A systematic contribution to the binding energy of nuclei

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A systematic contribution to the ground state energy coming from the Coulomb interaction between nucleons is considered. Besides the Hartree and Fock terms there is a significant Coulomb correlation term due to the correlated motion of nucleons under the influence of a strong interaction between nucleons. The correlation term is strongly enhanced by the presence of the surface, and this mechanism accounts for a main part of the Okamoto–Nolen–Schiffer anomaly in the binding energy differences. The contribution to the bulk energy and surface tension is considered. © *1996 American Institute of Physics.*

The Okamoto–NOlen–Schiffer anomaly in the binding energy differences of mirror nuclei[1] has attracted much interest during the last 3 decades. Most of the earlier attempts at resolving the anomaly addressed many-body effects suspected of being at the root of the problem (see Refs. 2–5). During the last few years, efforts have shifted towards trying to explain the magnitude of the anomaly in terms of the charge-symmetry-breaking (CSB) nuclear forces.[4,6,7] A correction arising from CSB forces, taken within the usual perturbative estimate, has a volume character, and its main term should be proportional to the number of protons (or neutrons). The correction we are discussing in this letter has a completely different mass dependence and is proportional to the nuclear surface, i.e., in case of the Coulomb interaction is $\propto Z^{2/3}$. We shall show that there is a systematic many-body mechanism which enhances the contribution due to the Coulomb interaction, in particular, and which is based on a common feature of a self-sustaining system: the presence of a surface.

The ground state energy E of a nucleus can be written in terms of the density functional approach[8,9] as follows

$$E=F_0[\rho_p(\mathbf{r}),\rho_n(\mathbf{r})]+F_c[\rho_p(\mathbf{r}),\rho_n(\mathbf{r})]. \tag{1}$$

Here F_0 is the main part of the functional, which is due to isospin-symmetry-conserving forces that depend symmetrically on the densities ρ_p, ρ_n, while F_c is due to CSB forces, i.e., to the Coulomb interaction in our case, and $\rho_p(\mathbf{r})$, $\rho_n(\mathbf{r})$ are the single-particle densities of neutrons and protons, respectively. The well-known Skyrme functional[10] can be considered as a possible realization of F_0, and F_c is given by[8]

$$F_c[\rho_p(\mathbf{r})]=F_c^{HF}=\frac{e^2}{2}\int \rho_p(\mathbf{r}_1)\rho_p(\mathbf{r}_2)\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}d\mathbf{r}_1 d\mathbf{r}_2$$
$$-\frac{e^2}{2}\int [\mathrm{Im}\,\chi_p^0(\mathbf{r}_1,\mathbf{r}_2,\omega)+\pi\rho_p(\mathbf{r}_1)\delta(\mathbf{r}_1-\mathbf{r}_2)]\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\frac{d\mathbf{r}_1 d\mathbf{r}_2 d\omega}{\pi}. \tag{2}$$

Here the first term on the right-hand side is the Hartree term, the second is the Fock term, and $\chi_p^0(\mathbf{r}_1,\mathbf{r}_2,\omega)$ is the linear response function of noninteracting protons moving in a self-consistent field. In this case, F_c obviously depends only on ρ_p. When taken in the local-density approximation or in the Slater approximation, the second term is equal to $-(3/4)(3/\pi)^{1/3}\int \rho_p^{4/3}(\mathbf{r})d\mathbf{r}$(Ref. 8). The equilibrium densities and the ground-state energy E can be found by using the well-known procedure of solving the Hartree–Fock-like equations which are directly derived from Eq. (1) (Ref. 8 and 10). Now let us recall that the nucleons move in a correlated manner in the nucleus. That is, instead of the linear response function $\chi_p^0(\mathbf{r}_1,\mathbf{r}_2,\omega)$ we have to use the linear response function $\chi_p(\mathbf{r}_1,\mathbf{r}_2,\omega)$ calculated with $V(\mathbf{r}_1,\mathbf{r}_2)$ being the effective interaction associated with the strong nucleon–nucleon interaction.[5,9] As a result, we have to add on the right-hand side of Eq. (2) a third term F_c^{corr}, which comes from the difference $\chi_p - \chi_p^0$ and gives rise to the so-called Coulomb correlation energy, which is of first order in the Coulomb interaction:[11]

$$F_c^{\mathrm{corr}}[\rho_p(\mathbf{r})]=-\frac{e^2}{2}\int \mathrm{Im}[\chi_p(\mathbf{r}_1,\mathbf{r}_2,\omega)-\chi_p^0(\mathbf{r}_1,\mathbf{r}_2,\omega)$$
$$-\chi_p^0(\mathbf{r}_1,\mathbf{r}_2,\omega)]\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\frac{d\mathbf{r}_1 d\mathbf{r}_2 d\omega}{\pi}. \tag{3}$$

The systematic contribution to the binding energy which we are discussing here arises from the correlation part of the energy, Eq. (3). We shall discuss this correlation energy contribution as a function of the density first in infinite homogeneous nuclear matter, then in semi-infinite matter, and at last in finite systems. We shall study the correlation energy of infinite and semi-infinite matter within the well-known jellium model (as one does when considering the correlation energy of an electron gas[12]) in order to get rid of the Hartree part of the Coulomb energy.

In infinite nuclear matter χ_p has a simple algebraic structure, due to the transitional invariance of such a system. The correlation energy density ΔE_{corr} can be represented as follows (for the sake of simplicity here we have suppressed the spin–isospin coordinated).

$$\Delta E_{\mathrm{corr}}=-\frac{1}{(2\pi)^4}\int d^3q d\omega\ \mathrm{Im}\left[\chi_0(\omega)\frac{V\chi_0(\omega)}{1-V\chi_0(\omega)}\right]U, \tag{4}$$

where U is the Coulomb interaction $U = 4\pi e^2/q^2$. we shall calculate ΔE_{corr} from Eq. (4), using the Landau–Migdal parametrization for the residual interaction (neglecting the spin dependence and the momentum dependence)[5]

$$V=\frac{d\varepsilon_F}{d\rho_0}\left\{\left[f_{\mathrm{ex}}+\left(f_{\mathrm{in}}-f_{\mathrm{ex}}\frac{\rho(\mathbf{r}_1)}{\rho_0}\right)+\left[f'_{\mathrm{ex}}+(f'_{\mathrm{in}}-f'_{\mathrm{ex}})\frac{\rho(\mathbf{r}_1)}{\rho_0}\right]\vec{\tau}_1\cdot\vec{\tau}_2\right\}\delta(\mathbf{r}_1-\mathbf{r}_2), \tag{5}$$

where $f_{ex} \approx -2.5$, $f_{in} \approx -0.1 \ldots 0.0$, and $f'_{ex} \approx f'_{in} \approx 0.5$, ρ_0 is the equilibrium nuclear matter density, and $d\varepsilon_F/d\rho_0 \approx 300\text{MeV}\cdot\text{fm}^3$. The stability of nuclear matter requires that the Landau–Migdal parameters satisfy the Pomeranchuk stability conditions $f_{in} > -0.5$ and $f'_{in} > -0.5$. One can easily separate the correlation energy $\varepsilon_c(\rho_p) = \Delta E_{corr}/\rho_p$ into a contribution due to the isoscalar modes and one due to isovector modes. We refer to these as the isoscalar $\varepsilon_{corr}(\rho_p)$ and isovector $\varepsilon'_{corr}(\rho_p)$ correlation energies. For the case of the Coulomb interaction between protons in symmetrical nuclear matter ($\rho_p^0 = \rho_0/2$) the isoscalar and isovector Coulomb correlation energies are approximately[11]

$$\varepsilon_{corr}(\rho_p^0 = 0.05 \ \text{MeV}\cdot\text{fm}^{-3}, \quad \varepsilon'_{corr}(\rho_p^0) = -0.15 \ \text{MeV}\cdot\text{fm}^{-3}. \tag{6}$$

Since the residual interaction V has a strong density dependence and the *isoscalar* part is strongly attractive in the region of low densities, uniform nuclear matter becomes unstable around $\rho \approx 0.6\rho_0$. The *isoscalar* part of the linear response function χ has a pole at $\omega = 0$, at the point where the nuclear compressibility vanishes (and the spinodal instability sets in), and, as result, the *isoscalar* Coulomb correlation energy diverges [see Eq. (4)]. It is noteworthy that the instability occurs in the *isoscalar* channel, and even though the Coulomb interaction seemingly breaks the isospin symmetry and one might naively expect that the isovector collective modes would be perhaps more relevant, the major contribution occurs in the isoscalar channel. With decreasing density the isovector Coulomb correlation energy decreases monotonically in magnitude, and no singularity ever appears in this channel.

The above remarks allow us to draw at once several qualitative conclusions. First of all, the Z dependence of the various terms in Eqs. (2) and (4) for a finite system should read as follows:

$$\Delta E_H \sim Z^2, \quad \Delta E_{ex} \sim Z, \quad \Delta E_{corr} \sim a_v Z + a_s Z^{2/3}, \tag{7}$$

and most likely the major contribution to the Coulomb correlation energy will arise from the surface of a nucleus (i.e., $|a_v| \ll a_s$). Moreover, one can fairly well expect that $a_s > 0$, since in the surface region the residual interaction is attractive, [see Eq. (4)] while the Coulomb exchange contribution is negative, and one can expect a partial cancellation of these contributions.

Because of the above-mentioned instability in the isoscalar response at low densities, the surface region requires a more thorough treatment. It is convenient in this case to introduce a coordinate system with the z axis normal to the surface and to present χ_p in a mixed coordinate–momentum (z, $\mathbf{q}$) representation where $\mathbf{q}$ is the momentum parallel to the surface. The Coulomb correlation energy per unit surface area, or the surface tension σ_c, can be written as

$$[\Delta E_{corr}]_s = \sigma_c = \int dz \rho_p(z)[\varepsilon_c(\rho_p(z)) - \varepsilon_c(\rho_p(-\infty))], \tag{8}$$

$$\varepsilon_c(\rho_p(z)) = -\frac{1}{(2\pi)^3 \rho_p(z)} \int d\omega d^2q dz' U(\mathbf{q}, z') \times \text{Im}\left[\chi_p\left(\mathbf{q}, z + \frac{z'}{2}, z - \frac{z'}{2}, \omega\right) - \chi_p^0\left(\mathbf{q}, z + \frac{z'}{2}, z - \frac{z'}{2}, \omega\right)\right], \tag{9}$$

where $U(\mathbf{q},z')=2\pi e^2\exp(-q|z'|)/q$.

One can use now the local-density approximation (LDA) to construct the Coulomb correlation energy functional (3) of finite nuclei,

$$F_c^{\rm corr}[\rho_p(\mathbf{r})]=\int \varepsilon_c(\rho_p(\mathbf{r}))\rho_p(\mathbf{r})d\mathbf{r} \tag{10}$$

with $\varepsilon_c(\rho_p)$given by Eq. (9). We remark that the LDA has traditionally been used in condensed-matter physics and nuclear physics calculations.

For semi-infinite nuclear matter the isoscalar and isovector Coulomb correlation energies thus obtained have quite different behaviors. The isovector part, while larger than the isoscalar part in the interior, is much smaller and decreasing in the surface region. At the same time, the isoscalar component of the Coulomb correlation energy has a very prominent peak at the surface, as one might have expected from our earlier argument for the case of infinite homogeneous matter of low density. It is worthy of note that it is the peak that gives the main contribution to the surface tension σ_c and, as one could anticipate, to the binding energy differences of mirror nuclei. Using these results for semi-infinite nuclear matter, one can now extract the volume and surface terms in the Coulomb correlation energy [see Eqs. (6) and (8)], and thus one gets $a_v \approx -0.1 \pm 0.1$ MeV and $a_s \approx 1.0...1.2$ MeV, respectively. Since we have used a zero-range residual interaction, these numbers should be taken as upper bounds. the uncertainty in a_s and especially in a_v arises mostly from the uncertainties in the Landau–Migdal parameter $f_{\rm in}$. The available phenomenological estimates do not agree even on the sign, i.e., on whether the isoscalar residual interaction is attractive or repulsive, but in any case the actual value is rather small. In the bulk a collective mode (Landau zero sound) will exist only if the residual interaction is repulsive. The fact that, so far, there seem to be no conclusive experimental indications that volume collective modes exist in finite nuclei—only the existence of surface modes is well established—is an indirect indication that $f_{\rm in}$ is indeed small.

Now, using the density function given by Eqs. (1), (2), and (10), one can calculate the Coulomb displacement energies. We stress that the density functional has no double-counting uncertainty in computations of such terms as two- and many-body short- and long-range correlations, core excitations, and configuration mixing.[2,3]

We have considered four pairs of mirror nuclei mass differences: ^{15}O–^{15}N; ^{17}F–^{17}O; ^{39}Ca–^{39}K; ^{41}Sc–^{41}Ca. These differences have been calculated, using the *SIII*[13] interaction for the F_0 in Eq. (1), with F_c given by Eqs. (2) and (10). We have also included the electromagnetic corrections, the vacuum polarization, and the finite radius of a neutron and proton.[2,3] The results of the calculations are in a good agreement (within 70 keV) with the experiment.[2] The contribution of the Coulomb correlation energy to the Coulomb displacement energy is $\delta E_{\rm corr}$=0.33 MeV in the A=40 region, and $\delta E_{\rm corr}$ = 0.25 MeV in the A=16 region. We estimate the accuracy of the calculation of $\delta E_{\rm corr}$ to be 20%.

We have also carried out direct computations of $\delta E_{\rm corr}$ in order to check the quality of the local-density approximation used and to analyze this value in more detail. Since the enhancement of the Coulomb correlation energy is due to the existence of the surface,

and thus is determined by gross nuclear features, we can analyze this phenomenon within the framework of simple models. Here is a brief description of the chosen model and calculation. For both neutrons and protons we use the same single-particle Wood–Saxon potential (well depth $V_0 = -53$ MeV, radius $R_0 = 1.25\ A^{1/3}$ fm, diffuseness $a = 0.65$ fm, and an appropriate spin–orbit potential) and neglect the Coulomb field of the protons. We have calculated the linear response function χ_p in coordinate representation for multipolarities $l = 0,\ldots,12$. The residual interaction is chosen of the separable form,

$$V(\mathbf{r}_1,\mathbf{r}_2)=\lambda\sum_{lm}\frac{dV_0(r_1)}{dr}\frac{dV_0(r_2)}{dr}Y^*_{lm}(\Omega_1)Y_{lm}(\Omega_2),$$

where $V_0(r)$ is the single-particle potential. The parameter λ is chosen so that the dipole linear response has a pole at $\omega=0$, while the Coulomb correlation energy is given by Eq. (3). This type of residual interaction has been widely studied[8,14] and leads to a satisfactory description of nuclear collective modes. The calculated $\delta E_{\rm corr}$ are of the order 200–300 keV in either the oxygen or calcium region, i.e., are of the same order of magnitude as the Okamoto–Nolen–Schiffer anomaly.[2,3] Thus, the direct calculations of $\delta E_{\rm corr}$ are in a good agreement with the calculations of $\delta E_{\rm corr}$ based on the LDA [Eq. (10)].

As we have mentioned several times above, the Coulomb correlation energy is always positive and therefore partially cancels the Coulomb exchange energy. It can lead also to strong effects in barrier tunneling in heavy nuclei, giving an appreciable contribution to the surface tension, as can be seen from the calculated value $a_s \approx 1$ MeV.

We do not claim that the effect we have described here, the strong enhancement of the Coulomb correlation energy due to the existence of a nuclear surface, is fully responsible for this anomaly. One must of course consider the contribution of the CSB nuclear forces as well, and very likely a similar enhancement mechanism for their contribution. A preliminary analysis which we have performed shows that the mechanism we have described here can lead to a significant reduction of the estimated strength of the CSB nuclear forces.

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