Shell model calculation in the *S*-*D* subspace

Luo Yan-An and Jin-Quan Chen*
Department of Physics, Nanjing University, Nanjing, 210008, People's Republic of China

(Received 24 December 1997)

The nucleon-pair shell model truncated to the *S*-*D* subspace is applied to the barium isotopes ^{130}Ba–^{136}Ba. The effects of the single-particle energy splitting on collectivities are examined. The main features of the low-lying collective states of the nuclei, especially for nuclei with a larger number of pairs, are well reproduced by a shell model Hamiltonian with three parameters. [S0556-2813(98)05207-8]

PACS number(s): 21.60.Cs, 27.60.+j

The low-lying spectra of medium and heavy nuclei exhibit striking regularities which are characteristic of collective quadrupole states. How to describe these collective states in terms of the spherical shell model is a long-standing problem in nuclear structure theory. With the explosive growth of computational power, shell model calculations have been undergoing tremendous development as documented in [1]. Effective diagonalization of the shell model Hamiltonian in model space with dimensions in the millions becomes feasible [2,3]. Recently, impressive developments have been made in the quantum Monte Carlo method for the shell model [4] and the model space with dimension 10^{10} can be handled. Despite these impressive developments, the cases of the medium weight and heavy nuclei with configurations 10^{14}–10^{18} are still out of reach. For these nuclei one still needs to truncate the model space drastically. A crucial point is how to truncate the huge shell model space to a manageable subspace so that the shell model calculations for such nuclei are feasible and are simple enough for a clear understanding of these quadrupole collective states. The success of the interacting boson model (IBM) [5] has suggested a possible truncation, the truncation to the *S*-*D* subspace with *S*-*D* collective nucleon pairs as the building blocks [6]. Recently a formalism has been described for the nucleon-pair shell model (NPSM) in [7]. The building blocks of the model space are ''realistic'' collective nucleon pairs of angular momenta $J=0,2,\ldots$. The NPSM has the advantages that the diagonalization of the Hamiltonian is carried out exactly in the fermion space without any mapping procedure and it is flexible enough to include the weak coupling model [8] (when the few lowest eigenstates of a two-valence-nucleon system are taken as the building blocks), the broken pair approximation (when all nucleons but few are in the *S* pairs) [9], the favored pair model [10], and the fermion dynamical symmetry model (FDSM) [11] [when the single-particle (s.p.) energy splitting is neglected] as its special cases, and it allows for various truncations, ranging from the truncation to the *S*-*D* subspace up to to the full shell model space.

For applying the NPSM to the barium isotopes, we truncate the shell model space to the collective *S*-*D* space. In this paper we attempt to study the effects of the s.p. energy splitting and the goodness of the *S*-*D* subspace. It is known that the s.p. energy term H_0 comes from the mean field, the dominant part in a shell model Hamiltonian, which favors independent motion of nucleons, i.e., counters the nuclear collectivity. By artificially setting $H_0=0$, the collectivity is greatly overestimated. It is also known that the s.p. energy splitting is comparable or larger than the excitation energy of the collective 2_1^+ state. Therefore it is by no means obvious that the collectivity described in the favored pair model and FDSM [10,11] with degenerate s.p. energies will survive in the ''realistic'' *S*-*D* subspace where the s.p. energy splitting is fully taken into account, and it is worth to study the s.p. energy effects on the collectivity quantitatively.

Our Hamiltonian consists of the surface delta interaction (SDI) interaction between like nucleons and a *Q*-*Q* force between protons (π) and neutrons (ν),

$$H=H_0+V(\pi)+V(\nu)-\kappa Q_\pi^2\cdot Q_\nu^2,$$

$$V(\sigma)=-4\pi G_\sigma \sum_{i>j=1}^{n} \delta(\Omega_{ij}), \tag{1}$$

where H_0 is the single-particle energy term.

The *S*-*D* pairs are ''realistic'' pairs, denoted by $A_\mu^{r\dagger}$, $r=0,2$, taken from the 0_1^+ and 2_1^+ eigenstates of a two-valence-nucleon system with a single-particle energy term and the SDI term.

A complete set of normalized but nonorthogonal many-pair basis vectors are denoted by

$$\begin{aligned}|\tau,J_NM_N\rangle&=|r_1r_2\cdots r_n;\ J_1J_2\cdots J_n\rangle\\&=\text{const}\times A_{M_n}^{J_n\dagger}(r_i,J_i)|0\rangle,\end{aligned} \tag{2}$$

where $A_{M_n}^{J_n\dagger}(r_i,J_i)$ is the creation operator for *N* pairs $r_1,\ldots,r_n$, coupled successively to the total angular momentum J_n and with J_i as the angular momentum for the first *i* pairs,

$$\begin{aligned}A_{M_n}^{J_n\dagger}(r_i,J_i)&=A_{M_n}^{J_n\dagger}\\&=\{\cdots[(A^{r_1\dagger}\times A^{r_2\dagger})^{J_2}\times A^{r_3\dagger}]^{J_3}\\&\quad\times\cdots\times A^{r_n\dagger}\}_{M_n}^{J_n}.\end{aligned} \tag{3}$$

The analytic expressions of the matrix elements of the Hamiltonian are given in Ref. [7].

*Electronic address: jqchen@chenwang.nju.edu.cn

TABLE I. The single-particle (-hole) energies for protons (neutrons) of $^{133}_{51}\mathrm{Sb}_{82}$ ($^{131}_{50}\mathrm{Sn}_{81}$) taken from [12].

ϵ_π (MeV)	$g_{7/2}$	$d_{5/2}$	$d_{3/2}$	$h_{11/2}$	$s_{1/2}$
	0	0.963	2.69	2.76	2.99
ϵ_ν (MeV)	$d_{3/2}$	$h_{11/2}$	$s_{1/2}$	$d_{5/2}$	$g_{7/2}$
	0	0.242	0.332	1.655	2.343

To study the effect of the s.p. level splitting, we take the nucleus ^{132}Ba, and let H_0 vary stepwise, $H_0=0$, $\frac{1}{3}H_0^{\mathrm{expt}}$, $\frac{2}{3}H_0^{\mathrm{expt}}$, H_0^{expt}, $H_0^{\mathrm{expt}}=H_0^{\mathrm{expt}}(\pi)+H_0^{\mathrm{expt}}(\nu)$, where $H_0^{\mathrm{expt}}(\pi)$ and $H_0^{\mathrm{expt}}(\nu)$ are the s.p. energies of the nuclei $^{133}_{51}\mathrm{Sb}_{82}$, and $^{131}_{50}\mathrm{Sn}_{81}$, respectively, taken from [12] and listed in Table I. We also take $G_\pi=0.177$ MeV and $G_\nu=0.131$ MeV, which are to be compared with the value $G=0.15$ MeV in [13]. From [14], we know that $\kappa=K/A^{5/3}$, where K is a constant, and $K\cong 300$ MeV, which gives $\kappa\cong 0.1$ MeV; so we take $\kappa=0.1$ MeV.

The spectra and $B(E2)$ value vs H_0 are shown in Fig. 1. Evidently, the s.p. level splitting has a strong effect on the scale and pattern of the spectra, as well as the $B(E2)$ values. The energy of the 2_1^+ states increases with H_0, while the $B(E2)$ values decrease with H_0: i.e., *the greater the s.p. energy splitting, the weaker the collectivity, and the higher the excitation energy of the* 2_1^+ *state*. In other words, the s.p. energy splitting counters the collective motion. If one uses the $B(E2,2_1^+\to 0_1^+)$ value as a measure for the collectivity, from Fig. 1 it is seen that s.p. energy degeneracy assumption overestimates the collectivity by a factor of $0.234/0.099=2.36$. From this we can see the great influence of the s.p. energy splitting on the collectivity.

The term H_0 affects the excitation energies in two opposite ways. First, H_0 causes the nucleons to distribute unevenly over the s.p. levels, thereby reducing the effective short range force, and the energy gap, i.e., the energy required to create one or more D pairs, with the consequence that the excitation energy decreases with H_0; second, because of $H_0\neq 0$, it requires extra energies to lift nucleons from the ground state configuration to various excited configurations, causing the excitation energy to increase with the splitting. If the first effect dominates over the second, the excitation energy will decrease with the s.p. level splitting; otherwise, it will increase with the s.p. level splitting. For a given Hamiltonian, the outcome of the competition between the two effects varies with the excitation states. From Fig. 1 it is seen that for the high-lying states, the first effect is dominant and their excitation energies decrease with H_0, while for the low-lying states, especially the 2_1^+, the second effect is dominant, with the consequence that the whole spectra become more compressed for large s.p. level splitting.

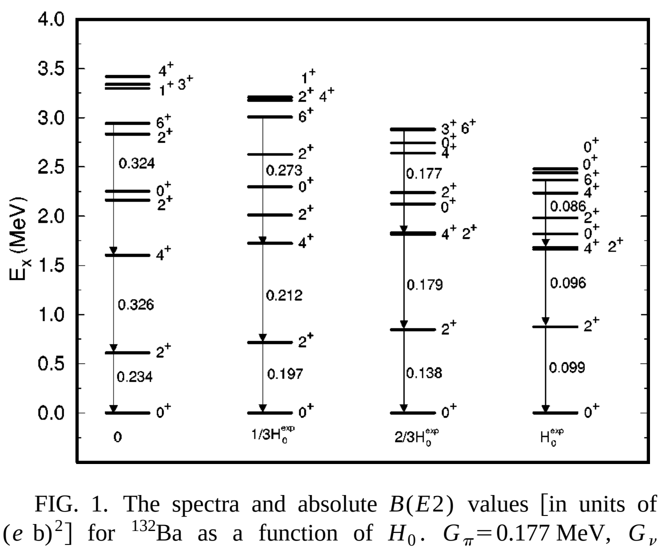

FIG. 1. The spectra and absolute $B(E2)$ values [in units of $(e\ \mathrm{b})^2$] for ^{132}Ba as a function of H_0. $G_\pi=0.177$ MeV, $G_\nu=0.131$ MeV, and $\kappa=0.1$ MeV.

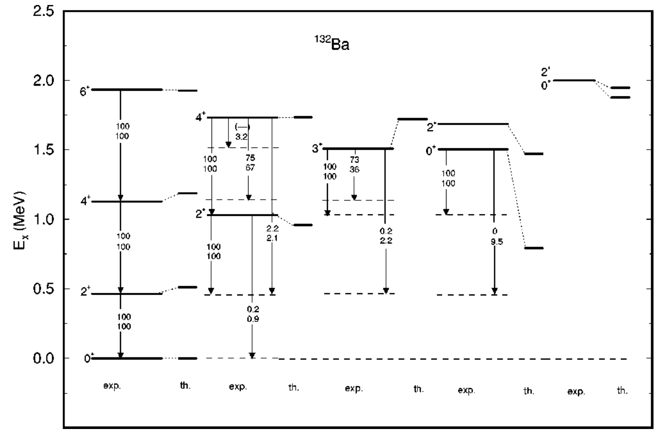

FIG. 2. The spectra and relative $B(E2)$ values for ^{132}Ba. The upper (lower) numbers are the measured (predicted) relative $B(E2)$ values. The experimental data are taken from [15] and [16].

For a more detailed fitting, we first take the nuclei ^{132}Ba. The results are shown in Fig. 2 with parameters $H_0=H_0^{\mathrm{expt}}$, $G_\pi=0.144$, $G_\nu=0.073$, and $\kappa=0.174$ (all in MeV). It is to be noted that here $G_\nu=0.073$ MeV is much smaller than $G_\pi=0.144$ MeV. The reason for this is that the s.p. energy splitting for protons is much larger than that for neutrons, and in order to counter the s.p. energy splitting effect on the collectivity, we need a much stronger SDI strength for protons.

Figure 2 shows that both the spectra and the relative $B(E2)$ values are well reproduced. The absolute $B(E2)$ value for $2_1^+\to 0_1^+$ with effective charge $e_\pi=e_\nu=1.5e$ is $0.081\ (e\ \mathrm{b})^2$, which is still only about one-half of the experimental value $0.172\ (e\ \mathrm{b})^2$. It indicates that the normalization due to the core polarization and other pairs is rather large.

The calculated and experimental spectra for ^{130}Ba–^{136}Ba are shown in Fig. 3, while the relative $B(E2)$ values are in Table II, with parameters in Table III. Figure 3 shows that the fittings are the worst for $^{136}_{56}\mathrm{Ba}_{80}$ with $N_\nu=1$ and the best for $^{130}_{56}\mathrm{Ba}_{74}$ with $N_\nu=4$. It indicates that the S-D truncation is not very good when the the number of nucleon pairs is too small. The reason for this is easily understood by the following arguments. The goodness of the S-D subspace depends on the relative value of the effective residual interaction $|V_{\mathrm{eff}}|$ and H_0. In the case of $R=H_0/|V_{\mathrm{eff}}|\gg 1$, the pairs with all possible angular momenta are almost degenerate and thus are on equal footing. In this case the nucleons move basically independently and obviously the S-D truncation will be very inadequate. With the decreasing of R, the S-D pairs will be favored more and more in energy, and the S-D pair approximation will get better. Since $|V_{\mathrm{eff}}|$ increases with N linearly

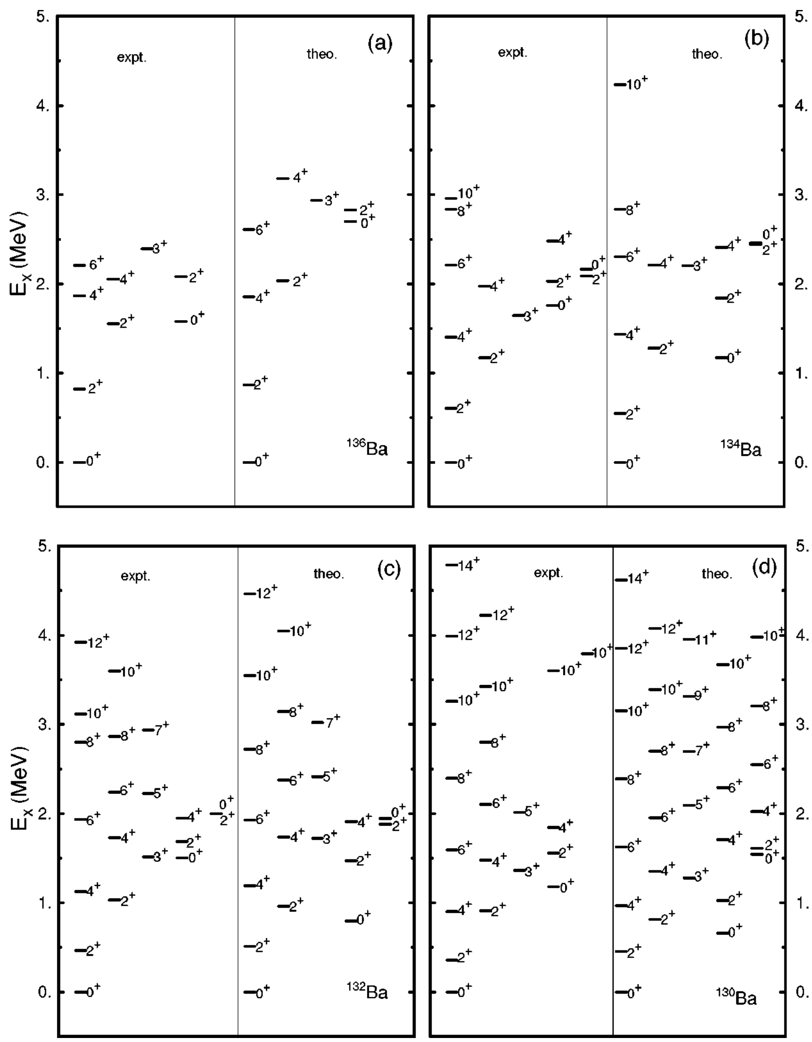

FIG. 3. The spectra for the even Ba isotopes. The experimental data are taken from [16].

or quadratically for the short and long range forces, respectively, one expects that the S-D truncation is better for larger N.

It implies that when N is small, the inclusion of the G pair might be necessary, as is shown in the weak coupling model calculation [8] by Ko *et al.*, in which they found that the wave functions of many low-lying states of the nuclei ^{210}Pb and ^{206}Pb given by the exact shell model calculation are reproduced surprisingly well by the model where S-D-G pairs instead of S-D pairs (or phonons in the language of [8])

TABLE II. The relative $B(E2)$ values for the even Ba isotopes. The experimental data are taken from [15].

	^{130}Ba		^{132}Ba		^{134}Ba		^{136}Ba	
$J_i \to J_f$	Expt.	Theory	Expt.	Theory	Expt.	Theory	Expt.	Theory
$2_2^+ \to 2_1^+$	100	100	100	100	100	100	100	100
$\to 0_1^+$	5.7	1.4	0.2	0.9	1.1	0.6	-	1.7
$3_1^+ \to 2_2^+$	100	100	100	100	100	100	100	100
$\to 4_1^+$	30	37	73	36	40	31	-	3.0
$\to 2_1^+$	1.5	1.4	0.2	2.2	1.0	2.1	-	0.5
$4_2^+ \to 2_2^+$	100	100	100	100	100	100	100	100
$\to 3_1^+$	-	13	-	3.2	14.5	1.0	-	85
$\to 4_1^+$	89	53	75	66.5	77	137	-	1.1
$\to 2_1^+$	3.9	2.9	2.2	2.1	2.5	19	-	114
$0_2^+ \to 2_2^+$	100	100	100	100	100	100	100	100
$\to 2_1^+$	-	12.8	0	9.5	4	3.9	-	2

TABLE III. The parameters used in the calculation.

Nucleus	G_π	G_ν	κ
^{136}Ba	0.176	0.050	0.290
^{134}Ba	0.169	0.060	0.212
^{132}Ba	0.144	0.073	0.174
^{130}Ba	0.107	0.074	0.172

are included. It will be very interesting to check the goodness of the S-D truncation for much larger values of N. However, the computing time will increase by two orders of magnitudes when N increases by one and it is impossible to go beyond $N_\pi = N_\nu = 4$ for rare earth nuclei by using a Pentium computer.

In summary, we carried out a microscopic calculation for the nuclei ^{130}Ba–^{136}Ba, starting from the spherical shell model with s.p. energy splitting fully taken into account. The three parameters in the Hamiltonian are determined by fitting to each nucleus and show smooth variations with nuclei, which is acceptable since it is not a realistic microscopic calculation yet. In the S-D subspace the s.p. energy term has profound effects on the scale and pattern of the spectra, and the $B(E2)$ values. The s.p. level splitting tends to weaken the collectivity significantly. The NPSM truncated to the ''realistic'' S-D subspace can account for the main feature of the low-lying collective states of the nuclei ^{130}Ba–^{136}Ba, especially for nuclei with a larger number of nucleon pairs. However, in order to bring the calculated $B(E2)$ absolute values close to the experimental ones, the normalization effect due to the non-S-D pairs and the polarization of the core has to be taken into account. This is in agreement with the conclusion of Ref. [17] that in spite of the drastic simplification it involves, the S-D space has included the basic dynamics for the low-lying quadrupole states already.

We would like to express our gratitude to B. Q. Chen for writing the efficient NPSM code, to X. W. Pan, Y. M. Zhao, and B. Q. Chen for doing some tentative calculations of the NPSM, and to F. Wang, K. T. Hecht, A. Klein, F. Iachello, H. Wu, J. Ginocchio, and S. Koonin for many stimulating discussions.

[1] *Contemporary Nuclear Shell Model*, edited by X. W. Pan *et al.*, Lecture Notes in Physics (Springer, Berlin, 1996).

[2] F. Andreozzi, L. Coraggio, A. Covello, A. Gargano, T. T. S. Kuo, and A. Porrino, Phys. Rev. C **56**, R16 (1997) and references therein.

[3] A. Holt, T. Engeland, E. Osnes, M. Hjorth-Jensen, and J. Suhonen, Nucl. Phys. **A618**, 107 (1997), and references therein.

[4] M. Honma, T. Mizusaki, and T. Otsuka, Phys. Rev. Lett. **75**, 1284 (1995); **77**, 3315 (1996).

[5] A. Arima and I. Iachello, Adv. Nucl. Phys. **13**, 139 (1983).

[6] T. Otsuka, A. Arima, F. Iachello, and I. Talmi, Phys. Lett. **76B**, 139 (1978); T. Otsuka, A. Arima, and F. Iachello, Nucl. Phys. **A309**, 1 (1978).

[7] J. Q. Chen, Nucl. Phys. **A626**, 686 (1997).

[8] C. M. Ko, T. T. S. Kuo, and J. B. McGrory, Phys. Rev. C **8**, 2379 (1973).

[9] K. Allaart, E. Boeker, G. Bonsignori, M. Savoia, and Y. K. Gambhir, Phys. Rep. **169**, 209 (1988).

[10] K. T. Hecht, J. B. McGrory, and J. P. Draayer, Nucl. Phys. **A197**, 369 (1972); T. Otsuka, Phys. Rev. Lett. **46**, 710 (1981); Nucl. Phys. **A368**, 244 (1981).

[11] C. L. Wu, D. H. Feng, X. G. Chen, J. Q. Chen, and M. Guidry, Phys. Rev. C **36**, 1157 (1987); C. L. Wu, D. H. Feng, and M. Guidry, Adv. Nucl. Phys. **21**, 227 (1994).

[12] B. Fogelberg and J. Blomquist, Nucl. Phys. **A429**, 205 (1984); W. J. Baldridge, Phys. Rev. C **18**, 530 (1978).

[13] S. Pittel, P. D. Duval, and B. R. Barrett, Ann. Phys. (N.Y.) **144**, 168 (1982).

[14] P. Vogel, in *Nuclear Physics*, Dubna Symposium (IAEA, Austria, 1968), p. 60.

[15] R. F. Casten and P. Von Brentano, Phys. Lett. **152B**, 22 (1985).

[16] M. Sakai, At. Data Nucl. Data Tables **31**, 401 (1984); S. Juutinen *et al.*, Phys. Rev. C **52**, 2946 (1995); K. Kirch *et al.*, Nucl. Phys. **A587**, 211 (1995).

[17] H. Nakada and T. Otsuka, Phys. Rev. C **55**, 748 (1997).