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Short note

Influence of Coulomb correlations on the location of drip line, single particle spectra and effective mass

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Abstract. A new systematic shift of the single-particle spectra of nuclei under the Coulomb interaction is considered. This shift results from the interplay between the Coulomb interaction and strong interaction, being greatly enhanced by the presence of the nuclear surface. This shift affects the position of the calculated proton drip line decreasing the maximal Z of a nucleus near the drip line by several units. The same mechanism is responsible for significant corrections to the mass difference of the mirror nuclei and to the effective proton mass.

PACS. 21.10.Sf Coulomb energies – 21.10.Dr Binding energies – 21.10.-k Nuclear energy levels

A study of the influence of the Coulomb interaction on the properties of atomic nuclei is of crucial importance. The main part of this influence is linked with the Hartree term of the Coulomb energy which is proportional to Z^2. Here Z is the number of protons of a nucleus. On the other hand, there exists a number of more subtle contributions to the Coulomb energy related to the interplay between the Coulomb interaction and nuclear forces. To illustrate it one can use the famous Okamoto — Nolen — Schiffer anomaly in the binding energy differences of mirror nuclei which has attracted much interest during the last 3 decades [1]. While it was shown that there is a new many-body mechanism, enhancing the contribution due to the Coulomb interaction and based on the common feature of a self-sustaining system, the presence of the surface. This contribution, allowing for the main part of the anomaly, has a specific Z dependence, being proportional to the nuclear surface $\sim Z^{2/3}$ [2].

The main goal of this Letter is a study of impact of this mechanism on the location of the proton drip line, single-particle proton excitations and the proton effective mass.

Within the density functional approach the ground state energy E of nucleus is given by [3]

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

Here F_0 is the main part of the functional dependent symmetrically on the densities ρ_p, ρ_n and related to isospin symmetry conserved forces. While F_c is due to the Coulomb interaction. We neglect easy to include terms: the contribution due to the proton-neutron mass difference and contribution of the charge symmetry breaking (CBS) forces [4]. The densities,

$$\rho_p(\mathbf{r}) = \sum_l n_p^l |\phi_p^l(\mathbf{r})|^2; \;\; \rho_n(\mathbf{r}) = \sum_l n_n^l |\phi_n^l(\mathbf{r})|^2, \qquad (2)$$

are the single particles densities of neutrons and protons, respectively, with n_p^l, ϕ_p^l and n_n^l, ϕ_n^l being the corresponding occupation numbers and single-particle wave functions. The well-known Skyrme functional can be considered as a possible realization of F_0, while in that case F_c is given by

$$\begin{aligned} F_c[\rho_p(\mathbf{r})] = {} & \frac{e^2}{2} \int \rho_p(\mathbf{r}_1)\rho_p(\mathbf{r}_2) \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \, d\mathbf{r}_1 d\mathbf{r}_2 \\ & - \frac{e^2}{2} \int [\chi_p^0(\mathbf{r}_1, \mathbf{r}_2, i\omega) + 2\pi\rho_p(\mathbf{r}_1)\delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(\omega)] \\ & \times \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} \frac{d\mathbf{r}_1 d\mathbf{r}_2 d\omega}{2\pi}. \end{aligned} \qquad (3)$$

Here the first term on r.h.s is the Hartree term, the second is the Fock term which, being taken in the Slater approximation, equals to

$$-(3/4)(3/\pi)^{1/3} e^2 \int \rho_p^{4/3}(\mathbf{r}) d\mathbf{r},$$

and $\chi_p^0(\mathbf{r}_1, \mathbf{r}_2, \omega)$ is the linear response function of the non-interacting protons moving in a self-consistent field. But

(3) is incorrect since it omits the term $F_c^{corr}[\rho_p(\mathbf{r})]$ that comes from the interplay between the Coulomb interaction and the effective interaction $R_{lm}(\mathbf{r}_1,\mathbf{r}_2)$ associated with the strong nucleon-nucleon interaction. In the first order in the Coulomb interaction, the Coulomb correlation energy F_c^{corr} is given by [2]

$$F_c^{corr}[\rho_p(\mathbf{r})] = -\frac{e^2}{2}\int[\chi_{pp}(\mathbf{r}_1,\mathbf{r}_2,i\omega)-\chi_p^0(\mathbf{r}_1,\mathbf{r}_2,i\omega)] \times\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\frac{d\mathbf{r}_1 d\mathbf{r}_2 d\omega}{2\pi}, \quad (4)$$

with $\chi_{pp}(\mathbf{r}_1,\mathbf{r}_2,\omega)$ being the linear response function of the protons of nucleus in question, disturbed by an external electric field. The main contribution to F_c^{corr} comes from the surface collective *isoscalar* excitations, the energies of that are much smaller then the energies of the isovector excitations. While in the case of homogeneous nuclear matter such a contribution is not strengthened, and as a result, the Coulomb correlation energy given by (4) is rather small. Thus, one can conclude that F_c^{corr} is of surface origin, being mainly defined by the *isoscalar* components of the effective interaction [2].

Now we turn to calculations of the shifts of the proton single particle energies ε_p^l under influence of the Coulomb correlation energy. To do it we employ the Landau equation [5]

$$\frac{\delta E}{\delta n_p^l} = \varepsilon_p^l. \quad (5)$$

It follows from (4,5) that the shift $\Delta\varepsilon_p^l$ related to the Coulomb correlation energy can be expressed as

$$\Delta\varepsilon_p^l = \frac{\delta F_c^{corr}}{\delta n_p^l} = -\frac{e^2}{2}\frac{\delta}{\delta n_p^l}\int[\chi_{pp}(\mathbf{r}_1,\mathbf{r}_2,i\omega)-\chi_p^0(\mathbf{r}_1,\mathbf{r}_2,i\omega)] \times\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\frac{d\mathbf{r}_1 d\mathbf{r}_2 d\omega}{2\pi}. \quad (6)$$

Here the variational derivative $\delta\chi_p^0/\delta n_p^l$ has the simple functional form

$$\frac{\delta\chi_p^0(\mathbf{r}_1,\mathbf{r}_2,\omega)}{\delta n_{\lambda_0}^p} = \big[G^p(\mathbf{r}_1,\mathbf{r}_2,\omega+\varepsilon_{\lambda_0}^p) + G^p(\mathbf{r}_1,\mathbf{r}_2,-\omega+\varepsilon_{\lambda_0}^p)\big] \times\phi_{\lambda_0}^{p*}(\mathbf{r}_1)\phi_{\lambda_0}^p(\mathbf{r}_2), \quad (7)$$

with $G^p(\mathbf{r}_1,\mathbf{r}_2,\omega)$ being the Green function of Z noninteracting protons moving in the single particle nuclear potential. While $\delta\chi_{pp}/\delta n_p^l$ is given by the matrix equation

$$\frac{\delta\chi_{lm}}{\delta n_p^l} = \frac{\delta\chi_l^0}{\delta n_p^l}\delta_{pm} + \sum_k\left[\frac{\delta\chi_l^0}{\delta n_p^l}R_{lk}\chi_{km}+\chi_l^0\frac{\delta R_{lk}}{\delta n_p^l}\chi_{km}+\chi_l^0 R_{lk}\frac{\delta\chi_{km}}{\delta n_p^l}\right], \quad (8)$$

with χ_{lm} being given by

$$\chi_{lm} = \chi_l^0\delta_{pm} + \sum_k\chi_l^0 R_{lk}\chi_{km}. \quad (9)$$

In (8,9) for the sake of brevity we omit the spatial integrations. The effective interaction is chosen of the separable form

$$R(\mathbf{r}_1,\mathbf{r}_2)_{lm} = \lambda\frac{dV_l(r_1)}{dr}\frac{dV_m(r_2)}{dr}\delta(\Omega_1-\Omega_2), \quad (10)$$

where $V_l(r)$ is the proton (neutron) single-particle potential. λ is chosen so that the dipole linear response has a pole at $\omega = 0$. This type of residual interaction has been widely studied [3,8] and leads to a satisfactory description of nuclear collective modes. The calculated $\Delta\varepsilon_p^l$ are of the order $(0.2-0.3)MeV$ in either medium nuclei region or heavy one, i.e. of the same magnitude as the Okamoto — Nolen — Schiffer anomaly. It is useful to check these results using simple approximations. The Coulomb correlation energy, given by (4), can be expressed within the local density approximation as

$$F_c^{corr}[\rho_p] = \int\rho_p(\mathbf{r})e_c(\rho(\mathbf{r}))d\mathbf{r}. \quad (11)$$

Here e_c is the Coulomb correlation energy per proton. Then the single-particle shift $\Delta\varepsilon_p^l$ may also be written in the following form

$$\Delta\varepsilon_p^l = \int\frac{\delta F_c^{corr}[\rho_p]}{\delta\rho_p}|\phi(\mathbf{r})_l|^2 d\mathbf{r}. \quad (12)$$

The correlation energy e_c has a very prominent positive peak at the surface [2]. For simple estimations of $\Delta\varepsilon_p$, when the single particle energy ε_p is located in the vicinity of the Fermi level, one can take $e_c(r) = -\beta\, a\, dF(r)/dr$, and $\rho_p(r) = \rho_0 F(r)$, with $\rho_0 = 0.08\ fm^{-3}$ being the proton number density in the central part of nucleus, while F is the Fermi function

$$F(r) = \frac{1}{1+\exp((r-R)/a)}. \quad (13)$$

Here R is the radius of a nucleus, the diffuseness a is chosen to be $0.6\ fm$, and coefficient $\beta \simeq 3MeV$. As a consequence of the taken approximation and after standard transformations of the Fermi integrals one gets for middle and heavy nuclei

$$\Delta\varepsilon_p \simeq \frac{\beta a}{R} \sim (0.3-0.4)MeV. \quad (14)$$

Since corrections of the order of $\beta(a/R)^2$ were dropped, (14) slightly overestimates the magnitude of the shift. It is seen from (14) that the contribution of the Coulomb correlation energy compensates the one arising from the Fock term. Thus, one can simply drop both the Fock term and F_c^{corr}, taking into account only the Hartree term. Such a procedure was postulated in [6,7]. Then, it is seen from (14) that a systematic upward shift of this magnitude of

the last occupied proton level in a nucleus near the proton drip line equivalent to a shift of the calculated proton drip line in the direction of decreasing Z by up to 5 units, see for example [9].

Consider the variation ΔM due to the Coulomb interaction of the proton effective mass M^* in the case of homogeneous nuclear matter. In that case, the single particle spectra depend on momentum p, while, as it follows from (5) the effective mass is given by [5]

$$\frac{1}{M^*} = \frac{1}{p_F}\frac{d\varepsilon_p(p)}{dp}|_{p=p_F}. \tag{15}$$

Here p_F is the Fermi momentum. To get the variation ΔM of the effective mass M^* one can use (15), replacing $\varepsilon_p(p)$ by the shift of the single particle energy defined by the Coulomb interaction. As a result, one gets [10]

$$\frac{\Delta M}{M^*(M^*+\Delta M)} = \frac{e^2 d}{p_F dp}\int \frac{\frac{\delta\chi_0(q,i\omega)}{\delta n_p}}{(1-R(q,i\omega)\chi_0(q,i\omega))^2}\frac{d\mathbf{q}d\omega}{q^2(2\pi)^3}. \tag{16}$$

Here M^* is the proton effective mass when the Coulomb interaction is switched off. The derivative d/dp is taken at $p = p_F$. We shall consider the variation ΔM when system under consideration is located in the vicinity of the point where its bulk incompressibility tends to zero. This resembles the conditions which take place around the nuclear surface. Thus, such a consideration gives possibility of a qualitative estimate of the variation ΔM under influence of the Coulomb interaction in finite nuclei. One can verify that

$$\frac{d}{dp}\frac{\delta}{\delta n_p}\chi_0(q,\omega)|_{p\to p_F} = -\frac{4\pi}{p_F^2}\delta(p_F-|\mathbf{p}+\mathbf{q}|)\delta(\omega)\mathbf{p}(\mathbf{p}+\mathbf{q}). \tag{17}$$

Upon substituting (17) into (16) one directly gets

$$\frac{1}{M^*+\Delta M} = \frac{1}{M^*} + \frac{e^2}{2\pi p_F} \times \int_{-1}^{1}\frac{x\,dx}{(1-x)[1-R(q(x),0)\chi_0(q(x),0)]^2}. \tag{18}$$

In (18) we have adopted the shorthand notation $q(x) = p_F\sqrt{2(1-x)}$. At the point the incompressibility vanishes the denominator $(1 - R\chi_0)$ vanishes as well when $x = 1\,(q = 0)$ and the integral (18) diverges and thus the effective mass vanishes $M^* + \Delta M \to 0$. NB, such a divergence appears only because of the presence of a surface in the naive local density approximation [2]. This result indicates that the Coulomb correlation energy in a self sustaining nuclear system affects the proton effective mass M^* in a nontrivial manner. In finite nuclei this divergence, which is related to the variation of the density at the surface, is smoothed out [2]. The net result is that the proton effective mass becomes smaller then the neutron effective mass and smaller than the effective mass evaluated in the absence of the Coulomb correlation energy. The relevance of such an effect on the properties of a high accuracy nuclear density functional was discussed in [7]. Here we give a theoretical ground for the origin of this effect.

In summary, we have considered the calculations of the single particle spectra in nuclei and the shift of the single particle levels under the influence of the Coulomb correlation energy. A major part of the Nolen–Schiffer anomaly is removed by this shift. At the same time the calculated drip line is moved in the direction of decreasing Z. We have also shown that the Coulomb correlation energy should be taken into account when computing correction to the effective proton mass. We did not include in our analysis however the CSB forces, which we left to a future analysis. They can lead to both volume and surface energy terms in the nuclear density functional.

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