Effect of variation of the single particle energies in the structure of $N=82$ isotones

Y. K. Gambhir and J. A. Sheikh
Department of Physics, Indian Institute of Technology, Bombay 400 076, India
(Received 13 February 1986)

The single particle energies extracted through the inverse gap equation method for each nucleus are used in the nuclear structure calculations within the framework of the broken pair approximation for $N=82$ even isotones. This makes a modest improvement of the trend of the level energies with particle number as compared to those obtained by using a fixed set of the single particle energies.

The nuclear shell-model calculations usually proceed with the notion that the observed nuclear properties are attributed only to the few valence nucleons outside the assumed inert core. The core just renormalizes some of the nucleon properties such as the nucleon charge, etc., and the two-body interaction matrix elements. The input parameters, viz., the single particle (s.p.) energies ($\epsilon_{\alpha\equiv nljm}$) of the valence levels and the effective two-body interaction matrix elements (TBME) relevant to the space are held fixed in the calculations for all the nuclei in the region. The input ϵ_j are taken either from the experiment where available or are calculated empirically, or are even treated as parameters. The effective TBME are obtained from the G matrix corrected for the renormalization contributions due to the core, or are calculated from the assumed phenomenological form of the interaction, or are adjusted to fit the experimental data. However, it is known that ϵ_j do vary with mass number, which is essentially a many-body effect. Unfortunately, it is very difficult to quantitatively ascertain this variation either from experiment or from theory. However, for some special cases such as single-closed shell (SCS) nuclei, it is possible to obtain ϵ_α for a specific nucleus through the inverse gap equation (IGE) (Refs. 1 and 2) procedure. The IGE method assumes that for SCS odd-A nuclei, the observed low-lying states with a given spin and parity corresponding to the valence s.p. orbitals are pure one- (or a mixture of one- and three-) quasiparticle excitations. This, together with the observed odd-even mass difference, then determines the quasiparticle energies (E_α). The knowledge of E_α in turn yields, by inverting the gap equation, the pairing strength (G) of the TBME and the physical gap parameter (Δ_α) of the Bardeen-Cooper-Schrieffer (BCS) theory apart from an overall normalization factor. The normalization is fixed through the number equation. The s.p. energies ϵ_α are then obtained by ascertaining whether a particular level is above or below the Fermi level from one-nucleon transfer reaction data. The results of IGE calculations are available[3] for $N=82$ isotones. In this paper we investigate the effect of variation of ϵ_α and G on the calculated spectrum of even $N=82$ isotones. We use the broken pair approximation (BPA) (Refs. 4 and 5) for the energy calculations. We restrict the protons outside the $Z=50, N=82$ inert core to occupy five valence levels ($1g_{7/2}, 2d_{5/2}, 2d_{3/2}, 3s_{1/2}, 1h_{11/2}$) and use the S-δ interaction between the valence protons. It is observed that the use of the input parameters ϵ_α and G obtained by the IGE procedure improves the results as compared to those obtained by using a fixed set of ϵ_α and G. We now describe briefly the method of calculation and then discuss the numerical results.

The IGE method assumes that the observed few low-lying excitations of odd-A SCS nuclei corresponding to the valence orbitals are described in terms of one- (a mixture of one- and three-) quasiparticle excitations. Half of the odd-even mass difference calculated from the nuclear mass tables is then added to the observed excitation energies to obtain the respective single-quasiparticle energies (E_α). The procedure to account for three-quasiparticle admixtures either by perturbation or through the iterative method is discussed in detail in Ref. 3. The relevant effect of three-quasiparticle admixtures in our context is to slightly modify the single-quasiparticle energies. Once E_α are known, the BCS gap equation becomes a real nonsymmetric eigenvalue problem

$$M\Delta' = \omega\Delta' . \tag{1}$$

The matrix M has the form

$$M_{ab} = \frac{1}{4}\left[\frac{(2j_b+1)}{(2j_a+1)}\right]^{1/2}\frac{G(aabb0)}{E_b} . \tag{2}$$

Here a denotes all but the magnetic quantum number m_α of the label α. The matrix M is made positive with the proper choice of the phase for the pairing TBME [$G(aabb0)$]. The inverse of the highest eigenvalue ω_0 of Eq. (1) gives the pairing strength (G) of the two-body effective interaction, while the corresponding eigenvectors Δ' (ω_0) having all positive components are related to the physical gap parameters of the BCS theory through an overall normalization factor. The normalization factor ξ satisfying the constraint $E_\alpha - \xi\Delta'_\alpha(\omega_0) \geq 0$ is fixed from the number equation. One needs to know whether a particular level is above or below the Fermi level before one can extract the single particle energies of the valence levels. This information can readily be ascertained from the respective one-nucleon transfer reaction data. The results of IGE calculations are available[3] for $N=82$ isotones, in which the observed spectra[6,7] of odd-A nuclei (shown in

 ©1986 The American Physical Society

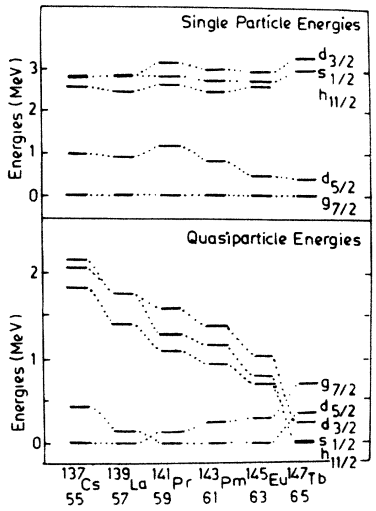

FIG. 1. The calculated proton s.p. energies and the quasiparticle energies (taken from Ref. 6) used in the IGE calculations for $N=82$ isotones.

Fig. 1) and the odd-even mass difference P (given in Table I), obtained from the mass tables,[8] have been used. The results of the analysis of one-nucleon transfer reaction data are then used in extracting the s.p. energies. The calculated s.p. energies are shown in Fig. 1 along with the quasiparticle energies which correspond to the lowest excitation energy of a given spin and parity. The calculated G, the strength of the pairing part of the interaction, and the fractional uncertainty Δp in the particle number are given in Table I, along with the odd-even mass difference P. The extracted s.p. energies and G do vary smoothly with mass number. In fact, the results indicate partial shell closure at $Z=64$ with a gap of about 2.56 MeV, supporting the semimagic nature of the $^{146}_{64}$Gd nucleus.

In the BPA the ground state $|\psi_0\rangle$ for p pairs of identical valence nucleons outside the core is assumed to be

$$|\psi_0\rangle \propto S_+^P |0\rangle \ . \tag{3}$$

Here the pair distributed operator S_+ is

$$S_+ = \sum_a \phi_a \left[\frac{(2j_a+1)}{2}\right]^{1/2} A_{00}^\dagger(aa) \ , \tag{4}$$

TABLE I. The odd-even mass difference p obtained from the observed binding energies (Ref. 8), the calculated G, the pairing strength of the TBME, and the fractional uncertainty Δp in the particle number P.

No. of valence protons	P (MeV)	G (MeV)	Δp
5	1.578	0.186	0.012
7	1.892	0.189	0.003
9	1.994	0.187	0.002
11	1.996	0.187	0.036
13	2.008	0.182	0.001
15	2.670	0.186	0.001

and $A_{JM}^\dagger$ is a two-particle creation operator with total angular momentum J and projection M. The expansion coefficients ϕ_a $(v_a/u_a, v_a^2+u_a^2=1)$ are determined by minimizing the expectation value of H with respect to the ground state $|\psi_0\rangle$. The BPA basis states are obtained by replacing one of the S_+ operators appearing in $|\psi_0\rangle$ by the $A_{JM}^\dagger(ab)$ operator. An orthonormal set of states for a given spin and parity J^π are constructed from these basis states for diagonalizing H. This yields the excitation energies and the corresponding wave functions.

It is to be pointed out that an accurate set of expansion coefficients (ϕ's) can also be obtained from the following iterative procedure, starting from any arbitrary set of ϕ's. The calculated BPA wave function for the ground state ($J=0$) is rewritten as

$$\sum_a x_a A_0^\dagger(aa)(S^\dagger)^{P-1}|0\rangle \ . \tag{5}$$

The new set of ϕ's are determined from the calculated x's by requiring that Eq. (5) has the same form as that of $|\psi_0\rangle$ [Eq. (3)]. The BPA calculations are again performed and the next set of ϕ's obtained. The procedure is rapidly converging; in practice two to three iterations are sufficient for an accurate determination of ϕ's. This avoids the need for determining ϕ's through the minimization.

Explicit numerical calculations have been carried out for $N=82$ isotones, restricting the valence protons outside the $Z=50, N=82$ core, in five ($1g_{7/2}$, $2d_{5/2}$, $2d_{3/2}$, $3s_{1/2}$, and $1h_{11/2}$) shell-model s.p. levels. Two sets of calculations have been performed. In the set labeled BPA, the s.p. energies ϵ_j with values 0.0, 0.96, 2.75, 2.83, and 2.54 MeV for $1g_{7/2}$, $2d_{5/2}$, $2d_{3/2}$, $3s_{1/2}$, and $1h_{11/2}$, respectively, and the strength $G=0.187$ MeV of the S-δ interaction are held fixed for all $N=82$ isotones. In the second set labeled BPA1 the specific values of ϵ_j and G obtained from the IGE for the respective nuclei are used. The calculated results for both sets are displayed in Fig. 2.

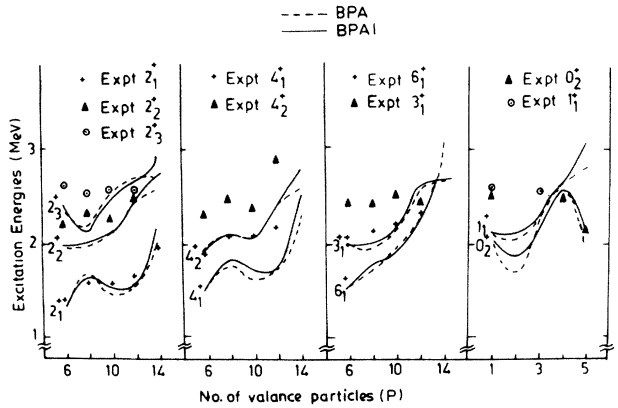

FIG. 2. The calculated and the experimental (Expt.) excitation energies in MeV. BPA represents the results obtained by using a fixed set of ϵ_a and G for all $N=82$ isotones, while BPA1 corresponds to the results obtained with the IGE values of ϵ_a and G for specific nuclei.

It is clear from the figure that the use of ϵ_j and G generally improves the results; even the 2_1^+ state in $P=8$ in BPA1 appears as the first excited state, which is not the case in the BPA. The calculated excitation energies for higher excited states are generally smaller both in the BPA1 and the BPA. This difference in energy is almost a constant for a given spin and parity, and it is of the same order of magnitude for all J^π states. However, the BPA1 agrees relatively better. Thus this makes a modest improvement of the trend of level energies with particle number as compared to those obtained by using a fixed set of s.p. energies. Therefore, specific s.p. energies relevant to a particular nucleus, if available, should be used in nuclear structure calculations.

We are grateful to S. P. Pandya, V. K. B. Kota, and C. R. Sarma for their interest in this work and to the Physical Research Laboratory, Ahmedabad, for providing the computer facility for a part of the calculations presented here.

[1]V. Gillet and M. Rho, Phys. Lett. **21**, 82 (1966).
[2]Y. K. Gambhir, Phys. Lett. **26B**, 695 (1968); Nucl. Phys. **A120**, 193 (1968).
[3]Y. K. Gambhir, Phys. Rev. Lett. **49**, 83 (1982).
[4]Y. K. Gambhir, A. Rimini, and T. Weber, Phys. Rev. **188**, 1573 (1969); Phys. Rev. C **3**, 1965 (1971).
[5]P. L. Ottaviani and M. Savoia, Phys. Rev. **178**, 1594 (1969); **187**, 1306 (1969); K. Allaart and E. Boeker, Nucl. Phys. **A168**, 630 (1971).
[6]B. H. Wildenthal, E. Newman, and R. L. Auble, Phys. Rev. C **3**, 1199 (1971).
[7]Y. Nagai *et al.*, Phys. Rev. Lett. **47**, 1259 (1981).
[8]A. H. Wapstra and K. Bos, At. Data Nucl. Data Tables **19**, 177 (1977).