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 and strong interactions, which is greatly enhanced in the nuclear surface region. 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

The main contribution of the Coulomb interaction in nuclei is given by the Hartree, which is proportional to Z^2. Here Z is the number of protons of a nucleus. However, 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 well known Nolen–Schiffer anomaly in the binding energy differences of mirror nuclei, which attracted so much interest during the last 3 decades [1]. Recently it was shown that there is a new many–body mechanism, which leads to an enhancement of the contribution of the Coulomb interaction in the nuclear surface region and which thus leads to a binding energy term with a $Z^{2/3}$–dependence [2]. The main goal of this Letter is to study the impact of this mechanism on the location of the proton drip line, the single–particle proton excitations and the proton effective mass.

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

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

Here F_0 is the main part of the functional, which is related to isospin symmetry conserving forces, and thus symmetric under the interchange $\rho_p(\mathbf{r}) \leftrightarrow \rho_n(\mathbf{r})$. F_c is due to the Coulomb interaction and also other isospin symmetry breaking forces. We shall focus here on Coulomb interaction and leave for a future analysis other easy to include terms, such as the contribution due to the proton–neutron mass difference and the contribution of the charge symmetry breaking (CSB) forces [3]. The densities,

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

are the single particles proton and neutron densities, where n_p^l, ϕ_p^l and n_n^l, ϕ_n^l stand for the corresponding occupation number probabilities and the single–particle wave functions. The popular Skyrme functional [4] can be considered as a possible realization of F_0, while F_c is usually taken as

$$F_c[\rho_p(\mathbf{r})] = \frac{e^2}{2}\int \rho_p(\mathbf{r}_1)\rho_p(\mathbf{r}_2)\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\,d\mathbf{r}_1 d\mathbf{r}_2 \tag{3}$$

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

Here the first term on r.h.s is the Hartree term, the second is the Fock term which in the Slater approximation becomes

$$-\frac{3}{4}\,(frac3\pi)^{1/3}\,e^2\int \rho_p^{3/4}(\mathbf{r})d\mathbf{r}.$$

$\chi_p^0(\mathbf{r}_1,\mathbf{r}_2,\omega)$ is the linear response function of the non–interacting protons, moving in a self–consistent field. However Eq. (2) is incorrect since it omits the contribution $F_c^{corr}[\rho_p(\mathbf{r})]$ due to the the interplay between the Coulomb interaction and the effective strong nucleon–nucleon interaction, which we shall denote $R_{lm}(\mathbf{r}_1,\mathbf{r}_2)$. In the first order in the Coulomb interaction, the Coulomb correlation energy F_c^{corr} is given by [2]

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

where $\chi_{pp}(\mathbf{r}_1,\mathbf{r}_2,\omega)$ is the linear proton–proton response function. The main contribution to F_c^{corr} is due to virtual isoscalar surface collective excitations. In homogeneous nuclear matter the Coulomb correlation energy given by Eq. (4) is rather small and there is no enhancement. However, for semi–infinite matter or finite nuclei one can show that the contribution to F_c^{corr} arising from the surface region dominates over the corresponding surface contribution F_c given by Eq. (3) alone. One can thus conclude that F_c^{corr} has a surface character mainly [2].

Let us turn now to the calculations of the proton single–particle energy shifts ε_p^l, due to the presence of the Coulomb correlation energy terms in the nuclear energy functional. Using Landau equation [5]

$$\varepsilon_p^l = \frac{\delta E}{\delta n_p^l} \tag{5}$$

and Eqs. (4,5) one can show that the proton single–particle energy shift $\Delta\varepsilon_p^l$ is given by

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

Here the variational derivative $\delta\chi^0_p/\delta n^l_p$ has the simple functional form

$$\frac{\delta\chi^0_p(\mathbf{r}_1,\mathbf{r}_2,\omega)}{\delta n^p_{\lambda_0}} = \left[G^p(\mathbf{r}_1,\mathbf{r}_2,\omega+\varepsilon^p_{\lambda_0}) + G^p(\mathbf{r}_1,\mathbf{r}_2,-\omega+\varepsilon^p_{\lambda_0})\right]\phi^{p*}_{\lambda_0}(\mathbf{r}_1)\phi^p_{\lambda_0}(\mathbf{r}_2), \tag{7}$$

with $G^p(\mathbf{r}_1,\mathbf{r}_2,\omega)$ being the Green function of Z noninteracting protons moving in the nuclear mean field potential. $\delta\chi_{pp}/\delta n^l_p$ can be obtained by solving the matrix equation

$$\frac{\delta\chi_{lm}}{\delta n^l_p} = \frac{\delta\chi^0_l}{\delta n^l_p}\delta_{pm} + \sum_k\left[\frac{\delta\chi^0_l}{\delta n^l_p}R_{lk}\chi_{km} + \chi^0_l\frac{\delta R_{lk}}{\delta n^l_p}\chi_{km} + \chi^0_l R_{lk}\frac{\delta\chi_{km}}{\delta n^l_p}\right], \tag{8}$$

with χ_{lm} being given by

$$\chi_{lm} = \chi^0_l\delta_{pm} + \sum_k \chi^0_l R_{lk}\chi_{km}. \tag{9}$$

The effective interaction is chosen of the separable form

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

where $V_l(r)$ is the proton (neutron) single–particle potential. λ is determined from the condition that the dipole linear response has a pole at $\omega = 0$. This type of residual interaction has been widely studied [4, 8] and leads to a satisfactory description of nuclear collective modes. The calculated $\Delta\varepsilon^l_p$ are of the order $(0.2-0.3)MeV$ in both medium and heavy nuclei region, which is thus of the same magnitude as the Nolen–Schiffer anomaly. It is useful to check these results using simple approximations. The Coulomb correlation energy, given by Eq. (4), can be expressed within the local density approximation as a local density functional

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

Here e_c is the Coulomb correlation energy per proton. The single–particle shift $\Delta\varepsilon^l_p$ is then given by

$$\Delta\varepsilon^l_p = \int \frac{\delta F^{corr}_c[\rho_p]}{\delta\rho_p}|\phi(\mathbf{r})_l|^2 d\mathbf{r}. \tag{12}$$

In Ref. [2] we have shown that he correlation energy e_c has a very prominent positive peak in the surface region. For simple numerical estimates of $\Delta\varepsilon_p$, when the single particle energy ε_p is close to the Fermi level, one can parametrize the Coulomb correlation energy per proton simply by $e_c(r) = -\beta\, a\, dF(r)/dr$, and use also $\rho_p(r) = \rho_0 F(r)$, with $\rho_0 = 0.08$ fm^{-3} the proton number density in the central part of nucleus, and F a Fermi function

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

Here R is the nuclear radius, the diffuseness a is chosen to be $0.6\ fm$, and the coefficient $\beta \simeq 3MeV$. After a few simple manipulations of the Fermi integrals one gets for middle and heavy nuclei

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

Since corrections of the order of $\beta(a/R)^2$ were dropped, Eq. (14) slightly overestimates the magnitude of the shift. 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 a few units of charge, see Ref. [9]. One can see from Eq. (14) that the contribution of the Coulomb correlation energy essentially compensates the corresponding contribution arising from the Fock term. A simple approximation scheme can in principle be adopted by dropping both the Fock term and F_c^{corr}, taking into account only the Hartree term. Such a procedure was postulated in Refs. [6, 7] where on overall high accuracy fit to nuclear masses and radii was sought. Such a simple approach however has little theoretical underpinning so far, since the Coulomb correlation energy has mostly a surface character, while the Coulomb exchange contribution has a predominantly volume origin.

Let us consider now the variation of the proton effective mass ΔM due to the Coulomb interaction. We shall derive the corresponding formula for the of the case of homogeneous nuclear matter, but specialize the final analysis in the nuclear surface region, within the framework of the local density approximation. In homogeneous nuclear matter the single–particle energy depends on momentum p, and as it follows from Eq. (5) the effective mass is given by [5]

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

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

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

Here M^* is the proton effective mass in the absence of the Coulomb interaction. 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 occurring around the nuclear surface [2]. One obtains then that

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

Upon substituting Eq. (17) into Eq. (16) one arrives at the following result

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

In Eq. (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 Ref. [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.

We thank G.F. Bertsch and G.A. Miller for discussion. This research was funded in part by DOE , INTAS under grant No. INTAS-OPEN-97-603, and RFBR under grant No. 98-02-16170. VRS would like to thank Department of Physics of the University of Washington, for hospitality, where part of this work was done.

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