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UNRESTRICTED SHAPES OF LIGHT NUCLEI IN THE LOCAL-DENSITY
APPROXIMATION: COMPARISON WITH JELLIUM CLUSTERS

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Unrestricted shapes of light nuclei in the local-density approximation: comparison with jellium clusters

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Abstract: The shapes of light nuclei are studied within density-functional theory. The Kohn–Sham method and the local-density approximation are used. No symmetry restrictions are imposed. A parallel study is made of monovalent atomic clusters described on the jellium model. The shapes obtained for nuclei with $Z = N = 2$ –22 show a striking similarity to those of atomic clusters of an equal number of valence electrons. Moments of inertia, when suitably normalized, are virtually identical. The calculated nuclear quadrupole moments are found insensitive to the effective interaction and in good agreement with experiment. Similar shape coexistence is established in both systems.

1. Introduction

The deformation of nuclei from spherical shape is most directly seen in the existence of nonvanishing quadrupole moments [1]. In leading order, the quadrupole moment comes from a $Y_2(\theta, \phi)$ shape of the nuclear surface. Quadrupole deformation is indeed the dominant kind of nuclear deformation, but hexadecapole deformations (Y_4) and even Y_6 de-

formations are experimentally known and theoretically studied [2]. The case of static odd multipole shapes, practically only Y_3 so far, is less certain [3]. The description in terms of a few low multipoles is clearly suitable for nuclei beyond the sd shell. Some light nuclei, however, can be understood as quasi-molecular structures composed of clusters of nucleons, particularly alpha particles [4].

In the independent-particle description of the shell model, deformation can be understood as resulting from the Pauli principle operating in partly filled shells; the summed single-particle energy is lowered by the onset of deformation. The explicit single-particle shell model for (quadrupole) deformed nuclei is the Nilsson model [5]. Nuclear shapes can be calculated quantitatively by mean-field methods: Hartree–Fock in a variety of forms and Nilsson–Strutinsky; for reviews see Refs. [6,7,2,8] and for a detailed exposition Ref. [9].

The Nilsson model was also the first model employed to describe the deformation of atomic clusters [10]. The description was successful in explaining the odd–even staggering in the abundance spectra and in the ionization potential. Later, also the Strutinsky averaging method has been used to study deformations in large metal clusters [11].

The differences between the electron gas and nuclear matter are that nuclear matter is much less compressible and its relative surface energy is much larger than that of the electron gas. Accordingly, one would expect that deformations in nuclear matter are smaller than in the electronic system.

The purpose of this paper is to study deformations in nuclei and metallic clusters on the same footing. It is clear that this can be done only by imposing approximations on both systems. To avoid the complications arising from the discrete ions in metal clusters, we use the so-called jellium model where the positive ions are approximated by a continuous background charge (for a review see Ref. [12]). In the case of nuclei we neglect the proton charge and the spin–orbit interaction and assume equal numbers of protons and neutrons. These restrictive assumptions are reasonably well justified since we study real nuclei with $A \leq 44$; the relevant magic numbers 2, 8, 20 are unaffected by the spin–orbit force and

isospin is an essentially good quantum number.

Furthermore, we use the density-functional theory with the Kohn-Sham method [13] and the local-density approximation to solve the many-body hamiltonian for the ground state (for a review see Ref. [14]). Both systems will then obey similar one-particle equations. Only the dependence of the mean-field potential on particle density will be different.

The results show that going from easily compressible electron liquid to nearly incompressible nuclear matter does not markedly change the degree or kind of deformation. This means, for example, that the intrinsic quadrupole moments depend essentially only on the density of nuclear matter. The calculated quadrupole moments turn out to be in good agreement with experiment.

2. The theoretical model

We apply the density-functional model to a nucleus as follows. To begin with, we only need to consider one kind of nucleon, say neutrons, since we assume the same number of protons and neglect the Coulomb repulsion. Of course, the protons are implicitly included in the calculation due to their interaction with neutrons.

The total energy of the neutrons in the nucleus can be written as a functional of the neutron density n ,

$$E = T_0[n] + V[n], \quad (1)$$

where T_0 is the kinetic energy for noninteracting neutrons and V includes the energy due to the interparticle interactions. The total energy of the nucleus is $2E$, since the energy of the protons is the same in our model.

In the Kohn-Sham method, the neutron density is written in terms of trial single-

particle wave functions ψ_i as a sum over the occupied states:

$$n(\mathbf{r}) = \sum_i |\psi_i(\mathbf{r})|^2. \quad (2)$$

This method includes the shell effects in the density-functional theory, since the kinetic energy is simply the sum of the kinetic energies of the occupied single-particle states ψ_i .

For the interaction part we apply the the local-density approximation. Let $e(n)$ be the total energy per neutron in homogeneous nuclear matter with equal neutron and proton densities. Then, if $t_0 = \frac{2}{3}\epsilon_F$ is the average kinetic energy per neutron,

$$v(n) = e(n) - t_0(n) \quad (3)$$

represents the potential energy per neutron of the homogeneous system. The local-density ansatz is that for an inhomogeneous system the potential-energy part can be written as

$$V[n] = \int d^3r n(\mathbf{r})v(n(\mathbf{r})). \quad (4)$$

Minimizing the total energy E with respect to the ψ_i leads to the well-known Kohn-Sham equations

$$-\frac{\hbar^2}{2m}\nabla^2\psi_i + V_{\text{eff}}\psi_i = \epsilon_i\psi_i, \quad (5)$$

where

$$V_{\text{eff}} = \frac{\delta V[n]}{\delta n(\mathbf{r})} \quad (6)$$

is the effective (density-dependent) single-particle potential.

For nuclear matter, the total energy of the homogeneous gas as a function of the gas density is not so well known. Thus we have used a simple approximation where the total energy per particle is expanded around the equilibrium density n_0 and write

$$\epsilon(n) = \alpha + \beta \left(\frac{n - n_0}{n_0} \right)^2, \quad (7)$$

where α is the usual volume energy in the semiempirical mass formula [1] and β is proportional to the incompressibility parameter K : $K = 18\beta$.

The justification for the approximation (7) is that, apart from the surface region, the density will be close to the equilibrium density. Accordingly the parabolic dependence is a good approximation. In our computations we use the parameter values $\alpha = -16$ MeV and $K = 288$ MeV. We have chosen the K value solely by requiring that the total energy

go to zero at zero density, i.e. $\beta = -\alpha$. This K value is somewhat larger than the value, about 200 MeV, usually given in the literature [1,9]. However, it is close to the estimate 301 MeV used by Myers and Swiatecki [15] in the Thomas–Fermi model for nuclei. The equilibrium density n_0 for neutrons was chosen to be $n_0 = 0.0693 \text{ fm}^{-3}$, corresponding to Wigner–Seitz radius $r_s = \left(\frac{4}{3}\pi n_0\right)^{-1/3} = 1.51 \text{ fm}$ for neutrons and $2^{-1/3}r_s = 1.20 \text{ fm}$ for nucleons. The effective potential V_{eff} is obtained from the total energy (7) according to Eqs. (3), (4) and (6).

From here on, we use the word particle for both neutrons and electrons. It is important to note that in the case of nuclei the particle density then means the neutron density, which is only one-half the density of nuclear matter, assumed symmetric.

For the electron system we use the ultimate jellium model [16], where the background density is completely deformable and always takes the same density as the electron gas. In this model the total energy includes, in analogy to Eq. (1), the kinetic and exchange–correlation energies. The Coulomb energy will be zero since the electron density is identical to the positive background density. For the correlation energy we can use any interpolation formula suggested in the literature [14] and immediately determine the effective potential as a function of the density. In the present calculations we have used the Perdew–Zunger interpolation formula [17] fitted to the numerical data of Ceperley and Alder [18].

In absolute magnitude, atomic and nuclear phenomena are vastly different. For qualitative comparison, however, we can define units which scale the parameters to comparable size. For the electron gas we use the atomic units with the Bohr radius $a_0 = 0.0529 \text{ nm}$ as the unit of length and $e^2/4\pi\epsilon_0 a_0 = 2 \text{ Ry} = 27.2 \text{ eV}$ as the unit of energy. For nuclear matter we choose the unit of length so that the equilibrium density n_0 for neutrons ($r_s = 1.51 \text{ fm}$) has the same numerical value as the equilibrium density of electrons in atomic units ($r_s = 4.18$); that unit is then $L \equiv 1.51 \text{ fm}/4.18 = 0.361 \text{ fm}$. The nuclear unit of energy we then define as $\hbar^2/m_n L^2 = 318 \text{ MeV}$.

In the above units, Fig. 1 shows the total energy per particle and the local effective po-

tential as functions of particle density for the homogeneous electron gas and homogeneous nuclear matter. The basic difference between the two systems is clearly seen. The incompressibility (proportional to the second derivative of the total energy) is much smaller in the electron gas than in nuclear matter. The effective potential is a monotonically decreasing function in the electronic case, while in nuclear matter it increases rapidly at high densities due to the hard cores of the nuclei.

We first solved the Kohn–Sham equations in the spherical cases of magic clusters, where the problem is mathematically one-dimensional. Fig. 2 shows the particle densities for nuclear and atomic clusters of 2, 8, 18* and 20 particles. The 18-particle cluster is denoted by a star because in this case the spherical cluster is an isomer (i.e. not the ground state). The variations in particle density, appropriately scaled, are seen to be larger for the electron clusters due to the larger compressibility. The density distribution of the corresponding homogeneous sphere is shown in each case for comparison.

The effect of the compressibility is even more prominent in large clusters. Fig. 3 shows the density profiles for spherical 92-particle clusters together with the effective potential. For the nuclear case this is fictitious since 92 is a magic number only in the absence of the spin–orbit interaction. In the jellium cluster the average density inside the cluster is larger than in the nucleus. Due to the large compressibility of the electron gas the surface tension can compress its density to a much higher value than the equilibrium density in a homogeneous gas. Consequently, the radius of the electron-gas cluster is slightly smaller than that of the nucleus (in the scaled units). Again the constant-density sphere is included for orientation.

The surface energies for nuclei and atomic clusters were estimated by computing the total energies of the spherical clusters with 20, 40 and 92 particles and fitting them to the total-energy, or mass, formula

$$E(N) = \alpha N + bN^{2/3}. \quad (8)$$

The coefficient α is simply the total energy per particle of the homogeneous system at

Fig. 1. Total energy per particle (upper panel) and local effective potential (lower panel) as functions of particle density for homogeneous nuclear matter (solid line) and for electron gas (dashed line). The electron-gas data are in atomic units and the nuclear data in scaled units explained in the text.

equilibrium density, and the coefficient b represents the surface energy. Table 1 gives the coefficients for the two systems, in atomic units for electrons and scaled units for neutrons. In the scaled units the surface energy of nuclear matter is twice as large as that of the electron gas. It should be noted that our model gives too small surface energies for both systems when compared with real systems. The experimental surface energy for sodium

Fig. 2. Particle-density profiles for spherical clusters of 2, 8, 18 and 20 particles. The solid line is the neutron density, the dashed line the electron density. The dotted line is the background density in the conventional jellium model. Units as in Fig. 1. The 18-particle cluster is denoted with a star (*) because the spherical shape shown is not the ground state.

Table 1

Parameters of the two systems, in atomic units for electrons and in scaled units for nuclei. By Eq. (7), α is the total energy per particle in the homogenous system at equilibrium density and β is related to the incompressibility; b is related to the surface energy through Eq. (8)

System	α	β	b
Jellium	-0.0777	0.0078	0.0149
Nucleus	-0.0505	0.0505	0.0289

and potassium atoms, respectively, gives $b = 0.025$ a.u. and $b = 0.021$ a.u. In nuclei the experimental value is $b = 0.046$ in the scaled units. This latter value takes into account that in our model the total number of nucleons is $A = 2N$ and $E(A) = 2E(n) = \alpha A + 2^{1/3}bA^{2/3}$.

The unrestricted shapes of the clusters were computed using a plane-wave basis. For details we refer to Ref. [16]. Here we only want to emphasize that no symmetry restrictions

Fig. 3. Density profile and effective potential for 92-particle clusters of nuclear matter (solid line) and electrons (dashed line). Units as in Fig. 1.

were imposed on the calculations. Several initial potentials were used for each cluster to guarantee that we obtained the true ground-state geometry. At most two different converged solutions (ground state and an isomer) were found for clusters containing up to 22 particles.

3. Results

Fig. 4 shows the ground-state geometries for jellium clusters and nuclei containing 2 to 22 particles. Generally, jellium clusters and nuclei containing the same number of particles have similar shapes. Inversion symmetry is broken in the jellium clusters of 10, 12, 16 and 18 electrons, whereas for nuclei this happens just barely for the 10- and 22-neutron clusters. The reason for the difference is the larger incompressibility and surface energy of nuclei. As

Fig. 4. Constant-density surfaces for electron clusters and nuclei. The density of the surface is 0.00125 atomic units (or scaled units for nuclei), which corresponds to 38% of the bulk density.

noted for jellium clusters in Ref. [16], any energy gain due to breaking inversion symmetry is extremely small, so that such shapes are “soft” to symmetry-restoring deformation. In nuclei, there is only weak evidence for any ground-state octupole deformations [3], with ^{229}Pa offering the best example.

Some of the atomic clusters can be interpreted as molecules consisting of magic clusters [16]. Thus the four-electron cluster can be viewed as a composite of two dimers. The corresponding nuclear cluster in Fig. 4 is quite similar and can be construed as ^8Be consisting of two alpha particles (for α clustering in light nuclei see Ref. [4]). For six particles we have a smooth oblate shape for electrons and neutrons alike; accordingly we do not have a three-alpha picture of ^{12}C . The 10-electron cluster can be thought of as consisting of an 8-electron cluster and a dimer, but the corresponding nuclear cluster (^{20}Ne) does not lend itself to a quasi-molecular interpretation. The general feature is that, due to their larger surface energy, nuclei deform somewhat less than atomic clusters and are therefore less susceptible to composite structure.

To quantify the differences between the shapes of jellium clusters and nuclei, we have computed the principal moments of inertia $\mathcal{I}_i$ for both systems. As in Ref. [16], we normalize the $\mathcal{I}_i$ so that their sum is 3, i.e.

$$\mathcal{I}_i \equiv 3 \int (r^2 - x_i^2) n(\mathbf{r}) d^3r / 2 \int r^2 n(\mathbf{r}) d^3r. \quad (9)$$

Fig. 5 shows them. The differences between the jellium clusters and nuclei are hardly noticeable. Even in the cases where inversion symmetry is broken in jellium clusters, there is no difference in the moments of inertia.

The total energy per particle is shown in Fig. 6. Both types of cluster show a similar odd-even staggering (odd clusters were computed only up to nine particles). Generally, the odd-even staggering is a much stronger effect than the variation caused by the shell structure. Only weak minima are seen at the magic sizes 8 and 20. To see more clearly the effects of the magic numbers, we have subtracted from the total energy the mass formula (7). The resulting energy difference is shown in Fig. 7 for the even clusters. The results

Fig. 5. Principal moments of inertia for nuclei (black squares) and jellium clusters (open squares). The sum of the three moments of inertia is normalized to be 3.

for nuclear matter and the electron gas are seen to be nearly identical. The clusters of 2, 8 and 20 particles represent deep minima relative to their neighbours. In addition, the size 14 shows a clear minimum, which indicates that this strongly deformed prolate cluster is “semimagic”.

The clusters of 14, 18, 20 and 22 particles have stable isomers. The isomers of the electronic clusters are discussed in detail in Ref. [16]. Here we wish to emphasize that similar isomers, representing shape coexistence, are obtained also for the nuclear clusters. Such shape coexistence is well established as a general feature of nuclei [2]. As in the case of the ground states, the shapes and especially the moments of inertia of the isomeric states are nearly equivalent in nuclear and electronic clusters.

The calculated shapes of the nuclei can be used to determine the intrinsic quadrupole moment Q_0 for the ground state. It is computed from the particle density according to

$$Q_0 = \sqrt{16\pi/5} \int r^2 Y_{20}(\theta, \phi) n(\mathbf{r}) d^3r. \quad (10)$$

Again, as in the case of the moments of inertia, the results for nuclei and jellium clusters are the same to within a few percent when they are scaled with the bulk density. This

Fig. 6. Total energy per particle for nuclei (black squares) and electron clusters (open squares). Units as in Fig. 1. The energies for the small odd clusters are shown as crosses.

Fig. 7. The difference of the total energy from the mass formula, Eq. (7). Open circles show electrons in atomic units and black dots nuclei in scaled units (see the text). Only even clusters are shown.

means that the quadrupole moment is totally insensitive to the interaction between the fermions in question. In other words, we can predict the quadrupole moments of small nuclei by knowing only the density of nuclear matter; no detailed knowledge is needed about the nuclear forces since they do not enter the computation.

Fig. 8 shows the calculated intrinsic quadrupole moments for even nuclei together with the experimental estimates. Unlike the spectroscopic quadrupole moment Q , the intrinsic quadrupole moment Q_0 is a model-dependent quantity that cannot be measured directly. We have estimated Q_0 from the measured quadrupole moment of the 2_1^+ state using the axially symmetric rigid-rotor model [1],

$$Q = \frac{3K^2 - J(J+1)}{(J+1)(2J+3)} Q_0, \quad (11)$$

where in our case $K = 0$ and $J = 2$. The experimental values for the quadrupole moments $Q(2_1^+)$ are taken from Ref. [19].

Another way to estimate the intrinsic quadrupole moment Q_0 also relies on the simple rigid-rotor model [1,20]. On that model, the E2 transition probabilities contain Q_0 . Particularly well known are the excitation probabilities $B(E2; 0_1^+ \rightarrow 2_1^+) \equiv B(E2)^\dagger$, whence

$$|Q_0| = \left[\frac{16\pi}{5} \frac{B(E2)^\dagger}{e^2} \right]^{1/2}. \quad (12)$$

The experimental values for $B(E2)^\dagger$ are taken from reference Ref. [20]. This method does not determine the sign of Q_0 . We have adopted the sign as determined from Eq. (11).

Fig. 8 shows that the calculated values of Q_0 are in excellent agreement with the experimental ones, except for $N = 14$ and $N = 16$ where the sign is wrong. In the case of $N = 14$ the experimental value is close to that for the oblate isomer found by the theoretical model. The $N = 16$ cluster does not have any isomers, but the cluster is extremely soft to deformation [16]. In this case it is expected that the simple model determining the intrinsic quadrupole moment according to Eqs. (11) and (12) is not valid. It should be emphasized that the intrinsic quadrupole moment is calculated from a very simple local-density model, which is not at all sensitive to the compressibility or surface energy

Fig. 8. Intrinsic quadrupole moments Q_0 of light nuclei. Black dots connected with the line are theoretical values for the ground state. The theoretical value for the $N = 14$ isomer is shown as a black square. The open circles are experimental Q_0 values determined from the quadrupole moments of the 2_1^+ states. The triangles are experimental values based on the E2 excitation probability. The experimental values [19] are for $Z = N$ nuclei, except for $N = 4$ where the nearest available value is taken from ^{10}Be .

used.

4. Discussion and conclusions

Deformation of metal clusters and nuclei can be studied by solving the same equations. The only difference is the density dependence of the local effective potential, which reflects the compressibility of the fermion gas in question. A smaller compressibility leads to a larger surface energy. Since deformation from spherical shape increases the surface area,

one would expect that the degree of deformation is sensitive to the surface energy. However, electron-gas clusters and nuclei of the same particle number are very similar in shape, so that the dependence on surface energy is only slight.

Our results agree well with the Hartree-Fock calculations reviewed by Ripka [6] and Svenne [7]. Their contour plots for the densities of ^{12}C (oblate), ^{20}Ne (prolate) and ^{24}Mg (triaxial) agree with the shapes in our Fig. 4 for the corresponding nuclei ($N = 6, 10, 12$). However, for ^{28}Si we have a prolate ground state and an oblate isomer ($N = 14$), while the Hartree-Fock results are just opposite. This is the sign discrepancy of the quadrupole moment discussed above.

It is of interest to compare our results with those from atomistic models of metal clusters. The ground-state geometries for the smallest clusters of alkali metals have been computed using *ab initio* configuration-interaction methods [21] and the local-density approximation with pseudopotentials [22]. Up to eight atoms, the geometries agree qualitatively with those obtained with the jellium model. A four-atom cluster is a rhombus, which is an atomistic realization of the prolate shape. The six-atom cluster is a nearly planar pentagon with one atom in the centre. This resembles closely the oblate shape resulting from the jellium calculation. Unfortunately there are hardly any calculations for the strongly deformed clusters of 14 or 18 particles, which we find to be prolate and oblate, respectively. However, recent calculations indicate that for Na_{14} the prolate geometry as well as the oblate isomer are stable even at high temperatures [23].

The simplest atomistic model, the Hückel model, also predicts that the 14-electron cluster is strongly deformed and prolate, whereas the cluster with 18 electrons is oblate [24]. These atomistic computations indicate that even when the single-particle wave functions are molecular orbitals they form shapes similar to those produced by the continuum models.

The simple model of this paper, based on the local-density approximation, can be used for other fermion systems as well. The ultimate jellium model serves as an approximation

for electron-positron clusters. A better approximation for this system could be obtained by adding a local electron-positron correlation. A similar model can be constructed for an electron-hole plasma in semiconductors. These systems are expected to resemble closely the ultimate jellium. On the other hand ^3He has a small compressibility like nuclear matter [25,26] and is expected to form similar clusters. However, our present model suggests that the deformation of small clusters is similar in all fermion systems.

In conclusion, we have used a simple model to study the deformation from a spherical shape in small nuclei and in jellium clusters. We have shown that cluster shapes are determined by the number of particles and they depend only weakly on the density dependence of the effective potential. Especially the intrinsic quadrupole moment is insensitive to the details of the model and can be estimated by knowing only the density of nuclear matter.

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