РОССИЙСКАЯ АКАДЕМИЯ НАУК

ПИСЬМА
В ЖУРНАЛ ЭКСПЕРИМЕНТАЛЬНОЙ
И ТЕОРЕТИЧЕСКОЙ ФИЗИКИ

ОСНОВАН В 1965 ГОДУ *ТОМ 62, ВЫПУСК 11*
ВЫХОДИТ 24 РАЗА В ГОД *10 ДЕКАБРЯ, 1995*

Журнал поддерживается в 1995 году Российским фондом фундаментальных исследований по проекту № 95-02-91030.

Pis'ma v ZhETF, vol.62, iss.11, pp.833 - 838

A SYSTEMATIC CONTRIBUTION TO THE BINDING ENERGY OF NUCLEI

A.Bulgac[1)], *V.R.Shaginyan*[+2)]

Department of Physics, Box 351560, University of Washington, Seattle, WA 98195-1560, USA

[+] *St. Petersburg Nuclear Physics Institute RAS, 188350 Gatchina, Russia*

Submitted 31 October 1995

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 acting 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.

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 of resolving the anomaly addressed many-body effects suspected of being at the root of the problem, see Refs. [2–5]. During the last years the 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 CBS 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

[1)]e-mail: bulgac@phys.washington.edu
[2)]e-mail: vrshag@lnpi.spb.su

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 the common feature of a self-sustaining system, the presence of the surface.

The ground state energy E of 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 related to isospin symmetry conserved forces dependent symmetrically on the densities ρ_p, ρ_n. F_c is related with CSB forces, that is the Coulomb interaction in our case, the densities $\rho_p(\mathbf{r})$, $\rho_n(\mathbf{r})$ are the single particles 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]

$$F_c[\rho_p(\mathbf{r})] = F_c^{HF} = \frac{e^2}{2}\int \rho_p(\mathbf{r}_1)\rho_p(\mathbf{r}_2)\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\,d\mathbf{r}_1 d\mathbf{r}_2 - \tag{2}$$

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

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

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

The systematic contribution to the binding energy we are discussing here, arises from the correlation part of the energy, Eq. (3). We shall discuss this correlation energy contribution first in infinite homogeneous nuclear matter as a function of the density, 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 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 translation invariance of such a system. The correlation energy density ΔE_{corr}

can be represented as follows (for sake of simplicity we have suppressed here the spin–isospin coordinates)

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

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

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

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 $d\varepsilon_F/d\rho_0 \approx 300\,\mathrm{MeV}\cdot\mathrm{fm}^3$. 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 respectively isovector $\varepsilon'_{corr}(\rho_p)$ correlation energy. 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 equal to [11]

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

Since the residual interaction V has a strong density dependence and in the region of low densities the *isoscalar* part is strongly attractive, the uniform nuclear matter becomes unstable around $\rho \simeq 0.6\rho_0$. 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 to remember 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 various terms in Eqs. (2), (4) for a finite systems should read as follows

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

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 Rel. (4), while the Coulomb exchange contribution is negative and one can expect a partial cancelation 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 present χ_p in a mixed coordinate–momentum representation, z and q, where q is the momentum parallel to the surface. The Coulomb correlation energy per unit surface, or the surface tension σ_c, can be written as

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

$$\varepsilon_c(\rho_p(z)) = -\frac{1}{(2\pi)^3 \rho_p(z)} \int d\omega d^2q dz' U(\mathrm{q}, z') \times \tag{9}$$

$$\times \mathrm{Im}\left[\chi_p(\mathrm{q}, z + \frac{z'}{2}, z - \frac{z'}{2}, \omega) - \chi_p^0(\mathrm{q}, z + \frac{z'}{2}, z - \frac{z'}{2}, \omega)\right]$$

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

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

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

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

The isoscalar and isovector Coulomb correlation energies for semi–infinite nuclear matter thus obtained have a quite different behavior. The isovector part, while larger in the interior as compared to isoscalar part, 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 worth to 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), (8), and thus one gets $a_v \approx -0.1 \pm 0.1$ MeV and $a_s \approx 1.0 \ldots 1.2$ 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_{in}. 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. 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, which is an indirect indication that f_{in} is small indeed.

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

We have considered the 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

SIII [13] interaction for the F_0 in Eq. (1), with F_c given by Eqs. (2), (10). We have included also 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 $\delta E_{corr} = 0.33\,\mathrm{MeV}$ in the $A = 40$ region, and $\delta E_{corr} = 0.25$ MeV in the $A = 16$ region. We estimate the accuracy of the calculation of δE_{corr} within 20%.

We have also carried out direct computations of δE_{corr} with aim to check the quality of the used local density approximation and to discuss in more details this value. 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 limit our analysis of 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 $R_0 = 1.25\,\mathrm{A}^{1/3}$ fm, diffuseness $a = 0.65$ fm and 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,

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

where $V_0(r)$ is the single-particle potential. 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 [14, 8] and leads to a satisfactory description of nuclear collective modes. The calculated δE_{corr} are of the order 200 ... 300 keV in either oxygen or calcium region, i.e. of the same magnitude as the Okamoto–Nolen–Schiffer anomaly [2, 3]. Thus, the direct calculations of δE_{corr} are in a good agreement with the calculations of δE_{corr} which have been based on 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 the appreciable contribution to the surface tension, as it can be seen from the found value of $a_s \approx 1$ 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 has of course to 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 CSB nuclear forces.

We wish to thank G.F.Bertsch, E.M.Henley, V.A.Khodel, G.A.Miller, J.A.Nolen and L.Wilets for fruitful conversations and comments. This research was supported in part by the Russian Foundation for Fundamental Investigations under Grant 95-02-04481 and by the International Science Foundation under Grant ML8300. One of us (V.R.S.) would like to thank the Institute for Nuclear Theory for

hospitality, where part of this work was done. Partial DOE and NSF support is greatly appreciated.

---

1. J.A.Nolen, Jr. and J.P.Schiffer, Ann. Rev. Nucl. Sci. **19**, 471 (1964).
2. S.Shlomo, Rep. Prog. Phys. **41**, 957 (1978); S.Shlomo and M.G.Love, Physica Scripta **26**, 280 (1982).
3. N.Auerbach, Phys. Rep. **98**, 273 (1983).
4. E.M.Henley and G.A.Miller, In: *Mesons in Nuclei*, Eds. M. Rho and D.H. Wilkinson, North-Holland, Amsterdam, 1979.
5. A.B.Migdal, *Theory of Finite Fermi Systems and Applications to Atomic Nuclei*, Wiley Interscience, New York, 1967 and see also the second edition in Russian, Nauka, Moscow, 1983.
6. E.G.Drukarev and M.G.Ryskin, Nucl. Phys. **A 372**, 560 (1994).
7. K.Saito and A.W.Thomas, Phys. Lett. **B 335**, 17 (1994); M.H.Shahnas, Phys. Rev. **C 50**, 2346 (1994); R.B.Wiringa, V.G.J.Stoks and R.Schiavilla, Phys. Rev. **C**, in press; B.S.Pudliner, V.R.Pandharipande, J.Carlson and R.B.Wiringa, Los Alamos preprint library nucl-th 9502031.
8. P.Ring and P.Schuk, *The Nuclear Many-Body Problem*, Springer-Verlag, New York, 1980.
9. V.A.Khodel, V.R.Shaginyan, and V.V.Khodel, Phys. Rep. **249**, 1 (1994).
10. D.Vautherin and D.M.Brink, Phys. Rev. **C 5**, 626 (1972).
11. V.R.Shaginyan, Yad. Fiz. **39**, 349 (1984).
12. M.Gell-Mann and K.A.Brueckner, Phys. Rev. **106**, 364 (1957); N.D.Lang and W.Kohn, Phys. Rev. **B 3**, 1215 (1971).
13. M.Beiner, H.Flocard, Nguen Van Giai, and P.Quentin, Nucl. Phys. **A 238**, 29 (1975).
14. A.Bohr and B.R.Mottelson, *Nuclear Structure*, vol. II ch. 6, Benjamin, New York, Amsterdam, 1974.