more \( S \) operators are replaced by \( A^\dagger \) operators, the space gradually approaches closer and closer to the exact shell model space. Ultimately when all \( S \) operators are replaced by an equal number of \( A^\dagger \) operators the space becomes identical to the exact shell model space.

To evaluate the matrix elements of the Hamiltonian \( H \) between the GBPA states (3), we rewrite \( H \) as

\[
H = H_0 + H_{pp} + H_{nn} + H_{np},
\]

(4)

where \( H_0 \) denotes the constant term and the other terms follow in their usual notations. The structure of \( H_{pp} \) (or \( H_{nn} \)) in a second quantized version is such that all the annihilation operators appear on the left and all the creation operators appear on the right. This is achieved by using the anticommutation property of the operators and treating the neutron and proton operators as independent. Explicitly, \( H_{pp} \) (or \( H_{nn} \)) contain the operators of the type \( a^\dagger a^\dagger \) and \( AA^\dagger \). Therefore, the matrix elements of the Hamiltonian involve the products of the overlaps of the BPA basis states

\[
\langle \tau^\dagger_{p,1} A^{\dagger}_{2,2} A^{\dagger}_{p,2} | 0 \rangle, \langle \tau^\dagger_{p,1} A_{2,2} A_{p,2} | 0 \rangle
\]

of identical nucleons. The explicit general expression for the overlap integral (\( \mathcal{D} \)) of the BPA states is given in Ref. 4. The contribution of \( H_{pp} \) (or \( H_{nn} \)) is exactly identical to that of identical nucleon case (explicit expression is given in Ref. 4) apart from a multiplication factor. Similarly, the \( H_{np} \) part is evaluated. The expressions for quadrupole and magnetic moments and transitions rates are derived following the same procedure. These expressions are similar in form as those of the identical nucleon case (given in Ref. 4) apart from a multiplication factor.

To test the computer code (written by us) suitable for GBPA calculations, as a first step, it is desirable to reproduce the exact shell model results for four valence particles (two protons and two neutrons). We choose \( ^{92}\text{Zr} \) nucleus for this purpose because its shell model results in terms of two-valence protons (confined to \( 2p_{1/2}, 1g_{9/2} \) orbitals) and two-valence neutrons (restricted to \( 2d_{5/2}, 3s_{1/2} \) orbitals) outside the \( ^{88}\text{Sr} \) core are available.\(^7\)

These results are reproduced using identical input information, thereby testifying to the correctness of our computer code. The phenomenological set of interaction matrix elements are employed in this calculation. The single particle energy difference \( \Delta E = \delta_{21/2} - \delta_{15/2} \) and the effective \( p-p \) interaction matrix elements are determined by directly fitting the observed spectra of \( N = 50 \) nuclei, while \( \Delta E = \delta_{25/2} - \delta_{29/2} \) and effective \( n-n \) and \( n-p \) interaction matrix elements are determined again by directly fitting the experimental energy levels of \( ^{90}\text{Y}, ^{90}_{-0.06}\text{Zr}, \) and \( ^{92}_{0.03,0.04}\text{Nb} \) nuclei, in the shell model. The details of the fitting procedure are
given respectively in Ref. 7 and Ref. 8.

The present calculation involves the following steps:

1. The pairing-model (BCS) gap and number equations are solved separately for protons and for neutrons to obtain the ground state parameters \((v_u, v_d)\) appearing in \(\tau_0^+|0\rangle\) and \(\tau_0^-|0\rangle\), respectively.

2. An orthonormal basis set for \(2p\)-protons and \(2n\)-neutrons in the valence shells, is constructed in terms of

   \[ [\tau_{p-1}^+ a_{p}^{+}\otimes\tau_{n+1}^+ a_{n}^{+}|0\rangle]_n \]

   basis states.

3. The total Hamiltonian \(H\) is then diagonalized in the space spanned by the orthonormal set obtained in (2). The calculated energy spectra (GBPA) for \(^{92\text{--}150}\text{Zr}\), even-even nuclei are shown in the Figs.

1–3, along with their observed (Expt) and shell-model (SM) spectra where available. The figures also contain the pure (BPA) proton (Protons) and pure (BPA) neutron (Neutrons) spectra, to facilitate the discussion. The latter results [protons (neutrons)] are obtained just by diagonalizing \(H_{\text{np}} (H_{\text{nn}})\) in the proton (neutron) subspace. Inspection of the Figs. 1–3 reveals that the GBPA and the SM results are in good agreement. The slight discrepancies exist for the levels with high excitation energy of \(^{92}\text{Zr}\) nucleus. This probably is due to the fact that at such excitation energies the neutron configurations with higher seniority not included in the GBPA, start becoming important. Further, this is even more so in the present calculation because of highly truncated nature of the configuration space used. The GBPA is expected to reproduce the SM results even better in the enlarged space. Unfortunately, such SM calculations in the enlarged space are not available and even do not seem to be feasible in near future and therefore leaves the present approximation (GBPA) as one of the viable alternatives. On the whole, one can then conclude that the GBPA is a satisfactory and a useful practical approximation to the shell model. The figures further reveal that the GBPA spectra is approximately similar to that obtained by adding BPA protons and BPA neutrons spectra. This fact indicates the weak nature of \(H_{\text{np}}\) part of the interaction, which in fact is expected as neutrons and protons fill different major shells.

In conclusion we remark that GBPA, which is quite feasible to carry out in practice, holds a great promise for large number of nuclei wherein the shell model calculations cannot simply be performed.

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