Quadrupole-quadrupole interaction calculations which include N=2 mixing

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Abstract

We carry out a study of the study of the Q · Q interaction in a model space which consists of several nucleons in an open shell and all 2\hbar\omega exciations. This interaction is \(-t\frac{3}{2}Q \cdot Q\), where for \(t=1\) we get the ‘accepted strength’. In the 0\(p\) space, the spectrum would scale with \(t\). In this space, the \(2^+_1\) and \(2^+_2\) states of \(^{10}\text{Be}\) are degenerate, as are the [330] and [411] sets of \(J = 0^+, 1^+\) and \(2^+\) triplets. When \(2\hbar\omega\) admixtures are included, the degeneracies are removed. For \(t \geq 1.8\) we have new ground state and a new \(2^+_1\) state. These are states in which two particles are excited from the 0\(p\) to the 1\(s - 0d\) shell. There is no mixing of these 2p-2h states with the other states. For these 2p-2h states the occupancy for 0s,0p,1s-0d and 1p-of are 4,4,2 and 0 respectively.
I. INTRODUCTION

In this work we will study the behaviour of the Q·Q interaction in a nucleus as a function of the strength of the interaction. Although this is a model study it helps to make things concrete by focusing on a particular nucleus. We choose $^{10}$Be. This nucleus is of particular interest because in a 0p space calculation with Q·Q there are some interesting degeneracies. For example, the $2^+_1$ and $2^+_2$ states are degenerate, and both have orbital symmetry [400]. The $L = 1$ $S = 1$ states with orbital symmetry [330] and [411] are degenerate. Thus we have two sets of degenerate triplets $J = 0^+, 1^+$ and $2^+$ emanating from the above two orbital configurations. These degeneracies can easily be found by applying the $SU(3)$ formula:

$$E(\lambda \mu) = \bar{\chi} \left[-4(\lambda^2 + \mu^2 + \lambda\mu + 3(\lambda + \mu)) + 3L(L + 1)\right]$$

If we write the interaction as $\chi Q \cdot Q$ then, in the 0p space and when we change $\chi$, the degeneracies will not be removed. All that will happen is that the energies of all states will be proportional to $\chi$, and so the spectrum will be blown up or shrunk as $\chi$ is made larger or smaller.

What happens though if we include contributions from other major shells? The Q·Q interaction will not connect $\Delta N = 1$ states because of parity arguments, but there will be $\Delta N = 2$ admixtures. Indeed, the concept of an $E2$ effective charge is often illustrated by using a Q·Q interaction to obtain $\Delta N = 2$ admixtures.

II. THE HAMILTONIAN AND CHOICE OF PARAMETERS

It has been shown by Bes and Sorensen [1] that if in the valence space (0p) the appropriate Q·Q interaction is $-\chi_0 Q \cdot Q$, then in a space which includes $\Delta N = 2$ excitations the appropriate strength is $-\frac{\chi_0}{2} Q \cdot Q$. We wish to vary the interaction, and we therefore parameterize it as

$$V = -t \left(\frac{\chi_0}{2}\right) Q \cdot Q$$
so that for $t = 1$ we have the standard choice of Bes and Sorensen [1]. For $^{10}Be$, we have $\chi_0 = 0.36146 \ MeV \ fm^{-1}$.

The Hamiltonian we use is

$$H = \sum_i T_i + \frac{1}{2} m \omega^2 r_i^2 - \sum_{i<j} t \frac{\chi_0}{2} Q(i) \cdot Q(j)$$

We perform shell model calculations using the OXBASH shell model code [2] in the space $(0p)^6$ plus 2$h\omega$ excitations. As mentioned in the introduction, when harmonic oscillator wave functions are used in a single major shell, the single particle terms in the above Hamiltonian are constant, so that the only part of the Hamiltonian that affects the spectra is the two-body term. The separation of energies is linear in $t$ - the wave functions are unaffected by the choice of (positive) $t$.

However, when $\Delta N = 2$ excitations are allowed, the linear terms are no longer constant, and the behaviour as a function of $t$ is more complicated. We will now study this behaviour as a function of $t$ in $^{10}Be$.

### A. Removal of Degeneracies

In Table I we present $t = 1$ results for $^{10}Be$ in a large space $(0p)^6$ plus all $2h\omega$ excitations. We present the results for the energies of $J = 1^+$ and $2^+ T = 1$ states, as well as $B(M1)$ and $B(E2)$ transitions from the ground state to these states. More precisely, it is the isovector $B(M1)$ in units of $\mu_N^2$ and isoscalar $B(E2)$ ($e_p = 1$, $e_n = 1$) in units of $e^2 fm^4$.

We see that there are many degeneracies still present in the large space e.g. four $J = 1^+ T = 1$ states at 12.12 $MeV$ and three at 13.90 $MeV$, as well as three $J = 2^+ T = 1$ states at 12.12 $MeV$. These degeneracies clearly correspond to various $S$, $T$ combinations for states of given $L$ and orbital symmetry [f].

However, other ‘accidental’ degeneracies which were present in the small space $(0p)^6$ are no longer present. The $J = 1^+_1$ and $1^+_2$ states at 3.74 $MeV$ and 7.31 $MeV$ are linear combinations of the $L = 1$ [330] and $L = 1$ [411] configurations (actually they are parts of
\( J = 0^+, 1^+, 2^+ \) triplets). In the small space, these two \( J = 1^+ \) states (or triplets) were degenerate - now one of the states is almost at twice the excitation energy of the other.

The \( 2^+_1 \) and \( 2^+_2 \) states are no longer degenerate. The \( 2^+_1 \) state is at 2.19 MeV with \( B(E2) \uparrow \) from the ground state of 63.8 \( e^2 fm^4 \), whilst the \( 2^+_2 \) state is at 3.40 MeV with \( B(E2) \uparrow = 113.4 \ e^2 fm^4 \). Note that, contrary to experiment, the second \( 2^+ \) state is the one most strongly excited. When a reasonable spin-orbit interaction is added to the Hamiltonian the situation is corrected.

It should be pointed out that in perturbation theory, in which only the direct part of the particle-hole interaction of \( Q \cdot Q \) is used to renormalize the interaction between two particles in the valence space, the degeneracies above would not be removed. The relevant diagram is the familiar Bertsch-Kuo-Brown bubble (or phonon) exchange between two nucleons [3,4]. For a simple \( Q \cdot Q \) interaction, this diagram simply renormalizes the strength of the \( Q \cdot Q \) interaction. Clearly, changing the strength in the valence space will not remove the degeneracies. Thus, the shell model diagonalization implicitly contains effects beyond the direct bubble diagram. Furthermore, these effects are quite important.

**B. Change in the Nature of the Ground State as \( t \) Increases**

We now vary \( t \) over the range \( 0 < t < 2 \). In Fig. 1 we plot as a dot-dash curve the value of \( E/t \) for the lowest \( 2^+ \) state, the one with finite but small \( B(E2) \) strength from ground. We also plot \( E/t \) as a solid line for the state with the strongest \( B(E2) \) from ground. It starts off at \( t = 1 \) as the second \( 2^+ \) state. In the \( 0p \) space, the \( 2^+_1 \) and \( 2^+_2 \) states would be degenerate, and the curve for \( E/t \) vs. \( t \) would be a horizontal line. However, in the \( 0p + 2\hbar \omega \) space there is a dependence on \( t \) (and more so for the solid curve).

But, for \( t \approx 1.8 \) and beyond, all the \( B(E2) \) strength from ground state goes to the new lowest \( 2^+ \) state. Furthermore, the value of \( E/t \) becomes constant for \( t \geq 1.8 \ i.e. \) the curve becomes horizontal. Clearly, the nature of the ground state changed beyond \( t = 1.7 \). We will now examine this change in more detail.
If the only thing that happened was that there was a new \( J = 0^+ \) ground state, then of course there would be a sudden change in the \( B(E2) \)’s from this new ground state to the \( 2^+ \) states. However, the static quadrupole moments of the \( 2^+ \) states themselves would not change.

For \( t = 1.1 \) the \( B(E2) \) to the \( 2^+_1 \) state is 40.61 e\(^2 fm^4 \) and to the \( 2^+_2 \) state 158.0 e\(^2 fm^4 \). The calculated static quadrupole moments are respectively \( 11.56 \) e\( fm^2 \) and \(-11.46 \) e\( fm^2 \).

As discussed by Fayache, Sharma and Zamick in Ref. [5], this is consistent with the two \( 2^+ \) states being prolate, with about the same intrinsic quadrupole moment \( Q_0 \), but the lower state would have \( K = 2 \) and the upper one \( K = 0 \). Indeed, for \( K = 0 \) \( Q(2^+) = -2/7Q_0 \), and for \( K = 2 \) \( Q(2^+) = +2/7Q_0 \).

The behaviour for \( t = 1.1 \) is maintained for \( t = 1.3 \) and 1.5, but for \( t = 1.7 \) and up to \( t = 1.75 \) there is a big drop in \( B(E2)_{0_1^+ \rightarrow 2_1^+} \). The other three quantities do not change, not even -strangely enough- \( Q(2_2^+) \).

Remember that for \( t = 1.75 \) we are still below the critical \( t \) for which the \( J = 0^+ \) ground state changes its nature. What is clearly happening is that a third \( 2^+ \) state has crossed over and came below what was formerly the \( 2^+_2 \) state. This is confirmed by noting that at \( t = 1.75 \) the \( B(E2)_{0_1^+ \rightarrow 2_2^+} \) is very large (162.1 e\(^2 fm^4 \)). Clearly, in going from \( t = 1.7 \) to \( t = 1.75 \), the \( 2^+_2 \) and \( 2^+_3 \) states have interchanged positions. The fact that the static quadrupole moments of the two states are about the same means that both states can be associated with two different prolate \( K = 0 \) bands which have the same deformation.

Next we consider \( t = 1.76 \). Here we are just beyond the critical \( t \), and the nature of the ground state has changed. Now the \( B(E2) \) to the \( 2^+_1 \) state is much weaker, and the \( B(E2) \) to the \( 2^+_2 \) state is strong. This suggests that the new \( 0^+ \) ground state and the new \( 2^+_2 \) state are members of a new rotational band, and that both of these states have come down in energy together.

When we go from \( t = 1.76 \) to \( t = 1.78 \) there is a big change, but the results stabilize beyond that. Now the \( B(E2) \) to the \( 2^+_1 \) state is the strongest (140 e\(^2 fm^4 \)), and the signs of the static quadrupole moments change. Now \( Q(2^+_1) \) is negative, and \( Q(2^+_2) \) is positive.
What is clearly happening is that there is another cross-over. What was formerly the $2^+_3$ state at $t = 1.7$ first crosses the the $2^+_2$ state at $t = 1.75$ (as mentioned above), and now crosses the $2^+_1$ state at $t = 1.78$. By $t = 1.78$ and beyond, the $0^+$ and $2^+$ members of a new band have become the lowest two states, and the results stabilize.

**III. INTERPRETATION OF THE NEW BAND: STATES WITH INTEGER OCCUPANCIES**

In Fig. 2 we plot the rapid descent of the $J = 0^+$ and $2^+$ members of the new rotational band. We start from $t = 1$, but if we project backward we see that for small $t$ the band emanates from the $2h\omega$ region. To better ascertain the nature of the new band, we give in Table III the occupancies of the single-particle levels that were used in this calculation *i.e.* $0s, 0p, 1s − 0d$ and $1p − 0f$.

At $t = 1.7$, just before the critical value, the $J = 0^+$ ground state is normal. The occupancy of the four major shells (in the order mentioned above) is 3.84, 5.78, 0.18 and 0.20. The first excited $0^+$ state at 0.585 MeV has occupancy 4, 4, 2 and 0. Clearly two nucleons have been excited from $0p$ to $1s − 0d$.

What is at first surprising is that, for this state, the occupancies are *precisely integers*. This is not an isolated example. It is also true at $t = 1.7$ for the second $2^+$ state at 4.33 MeV.

When we go to $t = 1.9$, we have passed the critical value, and things have settled down. The lowest $0^+$ and $2^+$ states are now the $2p − 2h$ states, both with the integer occupancies 4, 4, 2 and 0.

Whereas most states do not have integer occupancies, there are many which do. These are at higher energies. For example, for $t = 1.7$, there are other states with the occupancy 4, 4, 2, 0 at 21.64, 22.95, 22.97, 25.32 and 35.75 MeV. These are states with occupancy (3, 4, 1, 0) at 43.6 and 44.2 MeV. The latter correspond to lifting one nucleon through two major shells.
Why do we get such a simple behaviour for the $2p - 2h$ states? The answer involves a special feature of the $Q \cdot Q$ interaction: all matrix elements in which two particles in a major shell $N$ scatter into a major shell $N \pm 1$ vanish. This is due to a parity selection rule. For example, $\langle 0p 0p | Q \cdot Q | 0d 0d \rangle$ factors into $\langle 0p | Q | 0d \rangle \langle 0p | Q | 0d \rangle$, and each of these factors vanishes because of this parity rule.

Carrying the argument further, there can be no matrix element coupling the \((0s)^4 (0p)^4 (0d - 1s)^2\) configuration with other configurations such as \((0s)^4 (0p)^6\) or \((0s)^4 (0p)^5 (0f - 1p)\) etc...

Also, in our calculation we have limited the space to $2 \hbar \omega$ excitations. Once we create the state with occupancy \((4,4,2,0)\) our model space does not permit further excitations. This explains the integer occupancy. Presumably if we enlarged the space to include $4 \hbar \omega$ excitations we would no longer have the integer occupancies. It would also be of interest to study the $4p - 4h$ states.

This also explains why, as we increase $t$ towards 1.76, the descent of the new band is so simple. Since there is no mixing with the other configurations, the $2p - 2h \ J = 0^+$ and $2^+$ states can just slip down below the $(0p)^6$ states.

The rapid descent of the $2p - 2h$ states can be understood in terms of the Nilsson model. To form the $2p - 2h$ state, we take two nucleons from the $0p$ shell and put them in the Nilsson orbit \((Nm_3 \Lambda)\) with quantum numbers \((220)\). This orbit comes down rapidly in energy as the nuclear deformation is increased. The Nilsson one-body deformed Hamiltonian can be obtained from the $Q \cdot Q$ two-body interaction by replacing $Q \cdot Q$ by $Q \cdot \langle Q \rangle$ where $\langle Q \rangle$ is the quadrupole moment of the intrinsic state.

**IV. CLOSING REMARKS**

In this work, we have studied the properties of the interaction $-t \frac{10}{2} Q \cdot Q$ as a function of the coupling strength $t$ in an extended model space which includes all $2\hbar \omega$ excitations beyond the valence space. Using $^{10}Be$ as an example, we found that states that were
‘accidentally’ degenerate in the $0p$ valence space (e.g. $2_1^+$ and $2_2^+$ of orbital symmetry [42], or the $J = 0^+, 1^+, 2^+$ triplets of orbital symmetries [411] and [33]), are no longer degenerate in the extended space. This means that the $2\hbar\omega$ admixtures do more than renormalize the coupling strength of $Q \cdot Q$.

The extended model space allows for $2p - 2h$ admixtures and indeed, for sufficiently large $t$ ($t \geq 1.8$), the $J = 0^+$ and $2^+$ members of this new band become the new $0^+_1$ and $2^+_1$ states. We find that this band, unlike the ‘normal’ ground state band for $t < 1.7$, has integer occupancies 4, 4, 2 and 0 for $0s$, $0p$, $1s - 0d$ and $1f - 0p$ respectively. There is no mixing between the new $2p - 2h$ band and the $0p - 0h$ band. This is a special feature of the $Q \cdot Q$ interaction.

On a speculative level we may argue that, for the $2p - 2h$ band above, we should use a value of $t$ considerably larger than 1. We don’t have enough model space to renormalize the two-body interaction in this band. Just as the interaction between the $(0p)^6$ states gets renormalized by the configurations in which one nucleon is excited through 2 major shells, so the interaction for the $2p - 2h$ state would get renormalized by allowing at least one nucleon to be excited through 2 major shells. But this would be a $4\hbar\omega$ state which, for practical reasons, we don’t have in our model space.

We can use the $Q \cdot Q$ interaction to place these $2p - 2h$ bands at the correct energies, but we will need other components of the realistic nucleon-nucleon interaction in order to mix these bands with the $0p - 0h$ bands. For example, we could use the dipole-dipole or octupole-octupole parts of the nucleon-nucleon interaction. Alternatively one can work directly with realistic interactions.

There has been much progress in large-basis shell model calculations in light nuclei. For example, there is the work of W.C. Haxton and C. Johnson [8] where they actually get the superdeformed $4p - 4h$ state in $^{16}O$ at a reasonable energy, although perhaps not with the full quadrupole collectivity. There is also the work of Zheng et.al. [7] where up to $8\hbar\omega$ excitations have been included in calculations of nuclei ranging from $^4He$ to $^7Li$. Also, Zamick, Zheng and Fayache [8] required multi-shell admixtures to demonstrate the
'self-weakening mechanism' of the tensor interaction in nuclei.

Nevertheless, schematic interactions like $Q \cdot Q$ still play a primary role in describing nuclear collectivity throughout the periodic table. They are of special importance for highly deformed intruder states.

Surprisingly, there have been very few studies of schematic interactions in multi-shell spaces. In the Elliott $SU(3)$ model, momentum terms have been introduced to prevent $N = 2$ admixtures in the valence space. This has lead to great simplicities and beautiful results. There have been R.P.A. studies with $Q \cdot Q$ which involve $N = 2$ mixing. These studies give $E2$ effective charge renormalizations in the valence space and also the energies of the giant quadrupole resonances, but they will not give us the highly deformed states such as the $2p - 2h$ state that we have found here. We therefore feel that careful studies of the schematic interactions in multi-shell spaces are important, and we hope that others will agree.

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FIGURES

FIG. 1. The ratio $E(2^+)/t$ for the $2^+$ state with the strongest $B(E2)$ (solid line, usually the second $2^+$ state), and the same ratio for the lowest $2^+$ state (dash-dot line). For $t > 1.77$ all the strength goes into one state (solid line).

FIG. 2. The energies of the $0^+$ and $2^+$ members of a $2p - 2h$ band, which descend rapidly as $t$ is increased. This band becomes the ground state band beyond $t = 1.78$, and in this model space has integer occupancy (4,4,2,0).
TABLE I. Energies of States in $^{10}$Be in a Large Space Calculation and Transitions from the Ground State

| $E(J = 1^+ T = 1)$ (MeV) | $B(M1) \uparrow^a (\mu_N^2)$ |
|---------------------------|-------------------------------|
| 3.74                      | 0.0                           |
| 7.31                      | 0.0                           |
| 12.12                     | $0.071^b$                     |
| 13.90$^c$                 | 0.0                           |
| 22.10                     | 0.0                           |

| $E(J = 2^+ T = 1)$ (MeV) | $B(E2) \uparrow^d (e^2 fm^4)$ |
|---------------------------|-------------------------------|
| 2.19                      | 4.954                         |
| 3.40                      | 47.170                        |
| 3.74                      | 0.0                           |
| 7.31                      | 0.0                           |
| 9.16                      | 0.0                           |
| 10.92                     | 0.0                           |
| 11.92                     | 0.0                           |
| 12.12                     | 0.1321                        |
| 13.90                     | 0.0                           |

$^a$ Isovector $B(M1)$ from the ground state to excited $J = 1^+$ states.

$^b$ Sum of transitions to a four-fold degenerate state at 12.12 MeV.

$^c$ This state is three-fold degenerate.

$^d$ Physical $B(E2)$ transitions (with $e_p = 1.0$, $e_n = 0$) from the ground state to excited $J = 2^+$ states.
TABLE II. The $B(E2)$'s (in $e^2 fm^4$) and Static Quadrupole Moments $Q$ (in $efm^2$) of the $2^+_1$ and $2^+_2$ states in $^{10}_Be$ for selected values of $t$. 

| $t$  | $B(E2)_{0^+ \rightarrow 2^+_1}$ | $Q(2^+_1)$ | $B(E2)_{0^+ \rightarrow 2^+_2}$ | $Q(2^+_2)$ |
|------|-------------------------------|------------|-------------------------------|------------|
| 1.1  | 34.2                          | 10.77      | 128.4                         | -10.71     |
| 1.3  | 43.9                          | 11.90      | 172.4                         | -11.78     |
| 1.5  | 46.4                          | 12.12      | 186.6                         | -11.98     |
| 1.7  | 48.3                          | 12.25      | 194.4                         | -10.85     |
| 1.75 | 42.1                          | 12.25      | 23.2                          | -10.83     |
| 1.76 | 5.1                           | 12.21      | 120.2                         | -10.78     |
| 1.78 | 139.9                         | -10.84     | 0                             | 12.28      |
| 1.8  | 139.9                         | -10.84     | 0                             | 12.28      |
| 2.0  | 139.9                         | -10.85     | 0                             | 12.34      |
| $t$ | $J^\pi$ | $E$  | 0s  | 0p  | 1s – 0d | 0f – 1p |
|-----|---------|------|-----|-----|---------|---------|
| 1.0 | 0$^+$   | 0.000| 3.92| 5.90| 0.08    | 0.10    |
|     | 0$^+$   | 3.746| 3.92| 5.88| 0.09    | 0.11    |
|     | 2$^+$   | 2.187| 3.92| 5.89| 0.09    | 0.10    |
|     | 2$^+$   | 3.400| 3.93| 5.90| 0.08    | 0.09    |
|     | 2$^+$   | 3.745| 3.92| 5.88| 0.09    | 0.11    |
| 1.3 | 0$^+$   | 0.000| 3.88| 5.84| 0.13    | 0.15    |
|     | 0$^+$   | 4.775| 3.89| 5.82| 0.13    | 0.16    |
|     | 2$^+$   | 2.783| 3.88| 5.83| 0.13    | 0.16    |
|     | 2$^+$   | 4.518| 3.89| 5.84| 0.13    | 0.15    |
|     | 2$^+$   | 4.775| 3.89| 5.82| 0.13    | 0.16    |
| 1.5 | 0$^+$   | 0.000| 3.86| 5.81| 0.16    | 0.18    |
|     | 0$^+$   | 2.890| 4    | 4    | 2       | 0       |
|     | 2$^+$   | 3.174| 3.86| 5.80| 0.16    | 0.18    |
|     | 2$^+$   | 5.191| 3.86| 5.79| 0.16    | 0.19    |
|     | 2$^+$   | 5.447| 3.86| 5.79| 0.16    | 0.19    |
| 1.7 | 0$^+$   | 0.000| 3.84| 5.78| 0.18    | 0.20    |
|     | 0$^+$   | 0.585| 4    | 4    | 2       | 0       |
|     | 2$^+$   | 3.562| 3.84| 5.77| 0.18    | 0.21    |
|     | 2$^+$   | 4.333| 4    | 4    | 2       | 0       |
|     | 2$^+$   | 5.805| 3.84| 5.75| 0.19    | 0.22    |
| 1.9 | 0$^+$   | 0.000| 4    | 4    | 2       | 0       |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| $^1_0$ | 1.564 | 3.82 | 5.76 | 0.20 | 0.22 |
| $^{2^+}$ | 4.190 | 4 | 4 | 2 | 0 |
| $^{2^+}$ | 5.512 | 3.82 | 5.74 | 0.20 | 0.23 |
| $^{2^+}$ | 7.934 | 3.82 | 5.72 | 0.21 | 0.25 |
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