Nuclear Deformation: A Proton-Neutron Effect?

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It is shown within the Hartree-Fock method with the Skyrme force that the quadrupole-quadrupole neutron-proton interaction gives the leading term in the nuclear deformation energy. The quadrupole-quadrupole coupling constants are derived and shown to agree with those obtained within the simple harmonic-oscillator model.

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The supposition that the long-range neutron-proton (n-p) interaction is the main reason for the nuclear deformation was formulated long ago within the nuclear shell model.[1-3] In terms of the conventional deformed-mean-field approach the n-p features are hidden in the parametrization of the neutron and the proton phenomenological one-body potentials. On the other hand, the self-consistent Hartree-Fock (HF) method with realistic effective two-body interaction allows for a transparent analysis of the n-p effects on the nuclear deformation. The results of such analysis are presented in this Letter.

Let us first discuss the model Hamiltonian with the quadrupole-quadrupole (Q-Q) interaction

$$\hat{H}=\hat{H}_0+\tfrac{1}{2}\kappa_0\hat{Q}_0\hat{Q}_0+\tfrac{1}{2}\kappa_1\hat{Q}_1\hat{Q}_1, \tag{1}$$

where $\hat{Q}_0=\hat{Q}_n+\hat{Q}_p$ and $\hat{Q}_1=\hat{Q}_n-\hat{Q}_p$ are the single-particle quadrupole isoscalar and isovector operators, respectively, κ_0 and κ_1 are the corresponding coupling constants, and $\hat{H}_0$ is a spherical single-particle Hamiltonian. Hamiltonian (1) can be employed in the description of low-frequency quadrupole vibrations (leading to a possible quadrupole instability and a stable deformation of the nuclear shape) or high-frequency quadrupole oscillations (giant quadrupole resonances). In the latter case the coupling constants κ_0 and κ_1 can be estimated[4] by use of the harmonic-oscillator Hamiltonian with the frequency ω_0 for $\hat{H}_0$. The result is[5]

$$\frac{16\pi}{5}\kappa_0=-\frac{4\pi}{5}\frac{M\omega_0^2}{A\langle r^2\rangle},\quad \frac{16\pi}{5}\kappa_1=\frac{\pi V_1}{A\langle r^4\rangle}, \tag{2}$$

where V_1 is the symmetry potential.

When we calculate the low-frequency quadrupole oscillations the quadrupole polarizability should be taken into account.[4] Consequently, the strength coefficients in Eq. (2) should be renormalized by factors $(1+\chi_0)$ and $(1+\chi_1)$, where χ_0 and χ_1 are the polarizability coefficients for isoscalar and isovector quadrupole modes, respectively. They can be estimated with the random-phase approximation and the experimental frequencies of the giant isoscalar and isovector resonances (see Sect. 6 of Ref. 4), which gives $\chi_0\approx 1$ and $\chi_1\approx -0.64$. Combining this with Eq. (2) and assuming[4] $V_1=130$ MeV, $M\omega_0^2=40.55A^{-2/3}$ MeV fm^{-2}, $\langle r^2\rangle=0.87A^{2/3}$ fm^2, and $\langle r^4\rangle=0.95A^{4/3}$ fm^4, one obtains the values of κ_0 and κ_1,

$$\kappa_0=-23.3A^{-7/3}\text{ MeV fm}^{-4},\qquad \kappa_1=15.4A^{-7/3}\text{ MeV fm}^{-4}, \tag{3}$$

which gives the mass-independent ratio

$$\kappa_1/\kappa_0\approx -0.66. \tag{4}$$

In the next step we rearrange the quadrupole part of Hamiltonian (1) in the following way:

$$\tfrac{1}{2}\kappa_0\hat{Q}_0\hat{Q}_0+\tfrac{1}{2}\kappa_1\hat{Q}_1\hat{Q}_1 =\tfrac{1}{2}\kappa_{nn}\hat{Q}_n\hat{Q}_n+\tfrac{1}{2}\kappa_{pp}\hat{Q}_p\hat{Q}_p+\kappa_{np}\hat{Q}_n\hat{Q}_p, \tag{5}$$

with $\kappa_{nn}=\kappa_{pp}=\kappa_0+\kappa_1$ and $\kappa_{np}=\kappa_0-\kappa_1$. Using Eq. (4) one obtains the ratio of the coupling constants

$$\kappa_{nn}/\kappa_{np}=\kappa_{pp}/\kappa_{np}\approx 0.2, \tag{6}$$

i.e., the n-p part of the Q-Q interaction is about 5 times larger than the n-n or the p-p parts. We can thus conclude that the $\hat{Q}_n\hat{Q}_p$ force may indeed be viewed as being responsible for the development of the nuclear deformation.

Since the isovector coupling constant κ_1 is positive, the equilibrium neutron and proton deformations tend to be similar, i.e., $Q_n\approx Q_p$ and $Q_0\gg Q_1$. Hence, by neglect of the like-particle interaction the readjustment of κ_{np} of the order of 20% is necessary. On the other hand, the isovector term is much smaller than the isoscalar term, which justifies the use of the $\hat{Q}_0\hat{Q}_0$ interaction in all models which incorporate the assumption of equal neutron and proton deformations.

Let us now discuss the self-consistent mean-field theory for which the energy of a fermion system has the form

$$E=\mathrm{Tr}(T\rho)+\tfrac{1}{2}\mathrm{Tr}\Gamma\rho+E_{\text{pair}}, \tag{7}$$

where ρ is the one-body density matrix, T is the kinetic energy operator, Γ is the one-body potential-energy operator, related to the two-body interaction V by $\Gamma = \mathrm{Tr} V\rho$, and E_{pair} is the energy of pairing correlations. The potential energy $\frac{1}{2}\mathrm{Tr}\Gamma\rho$ can be split into three parts

$$\tfrac{1}{2}\mathrm{Tr}\Gamma\rho = E^{nn} + E^{pp} + E^{np}, \tag{8}$$

where $E^{\tau\tau'} = \mathrm{Tr}[\rho^{\tau}\mathrm{Tr}(V\rho^{\tau'})]/(1+\delta_{\tau\tau'})$, and $\tau,\tau' = p$ or n. In order to study the quadrupole deformation energy one can decompose the proton and neutron density matrices into different multipole components[6]

$$\rho^{\tau} = \rho_0^{\tau} + \rho_2^{\tau} + \rho_4^{\tau} + \cdots, \tag{9}$$

where ρ_J^{τ} is the rank-J tensor operator. In the present study we consider the axial, reflection symmetric shapes, and therefore expansion (9) contains only the even-J terms and the magnetic quantum numbers (not shown explicitly) are equal to zero. Expansion (9) allows us to express the potential energy as the sum

$$E^{\tau\tau'} = E_0^{\tau\tau'} + E_2^{\tau\tau'} + E_4^{\tau\tau'} + \cdots, \tag{10}$$

where

$$(1+\delta_{\tau\tau'})E_J^{\tau\tau'} = \mathrm{Tr}\Gamma^{\tau}\rho_J^{\tau'} = \mathrm{Tr}\Gamma_J^{\tau}\rho_J^{\tau'}$$

and Γ_J^{τ} is the rank-J multipole component of $\Gamma^{\tau} = \mathrm{Tr}V\rho^{\tau}$. Finally, energy (7) can be written as

$$E = E_0^{\mathrm{tot}} + E_2^{nn} + E_2^{pp} + E_2^{np} + \cdots, \tag{11}$$

where $E_o^{\mathrm{tot}} = \mathrm{Tr}(T\rho) + E_0 + E_{\mathrm{pair}}$ is the total monopole energy of the system, composed of the kinetic energy, monopole potential energy, and pairing energy.[7] The energies $E_J^{\tau\tau'}$ for $J > 2$ are usually very small[6] and will be neglected in the following discussion.

We have chosen the germanium isotopes $^{60-82}$Ge for our analysis because these nuclei show interesting prolate-oblate and spherical-deformed competition of shapes. The deformed states of these nuclei were obtained with the constrained HF method with the Skyrme S III interaction. The pairing correlations were included by means of the BCS approximation with constant gap parameters.[8] The isoscalar quadrupole moment $\hat{Q}_0$ was used as the constraining operator.

The dependence of the deformation energy $\delta E = E - E(Q_0 = 0)$ on the quadrupole moment $Q_0 = \langle \hat{Q}_0 \rangle$ is shown in Fig. 1 for the considered germanium isotopes. The deformation energies exhibit a characteristic pattern, which can be easily related to the shell structure for neutron numbers between $N = 28$ and $N = 50$. From the nearly spherical semimagic isotope ^{60}Ge one observes a sequence of deformed nuclei ending at the spherical semimagic isotope of ^{82}Ge. The effect of the shell closure at $N = 40$ is clearly visible.

The quadrupole energies E_2^{nn}, E_2^{pp}, and E_2^{np} and the monopole energy relative to the spherical point, $\delta E_0^{\mathrm{tot}} = E_0^{\mathrm{tot}} - E_0^{\mathrm{tot}}(Q_0 = 0)$, are presented in Fig. 2 as functions of the quadrupole moment Q_0 for ^{72}Ge. In the inset of Fig. 2 the isospin components E_0^{nn}, E_0^{pp}, and E_0^{np} of the monopole potential energy are shown as functions of the mass number A for $Q_0 = 0$. It is seen that the unlike-particle potential energy E_0^{np} is about 5 times

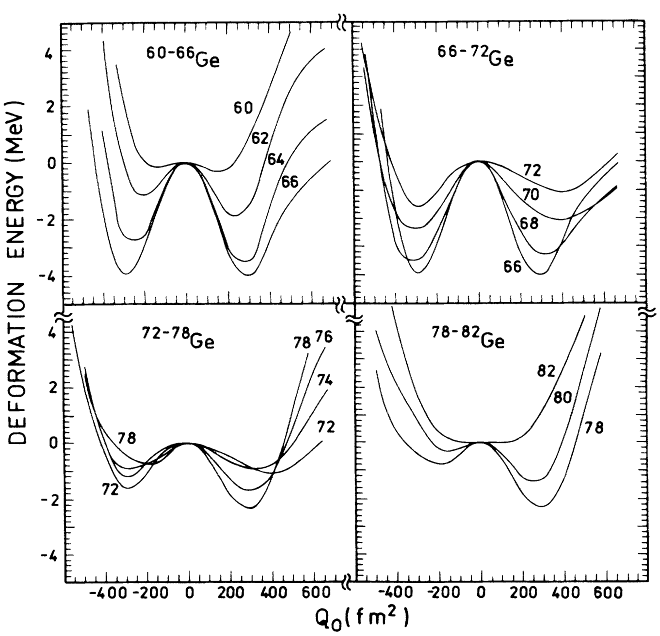

FIG. 1. Hartree-Fock deformation energies $\delta E = E - E(Q_0 = 0)$ for the doubly even $^{60-82}$Ge isotopes as functions of the quadrupole moment Q_0.

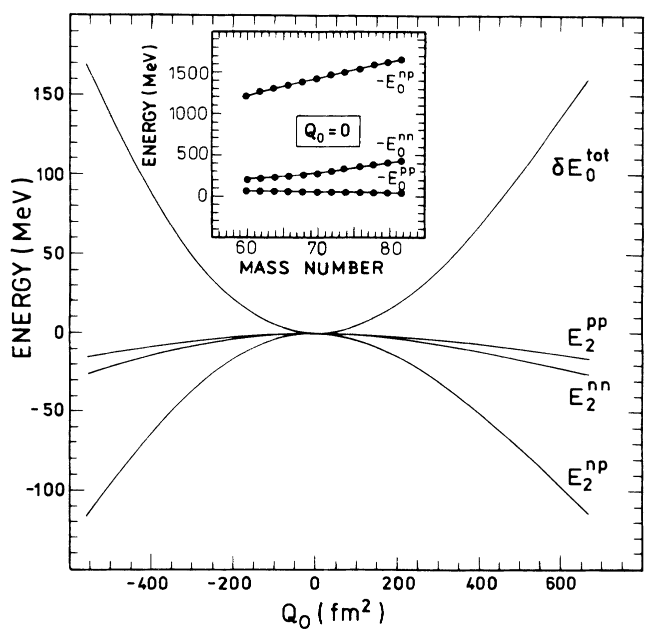

FIG. 2. The total monopole, $\delta E_0^{\mathrm{tot}}$, and the quadrupole, E_2^{nn}, E_2^{pp}, and E_2^{np}, energies for ^{72}Ge as functions of the quadrupole moment Q_0. In the inset, the potential monopole energies E_0^{nn}, E_0^{pp}, and E_0^{np} are shown for $Q_0 = 0$ as functions of the mass number.

larger than the sum of like-particle potential energies. Hence the nuclear binding results mainly from the n-p effective interaction. The quadrupole n-p energy is also much larger than the n-n and the p-p quadrupole energies. The monopole energy δE_0^{tot} increases with $|Q_0|$ and all the quadrupole energies decrease with $|Q_0|$. The total deformation energy of the order of a few megaelectronvolts shown in Fig. 1 originates from a cancellation between the monopole and the quadrupole energy. Since the E_2^{np} term is the component most decreasing with $|Q_0|$, one can say that the nuclear deformation is caused by the quadrupole n-p interaction. Similar conclusions can be drawn for all germanium isotopes studied here.

Comparing expression of the HF energy, Eq. (11), with Hamiltonian (1) expressed in terms of the n-n, p-p, and n-p interactions, Eq. (5), one can identify the energy E_0^{tot} with the mean value of $\hat{H}_0$ and the quadrupole energies $E_2^{\tau\tau'}$ with the corresponding mean values of the isospin components of the Q-Q interaction. Based on such identification the coupling constants can be determined from the HF results as $\kappa_{nn}=2E_2^{nn}/Q_n^2$, $\kappa_{pp}=2E_2^{pp}/Q_p^2$, $\kappa_{np}=E_2^{np}/(Q_nQ_p)$, where $Q_n=\langle\hat{Q}_n\rangle$ and $Q_p=\langle\hat{Q}_p\rangle$. The values of κ_{nn}, κ_{pp}, and κ_{np}, calculated at $Q_0=-75$ fm^2, have been used to determine the isoscalar and isovector coupling constants, κ_0 and κ_1. They are plotted in Fig. 3 together with the harmonic-oscillator estimates of Eq. (3) as functions of A. The fair agreement between simple estimates (4), which give a good fit to the quadrupole giant-resonance energies, and the HF results indicates that the Skyrme force contains the correct Q-Q component, and thus is able to describe both the low- and high-energy quadrupole oscillations.[9]

In order to illustrate the cancellation between the monopole and the quadrupole energies (Fig. 2), we have plotted in Fig. 3 the stiffness of the monopole energy defined as $C_0=2\ \delta E_0^{\text{tot}}/Q_0^2$. As seen in Fig. 3, the stiffness C_0 is very close in magnitude to κ_0 and has the opposite sign. Their sum is an order of magnitude smaller than each of them, and for small deformations it is close to the stiffness of the deformation energy $C=2\times\delta E/Q_0^2\approx C_0+\kappa_0$, which is plotted in Fig. 4 (at $Q_0=-75$ fm^2) together with the equilibrium deformation energy $\delta E^{\text{eq}}=E(Q_0^{\text{eq}})-E(Q_0=0)$ calculated at the prolate minima. It is seen that C and δE^{eq} are strongly correlated and nicely reflect the shell closures at $N=28$, 40, and 50.

Recently, a very systematic behavior of the low-energy nuclear data when plotted against the product N_nN_p of numbers of valence neutron and proton pairs has been shown.[10] The correlation between N_nN_p and the quadrupole collectivity is usually understood as an indication that the n-p interaction is the main factor determining the nuclear deformation. Moreover, the expression

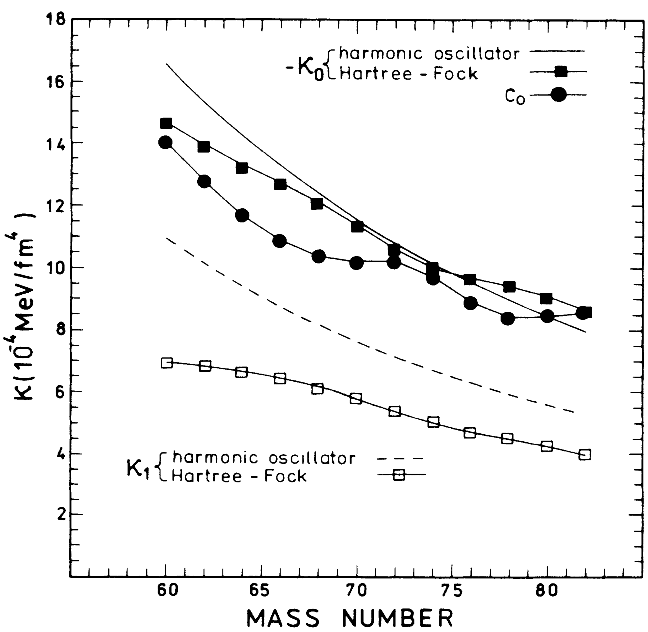

FIG. 3. The Q-Q isoscalar and isovector coupling constants obtained within the HF method (filled and open squares) shown as functions of the mass number for the germanium isotopes, and compared to the harmonic-oscillator estimates of Eq. (3) (solid and broken lines). The stiffness of the monopole energy, $C_0=2\ \delta E_0^{\text{tot}}/Q_0^2$, is also shown (filled circles).

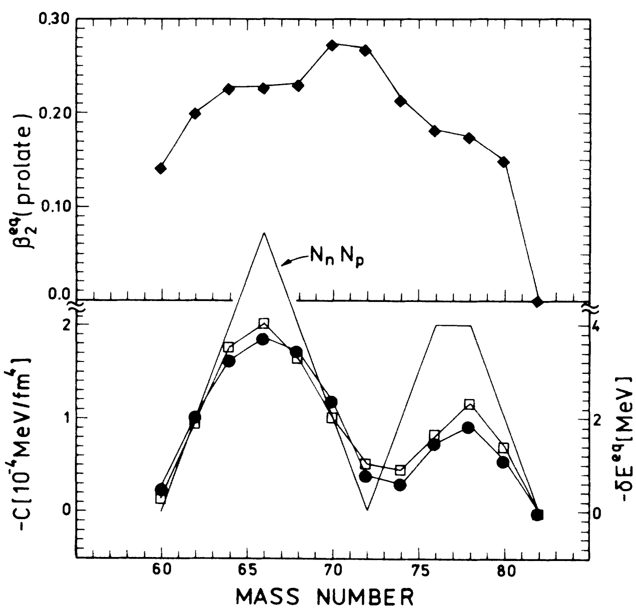

FIG. 4. Hartree-Fock equilibrium deformation energy $\delta E^{\text{eq}}=E(Q_0^{\text{eq}})-E(Q_0=0)$ for prolate minima (squares, scale to the right) and the stiffness $C=2\delta E/Q_0^2$ (calculated at $Q_0=-75$ fm^2, circles, scale to the left) shown as functions of the mass number for the germanium isotopes. The product of numbers of valence proton and neutron pairs N_nN_p is plotted in arbitrary units (solid line). The prolate equilibrium deformations β_2^{eq} determined from Q_0^{eq} are also shown in the upper part of the figure.

N_nN_p is considered as an estimate of the equilibrium deformation energy.[11] This conclusion is qualitatively supported by the results of Fig. 4, where the product N_nN_p plotted against A shows the same pattern as δE^{eq} and the stiffness C. On the other hand, the values of the prolate equilibrium deformations β_2^{eq}, determined from the Hf equilibrium quadrupole moments Q_0^{eq}, Fig. 4, show clear maximum at $N=40$.

In trying to decide which part of the energy, Eq. (11), makes a given isotope spherical or deformed one should observe that the monopole stiffness C_0 reflects the shell structure in a much stronger way than the isoscalar coupling constant κ_0 (see Fig. 3). The shell fluctuation of C and δE^{eq} should thus be mainly attributed to the fluctuations of C_0, while the Q-Q interaction provides a steady deformation-driving factor. Hence the fact that the equilibrium deformation energy is correlated with the product N_nN_p *is not* an immediate consequence of the dominance of the $\hat{Q}_n\hat{Q}_p$ term in the quadrupole energy. The increase of the monopole energy with $|Q_0|$ and its shell fluctuations constitute more important factors in establishing such a correlation.

In summary, the importance of the n-p Q-Q interaction in generating the nuclear deformation is supported by the self-consistent calculations employing the HF method with the Skyrme interaction. The coupling constants derived from this approach are very close to the estimates of the harmonic-oscillator model. Strong correlation between equilibrium deformation energy and the product of numbers of valence neutron and proton pairs N_nN_p is found. It is shown, however, that this correlation should be primarily attributed to the fluctuations of the monopole energy of the nucleus, while the strength of the $\hat{Q}_n\hat{Q}_p$ interaction does not show any obvious correlation with the shell structure.

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[7]Note that since the kinetic energy T is the scalar operator one has $\mathrm{Tr}(T\rho)=\mathrm{Tr}(T\rho_0)$. Similarly, the pairing energy, $E_{\mathrm{pair}}=\frac{1}{2}\Delta\mathrm{Tr}(\kappa)$, depends only on the monopole part of the pairing tensor κ (Δ is the pairing gap parameter).

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