The First-Order E2 Core Polarization Charge of $^{41}$Ca in Woods-Saxon Shell Model

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The core polarization charge of the E2 transition from the first excited $3/2^-$ state to the $7/2^-$ ground state of $^{41}$Ca is calculated in the first-order perturbation theory by using the wave functions of a Woods-Saxon potential and compared with the results of harmonic oscillator potential. The contributions from the particle-hole excitations to continuum particle states, which constitute the major part of the excitations, are calculated explicitly. The resultant first-order core polarization charge in the Woods-Saxon shell model with a $δ$-function type effective interaction $0.233e$ is smaller than the one of the harmonic oscillator shell model $0.311e$. The effects of the continuum states are discussed in comparison with the harmonic oscillator shell model.

§ 1. Introduction

A realistic shell model potential of a nucleus has finite number of bound states and continuum states. However the harmonic oscillator (HO) potential which is employed usually in nuclear structure studies has bound states only. It is very interesting to study the effects of this special feature of a realistic shell model potential on the explanation of the various properties of nuclei. The main purposes of this paper are detailed investigation of the effects of the continuum states on the first-order core polarization charge of the E2 transition from the first excited $3/2^-$ state to the $7/2^-$ ground state of $^{41}$Ca in a Woods-Saxon (WS) shell model, as a simple example of the realistic shell model. The results are compared with those of the HO shell model calculation.

The E2 effective charge of $^{41}$Ca has been extensively investigated and these works revealed importance of the core polarization effect. We can refer to the paper of Brown et al. for the detailed discussion on the effective charge.

The first-order core polarization charge of a neutron in the above stated E2 transition of $^{41}$Ca is determined by the seventeen one particle-one hole excitations of protons in HO shell model calculation. In a WS shell model, among the particle states of these excitations all states except for the $1f_{7/2}$ state are continuum states and $f_{7/2}$ continuum state is also a possible candidate for the particle state in addition to the bound $1f_{7/2}$ state. Moreover a proton in $1s_{1/2}$ hole state can be excited to $d_{5/2}$ and $d_{3/2}$ continuum particle states.

The radial part of the single-particle wave function of a WS potential depends on $j$ and the charge state $τ$ as well as $n$ and $l$ in contrast with the case of HO
potential. This makes the calculation of the core polarization charge very complicated, together with the state dependence of the energy denominator in perturbation calculation. In § 2 a WS potential of \(^{41}\)Ca is introduced and some discussions on the method of solution of the eigenstates are given. The formulas of the first-order E2 core polarization charge of \(^{41}\)Ca are derived in § 3.1 and the results of the numerical calculations are discussed in comparison with the ones in a HO shell model in § 3.2. A short comment on the method of numerical integral over the energy of continuum state is also given in this section. Brief conclusions are given in § 4.

§ 2. Woods-Saxon potential of \(^{41}\)Ca and its eigenstates

We use the following WS potential:

\[
V(r) = -V_1 f_1(r) + \left(1/2\right) \left[ j(j+1) - l(l+1) - 3/4 \right] \\
\times \left( V_2 r^2 / r \right) \frac{df_1(r)}{dr} + \left( (1 + \tau_3) / 2 \right) V_C(r),
\]

where \(V_C(r)\) is a Coulomb potential of a uniformly charged sphere of radius \(R_0\) that is

\[
V_C(r) = \begin{cases} 
\left( (Z - 1) e^2 / (2R_0) \right) (3 - (r/R_0)^2), & (r \leq R_0) \\
(Z - 1) e^2 / r, & (r > R_0)
\end{cases}
\]

and \(\tau_3 = 1\) for proton and \(\tau_3 = -1\) for neutron. In these expressions

\[
f_i(r) = 1 / \left[ 1 + \exp \left( (r - R_i) / a_i \right) \right], \\
V_i = V_{i0} + V_{i1} (N - Z) / (N + Z),
\]

\(R_i = r_i A^{1/3}\).

Bohr and Mottelson’s values of the parameters of the WS potential are used:

\[
V_{i0} = 51, \quad V_{i1} = -33, \quad V_{i2} = 22, \quad V_{i3} = -14, \quad (\text{MeV})
\]

\[
a_i = 0.67, \quad r_i = 1.27. \quad (\text{fm})
\]

The factor \(1/r\) of the spin-orbit part of \(V(r)\) becomes singular for \(r \to 0\) in the states with \(l \neq 0\). This singularity is managed following Blomqvist and Wahlborn.

The radial equation is solved in three regions: (I) \(0 \leq r \leq b\), (II) \(b \leq r \leq r_z\) and (III) \(r_z \leq r\). In the region (I), \(V(r)\) is fixed as \(V(b)\) and \(b = 0.3 \text{ fm}^{\circ}\) and in the region (III), \(V(r)\) is approximated to \(V(r) \approx (1 + \tau_3) / 2 V_C(r)\) and \(r_z\) is determined so as to be |\(V(r) - (1 + \tau_3) / 2 V_C(r)\)| < \(10^{-8}\) MeV, and the phase shift \(\delta_U(\varepsilon)\) to be \(r_z\)-independent. The equation in the region (II) is solved numerically. Milne’s progressor and corrector method of numerical integration is used and the starting values are determined by four starter formulas. The phase of the wave
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The single-particle levels of $^4\text{Ca}$ of WS potential with Bohr and Mottelson's parameters and the empirical ones of $^4\text{Ca}$. The proton resonance energies are shown by the dotted lines.

Fig. 1. The single-particle levels of $^4\text{Ca}$ of WS potential with Bohr and Mottelson's parameters and the empirical ones of $^4\text{Ca}$. The proton resonance energies are shown by the dotted lines.

Fig. 2. The theoretical cross sections of the proton single-particle channels in $^4\text{Ca}$. All resonant channels and a non-resonant one are indicated.

function is defined so as to be positive near the origin. The eigenvalues and the phase shifts are determined through the conditions of continuity at the outermost loop in this region and the first-order derivative is calculated by using seven point formula. The standing wave solution is orthonormalized to $\delta$-function in energy:

$$\int dr R^*_{\nu j}(r) R_{\nu j}(r) = \delta(\varepsilon - \varepsilon').$$  \hspace{1cm} (4)

The calculated single-particle energies of $^4\text{Ca}$ are compared with the empirical ones in Fig. 1. The calculated r.m.s. charge radius of $^4\text{Ca}$ is 3.39 fm in compared with the empirical one 3.46 fm. According to our calculation, the proton states have resonances in $p_{3/2}$, $p_{1/2}$, $f_{5/2}$, $g_{9/2}$ and $g_{7/2}$ partial waves and these resonance energies are also indicated in Fig. 1. As an illustration of the energy dependences of phase shift for these partial waves, the theoretical cross sections of single-particle channels are shown in Fig. 2. In this figure, it can be seen that the $g_{7/2}$ resonance is very broad in comparison with the other resonances and this broadness comes from the fact that the resonance energy is much higher than the barrier height of an effective potential.
On the other hand, the $p_{3/2}$ state has an extremely sharp and strong resonance at the energy which is much lower than the effective potential barrier in the nuclear surface region, so that the wave function around the resonance energy behaves as if it were a bound state. These properties of the continuum states have important effects on the core polarization charge.

§ 3. The first-order E2 core polarization charge of $^{41}$Ca

3.1. Formulas

The particle-hole excitations of proton which contribute to the first-order core polarization charge of the E2 transition from the excited 3/2$^{-}$ state to the 7/2$^{-}$ ground state of $^{41}$Ca are shown in Fig. 3. The first-order core polarization charge of a valence neutron of the E2 transition can be expressed as a sum of the contribution of each proton excitation from a hole state $H$ to a particle state $P$:

$$\delta e_{n}^{WS}(E2; 2p_{3/2}(n) \rightarrow 1f_{7/2}(n)) = \sum_{H \rightarrow P} \delta e_{n}^{WS}(H \rightarrow P).$$  \hfill (6)

The $\delta e_{n}^{WS}(H \rightarrow P)$ can be written as

$$\begin{align*}
\delta e_{n}^{WS}(H \rightarrow P) &= \left\{ \begin{array}{ll}
\frac{eV}{4\pi \langle 2p_{3/2}(n) | r^2 | 1f_{7/2}(n) \rangle} & A I_{1}(n_{P}) I_{1}(n_{P}) \left[ \frac{1 + \alpha C}{\varepsilon_{P} - \varepsilon_{H} - 3.648} + \frac{1 - \alpha C}{\varepsilon_{P} - \varepsilon_{H} + 3.648} \right] \quad \text{(P for bound state)}, \\
\frac{eV}{4\pi \langle 2p_{3/2}(n) | r^2 | 1f_{7/2}(n) \rangle} & A \int d\varepsilon I_{1}(\varepsilon) I_{2}(\varepsilon) \left[ \frac{1 + \alpha C}{\varepsilon - \varepsilon_{H} - 3.648} + \frac{1 - \alpha C}{\varepsilon - \varepsilon_{H} + 3.648} \right] \quad \text{(P for continuum state)},
\end{array} \right.
\end{align*}$$  \hfill (7.1)

where the charge independent $\delta$-function type effective interaction$^{16}$ is used in order to compare with the result of HO calculation, and

$$V = 500 \text{ MeV} \cdot \text{fm}^3 \quad \text{and} \quad \alpha = 0.12.$$  \hfill (7.2)

The kinematical factor $A$ is given by

$$A = (2j_{H} + 1) (20j_{P} 1/2 | j_{P} 1/2)^{2},$$  \hfill (8)

and another kinematical factor $C$ comes from the $\sigma_{1} \cdot \sigma_{2}$ term in the effective interaction and cannot be expressed in a simple closed form. In Eqs. (7)

$$I_{1}(\varepsilon (or \ n_{P})) = \int_{0}^{\infty} dr \ r^{2} R_{\varepsilon(\sigma_{1} \cdot \sigma_{2})}^{**}(r) R_{n_{P} n_{P}^{*}}^{**}(r)$$  \hfill (9)
is an integral related to the E2 transition matrix element and

\[ I_s(\varepsilon_p \text{ or } n_p) \]

\[ = \int_0^{\infty} dr \frac{1}{r} R_p^{s_{1/2} \rightarrow n_p} (r) R_{n_p}^{s_{1/2} \rightarrow n} (r) R_{n}^{s_{1/2} \rightarrow n} (r) \]

is an integral related to the matrix element of the effective interaction. The superscripts \( n \) and \( p \) mean neutron and proton respectively, and \( \varepsilon \) is the energy of the continuum state.

In HO calculation, the approximations

\[ \varepsilon_p^{} \pm \varepsilon_H^{} = (\varepsilon_{2s_{1/2}}^{} \pm \varepsilon_{2p_{1/2}}^{}) = 2\hbar \omega \]

are used usually, and therefore Eqs. (7) can be simplified further as

\[ \delta e^{\text{HO}}_{\text{HO}} (H \rightarrow P) = \frac{eV}{4\pi^2 \rho |r|^2} I_1^{\text{HO}} (n_p) I_2^{\text{HO}} (n_p) \]

where the superscript HO means that the quantities are calculated by the HO radial wave function \( R_{\text{HO}} (r) \).

3.2. Calculations and Discussion

In HO calculation, the particle-hole excitations contributing to the first-order E2 core polarization charge are restricted to \( 2\hbar \omega \) excitations and this excitation energy is \( \sim 21 \) MeV in \(^{40}\text{Ca}\). On the other hand, in WS calculation the calculated single-particle energies are used and the energies of continuum states extend from zero to infinity.

The contributions from the excitations to the continuum states are determined through the \( \varepsilon \)-dependence of the product \( I_s(\varepsilon) I_s(\varepsilon) \) in Eq. (7·2), and the depend-
Fig. 4. Some examples of the energy dependences of the product $I_1(\epsilon)I_2(\epsilon)$ for the particle-hole excitations to resonant continuum states.

1 $1p1/2(p) \rightarrow p3/2(p) \times 1/10000$
2 $1p3/2(p) \rightarrow p1/2(p)$
3 $1p1/2(p) \rightarrow f5/2(p)$
4 $1d5/2(p) \rightarrow g9/2(p) \times 1/2$
5 $1d5/2(p) \rightarrow g7/2(p)$

Fig. 5. Some examples of the energy dependences of the product $I_1(\epsilon)I_2(\epsilon)$ for the particle-hole excitations to non-resonant continuum states. The scale of ordinate in this figure is ten times as small as that of Fig. 4.
ence tends to concentrate on a certain energy region peculiar to each excitation as can be seen in Figs. 4 and 5. This tendency is due to the fact that both of the centrifugal and Coulomb barrier prevent a wave function from penetrating inside of nucleus at low energy and the rapid oscillations of continuum wave function give rise to cancellation at higher energy. If there is a single-particle resonance, the concentration around the resonance energy becomes remarkably sharp except for $q_{12}$ state and the maximum value is an order of magnitude larger than that of the non-resonant case.

In the calculation of $\delta e_e^{\text{ws}}(H\rightarrow P)$ of the excitation to continuum state, the energy integrals are approximated by the integration up to the energy where the absolute value of the product $I_1(\varepsilon) I_2(\varepsilon)$ becomes less than 0.0001. Then the upper bounds of the integrals vary from about 30 to about 100 MeV depending on the excitation. In order to save computer time but to keep accuracy of calculations, the mesh intervals of the integral are determined through two steps in general. In the first step, $I_1(\varepsilon)$ and $I_2(\varepsilon)$ are calculated by using the numerically solved wave functions at some base points. These base points are settled in the intervals of $0.05\sim0.1$ MeV for resonance region and of $0.1\sim5$ MeV for remaining non-resonance region depending on the $\varepsilon$-dependences of $I_1(\varepsilon)$ and $I_2(\varepsilon)$. In the second step, the values of the product between two neighbouring base points are interpolated according to Lagrange’s five point formula and the final mesh intervals are $0.05$ MeV for resonance region and $0.1$ MeV for no resonance one. In the transitions to the $p_{3/2}$ particle state, special attention is paid for the determination of the energy intervals in these two steps around the resonance energy, because of the very sharp and strong resonance, and much smaller values are used. The energy integrals are performed by using Newton-Cotes’ ten point formula to each ten interval of the final mesh points.

The contributions of each particle-hole excitation in WS and HO shell model and the values of the kinematical factors $A$ and $C$ are listed in Table I. The contributions of the excitations from $1s_{1/2}$ are negligibly small. This can be explained as follows. The WS wave function of $1s_{1/2}$ is approximated very well by the $1s$ HO wave function, so that the $1s_{1/2}$ WS wave function multiplied by $r^2$ of E2 operator is the $1d$ HO wave function in very good approximation and then can be approximated by the $1d_{5/2}$ and/or $1d_{3/2}$ WS function. Therefore the matrix elements for the E2 transitions from $1s_{1/2}$ hole state to $d_{5/2}$ and $d_{3/2}$ continuum particle state can be approximated by the overlap integrals of the bound $1d_{5/2}$ and $1d_{3/2}$ state and the continuum $d_{5/2}$ and $d_{3/2}$ state, and become very small because of the orthogonality.

The contribution of the excitation to the bound particle state $1f_{7/2}$ is 0.0231e and is about 1.23 times the corresponding HO value. This 23% excess is caused by the exponential tail of the bound state wave function and the small calculated energy denominator. The contribution of the excitation to the $f_{7/2}$ continuum particle state is only 0.0006e.
Table 1. Comparison of the contributions of each particle-hole excitation calculated in WS shell model and the ones in HO shell model. The particle state attached an asterisk has a resonance in continuum. Ratio (\%) = 100 \times \Delta e_n^{WS}(H \rightarrow P)/\Delta e_n^{HO}(H \rightarrow P).

<table>
<thead>
<tr>
<th>Hole</th>
<th>Particle</th>
<th>A</th>
<th>C</th>
<th>\Delta e_n^{WS}(H \rightarrow P)</th>
<th>\Delta e_n^{HO}(H \rightarrow P)</th>
<th>Ratio (%)</th>
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<td>1s_{1/2}</td>
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<td>-2/3</td>
<td>0.0006</td>
<td>-</td>
<td>-</td>
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<tr>
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<td>d_{3/2}</td>
<td>4/5</td>
<td>1</td>
<td>0.0009</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>1p_{1/2}</td>
<td>f_{1/2}</td>
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<td>-2/3</td>
<td>0.0150</td>
<td>0.0167</td>
<td>97.4</td>
</tr>
<tr>
<td>1p_{1/2}</td>
<td>f_{3/2}</td>
<td>72/35</td>
<td>-2/3</td>
<td>0.0066</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>1p_{1/2}</td>
<td>g_{1/2}</td>
<td>4/5</td>
<td>1</td>
<td>0.0139</td>
<td>0.0154</td>
<td>90.3</td>
</tr>
<tr>
<td>1p_{1/2}</td>
<td>g_{3/2}</td>
<td>4/5</td>
<td>1</td>
<td>0.0152</td>
<td>0.0154</td>
<td>98.7</td>
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<tr>
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<td>2/3</td>
<td>0.0068</td>
<td>0.0190</td>
<td>62.4</td>
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<td>7/3</td>
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<td>0.0069</td>
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<td>2/3</td>
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<td>0.289</td>
<td>0.3107</td>
<td>91.1</td>
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Among the contributions of the excitations to resonant continuum particle states, the largest one is the 1d_{5/2} \rightarrow g_{5/2} excitation and is 1.06 times the corresponding HO value. This is due to the fact that the g_{5/2} resonance is very strong. On the other hand, the contribution of the 1d_{3/2} \rightarrow g_{3/2} excitation is small compared with that of the 1d_{5/2} \rightarrow g_{5/2} excitation because of the small kinematical factor A and of the broad and weak g_{3/2} resonance. The amplitude of the radial wave function of the g_{3/2} continuum state around the resonance energy is not so large, so that the energy integral of the product \langle f(s) \rangle_{L}^{2} divided by the energy denominator becomes small in general. This makes the excitation to the g_{3/2} continuum state disadvantageous. The reduction of the contribution of the 1d_{5/2} \rightarrow g_{5/2} excitation is also due to the same reason, in spite of the large kinematical factor A. The excitations to the p_{1/2}, p_{3/2} and f_{5/2} continuum state have similar but slightly smaller contributions than the corresponding HO values.

The contributions of the excitations to non-resonant continuum particle states are small in general, except for the diagonal transitions 1d_{5/2} \rightarrow d_{5/2} and 1d_{5/2} \rightarrow d_{3/2}. The
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product \(I_1(\varepsilon)I_2(\varepsilon)\) is small usually in this type of excitations. The \(\varepsilon\)-dependence of the product is mainly due to \(I_1(\varepsilon)\) and is determined by the delicate overlapping relations between the wave functions of bound states and those of continuum states.

The wave function of non-resonant continuum state following bound state has the first node in the neighbourhood of the point where the inner repulsive \(V_{\text{eff}}(r)\) is equal to the energy of the continuum state. The contribution to the matrix element of \(r^4\) from the inner region of this node is very small because of the very small amplitudes of the wave functions and the smallness of \(r^4\) itself, and the value of the matrix element is determined mainly by the integral in the outer region. It becomes, however, small in general due to the oscillation of the continuum wave function in the spread of the hole state one. On the other hand, the wave function of the corresponding particle state of HO potential is bound state and makes no cancellation resulting from such kind of oscillation. Thus the matrix element has a large value.

The noticeable result on the non-resonant excitations is the fact that the contributions of the excitations from \(d\)-hole states to \(d\)-continuum particle states are nearly equal to the ones of HO calculations. Among these excitations, the diagonal transitions \(1d_{5/2}\rightarrow d_{5/2}\) and \(1d_{3/2}\rightarrow d_{3/2}\) constitute the parts of the main contributions to the WS value of the core polarization charge. This is due to the fact that the second nodes of these \(d\)-state wave functions are pushed outside by the centrifugal force so that the cancellation is not so remarkable as the other cases of the non-resonant states.

The resultant first-order E2 core polarization charge of \(^{41}\text{Ca}\) in WS shell model is 0.283\(e\) and is 91\% of the HO value 0.311\(e\). In this WS value, the contributions of the excitations from \(1s_{1/2}\) hole state, those to \(1f_{7/2}\) bound and \(f_{7/2}\) continuum particle state, those to resonant continuum particle states and those to non-resonant continuum particle states are 0.5\%, 8.4\%, 69.2\% and 21.9\% respectively and therefore the excitations to the resonant states constitute the main part of the WS value and the contributions of the special excitations in WS shell model which do not occur in HO shell model are very small. The contributions of the corresponding excitations in HO shell model calculations are 0\%, 6.0\%, 69.0\% and 25.0\% of the total HO value respectively.

\section*{§ 4. Conclusions}

A few results of calculations of the first-order core polarization charge for the \(3/2^-\rightarrow 7/2^-\) E2 transition of \(^{41}\text{Ca}\) are listed in the following:

- Siegel-Zamick \(^{3}\) $\delta e_s = 0.415e$, $\hbar\omega = 10.0$ (MeV) KK-interaction
- Kuo-Osnes \(^{6}\) 0.381\(e\) 10.5 KB-interaction
- Brown et al. \(^{1}\) 0.307\(e\) 10.73 $\delta$-function int.
- ours 0.283\(e\) WS pot. (B-M) $\delta$-function int.
The result of Ref. 1) only can be compared directly with ours among these results. Our WS value is 92.2% of the HO value of Ref. 1). According to our calculations, we can point out two important features of the continuum shell model as conclusions. One of them is the general reduction of the matrix elements compared to the corresponding ones of HO shell model as is seen in Table I but for some exceptions. The reason of this reduction is, as stated in the last part of § 3.2, essentially due to the extra cancellations introduced by the continuum states wave functions, which have more nodes than the HO ones in the spread of the hole states wave functions. Especially excitations to non-resonant continuum states like $1d_{3/2} \rightarrow s_{1/2}$, $2s_{1/2} \rightarrow d_{3/2}$ and so on are reduced considerably, but these large reductions affect little on the final result because of their minor role played in the E2 core-polarization charge.

Another feature of the continuum shell model is the existence of the resonances in some particular partial waves. They enhance the matrix elements up to nearly the corresponding HO values in spite of the extra cancellations stated above, and the major part of the E2 core-polarization charge is determined by an excitation to the bound particle state and some ones to the resonant particle states, as can be seen in Table I. However this situation obscures the difference of the two shell models. Such quantities, like giant resonances, that are very sensitive to the mixing of the non-resonant continuum states will reveal the features of the continuum shell model more apparently. It is also considered that the effects of the ground state correlation and the higher order perturbation are important in the realistic shell model such as WS shell model and the properties of the effective interaction used also have important effect on the results.

The numerical calculations were carried out by FACOM 230/60 at the computer Center of Osaka City University and by FACOM M190 at the Data Processing Center of Kyoto University.

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