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The isospin-dependent quadrupole-quadrupole interaction used in shell model calculations – the effects of including $\Delta N = 2$ excitations and a two-body spin-orbit interaction term

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Abstract. The effect of the "B" term in the interaction $-\chi Q(1) \cdot Q(2)[1 + B\boldsymbol{\tau}(1) \cdot \boldsymbol{\tau}(2)]$ was previously considered in the $0p$ shell (small space). It is now studied in a larger space which additionally includes $\Delta N = 2$ excitations. When B is made sufficiently negative we still obtain for ^{10}Be, even in the larger space, an unphysical collapse of some of the low-lying states so that their energies are less than the energy of the conventional $J = 0^+$ ground state. This effect, however, occurs for values of B considerably more negative than was the case in the smaller space. It is shown that the inclusion of an additional two-body spin-orbit interaction term prevents this unrealistic collapse in both the large and small spaces.

1 Introduction and background

In a previous work [1], for a shell model calculation of ^{10}Be, a quadrupole-quadrupole interaction, of the form $-\chi Q \cdot Q[1 + B\boldsymbol{\tau}(1) \cdot \boldsymbol{\tau}(2)]$, was used which has a combination of the usual isospin-independent first term and the less common isospin-dependent second term. In that reference motivations were provided for the selection of both the specific interaction and the specific nucleus that were studied. The model space utilized was the $0p$ shell, and in particular the dependence on the parameter B (the strength of the isospin-dependent second term in the interaction) was studied.

For $B = 0$ we have a spin-isospin independent interaction, and for the $0p$ shell the Wigner Supermultiplet Theory applies [2]. We can also think of this $B = 0$ case in ^{10}Be as a very simple application of the Elliott model [3] to the $0p$ shell. Of course, the greatest interest in the latter model will be in the $1s$–$0d$ shell. The study of the addition (to the common isospin-independent $Q \cdot Q$ interaction) of the isospin dependent term $-\chi B\boldsymbol{\tau}(1) \cdot \boldsymbol{\tau}(2)$ can thus be regarded as an exploration of what happens when we deviate from the simple SU(3) limit. In another vein, a large negative value of B has been invoked in R.P.A. calculations to explain the splitting of the isovector and isoscalar giant quadrupole resonances. Will this same large negative B also give better results (for level energies and electromagnetic transition rates) in shell model calculations than the $B = 0$, SU(3) limit?

In the previous calculation of ^{10}Be in the $0p$ shell [1], the answer was a resounding no! In the $0p$ space calculation with $B = 0$, the ground state has $J = 0^+$ and orbital symmetry [42]. There is a two-fold degeneracy for the first excited state: two $J = 2^+$ states both with orbital symmetry [42], corresponding to $K = 0$ and $K = 2$. The focus of interest in [1] was also on two higher-lying degenerate $L = 1$ $S = 1$ states: one with orbital symmetry [33], and the other [411]; in each of these two cases from the $L = 1$ $S = 1$ configuration one obtains a triplet of states $J = 0,\ 1,\ 2$.

When a negative B of increasing magnitude was introduced (see Fig. 1 of this paper), the 2_1^+ state came down in energy in a nearly linear fashion as a function of B. The $B(E2)$ to this state was purely isovector, i.e. was proportional to $(e_p - e_n)^2$. Ultimately, at $B \approx -0.68$ this 2_1^+ state crossed below the 0_1^+ state and became the ground state.

However, coming down even faster as B was becoming more negative was a triplet of states with $J = 0^+,\ 1^+$ and 2^+ which for $B = 0$ was part of the degenerate [33] and [411] $L = 1$ $S = 1$ states mentioned above. Very quickly, after the 2_1^+ state became the ground state, as the magnitude of the negative B was further increased beyond

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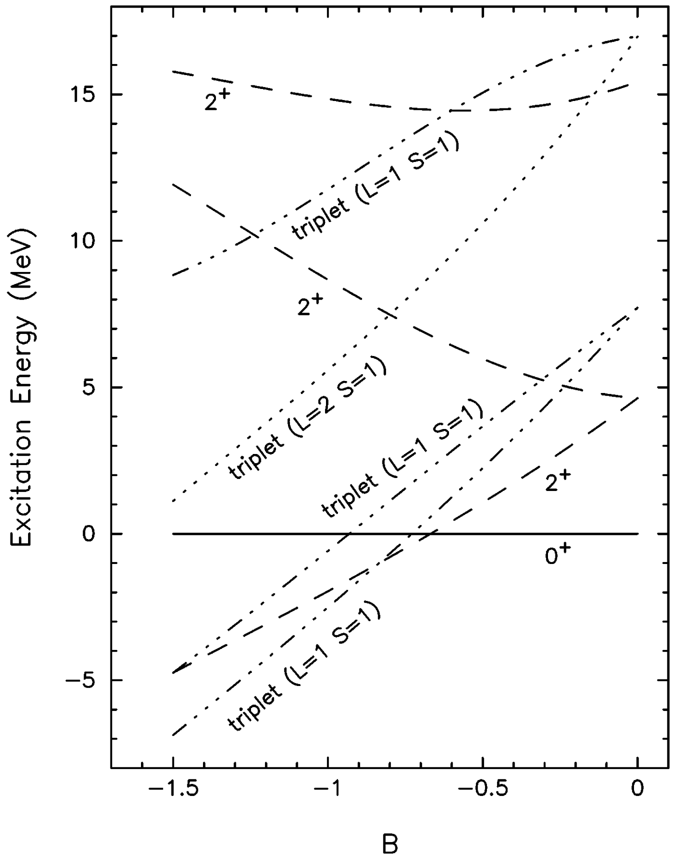

Fig. 1. The excitation energies of selected states in ^{10}Be, with respect to the 0_1^+ state, as a function of the isospin-dependent quadrupole-quadrupole interaction parameter B. The energy of the conventional 0_1^+ state is always taken to be 0 MeV and the energies of the other states are adjusted accordingly. Small Space with $x = 0.0$

$B \approx -0.68$ this triplet (which is some linear combination of states of symmetry [33] and [411]) became the ground state for $B \le -0.74$.

The "collapse" described in the last two paragraphs is physically unrealistic since all known even-even nuclei have the 0_1^+ level as their unique ground state.

The scope of this paper is outlined in Sect. 2. The results of previous work are summarized in Sect. 3. Sections 4 and 5 consider the effects of the isospin-dependent term and the spin-orbit term in the small space. The effects of enlarging the shell-model space are discussed in Sect. 6.

2 Outline of the calculations for ^{10}Be carried out in the present paper

In this paper, in the hope of preventing the aforementioned undesirable collapse, we extend the calculations of [1] in two ways. First, we increase the model space to include not only all the possible configurations in the $0p$ shell, but also all $2\hbar\omega$ (i.e. $\Delta N = 2$) excitations. We thus have a "small" space ($0p$ shell) and a "large" space ($0p + 2\hbar\omega$). Second, we study the effects of also including two body spin-orbit interactions. Our interaction is now $-\chi Q \cdot Q\,[1 + B\boldsymbol{\tau}(1)\cdot\boldsymbol{\tau}(2)] + xV_{s.o.}$ where x is a multiplicative constant and $V_{s.o.}$ is a two body spin-orbit interaction which was initially used and described by Zheng and Zamick [4]. Basically, for $x = 1$, the last term in the interaction gives a good fit to the free-space two-body spin-orbit part of a non-relativistic G matrix derived from a realistic interaction [Bonn A interaction]. The two-body spin-orbit interaction ($xV_{s.o.}$) behaves to a very large extent like an one-body spin-orbit interaction which depends on the nucleon member. For $x = 1$ the results quoted in Table 1 of [4] for the $p_{1/2}$–$p_{3/2}$ splitting are 3.38 MeV for a ^{4}He and 5.06 MeV for an ^{16}O core. There are, however, some arguments that inside a nucleus the spin-orbit interaction becomes stronger due to medium modifications in a relativistic formulation. Hence we shall also present results for $x = 1.5$.

The results of our calculations for the energies of the levels of ^{10}Be are presented in Figs. 1 – 6, which correspond respectively to the following calculations:

Fig.1:	Small space	$x = 0.0$	(no spin-orbit interaction)
Fig.2:	Small space	$x = 1.0$	(free space spin-orbit interaction)
Fig.3:	Small space	$x = 1.5$	(medium modified spin-orbit interaction)
Fig.4:	Large space	$x = 0.0$	(no spin-orbit interaction)
Fig.5:	Large space	$x = 1.0$	(free space spin-orbit interaction)
Fig.6:	Large space	$x = 1.5$	(medium modified spin-orbit interaction)

In all these six figures the energy of the conventional 0_1^+ state is always taken to be zero and the energies of all other states are given with respect to that state.

3 Small space results for ^{10}Be without the spin-orbit interaction term

In Fig. 1 we show a calculation of the energies of states in ^{10}Be as a function of the (negative) B in the small space (the $0p$ shell) and without any spin-orbit interaction. For $B = 0$ we have the supermultiplet or SU(3) limit in which the 2_1^+ and 2_2^+ states are degenerate at a calculated energy of 4.7 MeV. They correspond to [42] $K = 0$ and [4] $K = 2$ states. There are two degenerate $L = 1$ $S = 1$ states with quantum numbers [411] and [33] which are calculated to be at 7.8 MeV. For each of these $L = 1$ $S = 1$ configurations, we get a triplet of states with $J = 0^+$, 1^+, and 2^+.

We see from Fig. 1 that as the magnitude of the negative B is increased from $B = 0$ one of the [42] 2^+ states comes down rapidly in energy and becomes the ground state at $B \approx -0.68$. Having a 2^+ ground state is of course very unphysical. And that is not the only problem in Fig. 1. As B becomes more negative, dropping down there even faster than the 2_1^+ is one of the $L = 1$ $S = 1$ triplets (which had a higher energy than the 2_1^+ at $B = 0$). This degenerate triplet of $J = 0^+$, 1^+, 2^+ states becomes the ground state for $B \leq -0.74$. Basically, the results in Fig. 1 reproduce (in a redrawn form) those of the previous work by Fayache, Sharma and Zamick [1]. The unrealistic nature of these results clearly requires that modifications be made to our approach to the problem, modifications such as those which our present paper will provide.

4 The B dependence of the level energies for two identical particles in the $1p$ shell – ^{6}He or ^{6}Be

We can gain some insight into why for large negative values of B we get other states coming down in energy with respect to the normal $L = 0$ $S = 0$ $J = 0$ ground state. This we do by considering the simplest problem of two identical particles in the p shell, *i.e.* ^{6}He or ^{6}Be. This analysis also applies to two holes (*i.e.* to ^{14}C or ^{14}O).

With a spin-isospin independent interaction, the wavefunctions can be classified by LS coupling:

$$\text{Ground State } (L = 0\ S = 0)^{J=0^+}$$
$$\text{First Excited State } (L = 2\ S = 0)^{J=2^+}$$
$$\text{Triplet } (L = 1\ S = 1)^{J=0^+,1^+,2^+}$$

The above states all have isospin $T = 1$.

With an isospin-independent $Q \cdot Q$ interaction (i.e. for our interaction with $B = 0$), the energies are given by [3]

$$\langle -\chi Q \cdot Q\rangle_{\lambda\mu L} = \bar{\chi}[-4(\lambda^2 + \mu^2 + \lambda\mu + 3(\lambda + \mu)) + 3L(L + 1)]$$

where $\bar{\chi} = \chi\frac{5b^4}{32\pi}$ with b the harmonic oscillator length parameter ($b^2 = \frac{\hbar}{m\omega}$).

For the even L states $(\lambda\mu)$ is equal to (20); for $L = 1$ $(\lambda\mu)$=(01). With the $Q \cdot Q$ interaction with $B \neq 0$, $-\chi Q \cdot Q[1 + B\boldsymbol{\tau}(1) \cdot \boldsymbol{\tau}(2)]$, we replace $\bar{\chi}$ by $\bar{\chi}(1 + B)$ (since $\boldsymbol{\tau}(\mathbf{1}) \cdot \boldsymbol{\tau}(\mathbf{2}) = +1$ for $T = 1$). The energies are then

$$\begin{array}{ll} L = 0\ S = 0: & -40\bar{\chi}(1 + B) \\ L = 2\ S = 0: & -22\bar{\chi}(1 + B) \\ L = 1\ S = 1: & -10\bar{\chi}(1 + B) \end{array}$$

For $B \geq -1$, the $L = 0$ state is the lowest in energy, and the $L = 1$ $S = 1$ triplet is the highest in energy. For $B = -1$, all three states are degenerate at zero energy. For $B < -1$, there is a sign change of the overall coupling and the $L = 1$ $S = 1$ triplet becomes the ground state and the $L = 0$ $S = 0$ state is at the highest energy.

5 The inclusion of a two-body spin-orbit interaction term in the small space

In Fig. 2 we stay in the small ($0p$ shell) space but add to the interaction an additional two-body spin-orbit term with $x = 1$ as discussed in Sect. 2. The 2_1^+ and 2_2^+ states are no longer degenerate at $B = 0$. This corresponds to the experimental results. The observed data has the 2_1^+ at 3.368 MeV and the 2_2^+ at 5.960 MeV. The $B(E2)$ from the $J = 0_1^+$ ground state to the 2_1^+ is very strong with $B(E2) = 52\ e^2\text{fm}^4$.

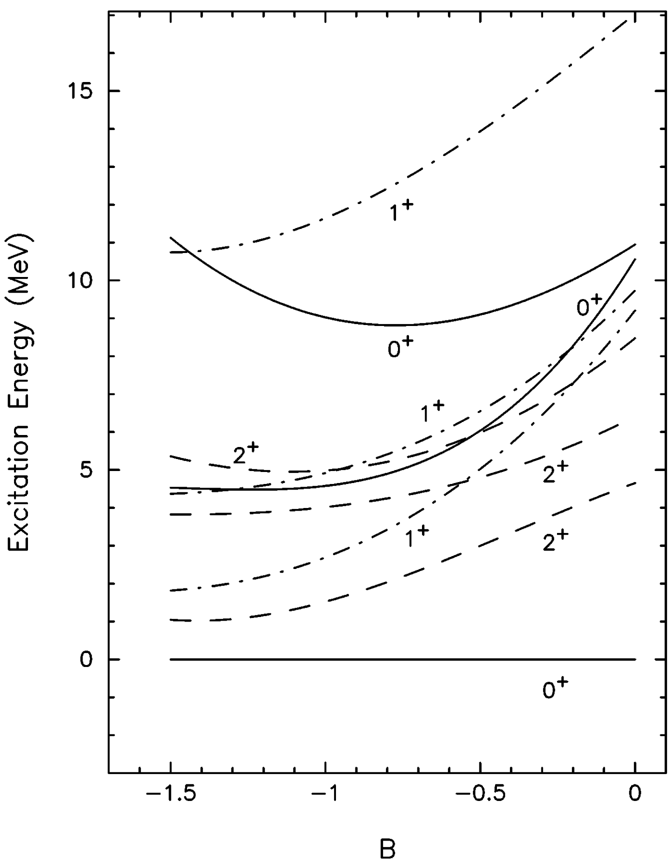

Fig. 2. Small Space with $x = 1.0$

As we increase the magnitude of (negative) B in Fig. 2, we no longer get the cross-over shown in Fig. 1, where for large negative values of B other states had lower energies than the conventional 0_1^+ state. The addition of the spin-orbit term has thus greatly stabilized the results. There is, however, one obvious disagreement with experiment; for $B \leq -0.55$ the lowest 1^+ state comes down to below the 2_2^+ state. This is not seen experimentally; indeed no low-lying 1^+ state has yet been observed in ^{10}Be and no $J = 1^+$ states are mentioned in the compilation of Ajzenberg-Selove [5].

Figure 3 was obtained by using a stronger (medium modified) spin-orbit interaction with $x = 1.5$ in the small space. Figure 3 is qualitatively similar to Fig. 2 (small space with $x = 1$) but in Fig. 3 the $J = 1^+$ state lies below the 2_2^+ state only for $B \leq -0.8$.

The results of this section suggest that it will be interesting to see what happens if we repeat our calculations for the spin-orbit strengths $x = 0$, 1.0 and 1.5 in a larger shell model space. This is done in Sect. 6.2.

6 Large space results for ^{10}Be

In this section, we extend our previous $0p$ space (small space) calculations of ^{10}Be, as described in Sects. 3 and 5,

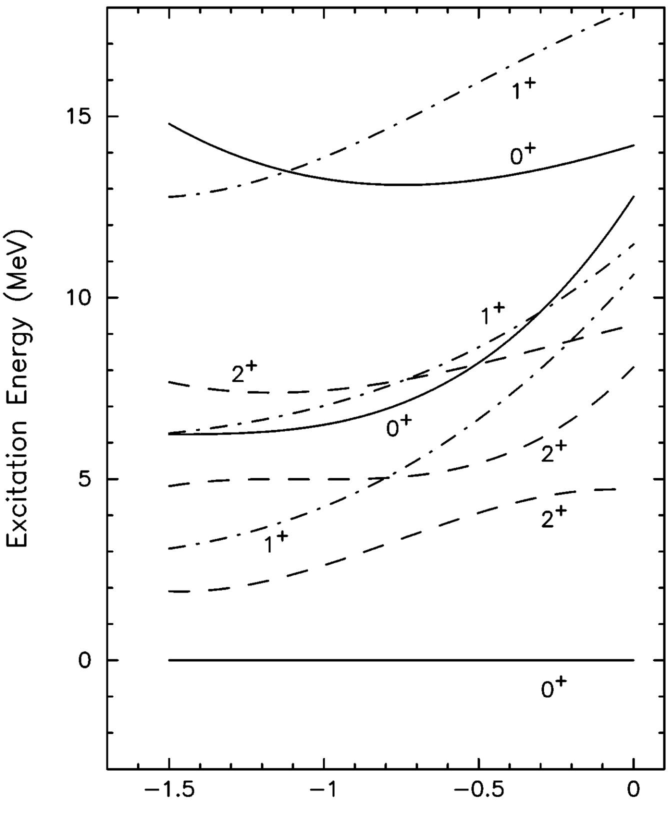

Fig. 3. Small Space with $x = 1.5$

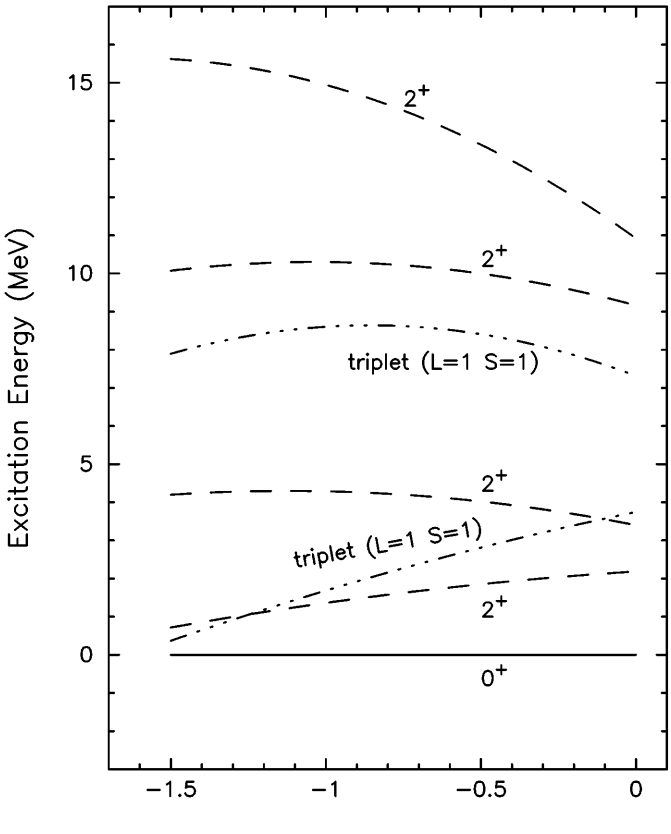

Fig. 4. Large Space with $x = 0.0$

to include all $\Delta N = 2$ (i.e., $2\hbar\omega$) excitations. The results are provided in Fig. 4 (with spin-orbit strength $x = 0$), Fig. 5 (with $x = 1$), and Fig. 6 (with $x = 1.5$). Although there are some differences between corresponding results (for the same value of x) between the small and large spaces, we can quickly assert that in the most important respects the results in the large space are remarkably similar to the corresponding small space results, albeit on a larger (i.e. expanded) scale of B.

6.1 Large space results with no spin-orbit interaction

We first consider in Fig. 4 the ^{10}Be case in the large space where there is no spin-orbit interaction term ($x = 0$).

We can compare in Figs. 1 and 4 (both for $x = 0$) the situations for $B = 0$ (i.e. a simple isospin independent $Q \cdot Q$ interaction). It is interesting then to note that when we extend the calculation with $x = 0$ to $\Delta N = 2$, some degeneracies are preserved and some are not. The supermultiplet degeneracies are preserved, i.e. for a given [f] the various (S, T) spin-isospin combinations are still degenerate. However, the 'accidental' degeneracies in the $0p$ space are not maintained in the larger space.

For example, the 2_1^+ and 2_2^+ states, which were degenerate in the $0p$ space, are no longer so in the extended space. The 2_1^+ state is calculated to be at 2.186 MeV, and the 2_2^+ state at 3.400 MeV. Most of the calculated $E2$ strength goes to the 2_2^+ state.

The two sets of triplets ($L = 1$ $S = 1$ $J = 0^+$, 1^+, 2^+) with orbital symmetry [33] and [411] are degenerate in the $0p$ space. This is because the $(\lambda\mu)$ values are (03) and (30) respectively and the SU(3) formula for the energy is symmetric in λ and μ. In the extended space, for $B = 0$, the states split in such a way that the excitation energy of one is about twice that of the other. The reason for the removal of this degeneracy may be that including $\Delta N = 2$ mixing is equivalent to having different oscillator frequencies in the x, y and z directions, as in the Nilsson model.

We next consider when $x = 0$ what happens to the excitation energies of the states in ^{10}Be as a function of an increasingly negative B in the large space (i.e. when we include not only all configurations in the $0p$ shell but also all $2\hbar\omega$ excitations as well). The results are shown in Fig. 4. In the lower part of that figure we follow the behaviour of the 2_1^+ state (dashed curve) and the $L = 1$ $S = 1$ degenerate triplet $J = 0^+, 1^+$ and 2^+ (triple dotted-dashed curve). We find that, although the overall scale for B has changed in going from the small space (Fig. 1) to the large space (Fig. 4), the two sets of results (both with $x = 0$, i.e. without the spin-orbit term) are qualitatively quite similar. That is to say, that the 2_1^+ state and the degenerate $L = 1$ $S = 1$ $J = 0^+$, 1^+, 2^+ triplet still both come down in energy in Fig. 4 as B becomes

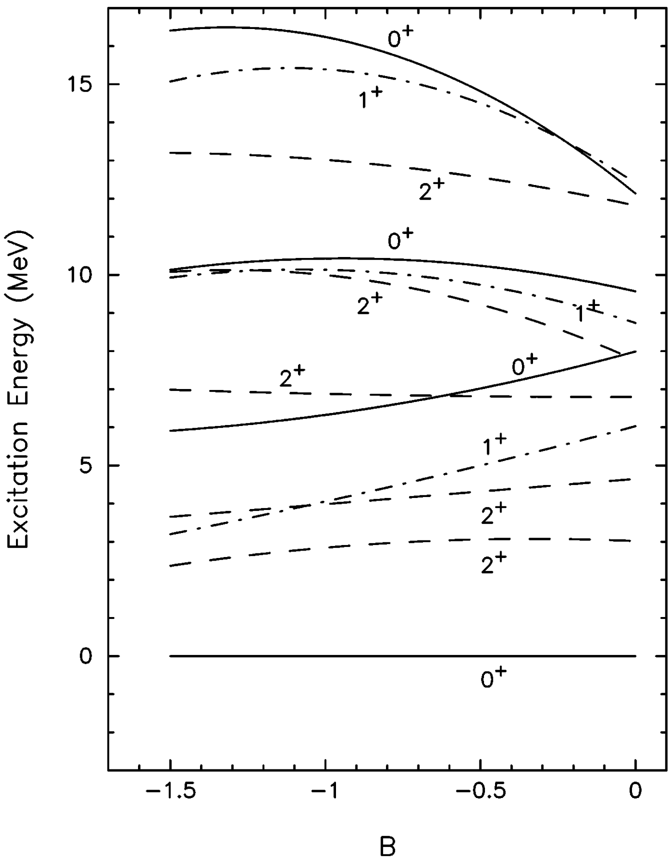

Fig. 5. Large Space with $x = 1.0$

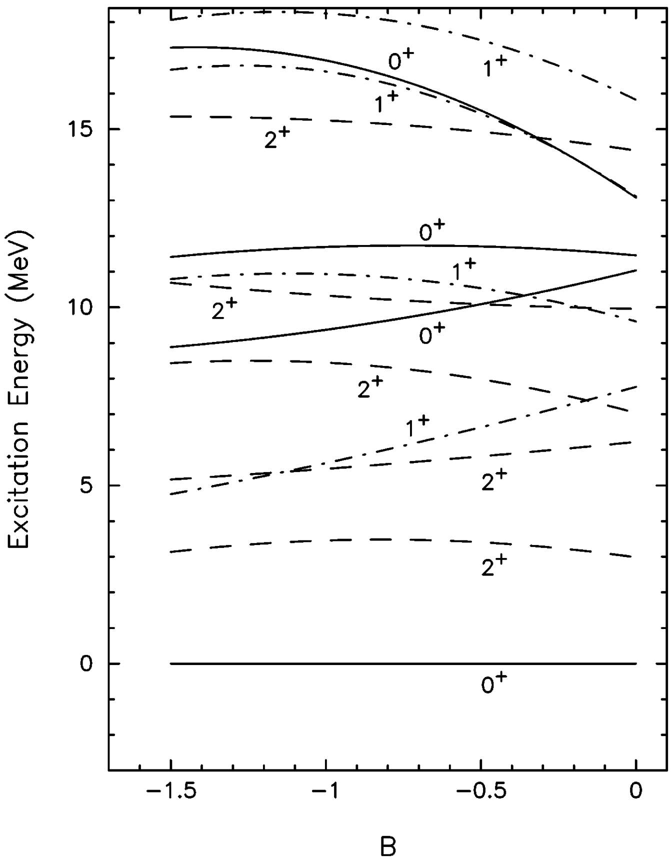

Fig. 6. Large Space with $x = 1.5$

more negative. Here in the large space, however, the $L = 1$ $S = 1$ triplet, which has a larger slope, beats out the 2_1^+ state, is the first to cross the 0^+ state at $B \approx -1.6$, and becomes the ground state for $B \leq -1.6$.

A very important point is that we notice a change of scale for the value of B at the crossover of the 0_1^+ state by somewhat more than a factor of two (-0.68 vs -1.60) in going from the small space to the large one. There has been considerable discussion of this in the literature, e.g. by Bes, Broglia and Nilsson [6], of how to relate values of B in large and in small model space. These authors point out that the "renormalized" B in a small space is considerably smaller than the "bare" B in the large space. For example, they suggest that corresponding to a bare value of $B = -3.6$ in the large space, the renormalized value to be used in a small space is only $B \approx -0.6$.

Another change in going from the small space to the large space concerns the isoscalar and isovector $B(E2)$'s. In the small space the 2_1^+, which came down in energy as B was made increasingly negative, was a purely "isovector" state [1]. That is to say the value of $B(E2, e_p, e_n)$ from the ground state to that 2_1^+ state was zero if $e_p = e_n$ but was large if $e_p = -e_n$. In the large space, the corresponding 2_1^+ state is not purely isovector. At $B = 0$, the 2_1^+ state is at 2.186 MeV and the 2_2^+ state at 3.400 MeV. The calculated isoscalar $B(E2)$'s ($e_p = e_n = 1$) are respectively 63.76 and 113.34 $e^2\text{fm}^4$; the isovector $B(E2)$'s ($e_p = 1, e_n = -1$) are respectively 12.49 and 9.52 $e^2\text{fm}^4$.

When $B = -1.5$ (just before the collapse), the lowest 2^+ state is at 0.370 MeV and is part of the $L = 1$ $S = 1$ triplet that is coming down towards the 0_1^+ state. That lowest 2^+ state has zero isoscalar and zero isovector strength. The two lowest 2^+ states when $B = 0$ are now (at $B = -1.5$) the second and third 2^+ states and are respectively at 0.717 and 4.199 MeV. The isoscalar $B(E2)$'s are 32.86 and 168.4 $e^2\text{fm}^4$, respectively; the isovector $B(E2)$'s are 13.28 and 0.193 $e^2\text{fm}^4$.

6.2 Large space results when the spin-orbit interaction term is added

When the spin-orbit interaction is added to our original interaction the results are stabilized just as they were in the small space. This can be seen in Fig. 5 (for $x = 1$) and in Fig. 6 (for $x = 1.5$). Whereas for $x = 0$ in the large space there is a collapse of the 2_1^+ state as well as of the triplet $L = 1$ $S = 1$ state near $B = -1.5$, this collapse disappears in the large space when the spin-orbit interaction is turned on. The only obvious unphysical behavior is the coming down of the $J = 1^+$ state below the 2_2^+ state. This occures for $B \leq -1.0$ for $x = 1$ (Fig. 5) and for $B \leq -1.2$ for $x = 1.5$ (Fig. 6). Again these values are larger in magnitude than the corresponding values in the small space ($B \leq -0.55$ in Fig. 2 and $B \leq -0.8$ in Fig. 3 respectively), but we would have expected still larger values in the large space following the prescription of [6]. Studying the behavior of the calculated 1_1^+ state in ^{10}Be is a good way to get a handle on the relative strengths of the opposing effects of making B increasingly negative and of increasing the strength x of the spin-orbit term. The latter increases the 1_1^+ energy, the former decreases it. Thus, for a known fixed value of the spin-orbit strength, we could in principle obtain an estimate for the value of B if we knew the excitation energy of the 1_1^+ state. This state could be experimentally identified because of the strong $B(M1)\uparrow$ for the $0_1^+ \rightarrow 1_1^+$ transition strength; in our large space calculations we predict it to be 3.53 μ_N^2 for $x = 1.5$, $B = 0$ and 3.86 μ_N^2 for $x = 1.5$, $B = -1.5$.

7 Closing remarks

In this paper we were able to eliminate the physically unrealistic results that were obtained in [1]. There, in the small $0p$ space, with the interaction $-\chi Q(1) \cdot Q(2)[1 + B\boldsymbol{\tau}(1) \cdot \boldsymbol{\tau}(2)]$, unphysical results were obtained for the excitation energies of the states of ^{10}Be. For the large negative values of B that are needed to give the correct splittings of the isovector and isoscalar giant quadrupole resonances, the 0_1^+ is no longer the ground state.

The first remedy that we investigated in this paper was to expand the $0p$ shell model space by adding to it all possible $2\hbar\omega$ excitations. We found that this approach did not remove the problem. The magnitude of the value of the negative B at which the crossover of the 0_1^+ occured in the large space was considerably larger than the corresponding magnitude in the small space, though smaller than would have been expected from the prescription of [6].

The second remedy that we tried in this paper involved adding to our original interaction a realistic two-body spin-orbit term. When this was done the collapse was eliminated in both the small ($0p$) and the large ($0p + 2\hbar\omega$) spaces.

Some additional remarks and caveats are in order. It was noted by Fayache, Sharma and Zamick [7] that the isovector scissors mode in ^{10}Be is at quite a high energy, $E \approx 22$ MeV. One cannot obtain such a high energy for this state with an isospin-independent $Q \cdot Q$ interaction whose strength is chosen so that the 2_1^+ energy comes out correctly. Adding a negative B term to the $Q \cdot Q$ interaction helps to raise the energy of the scissors mode state. On the other hand, when one examines realistic interactions, by focusing on their long range parts, one does see the emergence of a $Q \cdot Q$ interaction but the large B term is not present. The microscopic origin of such a term is not understood. Recently, there has been an analysis by Nojarov, Faessler and Dingfelder [8] and by Nojarov [9] of the isovector part of the optical potential and they feel that it should be weaker than in previous analyses.

In conclusion, we have shown that by adding a realistic two-body spin-orbit interaction one can remove the low-energy instabilities that arise when one adds an isospin-dependent term to the quadrupole-quadrupole interaction (a term which helps to get the correct isospin splitting of giant quadrupole resonances and to raise the energies of scissors mode states). In other words, it makes no sense to use the interaction $-\chi Q \cdot Q[1 + B\boldsymbol{\tau}(1) \cdot \boldsymbol{\tau}(2)]$ with large negative B, unless one also adds spin-orbit terms.

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