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Density-dependent relativistic Hartree–Fock approach

Wen-Hui Long [a,b], Nguyen Van Giai [b], Jie Meng [a,c,d,*]

[a] *School of Physics, Peking University, Beijing 100871, China*

[b] *Institut de Physique Nucléaire, CNRS-IN2P3, Université Paris-Sud, 91406 Orsay, France*

[c] *Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100080, China*

[d] *Center of Theoretical Nuclear Physics, National Laboratory of Heavy Ion Accelerator, Lanzhou 730000, China*

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Abstract

A new relativistic Hartree–Fock approach with density-dependent σ, ω, ρ and π meson–nucleon couplings for finite nuclei and nuclear matter is presented. Good description for finite nuclei and nuclear matter is achieved with a number of adjustable parameters comparable to that of the relativistic mean field approach. With the Fock terms, the contribution of the π-meson is included and the description for the nucleon effective mass and its isospin and energy dependence is improved.

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The relativistic mean field (RMF) theory [1,2] has received much attention due to its successful description of numerous nuclear phenomena [3–9]. In its most widely employed versions, i.e., with either self-coupling interactions or density-dependent meson–nucleon couplings, the RMF theory with a limited number of parameters can describe very well a very large amount of data: saturation properties of nuclear matter [10], nuclear binding energies and radii, the isotopic shifts in the Pb-region [11]. It gives a natural description of the nuclear spin–orbit potential [12], and explains the origin of the pseudospin symmetry [13,14] and spin symmetry of the anti-nucleon spectrum [15] as a relativistic symmetry [15–18]. In spite of these successes, there are still a number of questions needed to be answered in the RMF theory: the contributions due to the exchange (Fock) terms and the pseudo-vector π-meson.

There exist attempts to include the exchange terms in the relativistic description of nuclear matter and finite nuclei. The earlier relativistic Hartree–Fock (RHF) method led to underbound nuclei due to the missing of the meson self-interactions [19]. Further developments were made by taking into account approximately the non-linear self-couplings of the σ-field [20] or by introducing the products of six and eight nucleon spinors in the zero-range limit [21]. Although some improvements were obtained, the RHF method is still not comparable with the RMF theory in the quantitative description of nuclear systems. The relativistic point coupling model has been used to investigate nuclear systems [22] and the consequences of Fierz transformations acting upon the contact interactions for nucleon fields occurring in relativistic point coupling models has been investigated in Hartree approximation, which yield the same models but in Hartree–Fock approximation instead [23,24]. It has been suggested that the Hartree–Fock approximation may constitute a physically more realistic framework for power counting and QCD scaling than the Hartree approximation.

In this work, a new RHF approach which contains density-dependent meson–nucleon couplings is developed. With a number of adjustable parameters comparable to that of RMF Lagrangians, this density-dependent RHF (DDRHF) theory can give a good description of nuclear systems without dropping the Fock terms. Furthermore, important features like the behavior of neutron and proton effective masses [25] can be interpreted well in DDRHF in comparison with the results of non-relativistic Brueckner–Hartree–Fock (BHF) [26] and Dirac–Brueckner–Hartree–Fock (DBHF) calculations [27,28].

* Corresponding author.
E-mail address: mengj@pku.edu.cn (J. Meng).

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The most important parts of the nuclear force are the short-range repulsive and medium-range attractive components. In analogy with the strong interaction in free space which is described by meson exchanges, it is convenient to represent the strong interaction in nuclear medium by the exchange of effective isoscalar and isovector mesons. The description of nucleon and meson degrees of freedom has to rely ultimately on the relativistic quantum field approach. According to this spirit, we start from an effective Lagrangian density $\mathcal{L}$ constructed with the degrees of freedom associated with the nucleon field (ψ), two isoscalar meson fields (σ and ω), two isovector meson fields (π and ρ) and the photon field (A). The parameters of the model are the effective meson masses and meson–nucleon couplings.

With the general Legendre transformation

$$\mathcal{H} = T^{00} = \frac{\partial \mathcal{L}}{\partial \dot{\phi}_i}\dot{\phi}_i - \mathcal{L}, \tag{1}$$

one can obtain the effective Hamiltonian from the Lagrangian density $\mathcal{L}$ as

$$\mathcal{H} = \bar{\psi}(-i\boldsymbol{\gamma}\cdot\nabla + M)\psi + \frac{1}{2}\int d^4x_2 \sum_{\substack{i=\sigma,\omega\\ \rho,\pi,A}} \bar{\psi}(x_1)\bar{\psi}(x_2)\Gamma_i D_i(x_1,x_2)\psi(x_2)\psi(x_1), \tag{2}$$

where $D_i(x_1,x_2)$ represent the corresponding meson propagators, and the interaction vertices Γ_i are defined as,

$$\Gamma_\sigma(1,2) \equiv -g_\sigma(1)g_\sigma(2), \tag{3a}$$

$$\Gamma_\omega(1,2) \equiv +g_\omega(1)\gamma_\mu(1)g_\omega(2)\gamma^\mu(2), \tag{3b}$$

$$\Gamma_\rho(1,2) \equiv +g_\rho(1)\gamma_\mu(1)\vec{\tau}(1)\cdot g_\rho(2)\gamma^\mu(2)\vec{\tau}(2), \tag{3c}$$

$$\Gamma_\pi(1,2) \equiv -\left[\frac{f_\pi}{m_\pi}\vec{\tau}\gamma_5\gamma_\mu\partial^\mu\right]_1 \cdot \left[\frac{f_\pi}{m_\pi}\vec{\tau}\gamma_5\gamma_\nu\partial^\nu\right]_2, \tag{3d}$$

$$\Gamma_A(1,2) \equiv +\frac{e^2}{4}\left[\gamma_\mu(1-\tau_3)\right]_1\left[\gamma^\mu(1-\tau_3)\right]_2. \tag{3e}$$

Following the experience and success in DDRMF [8,29–34], the meson–nucleon couplings g_σ, g_ω, g_ρ and f_π are taken as functions of the baryonic density ρ_b. For σ- and ω-meson, the density-dependence of the couplings g_σ and g_ω are chosen as

$$g_i(\rho_b) = g_i(\rho_0)f_i(\xi), \tag{4}$$

where $i = \sigma, \omega$, and

$$f_i(\xi) = a_i\frac{1+b_i(\xi+d_i)^2}{1+c_i(\xi+d_i)^2}, \tag{5}$$

is a function of $\xi = \rho_b/\rho_0$, and ρ_0 denotes the baryonic saturation density of nuclear matter. In addition, five constraint conditions $f_i(1) = 1$, $f''_\sigma(1) = f''_\omega(1)$, and $f''_i(0) = 0$ are introduced to reduce the number of free parameters. For simplicity, the exponential density-dependence is adopted for f_π as well as g_ρ [35]:

$$g_\rho(\rho_b) = g_\rho(0)e^{-a_\rho\xi}, \tag{6a}$$

$$f_\pi(\rho_b) = f_\pi(0)e^{-a_\pi\xi}. \tag{6b}$$

The coupling constants $g_\rho(0)$ and $f_\pi(0)$ are fixed to their values in free space. One reason to do so is just to reduce the number of free parameters and another reason is that the inclusion of Fock terms allows such choice. There are in total 8 free parameters, i.e., m_σ, $g_\sigma(\rho_0)$, $g_\omega(\rho_0)$, a_ρ, a_π, and three others from the density-dependence of g_σ and g_ω. A new parametrization called PKO1 is found (see Table 1) by fitting the masses of the nuclei ^{16}O, ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{68}Ni, ^{90}Zr, ^{116}Sn, ^{132}Sn, ^{182}Pb, ^{194}Pb, ^{208}Pb and ^{214}Pb, and the values of the baryonic saturation density ρ_0, the compression modulus K and the symmetry energy J of nuclear matter at the saturation point.

It should be emphasized that here the effective interaction PKO1 is obtained by fitting the empirical properties of nuclei and the nuclear matter at the saturation point. In Table 1 one finds $a_\rho = 0.076$ and $a_\pi = 1.232$. This means that $g_\rho(1)/g_\rho(0) = 0.93$ and $f_\pi(1)/f_\pi(0) = 0.36$, i.e., the contribution from the pion is strongly reduced as compared to that in free space. In fact, the effect of pion has been taken into account effectively via the other mesons. It will be refined in the future if more information is used to constrain the density dependence of the effective interaction in the medium.

The PKO1 parameter set gives the following nuclear matter bulk properties: compression modulus $K = 250.24$ MeV, symmetry energy $J = 34.37$ MeV, binding energy per particle $E/A = -15.996$ MeV, saturation baryonic density $\rho_0 = 0.1520\ \text{fm}^{-3}$.

For finite nuclei, the self-consistent Dirac equations are solved in coordinate space with techniques similar to those used in RMF [36,37]. The non-local exchange (Fock) potentials are treated exactly as in Ref. [19]. Calculations are carried out for a set of selected nuclei (S.N.), i.e., ^{16}O, ^{40}Ca, ^{48}Ca, ^{56}Ni, ^{58}Ni, ^{68}Ni, ^{90}Zr, ^{112}Sn, ^{116}Sn, ^{124}Sn, ^{132}Sn, ^{182}Pb, ^{194}Pb, ^{204}Pb, ^{208}Pb, ^{214}Pb, and ^{210}Po, as well as the Sn and Pb isotopic chains. For the open shell nuclei, the pairing correlations are treated by the BCS method with a density-dependent delta force [38]. A detailed comparison with the predictions of some typical RMF parameterizations: PK1 [34], PKDD [34], NL3 [39] and DD-ME1 [33] are summarized in Table 2 where the root mean square (rms) deviations from the data are shown. As one can see in Table 2, the DDRHF approach with PKO1 provides a good quantitative description of finite nuclei, sometimes better than the RMF approach. It should be emphasized that this is the first time for the RHF approach to provide such a good quantitative description for the finite nuclei and nuclear matter.

From previous discussion, one can find that good description of nuclear systems comparable to that of RMF can be obtained without dropping the Fock terms. Taking ^{208}Pb as an example, shown in Fig. 1 are the neutron energy densities from Hartree

Table 1
The effective interaction PKO1 for DDRHF with $M = 938.9$ MeV, $m_\omega = 783.0$ MeV, $m_\rho = 769.0$ MeV, $m_\pi = 138.0$ MeV

m_σ	525.7691	a_σ	1.3845	a_ω	1.4033
g_σ	8.8332	b_σ	1.5132	b_ω	2.0087
g_ω	10.7299	c_σ	2.2966	c_ω	3.0467
$g_\rho(0)$	2.6290	d_σ	0.3810	d_ω	0.3308
$f_\pi(0)$	1.0000	a_ρ	0.0768	a_π	1.2320

Table 2
The rms deviations Δ from the data for the RHF calculations with PKO1 in comparison with that of RMF with PK1, PKDD, NL3 and DD-ME1. The rows from two to ten respectively correspond to: the binding energies E_b of the selected nuclei (S.N.) and the even–even nuclei in Pb and Sn chains; two-neutron separation energies S_{2n} of Pb and Sn isotopes; charge radii r_c of the S.N. and Pb isotopes; isotope shifts (I.S.) of Pb isotopes; spin–orbit (S.O.) splittings of doubly magic nuclei

		PKO1	PK1	PKDD	NL3	DD-ME1
Δ_{E_b}	S.N.	1.6177	1.8825	2.3620	2.2506	2.7561
	Pb	1.8995	2.0336	2.7007	2.0021	2.1491
	Sn	1.2665	1.9552	2.4567	1.6551	0.9168
$\Delta_{S_{2n}}$	Pb	0.6831	0.9192	1.3139	0.9359	1.2191
	Sn	0.6813	0.7762	1.0629	0.8463	0.7646
Δ_{r_c}	S.N.	0.0269	0.0204	0.0188	0.0177	0.0163
	Pb	0.0056	0.0061	0.0060	0.0143	0.0150
$\Delta_{\text{I.S.}}$	Pb	0.0760	0.0784	0.0784	0.0679	0.0567
$\Delta_{\text{S.O.}}$	O	0.1761	0.2879	0.6817	0.2195	0.1107
	Ca	0.5078	0.6638	0.8159	0.7184	0.6041
	Ni	0.3959	0.9923	1.3287	1.3315	0.9029
	Sn	0.1650	0.3300	0.6913	0.4757	0.5408
	Pb	0.2014	0.3902	0.6370	0.4604	0.4588

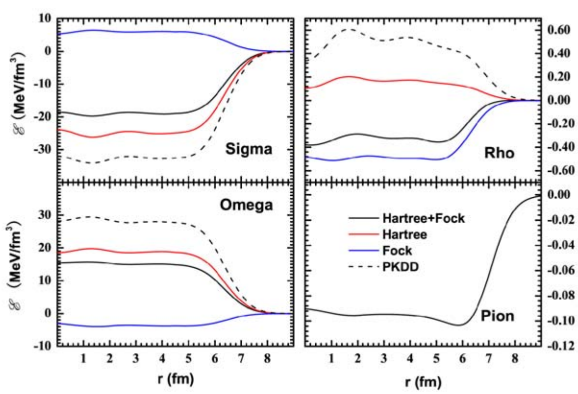

Fig. 1. Energy density contributions from Hartree and Fock terms in different channels for neutrons in ^{208}Pb given by DDRHF with PKO1, in comparison with RMF with PKDD.

and Fock terms in different meson channels in DDRHF, compared with the results of RMF with PKDD [34]. There exist significant and remarkable differences between DDRHF and RMF results.

Although the attractive and repulsive parts of the nuclear force are mainly provided by σ- and ω-mesons respectively, the contributions in DDRHF are much less than their corresponding ones in RMF, as shown in Fig. 1. For the isovector channels, the isovector ρ- and π-mesons in the DDRHF approach become attractive due to the strong Fock terms. While in the standard RMF with σ-, ω- and ρ-mesons, the isospin part of nuclear force is provided only by the direct part of ρ-meson, which gives the repulsive interaction for the neutrons. Furthermore it should be emphasized that one of the advantage of the DDRHF is the inclusion of the π-meson which is very important at large distance in DDRHF.

An important difference between the RHF and RMF approaches is the nucleon effective mass. In the medium, particles or quasi-particles behave as if their mass is different from their bare mass due to interactions with surrounding particles, which is reflected in the level density as an example. In Ref. [25], the nucleon effective mass has been discussed and it is shown that there are two sources of modification of the bare mass: the non-locality of the mean field which gives rise to the so-called k-mass M_k^*, and the energy dependence of the mean field which leads to the E-mass M_E^*. The total effective mass M^* is related to M_k^* and M_E^*. One can already note that the RMF (RHF) mean field is local (non-local) in coordinate space and therefore, it can be expected that their effective masses will differ. It should be also emphasized that, in RMF theory appears the Lorentz scalar mass $M_S = M + \Sigma_S$ where Σ_S is the scalar self-energy. It should not be confused with any of the M^* and one should refer to it as the scalar mass, or Dirac mass.

In the non-relativistic framework, the energy–momentum relation

$$\frac{1}{2M}k^2 + V(k;\epsilon) = \epsilon \tag{7}$$

leads to the effective mass M^* [25]:

$$\frac{M^*}{M} \equiv 1 - \frac{dV(k(\epsilon);\epsilon)}{d\epsilon}, \tag{8}$$

where $\epsilon = E - M$ is the single-particle energy and $V(k;\epsilon)$ is the momentum- and energy-dependent mean field.

In a relativistic framework like RMF or RHF, the energy–momentum relation is,

$$(\boldsymbol{k} + \hat{\boldsymbol{k}}\Sigma_V)^2 + (M + \Sigma_S)^2 = (E - \Sigma_0)^2, \tag{9}$$

where Σ_S, Σ_V, and Σ_0 are respectively the scalar, spacelike- and timelike-vector components of the self-energy. Its Schrödinger-type form can be derived as:

$$\frac{1}{2M}k^2 + V(k;\epsilon) - \frac{\epsilon^2}{2M} = \epsilon, \tag{10}$$

which give the effective masses M_{R}^*,

$$\frac{M_{\mathrm{R}}^*}{M} = 1 - \frac{d}{d\epsilon}\left[V\big(k(\epsilon);\epsilon\big) - \frac{\epsilon^2}{2M}\right] \tag{11}$$

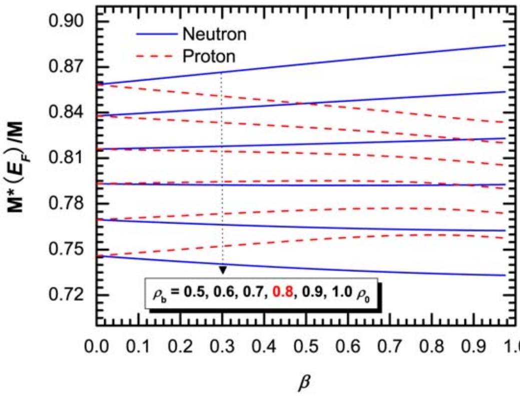

Fig. 2. Neutron and proton effective masses $M^*_{\rm NR}$ at their corresponding Fermi energy E_F calculated in DDRHF with PKO1 as functions of $\beta = (N - Z)/A$ for different baryonic densities.

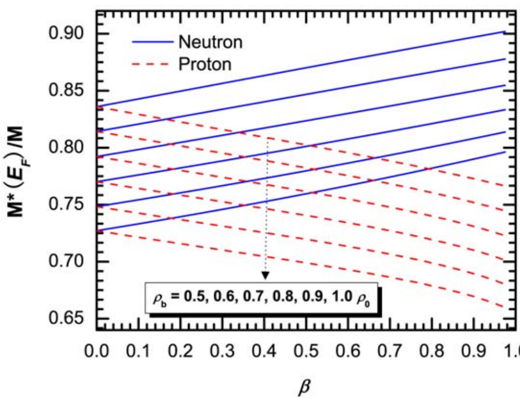

Fig. 3. Same as Fig. 2, but for $M^*_{\rm R}$.

and $M^*_{\rm NR} = M^*_{\rm R} - \epsilon$ in the non-relativistic approximation by neglecting the last term at the left side of Eq. (10). One can see that $M^*_{\rm NR}$ is the effective mass in Refs. [25,27] and M^*_R the group mass in Ref. [25], and they are the same in the non-relativistic approach. In the relativistic approach they can be significantly different, as shown in the following.

The neutron and proton effective masses $M^*_{\rm NR}$ and $M^*_{\rm R}$ at their corresponding Fermi energy E_F from the DDRHF calculations with PKO1 are respectively shown as functions of $\beta = (N - Z)/A$ in Figs. 2 and 3 for different density ρ_b. At lower density, the RHF gives the trend that $M^*_{{\rm NR},n}(E_{F,n}) > M^*_{{\rm NR},p}(E_{F,p})$ but this trend is reversed around $0.8\rho_0$. For $M^*_{\rm R}$, one always have $M^*_{{\rm R},n}(E_{F,n}) > M^*_{{\rm R},p}(E_{F,p})$ for all densities.

In contrast, for RMF, the relatively simple expressions tell us that one always have $M^*_{{\rm NR},n} < M^*_{{\rm NR},p}$ and $M^*_{{\rm R},n}(E_{F,n}) > M^*_{{\rm R},p}(E_{F,p})$ for neutron rich system. This difference between RHF and RMF is related to the presence of exchange (Fock) terms which bring non-locality effects to the RHF self-energies. It is worthwhile to mention that in Brueckner–Hartree–Fock studies it is found that $M^*_n(E_{F,n}) > M^*_p(E_{F,p})$ [28,40], but at larger density ($\rho_b = 0.17\ {\rm fm}^{-3}$) [40].

Another significant difference between RMF and DDRHF predictions is the energy dependence of $M^*_{\rm NR}$. In RMF, $M^*_{\rm NR}$ is a constant whereas it is a function of E or k in RHF. In Fig. 4,

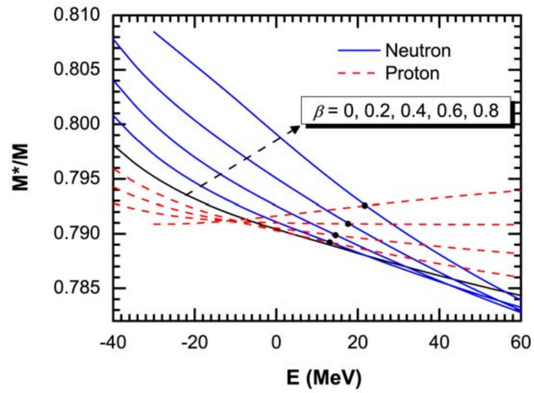

Fig. 4. The energy dependence of the effective mass $M^*_{\rm NR}$ calculated in RHF with PKO1, for $\rho = 0.8\rho_0$ and different values of neutron excess β.

the energy dependence of $M^*_{\rm NR}$ for different β at $\rho_b = 0.8\rho_0$ is shown. The neutron effective mass tends to decrease with the energy whereas the proton mass is more constant or slightly increases in neutron rich matter.

One can see that the neutron effective masses are larger than the proton ones at low energy, i.e., $M^*_{{\rm NR},n}(E) > M^*_{{\rm NR},p}(E)$, and depending on the β, a different feature appears at energy $E \sim 15$–20 MeV (solid points). It was also found in Dirac–Brueckner–Hartree–Fock calculations that $M^*_{{\rm NR},n}(E) > M^*_{{\rm NR},p}(E)$ [27], but at higher energy ($E = 50$ MeV). Combining with the discussion of Fig. 2, one can conclude that the DDRHF will predict $M^*_{{\rm NR},n} > M^*_{{\rm NR},p}$ at low energy or low density in neutron rich system while $M^*_{{\rm NR},n} < M^*_{{\rm NR},p}$ for the RMF.

In summary, it has been demonstrated that one can go beyond the standard relativistic mean field approach to include the exchange (Fock) terms and the new couplings such as pion–nucleon couplings which are effective only through exchange terms. These exchange terms are the cause of subtle effects such as the isospin dependence of the effective masses. The same (or even better) quantitative description of nuclear properties comparable to RMF can be achieved with a comparable number of adjusted parameters. It will open the door to the future investigation of nuclei by the relativistic Hartree–Fock–Bogoliubov approach and the relativistic RPA on top of RHF approximation.

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