Core polarization for the electric quadrupole moment of neutron-rich Aluminum isotopes

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The core polarization effect for the electric quadrupole moment of the neutron-rich $^{31}$Al, $^{33}$Al and $^{35}$Al isotopes in the vicinity of the island of inversion are investigated by means of the microscopic particle-vibration coupling model in which the Skyrme Hartee-Fock-Bogoliubov and quasiparticle-random-phase approximation are used to calculate the single-quasiparticle wave functions and the excitation modes. It is found that the polarization charge for the proton $1d_{5/2}$ hole state in $^{33}$Al is quite sensitive to coupling to the neutrons in the $pf$-shell associated with the pairing correlations, and that the polarization charge in $^{35}$Al becomes larger due to the stronger collectivity of the low-lying quadrupole vibrational mode in the neighboring $^{36}$Si nucleus.

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I. INTRODUCTION

The nuclear structure far from the $\beta$-stability line has been studied very actively with the development of the new-generation radioactive-isotope beam techniques together with of the microscopic nuclear models applicable to drip-line nuclei carried out by the high performance computers.

The ground state properties and the dynamical properties such as low-energy excitation modes and giant resonances in the medium-mass to the heavier nuclei have been successfully described by the self-consistent mean-field theory or the nuclear density-functional theory (DFT) [1]. The nuclear DFT has been applied to mean-field theory or the nuclear density-functional theory [1].

In this paper, we investigate the ground-state properties and the dynamical properties of the neutron-rich $^{33}$Al isotopes in the vicinity of the island of inversion are investigated by means of the microscopic particle-vibration coupling model in which the Skyrme Hartee-Fock-Bogoliubov and quasiparticle-random-phase approximation are used to calculate the single-quasiparticle wave functions and the excitation modes. It is found that the polarization charge for the proton $1d_{5/2}$ hole state in $^{33}$Al is quite sensitive to coupling to the neutrons in the $pf$-shell associated with the pairing correlations, and that the polarization charge in $^{35}$Al becomes larger due to the stronger collectivity of the low-lying quadrupole vibrational mode in the neighboring $^{36}$Si nucleus.

The article is organized as follows: In Sec. [II] the method is explained. In Sec. [III] we perform the numerical calculations and investigate the core polarization for the electric quadrupole moments in $^{31,33,35}$Al. Sec. [IV] contains the conclusions.

II. METHOD

A. Microscopic particle-vibration coupling model

The nuclear Hamiltonian of a PVC model [12] on top of the Skyrme-Hartee-Fock-Bogoliubov (HFB) and QRPA is written as

$$\hat{H} = \sum_i E_i \hat{\beta}_i^\dagger \hat{\beta}_i + \sum_\lambda \hbar \omega_\lambda \hat{B}_\lambda^\dagger \hat{B}_\lambda + \hat{H}_{\text{couple}}. \quad (1)$$

Here $E_i$ is the quasiparticle energy obtained as a self-consistent solution of the Skyrme-HFB equation, $\hat{\beta}_i^\dagger$, $\hat{\beta}_i$ the quasiparticle creation and annihilation operators. The nucleon creation operator $\hat{\psi}_i^\dagger (r)$ is then represented using the quasiparticle wave functions as

$$\hat{\psi}_i^\dagger (r) = \sum_i \varphi_{1,i}(r) \beta_i^\dagger + \varphi_{2,i}(r) \beta_i. \quad (2)$$

The phonon energy $\hbar \omega_\lambda$ is a solution of the QRPA equation on top of the Skyrme-HFB, and $\hat{B}_\lambda^\dagger$, $\hat{B}_\lambda$ the phonon creation and annihilation operators. We solve the Skyrme-HFB+QRPA equations in the $m$-scheme. Details of the calculation scheme is given in Ref. [6].

Let us now consider the change of the density $\rho(r)$ due to the collective vibrations as $\rho(r) \rightarrow \rho(r) + \delta \rho(r, t)$. The nuclear potential $U[\rho(r)]$ is accordingly changed as $U[\rho(r)] \rightarrow U[\rho(r) + \delta \rho(r, t)]$. To first order in the change of the density, the difference of the nuclear potential is evaluated to be

$$U[\rho(r) + \delta \rho(r, t)] - U[\rho(r)] = \int \delta \rho(r, t) \frac{\delta U[\rho(r)]}{\delta \rho(r')} \delta \rho(r', t). \quad (3)$$

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Then, the PVC Hamiltonian has a form of
\[
\hat{H}_{\text{couple}} = \int dr dr' \frac{\delta U[\rho(r)]}{\delta \phi(r')} \delta \phi(r', t) \hat{\psi}^\dagger(r) \hat{\psi}(r).
\]
(4)

We introduce the vacuum defined by the product of the HFB vacuum and the QRPA vacuum;
\[
\hat{\beta}_i(0) = 0, \quad \hat{B}_\lambda(0) = 0.
\]
(5)
The density variation \(\delta \phi(r, t)\) can be written in a second quantized form using the QRPA modes as
\[
\delta \phi(r) = \sum_\lambda \left[ \delta \phi_\lambda(r) \hat{B}_\lambda^\dagger + \delta \phi^*_\lambda(r) \hat{B}_\lambda \right],
\]
(6)
where \(\delta \phi_\lambda(r)\) is a transition density to the QRPA state \(|\lambda\rangle = \hat{B}_\lambda^\dagger |0\rangle\).

The \(\hat{\beta}_i^\dagger \hat{\beta}_j^\dagger\) and \(\hat{\beta}_i \hat{\beta}_j\) parts in \(\psi(r')\psi(r)\) are taken into account in the QRPA phonons [16]. Consequently, the PVC Hamiltonian in the leading order reads
\[
\hat{H}_{\text{couple}} = \sum_{\lambda, ij} \int dr dr' \frac{\delta U[\rho(r)]}{\delta \phi(r')} \left[ \delta \phi_\lambda(r') \hat{B}_\lambda^\dagger + \delta \phi^*_\lambda(r') \hat{B}_\lambda \right]
\]
\[
\times \left[ \varphi_{1,i}(r) \varphi_{1,j}^\dagger(r) - \varphi_{2,i}(r) \varphi_{2,j}^\dagger(r) \right] \beta_i \beta_j.
\]
(7)
The higher order effects can be treated systematically in the Nuclear Field Theory [17].

The coupling interaction in Eq. (7) is derived from the Skyrme density functional. In the present calculation, we approximate the momentum dependent terms in the Skyrme interaction by the Landau-Migdal (LM) form. This approximation is made only for the construction of the PVC Hamiltonian as in Refs. [13, 10]. The isoscalar (IS) and the isovector (IV) coupling interactions are expressed as
\[
\frac{\delta U[\rho(r)]}{\delta \phi(r')} \delta \phi_\lambda(r') = \begin{cases} 
\nu^{r=0}(r) \delta \phi_{\lambda}^{\text{IS}}(r') \delta(r - r') & \\
\nu^{r=1}(r) \delta \phi_{\lambda}^{\text{IV}}(r') \delta(r - r') - \tau_z r'_z & 
\end{cases}
\]
(8)
The explicit expressions for \(\nu^{r=0}(r) = F_0/N_0\) and \(\nu^{r=1}(r) = F_0'/N_0\) are given in Ref. [20].

**B. Description of odd-\(A\) systems**

In order to describe the odd-\(A\) nuclear systems, we diagonalize the Hamiltonian [11] within the subspace \(\{\hat{\beta}_i^\dagger |0\rangle, \hat{B}_\lambda^\dagger \hat{\beta}_j^\dagger |0\rangle\}\). Then, the resulting state vector is written as
\[
|\phi\rangle = \sum_i c_i \hat{\beta}_i^\dagger |0\rangle + \sum_{\lambda, ij} c_{\lambda, ij}^\dagger \hat{B}_\lambda^\dagger \hat{\beta}_j^\dagger |0\rangle.
\]
(9)
The operator for the quadrupole moment can be written as
\[
\hat{Q} = \langle \hat{Q} \rangle + \sum_{ij \in \pi} Q_{ij} \hat{\beta}_i^\dagger \hat{\beta}_j + \sum_\lambda (Q_\lambda \hat{B}_\lambda^\dagger + Q_\lambda \hat{B}_\lambda),
\]
(10)
where
\[
Q_{ij} = \langle 0 | \hat{\beta}_i \hat{Q} \hat{\beta}_j^\dagger |0\rangle = \int dr (3 \langle z^2 - r^2 \rangle \varphi_{1,i}(r) \varphi_{1,j}^\dagger(r) - \varphi_{2,i}(r) \varphi_{2,j}^\dagger(r)),
\]
(11a)
\[
Q_\lambda = \langle 0 | \hat{B}_\lambda \hat{Q} |0\rangle = \int dr (3 \langle z^2 - r^2 \rangle \delta \phi^*_\lambda(r)),
\]
(11b)
and \(\langle \hat{Q} \rangle\) is the vacuum expectation value.

The electric \(Q\) moment of the eigenstate \(|\phi\rangle\) is then calculated as
\[
\langle \phi | e \hat{Q} | \phi \rangle = e \left\{ \langle \hat{Q} \rangle + \sum_i \left[ (c_i^0)^2 Q_{ii} + 2 c_i^0 \sum_\lambda c_{\lambda,i} Q_\lambda \right] + \sum_{\lambda, jk} c_{\lambda,jk}^2 Q_{jk} \right\},
\]
(12)
We apply this model to odd-\(Z\) nuclei to calculate the proton polarization charge of the state \(|i\rangle\) for the \(Q\) moment, which is defined as
\[
e_{\text{pol}}^\pi = e \left( \frac{\langle \phi | e \hat{Q} | \phi \rangle}{\langle i | \hat{Q} | i \rangle} - 1 \right),
\]
(13)
where \(\langle i | \hat{Q} | i \rangle = \langle \hat{Q} \rangle + Q_{ii}\).

**C. Parameters**

For the mean-field Hamiltonian, we employ the SkM* interaction [21] in the present numerical applications. We use the lattice mesh size \(\Delta \rho = \Delta z = 0.6\) fm and a box boundary condition at \(\rho_{\text{max}} = 9.9\) fm, \(z_{\text{max}} = 9.6\) fm. The quasiparticle energy cutoff is chosen at \(E_{\text{qp,cut}} = 60\) MeV and the quasiparticle states up to \(\Omega^\pi = 15/2^+\) are included. The pairing strength parameter is determined so as to reproduce the experimental pairing gap for neutrons in \(^{34}\text{Mg}\) (\(\Delta_{\nu,\exp} = 1.7\) MeV) obtained by the three-point formula [22]. The strength \(t'_0 = -295\) MeV fm\(^3\) for the mixed-type pairing interaction with the exponent of the density-dependence \(\gamma = 1\) leads to the pairing gap \(\langle \Delta_{\nu} \rangle = 1.71\) MeV in \(^{34}\text{Mg}\) [4]. On top of the Skyrme-HFB, we solve the QRPA equation within the space of the two-quasiparticle excitation of \(E_\alpha + E_\beta \leq 60\) MeV. The momentum-dependent terms in the residual interaction are exactly treated.

The density-dependent Landau parameters \(F_0\) and \(F'_0\) for the PVC interaction are determined by the parameters of the SkM* interaction. As shown in Refs. [6, 23], the attraction of the LM interaction is stronger than that of the self-consistent interaction in which the momentum-dependent terms are treated exactly. Therefore, we multiply the overall factor \(f_{\text{LM}}\) for the PVC interaction. We use \(f_{\text{LM}} = 0.8\) and 0.9 for comparison. Accordingly, the difference of the results can be considered as a theoretical uncertainty.
III. RESULTS AND DISCUSSION

A. Properties of $^{32,34,36}\text{Si}$

We describe the odd-Z neutron-rich Al isotopes as a proton single-hole state coupled to the neighboring Si isotopes because the pairing gaps of protons in Si isotopes are zero. We summarize here the ground state properties and the structure of quadrupole excitations in $^{32,34,36}\text{Si}$.

In Table I the ground state properties are summarized. The neutron-rich Si isotopes under investigation are spherical although the calculated deformation parameters are not exactly zero ($\beta_2 = 0.02$ in $^{34}\text{Si}$). This is due to the artificial breaking of the spherical symmetry associated with the finite mesh size and the rectangular box, and thus it is considered as a numerical error. The average pairing gaps of neutrons are finite, while those of protons are zero. This indicates that the $^{34}\text{Si}$ has a neutron $2p - 2h$ configuration in its ground state. The neutron occupation number of the $1f_{7/2}$ orbital is 0.31, 0.78 and 2.21 in $^{32,34,36}\text{Si}$ and that of the $2p_{3/2}$ orbital is 0.10 in $^{36}\text{Si}$.

Figure 1 shows the response functions for the isoscalar (IS), isovector (IV) and proton quadrupole excitations. We can see a prominent peak at around 3 MeV in all of the isotopes under investigation. The isoscalar transition strengths are $B$(IS$2^+\rightarrow 2^+_1$) = 626, 637 and 1137 fm$^4$ in $^{32,34,36}\text{Si}$, corresponding to 104, 98 and 162 in Weisskopf unit. Besides the low-lying collective $2^+$ state, we can see the giant quadrupole resonances (GQR) at around 20 MeV and 30 MeV for the IS and IV excitations.

The $2^+_1$ state in $^{32}\text{Si}$ is mainly generated by the sd-shell configurations of neutron and proton. The microscopic structure of the $K^\pi = 0^+$ component is given by the two-quasiparticle excitations of $(\nu2s_{1/2} \otimes 1d_{3/2})$ with a weight of 0.04, $(\nu1d_{3/2})^2$ with 0.61, and $(\pi2s_{1/2} \otimes 1d_{5/2})$ with 0.30. The microscopic structure of the $K^\pi = 1^+$ and $2^+$ components is the same within the numerical accuracy as of the $K^\pi = 0^+$ component because of the spherical symmetry. The strength in the energy region $15 \leq h\omega \leq 25$ MeV exhausts 79.4% of the IS energy-weighted sum rule (EWSR) value. The IS strength in the low energy region up to 10 MeV exhausts 1.2% of EWSR. The IV strength is distributed in a wider energy range $20 \leq h\omega \leq 40$ MeV. The summed strength in this energy region exhausts 75.2% of the IV-EWSR value.

In $^{34}\text{Si}$ the neutron excitations into the pf-shell become appreciable for the $2^+_1$ state. The microscopic structure of the $K^\pi = 0^+$ component is given by the $(\nu1d_{3/2})^2$ excitation with a weight of 0.21, $(\nu1f_{7/2})^2$ with 0.10, and $(\pi2s_{1/2} \otimes 1d_{5/2})$ with 0.63. The strength in the energy region $15 \leq h\omega \leq 25$ MeV exhausts 79.8% of the IS-EWSR value, and the strength in the energy region $20 \leq h\omega \leq 40$ MeV exhausts 74.3% of the IV-EWSR value.

The $K^\pi = 0^+$ component of the $2^+_1$ state in $^{36}\text{Si}$ is mainly generated by the $(\nu1f_{7/2})^2$ excitation with a weight of 0.39, $(\nu2p_{3/2})^2$ with 0.08, and $(\pi2s_{1/2} \otimes 1d_{5/2})$ with 0.47. The strength in the energy region $15 \leq h\omega \leq 25$ MeV exhausts 77.6% of the IS-EWSR value, and the strength in the energy region $20 \leq h\omega \leq 40$ MeV exci-

### Table I: Ground state properties of $^{32,34,36}\text{Si}$ obtained by the deformed HFB calculation with the SkM* interaction and the mixed-type pairing interaction. Chemical potentials, average pairing gaps, root-mean-square radii for neutrons and protons are listed. The average pairing gaps of protons are zero in these isotopes. The average pairing gap is defined as $\langle \Delta \rangle = -\int dr \rho(\hat{\omega})/\int d\rho(\hat{\omega})$.

|   | $^{32}\text{Si}$ | $^{34}\text{Si}$ | $^{36}\text{Si}$ |
|---|----------------|----------------|----------------|
| $\lambda_\nu$ (MeV) | -7.76 | -6.60 | -5.51 |
| $\lambda_\pi$ (MeV) | -13.5 | -15.9 | -17.3 |
| $\langle \Delta \rangle_\nu$ (MeV) | 1.56 | 1.67 | 1.94 |
| $\sqrt{\langle r^2 \rangle_\nu}$ (fm) | 3.22 | 3.32 | 3.39 |
| $\sqrt{\langle r^2 \rangle_\pi}$ (fm) | 3.10 | 3.13 | 3.16 |
We take the QRPA states of the IS and IV modes in neutron-rich nuclei, we can see an appreciable IV strength in the lower energy region $10 \leq \hbar \omega \leq 20$ MeV. The summed strength in this energy region exhausts 10.4% of the IV-EWSR value.

B. Polarization charges in $^{31,33,35}$Al

For describing the $I^\pi = 5/2^+$ state of $^{31,33,35}$Al, we diagonalize the Hamiltonian $\mathbf{1}$ in the model space of the proton single-hole state of the $1d_{5/2}$ orbital $|\Omega^\pi = -5/2^+\rangle$ and the coupled states of $|\Omega^\pi = -5/2^+\rangle \otimes \omega_{K=0}$, $|(-3/2^+)^{-1} \otimes \omega_{K=1}\rangle$ and $|(-1/2^+)^{-1} \otimes \omega_{K=2}\rangle$. We take the QRPA states $|\omega_\lambda\rangle$ whose IS or IV quadrupole transition strengths possessing greater than in 1 W.u.

The dimension of the Hamiltonian $\mathbf{1}$ is 225 for $^{31}$Al. The $I^\pi = 5/2^+$ state of $^{31}$Al is constructed mainly by the one hole state and the hole coupled to the $2_1^+$ state as

$$|^{31}$Al; $I^\pi = 5/2^+, M = 5/2\rangle = 0.93((-5/2^+)^{-1}) + 0.21((-5/2^+)^{-1} \otimes 2_1^+ (K = 0)) - 0.23((-3/2^+)^{-1} \otimes 2_1^+ (K = 1)) + 0.16((-1/2^+)^{-1} \otimes 2_1^+ (K = 2)).$$

(14)

The amplitude associated with the other components are smaller than 0.1. The coupled states in Eq. (14) correspond to the $(\pi 1d_{5/2})^{-1} \otimes 2_1^+$ state in the $j-$scheme representation. The ratios of the amplitudes are identical to those of the Clebsch-Gordan coefficients $\frac{5/2}{22} \otimes \frac{5/2}{22}$, $\frac{5/2}{22} \otimes \frac{5/2}{22}$ and $\frac{5/2}{22} \otimes \frac{5/2}{22}$. The quadrupole moment of $^{31}$Al is then calculated using Eq. (12) as $13.6(13.9)\text{fm}^2$, where we use $f_{JM} = 0.8 (0.9)$. From this value, the polarizability charge of Eq. (13) is calculated as $\varepsilon_{\text{pol}} = 1.03e(1.08e)$. The result of the calculation overestimates slightly the experimental value of the Q moment $11.2 \pm 3.2\text{fm}^2$ [12].

For $^{33}$Al, the dimension of the Hamiltonian $\mathbf{1}$ is 250. As in $^{31}$Al, the wave function of $^{33}$Al is written by mainly the one hole state with a weight (the squared amplitude) of 0.90 and the hole coupled to the $2_1^+$ state with a weight of 0.08. The calculated values of the Q moment and the polarization charge are $13.0(13.4)\text{fm}^2$ and $\varepsilon_{\text{pol}} = 0.89e(0.96e)$, respectively. The quadrupole moments and polarization charges of $^{31}$Al and $^{33}$Al are not very different.

The dimension of the Hamiltonian $\mathbf{1}$ is 285 for $^{35}$Al. As in the case of $^{31}$Al and $^{33}$Al, the wave function of $^{35}$Al is written by the one hole state with a weight of 0.85 and the hole coupled to the $2_1^+$ state with 0.14. The contribution of the coupling to the $2_1^+$ state is larger than in $^{31,33}$Al. The calculated values of the Q moment and the polarization charge are $14.7(15.1)\text{fm}^2$ and $\varepsilon_{\text{pol}} = 1.12e(1.18e)$, respectively.

In order to see separately the effects of coupling to the low-lying modes and to the giant resonances on the polarization charge, we diagonalize the Hamiltonian $\mathbf{1}$ in the model space containing only the RPA modes with their energies larger than 10 MeV. The obtained polarization charges for the $1d_{5/2}$ orbital are $\varepsilon_{\text{pol}} = 0.20e(0.22e)$, $0.21e(0.24e)$ and $0.18e(0.20e)$ in $^{31}$Al, $^{33}$Al and $^{35}$Al, respectively. These values are close to the systematic value obtained in Ref. [24] ($0.21e$; 0.18e and 0.15e in $^{31,33,35}$Al), where the microscopic PVC calculations were performed including only the giant resonances on top of the self-consistent HF+RPA in light neutron-rich nuclei.

The enhancement of the polarization charge in $^{35}$Al is thus due to the strong collectivity of the low-lying quadrupole vibrational mode in the core nucleus $^{36}$Si because the effects of coupling to the giant resonances are not sensitive to the neutron number in Al isotopes under investigation.

C. Effects of the pairing correlations in $^{33}$Al

We investigate the effects of coupling to the $pf$-shell in $^{33}$Al. The dominant correlation in the present case is the pairing correlation because the core nucleus $^{34}$Si is calculated to be spherical at the HFB level.

Figure 2 shows the IS, IV and proton quadrupole transition strengths in $^{34}$Si obtained by solving the Skyrme HF+RPA equations without pairing correlations. The collectivity of low-lying states are tremendously weakened, while the structure of GQR is not very different to that obtained by solving the Skyrme HFB+QRPA equations shown in Fig. 1.

The $2_1^+$ state is constructed dominantly by the $(\pi 2s_{1/2} \otimes 1d_{5/2})$ excitation with a weight of 0.98. The strength $B(\text{IS}2; 0^+ \rightarrow 2_1^+)$ has only 237 fm$^4$. Using the RPA transition densities, we diagonalize the Hamiltonian $\mathbf{1}$ with a dimension of 241. The calculated wave func-
The proton quasiparticle of the $1d_{5/2}$ orbital, and the coupled states of a $sd$-shell quasi-proton to the quadrupole modes in $^{32}$Mg. In the present calculation with a dimension of 276, $^{33}$Al is constructed by the quasi-proton of the $1d_{5/2}$ level with a weight of 0.85, $|\pi 1d_{5/2} \otimes 2_1^+\rangle$ with 0.10, $|\pi 2s_{1/2} \otimes 2_1^+\rangle$ with 0.04, and $|\pi 1d_{3/2} \otimes 2_1^+\rangle$ with 0.01. The electric $Q$ moment of $^{33}$Al is then calculated as 12.4 (12.6) $\text{fm}^2$. This is consistent with the calculation in Sec. III.B.

**IV. CONCLUSION**

The polarization charges for the electric quadrupole moment of the neutron-rich Al isotopes at around $N = 20$ have been investigated by carrying out the microscopic particle-vibration coupling calculation in which the coordinate-space Skyrme-Hartree-Fock-Bogoliubov quasi-particle-random-phase approximation are employed to calculate the single-quasiparticle wave functions and the transition densities.

It has been found that the neutron pairing correlations are crucial to generate collectivity of the $2_1^+$ state in $^{34}$Si, and that the polarization charge of the proton hole state of the $1d_{5/2}$ orbital becomes small in the absence of the pairing correlation in $^{33}$Al. The effect of the neutron pairing correlation at $N = 20$ on the enhancement of the polarization charge in $^{33}$Al is very similar to the enhancement mechanism of the $B(E2)$ in $^{33}$Mg.

Effects of coupling to the giant resonances on the polarization charge are not very different in a small region of isotopes, and the low-lying collective modes have much effect on the polarization charge. Therefore, the polarization charge in $^{35}$Al is larger than in $^{31,33}$Al as a consequence of the stronger collectivity of the $2_1^+$ state in $^{36}$Si.

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