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Pygmy dipole resonances in the calcium isotopes

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We present microscopic density functional theory calculations of the total dipole absorption cross sections of the even-A calcium isotopes from ^{40}Ca through ^{48}Ca. The results reveal the onset of a collective dipole oscillation occurring at low energy and decoupled from the giant dipole resonance. The radial density fluctuations associated with this low-lying mode have the character of the pygmy dipole resonance predicted to exist in neutron rich nuclei.

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Recently, the availability of beams of light, unstable nuclei has elicited increased interest in the physics of neutron rich nuclei [1]. These nuclei display several features not readily observed in stable light nuclei with $N \approx Z$. One of these is the so-called "neutron halo" [2], which has been the focus of intense investigation [3]. Another is the "soft" [1,2] or "pygmy" [4] dipole resonance (PDR), which is thought to result from the excess neutron density vibrating out of phase with a stable core nucleus [5,6]. This paper presents results on the structure of that particular resonance obtained from a microscopic study of the the electric dipole response of the calcium isotopes.

We first present the density functional theory (DFT) formalism [7–9] used to determine both the ground state properties of the nuclei and their collective excitations. This theory is an elegant method for simplifying the many-body problem and has found a wide range of applications, primarily in atomic, molecular, and condensed matter physics [7,8]. In these contexts it is based on the rigorous theorem of Hohenberg and Kohn [10], which establishes the total energy as a functional of the electronic density; the density which minimizes the energy functional is then the true ground state density of the system.

Extensions of the theory to nuclear systems is hampered by the absence of an external potential confining the nucleons. Although some formal justification for the theory in the nuclear context has appeared [9], most applications are based on a heuristic generalization in which the energy is considered a functional of both the proton (ρ_p) and neutron (ρ_n) densities [11,12]. Such applications have demonstrated that the theory provides a reasonable description of ground state properties, but no applications to collective response have been presented yet.

The functional we employ is composed of several terms, which we write as

$$E[\rho_p,\rho_n]=E_k[\rho_p,\rho_n]+E_c[\rho_p]+E_n[\rho_p,\rho_n]+E_\nabla[\rho_p,\rho_n]. \quad (1)$$

Following the electronic example [13], we define $E_k[\rho_p,\rho_n]$ to be the kinetic energy of a collection of Z noninteracting protons and N noninteracting neutrons, which have densities ρ_p and ρ_n, respectively. This kinetic energy term can be expressed in the form

$$E_k[\rho_p,\rho_n]=\sum_{\lambda,\tau}\int d^3r\,\phi^*_{\lambda\tau}(\mathbf{r})\left(-\frac{\hbar^2}{2m}\nabla^2\right)\phi_{\lambda\tau}(\mathbf{r}) \quad (2)$$

in which the single-particle wave functions satisfy the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\phi_{\lambda\tau}(\mathbf{r})+v^\tau_{\rm eff}(\mathbf{r})\phi_{\lambda\tau}(\mathbf{r})=\epsilon_{\lambda\tau}\phi_{\lambda\tau}(\mathbf{r}). \quad (3)$$

The function $v^\tau_{\rm eff}(\mathbf{r})$ is a local effective potential confining the nucleons with isospin index τ, and $\epsilon_{\lambda\tau}$ is the corresponding single-particle eigenvalue. The above assumes the existence of such a local potential which allows the construction of the nucleon densities according to $\rho_\tau(\mathbf{r})=\Sigma_\lambda|\phi_{\lambda\tau}(\mathbf{r})|^2$.

The energy associated with the Coulomb interaction is simply

$$E_c[\rho_p]=\frac{e^2}{2}\int d\mathbf{r}\int d\mathbf{r}'\,\frac{\rho_p(\mathbf{r})\rho_p(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|} -e^2\left(\frac{3}{4}\right)\left(\frac{3}{\pi}\right)^{1/3}\int d\mathbf{r}\,\rho_p^{4/3}(\mathbf{r}). \quad (4)$$

The first term represents the classical Coulomb self-energy, while the second denotes a local approximation to exchange.

The $E_n[\rho_p,\rho_n]$ term encompasses part of the effects of the strong nuclear force as represented by the energy of infinite nuclear matter. Within a local density approximation [10] we have

$$E_n[\rho_p,\rho_n]=\int d\mathbf{r}\,\rho(\mathbf{r})\epsilon_n(\rho_p(\mathbf{r}),\rho_n(\mathbf{r})), \quad (5)$$

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where $\rho(\mathbf{r})=\rho_p(\mathbf{r})+\rho_n(\mathbf{r})$ and $\epsilon_n(\rho_p,\rho_n)$ is the energy per nucleon of infinite nuclear matter having the densities ρ_p and ρ_n. Following Brueckner *et al.* [11], we use the parametrization

$$\epsilon_n(\rho_p,\rho_n)=\sum_{i=1}^{3} b_i(1+a_i\alpha^2)\rho^{n_i}, \tag{6}$$

where α is the asymmetry parameter defined as $\alpha=(\rho_p-\rho_n)/(\rho_p+\rho_n)$. With $n_1=1$, $n_2=4/3$, and $n_3=5/3$, the coefficients a_i and b_i were obtained by fitting to the equation of state of ter Haar and Malfliet [14]; we find $a_1=-0.684$, $a_2=-0.943$, $a_3=-1.743$, $b_1=-779.5$, $b_2=1185.0$, and $b_3=-345.6$. These values give the energy in MeV when the density is expressed in units of fm^{-3}. The coefficients differ from those of Lombard [12], which were found to give unphysical interaction energies for high densities and large asymmetries.

The final term, $E_\nabla[\rho_p,\rho_n]$, is a correction for the inhomogeneities in a finite nucleus. It was taken in the form of a gradient correction [11,12]

$$E_\nabla[\rho_p,\rho_n]=\int d\mathbf{r}\,\{\eta|\nabla\rho(\mathbf{r})|^2+\kappa|\nabla(\rho(\mathbf{r})\alpha(\mathbf{r}))|^2\}, \tag{7}$$

which can be viewed as the leading terms in a systematic gradient expansion. This correction is essential since without it the nuclei are found to be severely overbound and contracted. The gradient coefficients η and κ are in principle functions of the nucleon densities, but in practice we have treated them as constants for each particular nucleus. For the ground state properties, κ plays a secondary role since the asymmetry α is typically small in the nuclei studied, and could be set to zero without adversely affecting our fits to the equilibrium properties. However, as we will see, κ cannot be neglected since it has an important effect on the dynamic response.

The equilibrium properties are determined by minimizing $E[\rho_p,\rho_n]$ with respect to the proton and neutron densities. This is achieved [13] by solving Eq. (3) self-consistently with $v^\tau_{\mathrm{eff}}(\mathbf{r})$ defined as the functional derivative of the interaction part of the energy functional in Eq. (1). To reproduce the experimental binding energies, the parameter η was adjusted accordingly; it was found to exhibit essentially a linear relationship with neutron excess, from a value of 50.7 MeV fm^5 for $^{40}\mathrm{Ca}$ to 32.5 MeV fm^5 for $^{48}\mathrm{Ca}$. For each of these isotopes the calculated rms radii fell within experimental uncertainty of the observed values [15], indicating that our method provides a realistic characterization of ground state properties.

Having determined the ground state proton and neutron densities for each of the calcium isotopes, we then performed linear response calculations to examine the effect of electric dipole perturbations. Within the DFT formalism [16,17], the variation in the equilibrium density is given by

$$\delta\rho_\tau(\mathbf{r},\omega)=\int d\mathbf{r}'\,\chi^\circ_\tau(\mathbf{r},\mathbf{r}',\omega)[\delta v_{\mathrm{ext}}(\mathbf{r}',\omega)+\delta v^\tau_{\mathrm{eff}}(\mathbf{r}',\omega)] \tag{8}$$

where $\delta v_{\mathrm{ext}}(\mathbf{r},\omega)$ is the externally applied perturbation at frequency ω and

$$\delta v^\tau_{\mathrm{eff}}(\mathbf{r},\omega)=\int d\mathbf{r}'\sum_{\tau'}\left.\frac{\delta v^\tau_{\mathrm{eff}}(\mathbf{r})}{\delta\rho_{\tau'}(\mathbf{r}')}\right|_{\rho^\circ_{\tau'}}\delta\rho_{\tau'}(\mathbf{r}',\omega) \tag{9}$$

accounts in an average way for the effects of the nucleon-nucleon interactions in the polarized state. In contrast to the usual nuclear random phase approximation calculations [18], this effect is incorporated through changes in the effective potential acting on the nucleons rather than by means of an effective (nonlocal) nucleon-nucleon interaction represented, for example, by the Skyrme interaction.

Finally, the noninteracting density response function appearing in Eq. (8) is given by

$$\chi^\circ_\tau(\mathbf{r},\mathbf{r}',\omega)=2\sum_i^{\mathrm{occ}}\sum_m \phi_i^*(\mathbf{r})\phi_m(\mathbf{r})\left(\frac{1}{\epsilon_m-\epsilon_i-\hbar\omega}+\frac{1}{\epsilon_m-\epsilon_i+\hbar\omega}\right)\phi_m^*(\mathbf{r}')\phi_i(\mathbf{r}'). \tag{10}$$

where the states $\phi_i(\mathbf{r})$ and $\phi_m(\mathbf{r})$ are eigenstates of the ground state Hamiltonian. The factor of 2 accounts for the assumed spin degeneracy of the occupied states. While the sum over m includes all eigenstates, transitions to occupied m states cancel and therefore do not contribute to the response function, as required by the Pauli exclusion principle. The response function is conveniently calculated by expressing it in terms of single-particle Green's functions [16,17], which in turn are constructed from regular and irregular solutions to the radial Schrödinger equation. In this way, both continuum and bound state excitations are included.

In our application to the study of electric dipole responses of the calcium nuclei, we employ the electric dipole operator as the external potential. Eliminating center-of-mass motion to avoid spurious isoscalar $E1$ resonances, the dipole operator is written

$$\delta v_{\mathrm{ext}}(\mathbf{r},\omega)=\sum_\tau q_\tau\left(\sum_m r\,Y_{1m}(\hat{r})\right), \tag{11}$$

with effective charges $q_p=eN/A$ for protons and $q_n=-eZ/A$ for neutrons. Note here that Eqs. (8) and (9) constitute a pair of integral equations for the density fluctuations $\delta\rho_\tau(\mathbf{r},\omega)$ and that by discretizing the radial variable, these integral equations are reduced to a set of linear equations which are solved numerically to obtain the density fluc-

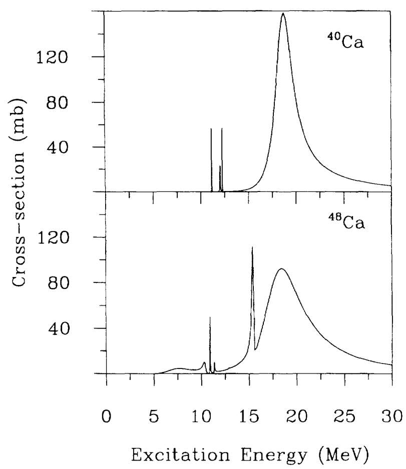

FIG. 1. Calculated total dipole absorption spectrum for ^{40}Ca and ^{48}Ca as a function of the excitation energy.

tuations. Once these have been determined, the total photoabsorption cross section is calculated using

$$\sigma_{\mathrm{abs}}(\omega)=\frac{4\pi\omega}{c}\int d\mathbf{r}\sum_{m} r\,Y_{1m}^{*}(\hat{r})\sum_{\tau} q_{\tau}\mathrm{Im}\;\delta\rho_{\tau}(\mathbf{r},\omega). \tag{12}$$

The $E1$ absorption spectra for ^{40}Ca and ^{48}Ca are displayed in Fig. 1. In both cases the dominant feature centered at approximately 19 MeV corresponds to the giant dipole resonance (GDR) and exhausts the Thomas-Reiche-Kuhn sum rule to within a few percent. Although the κ parameter in the gradient correction was not needed for the ground state calculations, it is required to position the GDR correctly. In the case of ^{40}Ca, the GDR appears at 15 MeV and is far too narrow when $\kappa=0$, while a value of $\kappa=363$ MeV fm^5 places the resonance close to the experimental position with a reasonable width. This effect can be easily understood in view of the fact that the gradient correction associated with κ tends to inhibit a large proton-neutron asymmetry in the surface region of the nucleus. Since this is precisely the character of the isovector GDR polarization, a finite κ value introduces an additional restoring force which acts to shift the GDR up in energy. On the other hand, for an isovector polarization in which the total density remains essentially constant, the parameter η has no effect. We have used the same value of κ for all the isotopes and find that the GDR remains close to 19 MeV as shown in Fig. 1 and consistent with experiment [19].

We also obtain, below the GDR, several narrow peaks which are derived from single-particle dipole transitions. More interestingly, we find a broad resonance for the neutron-rich isotopes in the energy range 5–10 MeV. In Fig. 2, we focus on this particular spectral range. The relative strength of the resonance increases as more neutrons are added to the valence f shell—a result quantified in Fig. 3, where we display, as a function of neutron excess, both the centroid position of the resonance and its integrated strength.

The smooth character of the resonance is evidence of a collective excitation of decidedly different character from the sharply peaked single-particle-like excitations. To better es-

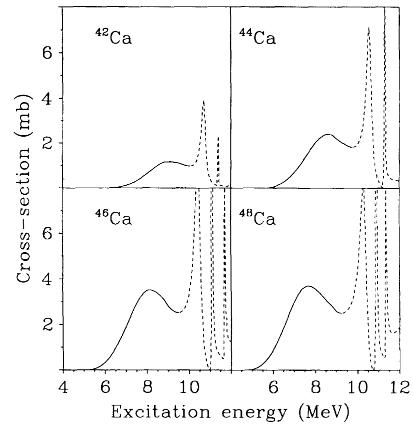

FIG. 2. Calculated low energy photoabsorption spectra for ^{42}Ca–^{48}Ca. The smooth broad peak seen in all isotopes and highlighted by a solid line is the part of the spectrum identified as the pygmy dipole resonance. The dashed portions correspond to single-particle-like excitations as distinct from the PDR.

tablish the character of this collective state we plot in Fig. 4 the variation of the polarization density along the nuclear axis for an excitation energy of about 8 MeV. This figure displays a neutron polarization which clearly can be interpreted as a *surface neutron density oscillating out of phase with a stable* ^{40}*Ca core*, thus consistent with the character of the collective excitation usually associated with the pygmy dipole resonance.

The possibility of a PDR in neutron-rich calcium isotopes has been investigated recently by Suzuki, Ikeda, and Sato [6] using a three-fluid model first introduced by Mohan, Danos, and Biedenharn [5]. In this model the valence neutrons are treated as a distinct component from the neutron fluid comprising the core of the nucleus. With this additional degree of freedom, both the GDR and PDR collective modes were obtained [5]. Suzuki, Ikeda, and Sato [6] imposed the additional constraint that the core neutrons oscillate together with the protons, thereby eliminating one degree of freedom and leaving only the PDR. In addition, these authors arbitrarily choose ^{46}Ca as their core and considered an exotic range of

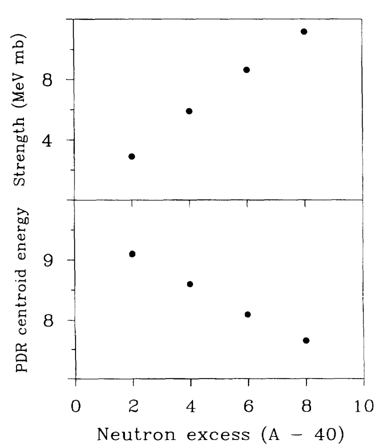

FIG. 3. Centroid energy and integrated strength of the pygmy dipole resonance calculated as a function of the number of neutrons excess to the ^{40}Ca core.

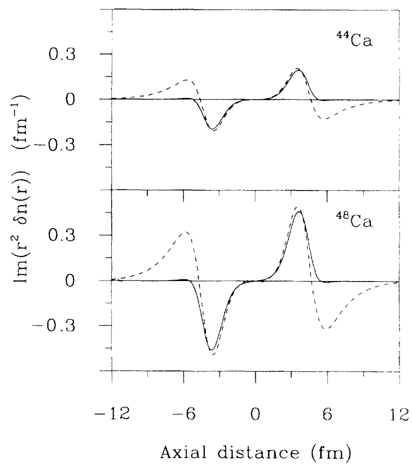

FIG. 4. Nucleon density variation calculated in the region of the pygmy resonance. ^{44}Ca is shown at 8 MeV, ^{48}Ca at 7.6 MeV. The solid line is for protons, the dashed line for neutrons.

isotopes reaching up to ^{61}Ca. Their model predicts the position of the the PDR to increase with neutron excess in contrast to our results which show the opposite behavior. One can understand such a result by invoking an analogy with a simple harmonic oscillator model where the resonance frequency is determined by the restoring force per particle. Since our PDR is associated with continuum excitations of the $1f$ neutrons, the separation energy is a measure of how tightly bound these neutrons are. Thus, as the threshold energy for $1f$ neutron emission decreases with increasing neutron excess, the centroid energy of the PDR should be expected to decrease with it, as we indeed find in our calculations.

Another quantitative disagreement with the hydrodynamic model is seen in the strength of the PDR. In our calculation for ^{48}Ca, for example, the PDR has a strength of $\leqslant 2\%$ of the total absorption cross section (most of which is concentrated in the GDR). On the other hand, the hydrodynamic estimate is about 10% for a system with a neutron excess of 8. However, these differences should not be overstated since the hydrodynamic description is after all a simplified picture with obvious limitations. In fact it was constructed specifically to yield the PDR, whereas in our calculation this collective mode arises naturally through the microscopic treatment of the full dipole response.

In conclusion, we have shown that the density functional formalism can provide a unified description of both ground state and collective nuclear properties. In the case of calcium isotopes with $N>Z$, we find a collective dipole mode at low energies—the so-called pygmy dipole resonance—which involves the oscillation of the neutron excess against a ^{40}Ca core. These results of course have a broader significance in the context of the PDR in heavier neutron-rich nuclei where their presence has already been ascertained [4], as well as in the physics of neutron halos [1]. This, we hope, will encourage experimental studies to explore the onset of collective resonances well below the GDR, especially now that higher resolution machines are becoming available.

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