Occupation probabilities from quadrupole moments in the Sn region

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It is shown that a simple BCS model with a quadrupole-quadrupole interaction provides a consistent description of the measured quadrupole moments of a sequence of odd mass Sn and Cd isotopes and allows the extraction of the neutron single particle occupation probabilities.

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I. INTRODUCTION.

In a recent high accuracy experimental study of electric quadrupole and magnetic dipole moments of a sequence of odd-mass Cd isotopes \cite{1} it was noted that the electric quadrupole moments of the $\frac{11}{2}^-$ states in the Cd isotopes vary linearly with neutron number and are very simply and very well described in terms of a $h_{11/2}$ orbital sequentially occupied in the seniority scheme with a large neutron effective charge $e_n = 2.5$. If this is so, the same simple physics should be manifest in the other presumed single quasi-particle states in Cd and, a-fortiori, in the the Sn isotopes which have a closed proton shell. The idea that the single neutron occupation probabilities can be so simply extracted from electromagnetic properties is sufficiently attractive to warrant a more detailed second look. The aim of this paper is to show that this can be done using a minimalist theoretical framework. Ultimately of course, large scale theoretical calculations, shell model or beyond-mean-field model, are required to describe the structure of these nuclei, including their electromagnetic properties. The aim of this paper is much more modest, but the picture is nevertheless useful for its simplicity.

II. THE MODEL.

As theoretical framework, I use the spherical BCS model with a weak-coupling approximation to include quadrupole collectivity. In this model, \cite{2} the states in the odd-even isotopes with dominantly single quasi-particle parentage can be written as:

$$ | j, m \rangle = | (1\text{qp})jm \rangle + C_2 | j \otimes 2^+; jm \rangle $$

where

$$ | (1\text{qp})jm \rangle = \alpha_{n\ell jm}^\dagger | 0 \rangle $$

and

$$ | j \otimes 2^+; jm \rangle = \sum_{m',M'} (j, m', 2, M' | j, m) \alpha_{n\ell jm'}^\dagger | 2^+, M' \rangle $$

with the usual relation between the quasi-particle operators $\alpha^\dagger$ and the particle operators $a^\dagger$

$$ \alpha_{n\ell jm}^\dagger = u_{n\ell j} a_{n\ell jm}^\dagger - (-)^{j-m} v_{n\ell j} a_{n\ell j-m} $$

The BCS ground state is $| 0 \rangle$, and $| 2^+ \rangle$ represents the first (collective) $2^+$ state which can usually be interpreted as a coherent superposition of two quasi-particle states. The coefficient $C_2$ is given in first-order perturbation theory by

$$ C_2 = -\langle (1\text{qp})jm | \hat{V} | j \otimes 2^+; jm \rangle / (E_2 - E_0) $$

I take the interaction potential $\hat{V}$ to be a quadrupole-quadrupole force \cite{3}

$$ \hat{V} = -\frac{1}{2} \chi_{pp} \sum_{\mu} (-)^{\mu} q_{\mu}(p) q_{-\mu}(p) - \frac{1}{2} \chi_{nn} \sum_{\mu} (-)^{\mu} q_{\mu}(n) q_{-\mu}(n) - \chi_{pn} \sum_{\mu} (-)^{\mu} q_{\mu}(p) q_{-\mu}(n) $$
where p,n refer to protons and neutrons respectively and the one-body quadrupole operator is

\[
q_\mu = \sum_{n^{\ell}m} \left( \int \psi^*_n r^2 Y_{2,\mu}(\theta, \phi) \psi_n d^3r \right) \cdot a^\dagger_{n^{\ell}m} a_{n^{\ell}m}.
\]

For a neutron quasi-particle, the expression for \( C_2 \) then becomes

\[
C_2 = \frac{1}{E_2 - E_0} \frac{1}{\sqrt{5(2j + 1)}} (u_{n^{\ell}j}^2 - v_{n^{\ell}j}^2) \langle \psi_{n^{\ell}j} | r^2 Y_2 | \psi_{n^{\ell}j} \rangle (2^+ || \chi_{nn} q(n) + \chi_{pn} q(p) || 0)
\]

**III. THE QUADRUPOLE MOMENTS**

To first order in \( C_2 \), the electric quadrupole moment of the weak coupling state in equation\[1\] is

\[
Q_{chg}(j) = \langle j, j | e_n q_0(n) + e_p q_0(p) | j, j \rangle
\]

\[
= \sqrt{\frac{16\pi}{5}} (2, 0, j, j) \left[ (u_j^2 - v_j^2) \frac{1}{\sqrt{2j + 1}} (\psi_j || e_n r^2 Y_2 || \psi_j) + 2C_2 \frac{1}{\sqrt{5}} (2^+ || e_n q(n) + e_p q(p) || 0) \right]
\]

\[
= \sqrt{\frac{16\pi}{5}} (2, 0, j, j) (u_j^2 - v_j^2) \frac{1}{\sqrt{2j + 1}} (\psi_j || r^2 Y_2 || \psi_j)
\]

\[
e_n + \frac{2}{5} \frac{1}{E_2 - E_0} (2^+ || e_n q(n) + e_p q(p) || 0) (2^+ || \chi_{nn} q(n) + \chi_{pn} q(p) || 0)
\]

(10)

Here \( e_n \) and \( e_p \) are the neutron and proton effective charges. In shell model calculations, their values are roughly \( e_n \approx 0.5e \) and \( e_p \approx 1.5e \) \[4, 5\], attributed mainly to the giant quadrupole resonance that is not explicitly included in the usual shell model. There are different ways of estimating the strength of the effective quadrupole-quadrupole force, however \( |\chi_{nn}| \) is always substantially smaller than \( |\chi_{pn}| \). Since a ratio \( \chi_{nn}/\chi_{pn} \approx 0.3 \) is obtained from Hartree-Fock calculations with a Skyrme interaction \[6, 7\], I feel justified in making the approximation that

\[
\langle 2^+ || e_n q(n) + e_p q(p) || 0 \rangle \propto \langle 2^+ || \chi_{nn} q(n) + \chi_{pn} q(p) || 0 \rangle
\]

(11)

For a neutron quasi-particle state, the quadrupole moment can then be written as

\[
Q_{chg}(j) = \sqrt{\frac{16\pi}{5}} (2, 0, j, j) \frac{1}{\sqrt{2j + 1}} (\psi_j || r^2 Y_2 || \psi_j) (u_j^2 - v_j^2) \left( e_n + \frac{2}{E_2 - E_0} \left( \frac{\bar{\chi}}{e_n} \right) B(E2; 0^+ \rightarrow 2^+) \right)
\]

\[
= Q_{sm}(j) (u_j^2 - v_j^2) \left( e_n + \frac{2}{E_2 - E_0} \left( \frac{\bar{\chi}}{e_n} \right) B(E2; 0^+ \rightarrow 2^+) \right)
\]

(12)

\[
= Q_{sm}(j) (u_j^2 - v_j^2) e_{n,tot}
\]

(13)

where the last equation defines the total effective charge \( e_{n,tot} \) and the shell model quadrupole moment is

\[
Q_{sm} = -\frac{1}{2} \frac{(2j - 1) J_{n^{\ell}j}^{(2)}}{J_{n^{\ell}j}^{(2)}}
\]

\[
J_{n^{\ell}j}^{(2)} = \int_0^\infty | R_{n^{\ell}j} |^2 r^4 dr
\]

(14)

Note that the spectroscopic quadrupole moment normally reported in experiments is \( Q_s = Q_{chg}/e \). Provided that the parameter \( \bar{\chi} \) can be estimated, equ.\[12\] can be used to simply extract the neutron occupation probabilities from experimental data on quadrupole moments and E2 transition probabilities.

**IV. THE Sn AND Cn ISOTOPIES**

The spectroscopic quadrupole moments and \( B(E2) \) values for the Sn and Cd isotopes have been measured over a range of masses between the magic neutron numbers \( N = 50 \) and \( N = 82 \). Table 1 summarizes the experimental
excitation energy and \(B(E2 \uparrow)\) value of the 2+ states in the even-even isotopes and Table 2 lists the measured spectroscopic quadrupole moments of the of the odd-neutron isotopes. The radial integrals \(I_{nl}^{(2)}\) are calculated using the shell model potential of reference 8. The strength of the quadrupole-quadrupole interaction is taken to be constant \(\chi = 0.3 \times 10^{-5}\text{ MeV fm}^{-4}\). This is chosen to yield reasonable values of \(u^2 - v^2\) for the 11/2\(^-\) states in the lightest Sn and Cd isotopes where the 0h\(_{11/2}\) is expected to be mostly empty and near \(N = 81\) where it should be filled. The factor \(B(E2)/\langle E_2 - E_0 \rangle\) is taken to be the average of the experimental values in the even neutron isotopes above and below the odd neutron isotope being studied. When both are not available, then the nearest \(B(E2)\) value and the average energy denominator is used. The extracted occupation functions \(u^2 - v^2\) are given in Table 2 and shown in Figs.1 and 2. The uncertainty in \(u^2 - v^2\) is estimated from the uncertainties in the experimental \(B(E2)\) and \(Q_s\), and does not include the uncertainty in \(\chi\), nor the uncertainty in \(e_n\).

| Z | A | \(E(2^+)\) [MeV] | \(B(E2; 0^+ \rightarrow 2^+) [e^2 b^2]\) | Reference | \(E(2^+)\) [MeV] | \(B(E2; 0^+ \rightarrow 2^+) [e^2 b^2]\) | Reference |
|---|---|---|---|---|---|---|---|
| 48 | 98 | 1.395 | 50 | 100 | \(\approx 3\) | \|8|
| 48 | 100 | 1.004 | 50 | 102 | 1.472 | \|8|
| 48 | 102 | 0.777 | 0.281 (45) | 50 | 104 | 1.26 | 0.163 (26) | 50 | 108 | 1.207 | 0.209 (32) | \|11|
| 48 | 104 | 0.658 | 0.390 (14) | 50 | 106 | 1.206 | 0.224 (16) | \|11|
| 48 | 106 | 0.633 | 0.410 (20) | 50 | 108 | 1.212 | 0.226 (18) | \|11|
| 48 | 108 | 0.633 | 0.430 (20) | 50 | 110 | 1.212 | 0.226 (18) | \|11|
| 48 | 110 | 0.658 | 0.450 (20) | 50 | 112 | 1.257 | 0.242 (8) | \|11|
| 48 | 112 | 0.617 | 0.510 (20) | 50 | 114 | 1.3 | 0.232 (8) | \|11|
| 48 | 114 | 0.558 | 0.545 (20) | 50 | 116 | 1.294 | 0.209 (6) | \|11|
| 48 | 116 | 0.514 | 0.560 (20) | 50 | 118 | 1.23 | 0.209 (8) | \|11|
| 48 | 118 | 0.488 | 0.568 (44) | 50 | 120 | 1.171 | 0.202 (4) | \|11|
| 48 | 120 | 0.506 | 0.48 (6) | 50 | 122 | 1.141 | 0.192 (4) | \|11|
| 48 | 122 | 0.569 | 0.41 (3) | 50 | 124 | 1.132 | 0.162 (6) | \|14|
| 48 | 124 | 0.613 | 0.35 (4) | 50 | 126 | 1.141 | 0.127 (8) | \|14|
| 48 | 126 | 0.652 | 0.22 (2) | 50 | 128 | 1.169 | 0.080 (5) | \|14|
| 48 | 128 | 0.645 | 0.16 (2) | 50 | 130 | 1.221 | 0.023 (5) | \|11|
| 48 | 130 | 1.325 | 50 | 132 | 4.041 | 0.11 (3) | \|16,17|

TABLE I. Experimental \(B(E2; 0^+ \rightarrow 2^+)\) of a sequence of Cd and Sn isotopes.

The extracted occupation probabilities are consistent with expectations with the exception of \(^{129}\text{Sn}\). Since the \(h_{11/2}\) orbital cannot be less than half filled in \(^{128}\text{Sn}\), the measured negative quadrupole moment of the 11/2\(^-\) level, even with a very large error bar, would imply a major change in structure compared to the other Sn isotopes but there is no other evidence for this happening. Leaving out \(^{128}\text{Sn}\), the total effective charge \(e_{n,tot}/e\) of the \(h_{11/2}\) quasiparticle states in the Sn isotopes, varies relatively weakly, ranging from 1.2 to 2.0, and the occupation probabilities are therefore a roughly linear function of the neutron number \(N\). This is very similar to the model advocated by Yordanov et al. 1. However, the Cd isotopes are more collective as evidenced by the lower energy and larger \(B(E2)\) of the 2+ states and consequently the \(h_{11/2}\) total effective charge \(e_{n,tot}/e\) is much larger and more variable, ranging from 2.5 to 9.5 near mid-shell. The occupation probabilities have a more complicated \(N\) dependence than assumed by Yordanov et al. 1 despite the remarkably linear \(N\) dependence of the quadrupole moments.

It is interesting that the data for the \(d_{5/2}\) quasiparticle state in the Cd isotopes clearly shows that this orbital fills more rapidly than the \(g_{7/2}\) orbital. The Sn data are consistent with this.

It is a limitation of laser spectroscopy that it can provide information only on the properties of the ground state and isomeric states. But a great strength is that it can do so with a consistent methodology for long chains of isotopes. Since occupation probabilities are monotonic though non-linear functions of \(N\) in pretty much all models, the data on each isotope propagates information along the whole chain. For example, in the Cd isotopes the occupation probability of the \(d_{5/2}\) orbital is close to 0.9 by \(N=63\) and this value will only increase with increasing \(N\); similarly, the occupation probability of the \(d_{3/2}\) orbital is down to 0.3 by \(N = 73\) and will only decrease with decreasing \(N\).

Since the coefficients \(|C_2|^2\) turn out to be small (always less than 0.03 for the Sn isotopes and less than 0.15 for the Cd isotopes and much less when \(|u^2 - v^2|\) is small), the weak coupling approximation is reasonable in the present case. However, calculating the quadrupole moments to first order in \(C_2\) also assumes that the quadrupole moment of the collective 2+ state in the even isotopes is not too large. Fortunately, this is so. Where experimental data are
available, $Q(2+)$ ranges from -0.28 b to -0.45 b in Cd and is substantially smaller in Sn. The resulting correction to the first order calculation would be less than 6% in the Cd isotopes and less than 2% in the Sn isotopes.

The value of $\bar{\chi}$ has a significant uncertainty but it doesn’t affect the shape of the curves in Figs.1 and 2 though it controls the scale of the vertical axis. The fact that a constant value works well for both isotope chains provides evidence for the validity of the approximation that $\chi_{nn}/\chi_{pn} \approx 1/3$ since the 2+ state is expected to be mainly a two neutron quasi-particle state in Sn but a mixed proton and neutron two quasi-particle state in Cd. However, the noticeable discontinuity at $^{120}$Cd just below the $N = 82$ neutron shell closure may indicate the limitation of the approximation. It may also be noted that the self-consistent estimate \cite{3, 7, 20} of the quadrupole interaction strengths

| $Z$ | $A$ | $E^*$ | $J^+$ | $nl\ell_j$ | $I_\alpha^{(2)}$ | $Q_\alpha^{(2)}$ | $(u^2 - v^2)$ | Reference(expt) |
|----|----|------|------|-------|------|-------|-------|----------------|
| 48 | 103 | 0     | 5/2+ | 1d$_{5/2}$ | 24.112 | -0.8(7) | 1.30(114) | [18] |
| 48 | 105 | 0     | 5/2+ | 1d$_{5/2}$ | 24.365 | 0.43(4) | -0.54(5) | [18] |
| 48 | 107 | 0     | 5/2+ | 1d$_{5/2}$ | 24.614 | 0.601(3) | -0.71(3) | [1] |
| 48 | 107 | 0.846 | 11/2 | 0h$_{11/2}$ | 28.143 | -0.94(10) | 0.72(8) | [18] |
| 48 | 109 | 0     | 5/2+ | 1d$_{5/2}$ | 24.864 | 0.604(1) | -0.69(3) | [1] |
| 48 | 109 | 0.464 | 11/2 | 0h$_{11/2}$ | 28.454 | -0.92(9) | 0.68(7) | [18] |
| 48 | 111 | 0.245 | 5/2+ | 1d$_{5/2}$ | 25.107 | 0.77(12) | -0.79(13) | [18] |
| 48 | 111 | 0.396 | 11/2 | 0h$_{11/2}$ | 28.771 | -0.747(4) | 0.50(2) | [1] |
| 48 | 113 | 0.264 | 11/2 | 0h$_{11/2}$ | 29.076 | -0.612(3) | 0.34(1) | [1] |
| 48 | 115 | 0.181 | 11/2 | 0h$_{11/2}$ | 29.387 | -0.476(5) | 0.23(1) | [1] |
| 48 | 117 | 0.136 | 11/2 | 0h$_{11/2}$ | 29.687 | -0.320(6) | 0.14(1) | [1] |
| 48 | 119 | 0.147 | 11/2 | 0h$_{11/2}$ | 29.988 | -0.135(3) | 0.06(1) | [1] |
| 48 | 121 | 0     | 3/2+ | 1d$_{3/2}$ | 27.671 | -0.274(7) | 0.33(3) | [1] |
| 48 | 121 | 0.215 | 11/2 | 0h$_{11/2}$ | 30.285 | 0.009(6) | -0.005(3) | [1] |
| 48 | 123 | 0     | 3/2+ | 1d$_{3/2}$ | 27.889 | 0.042(5) | -0.06(1) | [1] |
| 48 | 125 | 0     | 11/2 | 0h$_{11/2}$ | 30.587 | 0.135(4) | -0.10(4) | [1] |
| 48 | 128 | 0     | 3/2+ | 1d$_{3/2}$ | 28.902 | 0.209(4) | -0.43(4) | [1] |
| 48 | 125 | 0+ x | 11/2 | 0h$_{11/2}$ | 30.876 | 0.269(7) | -0.26(3) | [1] |
| 48 | 127 | 0     | 3/2+ | 1d$_{3/2}$ | 28.314 | 0.239(5) | -0.72(6) | [1] |
| 48 | 127 | 0+ x | 11/2 | 0h$_{11/2}$ | 31.170 | 0.342(10) | -0.49(4) | [1] |
| 48 | 129 | 0     | 3/2+ | 1d$_{3/2}$ | 28.970 | 0.132(7) | -0.56(6) | [1] |
| 48 | 129 | 0+ x | 11/2 | 0h$_{11/2}$ | 31.455 | 0.570(13) | -1.16(11) | [1] |
| 50 | 109 | 0     | 5/2+ | 1d$_{5/2}$ | 24.358 | 0.31(10) | -1.09(30) | [18] |
| 50 | 111 | 0     | 7/2+ | 0g$_{7/2}$ | 24.826 | 0.18(9) | -0.52(26) | [18] |
| 50 | 113 | 0.738 | 11/2 | 0h$_{11/2}$ | 28.754 | -0.41(4) | 0.91(9) | [18] |
| 50 | 115 | 0.613 | 7/2+ | 0g$_{7/2}$ | 25.357 | 0.26(3) | -0.80(9) | [18] |
| 50 | 115 | 0.714 | 11/2 | 0h$_{11/2}$ | 29.061 | -0.38(6) | 0.89(14) | [18] |
| 50 | 117 | 0.315 | 11/2 | 0h$_{11/2}$ | 29.365 | -0.42(5) | 0.99(12) | [18] |
| 50 | 119 | 0.024 | 3/2+ | 1d$_{3/2}$ | 26.833 | -0.112(7) | 0.54(4) | [18] |
| 50 | 119 | 0.09 | 11/2 | 0h$_{11/2}$ | 29.662 | -0.21(2) | 0.48(5) | [18] |
| 50 | 121 | 0     | 3/2+ | 1d$_{3/2}$ | 27.058 | -0.02(2) | 0.10(10) | [18] |
| 50 | 121 | 0.006 | 11/2 | 0h$_{11/2}$ | 29.967 | -0.14(3) | 0.32(7) | [18] |
| 50 | 123 | 0     | 11/2 | 0h$_{11/2}$ | 30.257 | 0.03(4) | -0.07(10) | [18] |
| 50 | 125 | 0     | 11/2 | 0h$_{11/2}$ | 30.555 | 0.14(21) | -0.38(57) | [19] |
| 50 | 127 | 0     | 11/2 | 0h$_{11/2}$ | 30.848 | 0.30(13) | -1.01(44) | [19] |
| 50 | 129 | 0.035 | 11/2 | 0h$_{11/2}$ | 31.136 | -0.18(17) | 0.87(82) | [19] |
| 50 | 131 | 0+ x | 11/2 | 0h$_{11/2}$ | 31.423 | 0.02(20) | -0.12(120) | [19] |

TABLE II. Experimental quadrupole moments, and deduced occupation functions $(u^2 - v^2)$ of a sequence of Cd and Sn isotopes for $\bar{\chi} = 0.3 \times 10^{-3}MeV - fm^{-4}$. For $^{113}$Sn(11/2−), $^{115}$Sn(7/2+), $^{115}$Sn(11/2−), $^{113}$Sn(11/2−) the signs shown in the table are based on systematics since only $|Q_\alpha|$ is known.
FIG. 1. (Color online) Occupation function \((u^2 - v^2)\) for the Cd isotopes for \(\bar{\chi} = 0.3 \times 10^{-3}\).

gives \(\chi_{nn} = 79A^{-7/3}\) and \(\chi_{pn} = 387A^{-7/3}\). Our value is smaller than the self consistent \(\chi_{nn}\) by a factor of roughly four, but this is perhaps not surprising since it multiplies an experimental \(B(E2)\) in equ. [12] which can include various renormalization effects.

V. CONCLUSIONS

I have shown that the measured electric quadrupole moments of a long chain of odd Cd and Sn isotopes can be simply understood in terms of a weak coupling model. In the model, the quadrupole moments are proportional to the occupation probability of the relevant orbitals which can therefore be extracted from the data. The formula for the quadrupole moment requires the empirical determination one strength parameter (which is held constant for the two isotope chains), but otherwise it involves experimental data and standard values for parameters such as effective charges.

The deduced occupation probabilities agree with expectations except for \(^{129}\)Sn. It would be interesting to repeat the experiments on the heavy Sn isotopes near the doubly closed shell \(^{132}\)Sn in order to decrease the large error bars for \(Q_s(h_{11/2})\) and to measure \(Q_s(d_{3/2})\).

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FIG. 2. (Color online) Occupation function \((u^2 - v^2)\) for the Sn isotopes for \(\chi = 0.3 \times 10^{-3}\).
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