Center-of-Mass Correction in a Relativistic Hartree Approximation

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We use the Peierls-Yoccoz projection method to evaluate the center-of-mass correction of a relativistic system of nucleons and sigma and omega mesons, described in a mean-field Hartree approach. This correction for ^{4}He, ^{16}O and ^{40}Ca is compared with the pure harmonic oscillator center-of-mass energy correction.

Keywords: Peierls-Yoccoz projection method; Center-of-mass correction

It is a well known fact that mean-field approximation to the nuclear many-body problem introduces center-of-mass (CM) spurious components in the solutions. In particular, Hartree-Fock self-consistent mean-fields obtained using realistic forces in a non-relativistic approach have been considered, and the corresponding CM corrections have been calculated for the energy [1, 2] as well as for other observables [3] in a fully microscopic way. For relativistic theories, as the widely used relativistic mean field theory [4] in the Hartree or Hartree-Fock approximations, the correction for the energy is usually estimated using the harmonic oscillator basis [5]. In this case, the treatment for the CM motion becomes trivial, though generally not consistent with the nuclear wavefunction obtained variationally.

In this paper we also address the problem of the CM energy correction in the framework of a relativistic Hartree approach, including both nucleon and meson degrees of freedom. We consider σ and ω mesons, without self-interactions, linearly coupled to nucleons. The CM correction is implemented by means of the Peierls-Yoccoz projection, assuming that the nucleus as a whole is a nonrelativistic system, though the nucleons inside are relativistic particles.

The mesons are explicitly included in the Lagrangian density, and their effect should, in principle, be also considered in the projection procedure. This issue was recently tackled in reference [6] for light nuclei, but a more systematic study is needed. In this paper we only take into account the nucleon contributions to the CM corrections. The calculations of the meson contribution are under way and the results will be reported elsewhere. Moreover, in this work we restrict our analysis to $N = Z$ closed-shell nuclei only. The Lagrangian density for a system of nucleons interacting with sigmas and omegas reads (we use the notation and definitions as in reference [7])

$$L = L_{\rm N}^{\rm free} + L_{\sigma}^{\rm free} + L_{\omega}^{\rm free} + L_{\rm NN\sigma}^{\rm int} + L_{\rm NN\omega}^{\rm int}, \qquad (1)$$

where N denotes the nucleon and σ, ω the mesons. The Lagrangians for the free fields are:

$$L_{\rm N}^{\rm free} = \overline{\psi}(x)(i\gamma^{\mu}\partial_{\mu} + M)\psi(x), \qquad (2)$$

$$L_{\sigma}^{\rm free} = -\frac{1}{2}\left[m_{\sigma}^2\varphi^2(x) - \partial_{\mu}\varphi(x)\partial^{\mu}\varphi(x)\right], \qquad (3)$$

$$L_{\omega}^{\rm free} = -\frac{1}{4}F_{\mu\nu}(x)F^{\mu\nu}(x) + \frac{1}{2}m_{\omega}^2\omega_{\nu}(x)\omega^{\nu}(x),$$

where

$$F_{\mu\nu} \equiv \partial_{\mu}\omega_{\nu}(x) - \partial_{\nu}\omega_{\mu}(x)$$

and M is the rest mass of the nucleon, and m_{σ} and m_{ω} the meson masses. The sigma and omega fields are denoted respectively by $\varphi(x)$ and $\omega^{\nu}(x)$, and the nucleon field by $\psi(x)$. For the interaction parts of the Lagrangian one has

$$L_{\rm NN\sigma}^{\rm int} = g_{\sigma}\overline{\psi}(x)\varphi(x)\psi(x) \qquad (4)$$

$$L_{\rm NN\omega}^{\rm int} = -g_{\omega}\overline{\psi}(x)\omega^{\nu}(x)\gamma_{\nu}\psi(x) + \frac{f_{\omega}}{4M}\overline{\psi}(x)\sigma^{\mu\nu}F_{\mu\nu}(x)\psi(x)\,. \qquad (5)$$

The nucleon field can be expanded as

$$\psi(x) = \sum_{\alpha} u_{\alpha}(\vec{r})e^{-iE_{\alpha}t}b_{\alpha} + \sum_{\alpha} v_{\alpha}(\vec{r})e^{iE_{\alpha}t}d_{\alpha}^{\dagger} \qquad (6)$$

$$\psi^{\dagger}(x) = \sum_{\alpha} u_{\alpha}^{\dagger}(\vec{r})e^{iE_{\alpha}t}b_{\alpha}^{\dagger} + \sum_{\alpha} v_{\alpha}^{\dagger}(\vec{r})e^{-iE_{\alpha}t}d_{\alpha}\,, \qquad (7)$$

where $u_{\alpha}(\vec{r})$ and $v_{\alpha}(\vec{r})$ form a complete set of Dirac spinors in the coordinate space, and b_{α} and $b_{\alpha}^{\dagger}$ are the creation and annihilation operators of a nucleon in the state α. By d_{α} and $d_{\alpha}^{\dagger}$ we denote the creation and the annihilation operators for the anti-nucleons in the same state α. Thus, starting from the above Lagrangian, and disregarding the tensor coupling, one obtains the following Hamiltonian, already restricted to the nucleon subspace [7]:

$$H = \sum_{\alpha\alpha'}\int f_{\alpha'}^{\dagger}(\vec{r})(-i\gamma^0\vec{\gamma}.\vec{\nabla} + \gamma_0 M)f_{\alpha}(\vec{r})d^3\vec{r}\,b_{\alpha'}^{\dagger}b_{\alpha} + \frac{1}{2}\sum_{\alpha,\alpha',\beta,\beta'}\int f_{\alpha'}^{\dagger}(\vec{r}_1)f_{\beta'}^{\dagger}(\vec{r}_2)V_{\alpha,\alpha'}(\mid\vec{r}_1 - \vec{r}_2\mid) \times f_{\beta}(\vec{r}_2)f_{\alpha}(\vec{r}_1)\,d^3r d^3r_1 d^3r_2\,b_{\alpha'}^{\dagger}b_{\beta'}^{\dagger}b_{\beta}b_{\alpha} \qquad (8)$$

with the potential given by

$$V_{\alpha,\alpha'}(|\,\vec{r}_1-\vec{r}_2\,|) \;=\; V_{\alpha,\alpha'}(r)=\sum_{i=\sigma,\omega}\frac{g_i^2}{4\pi}\gamma_0(1)\gamma_0(2)\Gamma_i(1,2) \times\frac{\exp\{-r[m_i^2-(E_\alpha-E_{\alpha'})^2]^{1/2}\}}{r}\,, \quad (9)$$

where $\Gamma_\sigma(1,2)=1$ and $\Gamma_\omega(1,2)=\gamma_\mu(1)\gamma^\mu(2)$ and E_α are the single-particle energies. In the model space, the state vector for a system of A-nucleons is approximated by

$$|\,\Psi>=b^\dagger_{\alpha_1}b^\dagger_{\alpha_2}\cdots b^\dagger_{\alpha_A}\,|\,0>\,, \quad (10)$$

where $\alpha_1,\ldots,\alpha_A$ are sets of single-particle quantum numbers and $|\,0>$ is the bare vacuum. In the Hartree approximation the single-particle energies and wave functions are obtained in the standard fashion by minimizing the ground state energy. We start from [7]

$$<\Psi\,|\,H\,|\,\Psi> \;=\; \sum_{\alpha=1}^{A}\int u^\dagger_\alpha(\vec{r})(-i\gamma^0\vec{\gamma}.\vec{\nabla}+\gamma^0 M)u_\alpha(\vec{r})d^3r +\frac{1}{2}\sum_{\alpha,\alpha'=1}^{A}\int u^\dagger_\alpha(\vec{r}_1)u^\dagger_{\alpha'}(\vec{r}_2)V_{\alpha,\alpha}(r)u_\alpha(\vec{r}_1)u_{\alpha'}(\vec{r}_2)d^3r_1\,d^3r_2\,, \quad (11)$$

where the first term corresponds to the kinetic energy and mass, and the second one to the direct potential. The spinors $u_\alpha(\vec{r})$ are explicitly given by

$$u_\alpha(\vec{r})=\begin{pmatrix} g_{nlj}(r)\varphi_{ljm}(\hat{r}) \\ \\ if_{nlj}(r)\vec{\sigma}.\hat{r}\varphi_{ljm}(\hat{r}) \end{pmatrix}\xi_{1/2,\tau_\alpha}\,, \quad (12)$$

where

$$\varphi_{ljm}(\vec{r})=\sum_{m_l,\mu}(lm_l\;\frac{1}{2}\mu\;|\;jm)Y_{l,m_l}(\hat{r})\chi_{1/2,\mu}\,. \quad (13)$$

We denote by $\chi_{1/2,\mu}$ and $\xi_{1/2,\tau_\alpha}$ the spin and isospin wave functions, respectively. For a closed shell nucleus the Hartree equations for the radial functions in both components of the Dirac spinor are given by

$$\frac{dF_\alpha(r)}{dr} \;=\; [M-E_\alpha+U^{(+)}_\alpha(r)]G_\alpha(r)+\frac{\kappa}{r}F_\alpha(r) \quad (14)$$

$$\frac{dG_\alpha(r)}{dr} \;=\; [M+E_\alpha+U^{(-)}_\alpha(r)]F_\alpha(r)-\frac{\kappa}{r}G_\alpha(r)\,, \quad (15)$$

where $\kappa=\mp(j+\frac{1}{2})$ for $j=l\pm\frac{1}{2}$ and $\alpha\equiv(n,l,j)$. In the previous equation we have introduced new radial functions related to the original ones through

$$g_\alpha=\frac{G_\alpha(r)}{r}, \quad (16)$$

$$f_\alpha=\frac{F_\alpha(r)}{r}. \quad (17)$$

We have also introduced

$$U^{(\pm)}_\alpha(r_1)=W^\sigma_\alpha(r_1)\pm W^\omega_\alpha(r_1) \quad (18)$$

and

$$W^k_\alpha(r_1)=\pm m_k\frac{g_k^2}{4\pi}\sum_\alpha 2(2j_\alpha+1)I^k_\alpha(r_1)\,, \quad (19)$$

where $k=\sigma,\omega$. The functions I^k_α are given by

$$I^k_\alpha(r_1)=\int_0^\infty dr_2\,j_0(\mathrm{i}m_k r_<)h^{(+)}_0(\mathrm{i}m_k r_>)[G^2_\alpha(r_2)\mp F^2_\alpha(r_2)]\,, \quad (20)$$

where m_k are the masses of the corresponding mesons. The $\pm$ signs in the above equations are related to the $\sigma(+)$ and $\omega(-)$ mesons. In (20) j_0 and $h^{(+)}_0$ are Bessel and Hankel spherical functions and $r_<$ ($r_>$) is the smaller (larger) value between r_1 and r_2. We solve the set of equations (14) to (19) by expanding the radial functions $f(r)$ and $g(r)$ in a harmonic oscillator basis, as explained in [5]. A fast convergence is achieved for all nuclei studied in this work.

Next, we want to obtain the center-of-mass correction to the energy using the model just described. It is well known, from the nuclear many-body problem, that the Hartree (or Hartree-Fock) approximation breaks translational invariance (see Ref. [1]) and that the broken symmetry can be recovered in the symmetry-breaking state by applying the Peierls-Yoccoz projection operator

$$\mathcal{P}_{\vec{p}}=\int\exp[\mathrm{i}(\hat{\vec{P}}-\vec{p})\cdot\vec{a}]\,d^3a, \quad (21)$$

which has the property

$$\mathcal{P}_{\vec{p}}\,\mathcal{P}_{\vec{p}\prime}=\delta(\vec{p}-\vec{p}\,')\mathcal{P}_{\vec{p}}. \quad (22)$$

In (21), $\hat{\vec{P}}$ is the total linear momentum operator and $\vec{p}$ the corresponding eigenvalue. Our approach consists in assuming that the physical nucleus state is obtained by projecting the product mean-field state into a zero momentum ($\vec{p}=\vec{0}$) state (projection after variation). Because the many-body Hamiltonian, expressed by (8) and (9), commutes with the projection operator, the total energy can be cast in the form:

$$E_{\vec{p}=0}=\frac{<\Psi\,|\,H\mathcal{P}_{\vec{p}=\vec{0}}\,|\,\Psi>}{<\Psi\,|\,\mathcal{P}_{\vec{p}=\vec{0}}\,|\,\Psi>}. \quad (23)$$

The denominator, $<\Psi\,|\,\mathcal{P}_{\vec{p}=\vec{0}}\,|\,\Psi>$, is a norm overlap matrix element. We start with the calculation of this overlap matrix normalization factor. The easiest way to compute this quantity is in momentum space. In configuration space the radial functions are expanded in the oscillator basis as

$$g_{nlj}(r)=\sum_{n=0}^{N}C_nR_{nlj}(r) \quad (24)$$

$$f_{nlj}(r)=\sum_{n=0}^{N'}\tilde{C}_nR_{nlj}(r). \quad (25)$$

where $N^{'}$ must be, at least, $N+1$ [5] and $C_n, \tilde{C}_n$ are expansion coefficients determined by the variational procedure. Inserting these expansions in equation (12) and going to the momentum space representation, we arrive, after a lengthy but straightforward calculation, to the following overlap kernel:

$$< \Psi \mid \mathcal{P}_{\vec{p}=\vec{0}} \mid \Psi >= \int < \Psi \mid \Psi(a) > d^3a = \int \det B \, d^3a. \tag{26}$$

The matrix is given by

$$B_{\alpha\beta} = 4\pi \sum_{\lambda} (\frac{1+(-)^{\lambda+l_\alpha+l_\beta}}{2}) [\mathrm{i}^{\lambda+l_\alpha-l_\beta} \int j_\lambda(pa) g^*_\alpha g_\beta p^2 dp + \mathrm{i}^{\lambda+\bar{l}_\alpha-\bar{l}_\beta} \int j_\lambda(pa) f^*_\alpha f_\beta p^2 dp] S_{\alpha\beta}. \tag{27}$$

where $\bar{l} = l \pm 1$ for $j = l \pm 1/2$ and

$$S_{\alpha\beta} = (-)^{m_\alpha + m_\beta + 1} \sqrt{\frac{2j_\alpha+1}{2j_\beta+1}} \frac{2\lambda+1}{4\pi} (j_\alpha - m_\alpha \lambda 0 | j_\beta - m_\beta)(j_\alpha 1/2 \lambda 0 | j_\beta 1/2) \delta_{\tau_\alpha, \tau_\beta} \tag{28}$$

In equation (27) we have explicitly used the fact that we are dealing with closed shell nuclei, so no angular dependence should appear in the overlap matrix. For the Hamiltonian kernel calculation, we have used the following general expressions[8]:

$$< \Psi \mid \hat{O} \mid \Psi(a) >=< \Psi \mid \Psi(a) > \sum_{\alpha\beta} < \alpha \mid \hat{O} \mid \beta(a) > B^{-1}_{\beta\alpha} \tag{29}$$

and

$$< \Psi \mid \hat{O}_{12} \mid \Psi(a) >= \frac{1}{2} < \Psi \mid \Psi(a) > \sum_{\alpha\beta\gamma\delta} < \alpha\beta \mid \hat{O}_{12} \mid \gamma(a)\delta(a) > B^{-1}_{\gamma\alpha} B^{-1}_{\delta\beta}, \tag{30}$$

where $\hat{O}$ and $\hat{O}_{12}$ are one and two body operators, respectively and only the direct term of the two-body operator has been kept. Using the same technique applied in the case of the overlap kernel, we find, for the kinetic term, $\hat{T} \equiv -\gamma_0 \vec{\gamma} \cdot \vec{P}$, in the Hamiltonian kernel,

$$< \alpha \mid \hat{T} \mid \beta(a) >=< \Psi \mid \Psi(a) > \sum_{\alpha\beta} T_{\alpha\beta} B^{-1}_{\beta\alpha}, \tag{31}$$

with

$$T_{\alpha\beta} = 4\pi \sum_{\lambda} (\frac{1+(-)^{\lambda+l_\alpha+l_\beta}}{2}) [\ -\mathrm{i}^{\lambda+1+l_\alpha-\bar{l}_\beta} \int j_\lambda(pa) g^*_\alpha g_\beta p^3 dp +$$
$$+\mathrm{i}^{\lambda+1+\bar{l}_\alpha-l_\beta} \int j_\lambda(pa) f^*_\alpha f_\beta p^3 dp] S_{\alpha\beta}\ . \tag{32}$$

For the mass term one finds

$$< \alpha \mid \gamma_0 M \mid \beta(a) >=< \Psi \mid \Psi(a) > \sum_{\alpha\beta} M_{\alpha\beta} B^{-1}_{\beta\alpha}, \tag{33}$$

with

$$M_{\alpha\beta} = 4\pi M \sum_{\lambda} (\frac{1+(-)^{\lambda+l_\alpha+l_\beta}}{2}) [\ \mathrm{i}^{\lambda+l_\alpha-l_\beta} \int j_\lambda(pa) g^*_\alpha g_\beta p^2 dp -$$
$$-\mathrm{i}^{\lambda+\bar{l}_\alpha-\bar{l}_\beta} \int j_\lambda(pa) f^*_\alpha f_\beta p^2 dp] S_{\alpha\beta}\ . \tag{34}$$

The calculation of the potential term is more involved and it turned out to be easier to perform it in configuration space. Our starting point is to substitute equation (9) with $\alpha = \alpha^{'}$ in eq.(30), since we are neglecting the Fock correction in the present approach [7]. Again, after a lengthy but straightforward calculation, we arrive at the following potential term:

$$< \psi \mid V_k \mid \psi(a) >= \frac{1}{2} g_k^2 m_k < \Psi \mid \Psi(a) > \sum_L \int dr_1\, dr_2\, r_1^2 r_2^2 j_L(\mathrm{i} m_k r_<) h_L(\mathrm{i} m_k r_>)$$
$$F^L(r_1, a) G^L(r_2, a), \tag{35}$$

where $k = \sigma, \omega$. The functions $F^L(r_1, a)$ and $G^L(r_2, a)$ have essentially the same structure, so that we have only to write

TABLE I: Ground-state energy, E, without the CM correction for the three double-closed shell nuclei considered in this work, the CM correction, $\Delta E_{\rm proj}$, calculated as described in the text, and the CM correction, $\Delta E_{\rm harm}$, calculated in the harmonic oscillator approximation.

Nucleus	$E\,[\mathrm{MeV}]$	$\Delta E_{\rm proj}\,[\mathrm{MeV}]$	$\Delta E_{\rm harm}\,[\mathrm{MeV}]$
^{4}He	-4.71	-13.22	-19.37
^{16}O	-93.66	-13.24	-12.20
^{40}Ca	-329.88	-11.24	-8.99

down the first one:

$$F^L(r,a) = \sum_{\alpha\beta} \int d(\cos\theta)[g^*_\alpha(r_-)g_\beta(r_+)\phi_{\alpha\beta}(\theta,\theta_-,\theta_+) + \\ + f^*_\alpha(r_-)f_\beta(r_+)\phi_{-\alpha-\beta}(\theta,\theta_-,\theta_+)]B^{-1}_{\beta\alpha}. \quad (36)$$

We have defined $r_\pm = \mid \vec{r}_\pm \mid$ with $\vec{r}_\pm = \vec{r} \pm \frac{\vec{a}}{2}$ and θ ($\theta_\pm$), which is the azimuthal angle associated with the position vector $\vec{r}$ ($\vec{r}_\pm$). The function ϕ is proportional to the product of three spherical harmonics with different (translated) arguments [9]. The minus sign, as in $-\alpha$, means that the orbital quantum number l_α is changed to $\bar{l}_\alpha$, *i.e.* the orbital angular momentum of the lower component.

With the previous expressions we have calculated the CM correction to the ground state energy for ^{4}He,^{16}O and ^{40}Ca and the results are shown in table I (to check the accuracy of our calculations we compared our ground state energies – column 1 of table I – with the TIMORA code[10]). For comparison, we also show the CM correction calculated in the simple harmonic approximation, as described in [5]. Except for the lightest nucleus (^{4}He), the harmonic approximation gives realistic values for the CM energy correction, as compared to the Peierls-Yoccoz projection values. However, as discussed in [2, 3], other observables, as the root mean square radius, form factors and spectroscopic factors should be investigated before a firm conclusion might be established. Moreover, as pointed out at the beginning, the meson degrees of freedom should be included in our calculation, and that work is already in progress.

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