Local density functional for isovector-meson exchange

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The local density approximation (LDA) for the exchange potential of QHD-I presented in a previous publication [R. N. Schmid, E. Engel, and R. M. Dreizler, Phys. Rev. C **52**, 164 (1995)] is extended to ρ mesons and pions to allow for realistic applications of the density functional approach to quantum hadrodynamics. Some results for spherical nuclei show that the LDA is an accurate approximation to the nonlocal Hartree-Fock–exchange potential also on the level of QHD-II.

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In a recent paper [1] (referred to as I in the following) we have specified a local exchange potential for nuclear structure calculations within the framework of the linear σ-ω model. It could be shown that the solution of the resulting exchange-only Kohn-Sham equations, constituting a density functional (DF) approach to meson-field theory, essentially reproduces the results of the computationally more involved Hartree-Fock (HF) approach. As a more realistic description of nuclear properties requires more sophisticated meson exchange models, such as, for instance, quantum hadrodynamics (QHD)-II, involving isovector mesons, we present here an extension of the DF approach incorporating the exchange contributions of both ρ mesons and pions in addition to those of the σ and ω mesons. Applications of this extended version of DF meson-exchange potentials yield good agreement with available HF data. This suggests that one may simplify nuclear structure calculations beyond the mean-field level by replacing the nonlocal HF potentials by their local DF equivalents.

The meson-exchange model to be investigated in the present contribution is specified by the Lagrangian (in the notations of Ref. [2])

$$\mathscr{L}=\mathscr{L}_F+\mathscr{L}_I,$$

$$\mathscr{L}_I=g_\sigma\bar{\Psi}\sigma\Psi-g_\omega\bar{\Psi}\omega^\mu\gamma_\mu\Psi-\frac{f_\pi}{m_\pi}\bar{\Psi}\gamma_5\gamma^\mu\boldsymbol{\tau}\Psi\,\partial_\mu\boldsymbol{\pi}$$
$$-g_\rho\bar{\Psi}\boldsymbol{\rho}_\mu\cdot\boldsymbol{\tau}\gamma^\mu\Psi-e\bar{\Psi}\gamma_\mu\frac{1}{2}(1+\tau_3)A^\mu\Psi. \tag{1}$$

Note that for pion exchange a pseudovector coupling is employed as it turned out to be more appropriate for the description of nuclear properties than the pseudoscalar coupling [3,4]. For ground states with a specified number of protons and neutrons, one obtains the following interaction terms in addition to those specified in Eq. (2.4) of Ref. [5]. The ρ mesons couple directly to the proton and neutron four-currents via an effective potential $V_\mu^{(\rho)}$, corresponding to both mean-field and exchange-correlation contributions,

$$g_\rho[j_p^\mu(\mathbf{x})-j_n^\mu(\mathbf{x})]V_\mu^{(\rho)}(\mathbf{x}). \tag{2}$$

In consequence, inclusion of the ρ meson does not introduce any new basic density or current variable in the DF formalism as compared to QHD-I. The interaction of the nucleons with pions leads to a scalar potential $V^{(\pi)}$, which couples to the divergence of the axial nuclear currents,

$$\left(\frac{f_\pi}{m_\pi}\right)[\boldsymbol{\nabla}\cdot\mathbf{j}_p^5(\mathbf{x})-\boldsymbol{\nabla}\cdot\mathbf{j}_n^5(\mathbf{x})]V^{(\pi)}(\mathbf{x}), \tag{3}$$

where $\mathbf{j}_q^5=\bar{\psi}_q\gamma^5\boldsymbol{\gamma}\psi_q$ and the discussion has again been restricted to ground states with definite charge. Thus in principle the set of basic variables of QHD-I (j_p^μ, j_n^μ, ρ_s) has to be extended by inclusion of one additional component $\boldsymbol{\nabla}\cdot[\mathbf{j}_p^5(\mathbf{x})-\mathbf{j}_n^5(\mathbf{x})]$.

The results of I were obtained in terms of the exchange-only limit of the local density approximation (LDA). In this approximation the density dependence of the exchange-correlation energy density of infinite nuclear matter, $e_{\rm xc}^{\rm INM}(\rho_s,\rho_p,\rho_n)$, is used for the actual inhomogeneous system of interest (i.e., nuclei),

$$E_{\rm xc}^{\rm LDA}[\rho_s,\rho_p,\rho_n]=\int d^3r\ e_{\rm xc}^{\rm INM}(\rho_s,\rho_p,\rho_n). \tag{4}$$

If one attempts to apply the same approximation to the QHD-II model specified by the Lagrangian (1), one is faced with the fact that the divergence of the pseudovector current vanishes in nuclear matter, so that on the level of the LDA the dependence of the exact $E_{\rm xc}$ on $\nabla\cdot(\mathbf{j}_p^5-\mathbf{j}_n^5)$ does not show up. In consequence, the pion exchange is only included in an indirect manner, by simply adding its $\rho_{p,n,s}$-dependent energy contribution to the exchange-correlation energy functional.

Restricting ourselves (as in I) to the exchange-only limit, we can specify the exchange-energy density as

$$e_x^{\rm INM}[\rho_p,\rho_n,\rho_s]=e_x^{{\rm INM},\sigma}(\rho_q,\rho_s)+e_x^{{\rm INM},\omega}(\rho_q,\rho_s)$$
$$+e_x^{{\rm INM},\pi}(\rho_q,\rho_s)+e_x^{{\rm INM},\rho}(\rho_q,\rho_s), \tag{5}$$

so that the corresponding LDA exchange potentials to be used in the Kohn-Sham (KS) equations [Eq. (6) of I] are given by

$$V_{q,x}^{\rm LDA}(\mathbf{x})=\frac{\partial}{\partial\rho_q(\mathbf{x})}e_x^{\rm INM}(\rho_p,\rho_n,\rho_s), \tag{6}$$

$$\phi_x^{\mathrm{LDA}}(\mathbf{x}) = -\frac{\partial}{\partial \rho_s(\mathbf{x})} e_x^{\mathrm{INM}}(\rho_p,\rho_n,\rho_s) \quad (7)$$

($q=p,n$) in complete analogy to the case of QHD-I.

The explicit forms of e_x^π and e_x^ρ involve the isospin decomposition [6],

$$e_x(\rho_p,\rho_n,\rho_s) = e(\rho_p,\rho_p,M^*) + e(\rho_n,\rho_n,M^*) + 4e(\rho_n,\rho_p,M^*), \quad (8)$$

where for ρ exchange $e(\rho_1,\rho_2,M^*)$ is given by [6]

$$e^\rho(\rho_1,\rho_2,M^*) = g_\rho^2 \frac{M^{*4}}{(2\pi)^4}\left\{ (\beta_1\eta_1 - \ln\xi_1)(\beta_2\eta_2 - \ln\xi_2) + \left(1 - \frac{w_\rho}{4}\right) I(w_\rho,\xi_1,\xi_2)\right\}, \quad (9)$$

with $w_\rho = m_\rho^2/M^{*2}$, while for the pion exchange one obtains

$$e^\pi(\rho_1,\rho_2,M^*) = \left(\frac{f_\pi}{m_\pi}\right)^2 \frac{M^{*6}}{(2\pi)^4}\{(\beta_1\eta_1 - \ln\xi_1)(\beta_2\eta_2 - \ln\xi_2) - w_\pi I(w_\pi,\xi_1,\xi_2)\}, \quad (10)$$

with $w_\pi = m_\pi^2/M^{*2}$. The additional parameters are $\beta_q = (3\pi^2\rho_q)^{1/3}/M^*$, $\eta_q = (1+\beta_q)^{1/2}$, and $\xi_q = \beta_q + \eta_q$, while M^* and $I(w,\xi_1,\xi_2)$ are defined as in I, Eqs. (10) and (17). Both functionals (9) and (10) (as well as those specified in I) are based on full meson propagators and thus include meson retardation. The Coulomb exchange has also been included on the level of the LDA, using the functional given by Eqs. (3.2a) and (3.3a) of Ref. [7] (neglecting retardation effects to allow for a comparison with standard HF results).

The results obtained by this exchange-only DF approach for some spherical nuclei are shown in Table I together with the corresponding HF values [2] (also including meson retardation) and experimental data (for technical details of our calculations see I). In order to allow for a meaningful comparison two different parameter sets have been used in the KS calculations: While the results from the nuclear matter based parameter set HF2 suggested by Zhang and Onley [2] represent the DF equivalent of their HF data, the values from the parameter set ZJO (this is parameter set 2 of Ref. [8]), which has been fitted to nuclear ground-state properties, fa-

TABLE I. Binding energies per nucleon (in MeV) and charge radii (in fm) from LDA KS calculations for several spherical nuclei using two different parameters sets (HF2 [2] — without center of mass correction, ZJO [8] — including center of mass correction) in comparison with HF calculations (using parameter set HF2 [2] — without center of mass correction) and experimental data (taken from Ref. [4]).

	$-E/A$				R_c			
	HF	LDA		Expt.	HF	LDA		Expt.
	HF2	HF2	ZJO		HF2	HF2	ZJO	
^{16}O	5.11	4.97	7.63	7.98	2.74	2.76	2.74	2.73
^{40}Ca	6.46	6.35	8.26	8.55	3.46	3.49	3.52	3.46
^{48}Ca	6.72	6.71	8.53	8.67	3.45	3.49	3.53	3.45
^{90}Zr	7.11	7.02	8.73	8.71	4.23	4.27	4.33	4.23
^{208}Pb	6.49	6.52	7.87	7.87	5.47	5.48	5.60	5.47
^{298}114			7.10				6.32	

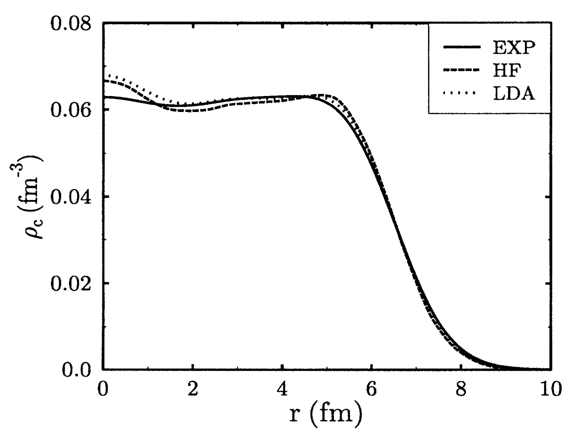

FIG. 1. Charge density distribution of ^{208}Pb from HF and KS calculations (with parameter set HF2 [2]) in comparison with experimental data [15].

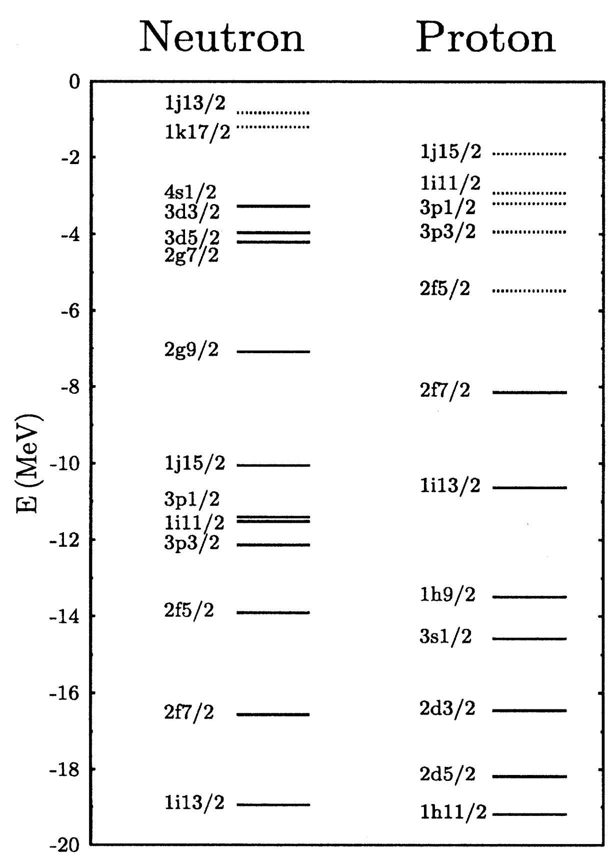

FIG. 2. Single-particle spectrum of ^{298}114 from KS calculation with parameter set ZJO [8] (solid lines indicate occupied levels, dashed lines unoccupied levels, and energies are in MeV).

cilitate a direct comparison with experiment. As Table I shows the DF results for both E/A and R_c are in good overall agreement with the HF values, demonstrating in particular the adequacy of the indirect inclusion of the pion exchange via (4–7), (8), and (10). As in the case of QHD-I the error of the LDA results decreases with increasing mass of the nucleus, as one would expect from an approximation based on the characteristics of nuclear matter. Though still small, the errors in the case of QHD-II are more pronounced for very small nuclei, which may be attributed to the inclusion of the pion: Due to the pion's rather small mass and the resulting enhanced range of interaction the LDA, being particularly suitable for short range interactions, is a somewhat less accurate approximation in this case.

Even though retardation effects have not been included in the parameter set ZJO [8], this set yields good results for the energies of finite nuclei in our DF approach as compared to the experimental values. Concerning charge radii the agreement is less satisfactory, but is nevertheless acceptable for a model without nonlinear self-interactions of the σ field. As is well known from least squares fits to nuclear ground-state properties on the mean-field level [9] the inclusion of these nonlinear terms is important for obtaining accurate results. It should be pointed out that the σ self-interaction may easily be included in the LDA via substitution of m_σ^2 by $m_\sigma^2 - b\phi + c\phi^2$ in the σ exchange energy [10]. However, we did not include the nonlinear contributions in the present calculations as no appropriate parametrization for this model on the HF level can be found in the literature.

A comparison of the charge density of ^{208}Pb obtained by the different approaches (using parameter set HF2) is given in Fig. 1. As in the case of QHD-I the agreement between the LDA and the HF density is excellent.

As a demonstration of the feasibility of the LDA approach we have investigated the superheavy nucleus $^{298}114$, for which relativistic HF calculations have not yet been reported. Our results for gross features like total energy and radii essentially agree with those obtained by both the nonrelativistic Skyrme-HF approach [11,12] and relativistic mean-field calculations including the nonlinear σ self-interaction [13] (compare also [14]). Figure 2 shows the single-particle spectrum of $^{298}114$ (calculated with the parametrization ZJO) which clearly displays the closed-shell character of $^{298}114$.

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