Density functional approach to quantum hadrodynamics: Local exchange potential for nuclear structure calculations

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Based on the density functional approach to quantum hadrodynamics a local effective exchange potential for use in nuclear structure calculations beyond the mean-field approximation has been developed. For a conceptual study of the density functional technique the resulting Kohn-Sham single-particle equations have been solved for several spherical nuclei within the linear σ-ω model. A detailed comparison with Hartree-Fock results is given.

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I. INTRODUCTION

Relativistic mean-field theory, introduced by Miller and Green [1] and Walecka [2], has been applied with considerable success to a variety of problems in nuclear structure physics. In particular, ground state properties of nuclei have been extensively studied in terms of different variants of the mean-field approximation, for example, by Horowitz and Serot [3] (for an overview see [4,5]).

In recent years there has been growing interest in many-body approaches beyond the mean-field limit. As the corresponding calculations can be quite involved, only a limited number of studies of nuclear properties for finite systems have been performed to date in terms of the Hartree-Fock (HF) approximation [6–9]. The computational demands, in particular for heavy nuclei, originating from the nonlocal character of the HF exchange potential complicate systematic investigations, involving, e.g., least-squares fits of the model parameters to empirical ground state data [8]. Only few efforts have been made to address the question of correlation effects for the case of finite nuclei [9–13]. The situation is more auspicious for the nuclear matter problem. Correlation effects have been studied extensively in the framework of the relativistic generalization of the Brueckner-Bethe approach [14–16]. The resulting Dirac-Brueckner (DB) method [17,18] may now be considered as state of the art for nuclear matter calculations. Due to the complicated nonlocal structure of the DB equations fully self-consistent calculations for finite systems do not (yet) seem possible [9]. For this reason effective approaches, parametrizing the correlation contributions in the form of a density dependent coupling constant, like density dependent mean-field and effective Dirac-Brueckner-Hartree-Fock schemes, have been developed [13,9].

This situation is somewhat similar to the difficulties one has to face in the *ab initio* description of Coulomb systems [19]. In this field, however, density functional (DF) methods have attracted considerable interest in recent years [20,19]. The high efficiency of DF calculations mainly originates from the local character of the density dependent exchange-correlation (xc) potential, the key ingredient of the basic, single-particle-type equations of DF theory (DFT) [21,22]. The success of DF methods in quantum chemical and condensed matter applications motivates their extension to relativistic nuclear physics. The foundations of a DFT approach to quantum hadrodynamics (QHD) have been given in Ref. [23] (to which we refer the reader for details) by generalizing the fundamental DF existence theorem to QHD and deriving the Kohn-Sham (KS) equations, which, in spite of their single-particle character, in principle contain *all* exchange and correlation effects.

The present contribution constitutes a more conceptual study of the KS approach to relativistic nuclear physics. In order to establish the basic elements of this technique and to analyze its properties we restrict ourselves to the exchange-only limit in the local density approximation (LDA) and to the simplest effective Lagrangian suggested in this context, i.e., the linear σ-ω model (QHD-I) [2]. Thus HF results [7,9] on the basis of QHD-I serve as a standard for comparisons. The exchange-only limit of the LDA potential is evaluated analytically and applied to finite nuclei. The question of correlation contributions (within the LDA) is indicated briefly as a unified approach to exchange and correlation effects would be the next logical step.

II. THE KOHN-SHAM APPROACH

A detailed discussion of the DFT approach to QHD-I and the derivation of the corresponding KS equations for the symmetric case has been given in [23]. A generalization to asymmetric systems (including Coulomb forces) is straightforward and will thus only be briefly summarized in the following. The DFT scheme is based on the fact that not only the properties of infinite nuclear matter (INM) but quite generally the ground state $|\Phi_0\rangle$ of any QHD system is uniquely determined by the proton and neutron ground state four-currents j_p^μ and j_n^μ and the ground state scalar density ρ_s, allowing one to un-

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derstand the ground state energy E_0 as a functional of these quantities:

$$E_0[\rho_s, j_p^\mu, j_n^\mu] = \langle \Phi_0[\rho_s, j_p^\mu, j_n^\mu] \mid \hat{H} \mid \Phi_0[\rho_s, j_p^\mu, j_n^\mu] \rangle \ .$$

Expressing the currents j_q^μ (where q characterizes either protons, $q = p$, or neutrons, $q = n$) and ρ_s in terms of auxiliary single-particle four-spinors $\varphi_{i,q}$,

$$\rho_s(\mathbf{x}) = \sum_{q=n,p} \left[\sum_{-M<\epsilon_{i,q}<\epsilon_{F,q}} \bar{\varphi}_{i,q}(\mathbf{x})\varphi_{i,q}(\mathbf{x}) \right], \tag{1}$$

$$j_q^\mu(\mathbf{x}) = \sum_{-M<\epsilon_{i,q}<\epsilon_{F,q}} \bar{\varphi}_{i,q}(\mathbf{x})\gamma^\mu\varphi_{i,q}(\mathbf{x}) \tag{2}$$

(within the no-sea approximation, i.e., neglecting all vacuum corrections) one can decompose E_0 as

$$E_0 = T_s + E_H + E_{\rm xc}, \tag{3}$$

where T_s represents the kinetic energy functional of noninteracting nucleons,

$$T_{s,q} = \int d^3x \sum_{-M<\epsilon_{i,q}<\epsilon_{F,q}} \varphi_{i,q}^+(\mathbf{x}) \ (-i\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \beta M) \ \varphi_{i,q}(\mathbf{x}). \tag{4}$$

E_H is the Hartree energy,

$$\begin{aligned} E_H = &-\frac{g_\sigma^2}{2}\int d^3x \ d^3y \ \frac{e^{-m_\sigma|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} \ \rho_s(\mathbf{x}) \ \rho_s(\mathbf{y}) \\ &+\frac{g_\omega^2}{2}\sum_{q=p,n}\int d^3x \ d^3y \ \frac{e^{-m_\omega|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} \ j_q^\mu(\mathbf{x}) \ j_{\mu,q}(\mathbf{y}) \\ &+\frac{e^2}{2}\int d^3x d^3y \frac{1}{4\pi|\mathbf{x}-\mathbf{y}|} j_p^\mu(\mathbf{x}) j_{\mu,p}(\mathbf{y}), \end{aligned} \tag{5}$$

and the exchange-correlation energy $E_{\rm xc}$ is defined via Eq. (3). Minimization of E_0 with respect to the $\varphi_{i,q}$ then leads to the single-particle equations (KS equations)

$$\Big\{ -i\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \beta\Big[M - \phi_H - \phi_{\rm xc} + \gamma_\mu(V_{q,H}^\mu + V_{q,{\rm xc}}^\mu)\Big]\Big\}\varphi_{i,q} = \epsilon_{i,q}\varphi_{i,q}, \tag{6}$$

where $\phi_H(\mathbf{x})$ and $V_{q,H}^\mu(\mathbf{x})$ are the usual Hartree potentials ($V_{p,H}^\mu$ includes the Coulomb contribution) and the local exchange-correlation potentials $\phi_{\rm xc}(\mathbf{x})$ and $V_{q,{\rm xc}}^\mu(\mathbf{x})$ are given by

$$V_{\mu,q,{\rm xc}}(\mathbf{x}) = \frac{\delta}{\delta j_q^\mu(\mathbf{x})} E_{\rm xc}[\rho_s, j_p^\mu, j_n^\mu], \tag{7}$$

$$\phi_{\rm xc}(\mathbf{x}) = -\frac{\delta}{\delta\rho_s(\mathbf{x})} E_{\rm xc}[\rho_s, j_p^\mu, j_n^\mu]. \tag{8}$$

Equations (1), (2), and (6)–(8) have to be solved self-consistently. We just remark that the standard mean-field approach is obtained from this scheme by simply neglecting $\phi_{\rm xc}(\mathbf{x})$ and $V_{q,{\rm xc}}^\mu(\mathbf{x})$. Knowledge of the exact $E_{\rm xc}[\rho_s, j_p^\mu, j_n^\mu]$ would in principle allow one to evaluate the exact ground state four-currents and scalar density as well as the exact ground state energy by solution of the KS equations (within the no-sea approximation or beyond). Reasonable approximations to $E_{\rm xc}[\rho_s, j_p^\mu, j_n^\mu]$, on the other hand, are expected to give reasonable currents, densities, and energies, as is the case for electronic systems [20,24].

III. EXCHANGE-CORRELATION ENERGY FUNCTIONAL

An exact representation of $E_{\rm xc}[\rho_s, j_p^\mu, j_n^\mu]$ can be obtained using the coupling constant integration method [23]. Unfortunately, the complexity of this representation does not allow its direct application. In order to obtain $E_{\rm xc}$ as an explicit density functional the standard approximation applied in the case of electronic systems [20,21] is the so-called local density approximation (LDA). In the present context the LDA amounts to utilizing the density dependence of the exchange-correlation energy density of nuclear matter, $e_{\rm xc}^{\rm INM}$, for the inhomogeneous system of interest, e.g., a nucleus, by locally replacing the nuclear matter densities by the actual densities $\rho_q(\mathbf{x}) = j_q^0(\mathbf{x})$ and $\rho_s(\mathbf{x})$,

$$E_{\rm xc}^{\rm LDA}[\rho_s, \rho_p, \rho_n] = \int d^3r \ \ e_{\rm xc}^{\rm INM}(\rho_s, \rho_p, \rho_n) \tag{9}$$

(the spatial components of the currents do not contribute in the LDA). However, usually $e_{\rm xc}^{\rm INM}$ is given as a function of the local effective mass $M^*(\mathbf{x}) = M - \phi_H(\mathbf{x}) - \phi_{\rm xc}(\mathbf{x})$ rather than ρ_s, $\tilde{e}_{\rm xc}^{\rm INM}(M^*, \rho_p, \rho_n)$. The connection between M^* and ρ_s is established by the standard mean-field relation

$$\rho_s = \frac{(M^*)^3}{2\pi^2}\sum_{q=p,n}[\beta_q\eta_q - \ln(\beta_q + \eta_q)], \tag{10}$$

where

$$\beta_q = (3\pi^2\rho_q)^{\frac{1}{3}}/M^*, \quad \eta_q = [1 + \beta_q^2]^{\frac{1}{2}} \ . \tag{11}$$

For nuclear matter, i.e., for homogeneous nonvanishing densities, M^* and ρ_s are completely equivalent as the uniqueness of (10) allows the elimination of M^* from $\tilde{e}_{\rm xc}^{\rm INM}(M^*, \rho_p, \rho_n)$ in favor of ρ_s. For inhomogeneous systems, however, the actual scalar density $\rho_s(\mathbf{x})$, Eq. (1), is not identical with the $\tilde{\rho}_s$ obtained from M^* via (10), although the differences are small in general. One can thus use a perturbative approach to $e_{\rm xc}^{\rm INM}(\rho_s, \rho_p, \rho_n)$ (for fixed ρ_p and ρ_n),

$$\begin{aligned} e_{\rm xc}^{\rm INM}(\rho_s) \approx &\ \tilde{e}_{\rm xc}^{\rm INM}(M^*) \\ &+\frac{d\tilde{e}_{\rm xc}^{\rm INM}}{dM^*}(M^*)\left(\frac{d\tilde{\rho}_s}{dM^*}(M^*)\right)^{-1}(\rho_s - \tilde{\rho}_s) \end{aligned} \tag{12}$$

in which the difference between ρ_s and $\tilde{\rho}_s$ has been taken into account to first order, wherever inversion of (10) leads to numerical difficulties as, e.g., in the asymptotic regime with its vanishing nuclear densities. In view of its close relationship to nuclear matter and its computational efficiency the LDA is an ideal starting point for applications of the KS approach to QHD and thus explicit

expressions for $e_{\rm xc}^{\rm INM}[M^*,\rho_p,\rho_n]$ will be summarized in the following.

The exchange-correlation energy of homogeneous nuclear matter has been studied by Chin [25]. The total $e_{\rm xc}^{\rm INM}$ separates into a scalar exchange component $e_{x,\sigma}^{\rm INM}$, a vector exchange term $e_{x,\omega}^{\rm INM}$, and a correlation contribution $e_c^{\rm INM}$,

$$e_{\rm xc}^{\rm INM}=\sum_{q=p,n}\left[e_{x,\sigma}^{\rm INM}(\beta_q,M^*)+e_{x,\omega}^{\rm INM}(\beta_q,M^*)\right]+e_c^{\rm INM}(\beta_p,\beta_n,M^*)\ . \tag{13}$$

Within the ring approximation (RPA) $e_c^{\rm INM}$ is given by (the notation follows Ref. [25])

$$e_c^{\rm INM/RPA}=-\frac{i}{2}\int\frac{d^4q}{(2\pi)^4}\left\{\ln(1-D'\Pi_L^D)+D'\Pi_L^D+2[\ln(1-D'\Pi_T^D)+D'\Pi_T^D]+\ln(1-\Delta'\Pi_s^D)+\Delta'\Pi_s^D+\ln\left[1-\frac{\Pi_M^2}{[(\Delta')^{-1}-\Pi_s^D][(D')^{-1}-\Pi_L^D]}\right]\right\}, \tag{14}$$

which has been evaluated numerically by Ji [26]. For the exchange energy densities one obtains

$$e_{x,\sigma}^{\rm INM}(\beta,M^*)=\frac{g_\sigma^2(M^*)^4}{(2\pi)^4}\left\{\frac{1}{4}(\beta\eta-\ln\xi)^2+\left(1-\frac{w_\sigma}{4}\right)I(w_\sigma,\xi,\xi)\right\}, \tag{15}$$

$$e_{x,\omega}^{\rm INM}(\beta,M^*)=\frac{g_\omega^2(M^*)^4}{(2\pi)^4}\left\{\frac{1}{2}(\beta\eta-\ln\xi)^2-\left(1+\frac{w_\omega}{2}\right)I(w_\omega,\xi,\xi)\right\}, \tag{16}$$

where $\xi=\beta+\eta$, $w_{\sigma,\omega}=m_{\sigma,\omega}^2/(M^*)^2$, and

$$I(w,\xi_1,\xi_2)=\int_1^{\xi_1}du\int_1^{\xi_2}dv\left(1-\frac{1}{u^2}\right)\left(1-\frac{1}{v^2}\right)\ln\frac{(uv-1)^2+uvw}{(u-v)^2+uvw} \tag{17}$$

[note that knowledge of $I(w,\xi_1,\xi_2)$ for $\xi_1\neq\xi_2$ is required for extensions of QHD-I]. The integral (17) has been calculated numerically by Chin [25] as well as Furnstahl and Serot [27]. However, $I(w,\xi_1,\xi_2)$ can also be evaluated analytically (the explicit result is given in the Appendix) which is particularly useful for application of (17) in self-consistent calculations.

Figure 1 shows the β dependence of $e_{x,\omega}^{\rm INM}$ for different values of w, i.e., M^*. To facilitate comparison with the well-known case of quantumelectrodynamics (see, for example, [28]) $e_{x,\omega}^{\rm INM}$ has been normalized with respect to $-g_\omega^2(M^*\beta)^4/(2\pi)^4$, i.e., its nonrelativistic and zero-mass limit. Figure 2 gives the corresponding behavior of $e_{x,\sigma}^{\rm INM}$ [normalized with respect to $g_\sigma^2(M^*\beta)^4/(2\pi)^4$]. Figures 1 and 2 clearly demonstrate the qualitative difference between massless and massive meson exchange: The short-range interaction of massive mesons leads to a much more pronounced reduction of the exchange energy density for vanishing β. For finite nuclei, however, the relevant w regimes are roughly given by $0.7<w_\omega$ and $0.2<w_\sigma$ in which only a weak w dependence of $e_{x,\omega}^{\rm INM}$ and $e_{x,\sigma}^{\rm INM}$ is found. While in the relevant β regime ($0<\beta<1$) the magnitude of the repulsive $e_{x,\sigma}^{\rm INM}$ increases with β, its attractive vector counterpart shows a clear maximum

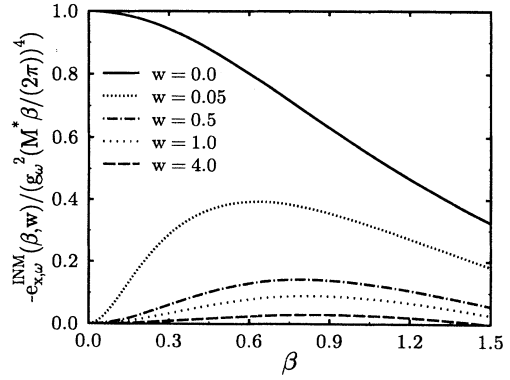

FIG. 1. Vector exchange energy density, Eq. (16), as a function of β, Eq. (11), for various values of w [normalized with respect to $-g_\omega^2(M^*\beta)^4/(2\pi)^4$].

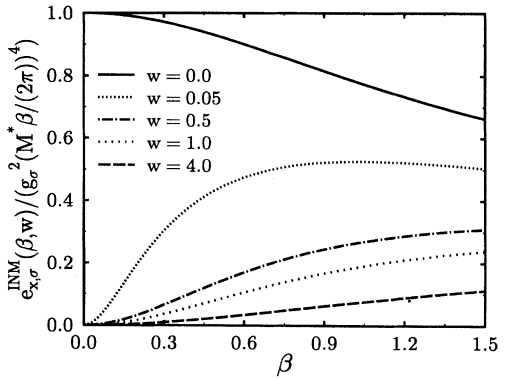

FIG. 2. Scalar exchange energy density, Eq. (15), as a function of β, Eq. (11), for various values of w [normalized with respect to $g_\sigma^2(M^*\beta)^4/(2\pi)^4$].

beyond which $e_{x,\omega}^{\mathrm{INM}}$ starts to approach its repulsive high-density limit (compare [25]).

IV. RESULTS FOR FINITE NUCLEI

In this first study of the KS approach to QHD we have restricted ourselves to the exchange-only limit [using the LDA, Eqs. (9), (15), and (16)], thereby obtaining a density functional equivalent of the HF approximation. While neglecting all correlation effects gives up the particular strength of the unified DFT approach to exchange and correlation, it nevertheless seems appropriate for a conceptual analysis of the local effective exchange potential resulting from the LDA. Moreover, in order to illustrate the essential features of this local potential the simplest model, i.e., QHD-I, is completely sufficient. Unfortunately, only a limited number of HF results on the basis of QHD-I are available in the literature [7,9], utilizing one particular parameter set (listed in Table I). In order to allow a comparison with these HF data, this parameter set has also been used in our KS calculations (as usual for finite nuclei the Coulomb interaction has been included).

Furthermore, it seems worth pointing out that the functionals (15) and (16) include meson retardation effects (on the level of the LDA), in contrast to the relevant HF calculations [7,9]. The importance of retardation corrections, however, has been examined by HF calculations for nuclear matter [29] as well as finite nuclei [30] within the framework of both QHD-I (without giving explicit results) and QHD-II. It has been concluded that due to the high meson masses involved these contributions are rather small for the case of QHD-I (for the binding energy the retardation correction amounts to less then 0.5%). Consequently a comparison of our "retarded" KS results with the "nonretarded" HF values of Refs. [7,9] seems justified.

The KS equations (6) have been solved by a basis expansion in terms of spherical harmonic oscillator functions. The same expansion technique has been used for the meson field equations determining Φ_H and V_H^0. Details of the numerical procedure can be found in [31]. All the results given in the following are based on an oscillator parameter of $\hbar\omega_0 = 41A^{-1/3}$ and 20 shells ($N_F = 20$). The numerical stability of our calculations has been verified by performing the convergence tests of Ref. [31].

Our results for spherical nuclei are summarized in Table II. Both nuclear radii and binding energies show an excellent overall agreement with the HF results. The largest discrepancy between HF and the LDA is found for light nuclei like ^{16}O, while the difference decreases with increasing nuclear size. This is exactly the behavior one would expect for an approximation based on nuclear matter like the LDA as surface effects become less important with increasing nuclear size as compared to bulk properties. It should be emphasized, however, that the small absolute difference of 0.1 MeV for ^{16}O clearly demonstrates the high accuracy of the LDA even for rather light nuclei. Moreover, the fact that nuclear radii from the LDA are more or less identical to their HF counterparts throughout the periodic table indicates that the LDA densities are very close to HF densities even in the surface regime. This is directly illustrated in Fig. 3 where the proton density of ^{114}Sn obtained by a LDA calculation is compared with the corresponding HF result [32], thus proving that the accuracy of the LDA for energies and radii is not based on a fortuitous cancellation of local errors.

For completeness we also give the KS single-particle spectrum of ^{40}Ca and ^{48}Ca in Table III. From a rigorous point of view, however, these KS eigenvalues do not have any physical significance (apart from the highest occupied level [21]) due to the auxiliary nature of the KS orbitals. Nevertheless, in the context of condensed matter problems the KS single-particle energies are often successfully used to identify band structures, indicating their usefulness from a pragmatic point of view. However, although the level schemes which we obtained for

TABLE I. QHD parameters from Ref. [7] used for all HF and KS calculations.

$m_\sigma = 440$ MeV	$g_\sigma^2 = 69.62$
$m_\omega = 783$ MeV	$g_\omega^2 = 153.81$
$M = 938.9$ MeV	

TABLE II. Binding energy (in MeV) and various rms radii (in fm) from HF and KS calculations for several spherical nuclei [34] (without center of mass correction).

	$-E/A$		R_c		R_n		R_p	
	HF	LDA	HF	LDA	HF	LDA	HF	LDA
^{16}O[a]	2.33	2.43	2.93	2.91		2.75		2.80
^{40}Ca[a]	4.32	4.37	3.59	3.59		3.42		3.50
^{48}Ca[a]	5.04	4.95	3.56	3.57		3.66		3.48
^{90}Zr		5.56		4.35		4.34		4.27
^{114}Sn[b]	5.54	5.56	4.63	4.65	4.68	4.68	4.56	4.58
^{146}Gd[b]	5.52	5.53	5.02	5.03	5.03	5.03	4.96	4.96
^{208}Pb		5.65		5.52		5.69		5.46

[a]HF results from Refs. [7,9].
[b]HF results from Ref. [35].

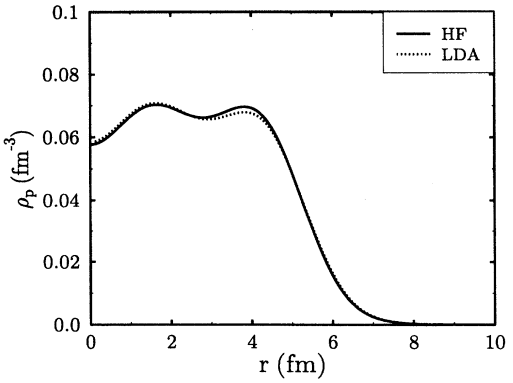

FIG. 3. Proton point densities for ^{114}Sn from HF [32] and LDA calculations (for the parameter set given in Table I).

TABLE III. Kohn-Sham single-particle energies ($-\epsilon_{i,q}$ in MeV) for ^{40}Ca and ^{48}Ca.

Level	^{40}Ca		^{48}Ca	
	Neutron	Proton	Neutron	Proton
$1s1/2$	53.23	44.76	57.00	50.09
$1p3/2$	36.01	28.04	40.36	34.38
$1p1/2$	30.25	22.29	35.81	29.70
$1d5/2$	20.16	12.70	24.23	19.01
$2s1/2$	14.02	6.84	16.82	11.37
$1d3/2$	11.96	4.71	16.16	10.92
$1f7/2$			9.54	

small and medium size nuclei (compare Table III) match the experimental data, a quantitative comparison of our eigenvalues with experimental single-particle energies is not appropriate at the present level of our calculations, as they are based on the linear σ-ω model.

V. SUMMARY AND OUTLOOK

Within the Kohn-Sham approach to density functional theory a local effective exchange potential has been derived. Its density dependence is based on the exchange energy of nuclear matter which here has been evaluated analytically in order to allow for efficient applications. As an illustration of the Kohn-Sham approach and a first study of its properties the resulting exchange-only Kohn-Sham equations have been applied to spherical nuclei (in the framework of the σ-ω model). A comparison with HF results demonstrates that this approach is able to accurately reproduce all features of the much more involved HF calculations, making density functional theory a very attractive alternative to other many-body techniques (even on the HF level).

For real applications the present approach has to be extended to more realistic nuclear models like QHD-II. On the other hand, the inclusion of correlation effects should reveal the real power of the KS approach illustrated here: Applications of the correlated Dirac-Fock-Brueckner method to finite nuclei seem to be restricted by the complex nonlocal potentials involved. Substantial simplifications will result from the use of local DF potentials, making the investigation of correlations effects in finite nuclei more amenable. In this respect the LDA for the ring contributions discussed in Sec. III might serve as a starting point. Moreover, on the level of the LDA the investigation of Dirac-Brueckner-type correlations should also be possible.

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APPENDIX: ANALYTICAL RESULT FOR THE EXCHANGE DIAGRAM

In this appendix we give the analytic result for the integral (17),

$$I(w,\xi_1,\xi_2) = \frac{w-2}{2}(\ln\xi_1\ln\xi_2 - \beta_1\eta_1\ln\xi_2 - \beta_2\eta_2\ln\xi_1) - \beta_1\beta_2 + \frac{1}{4}\left[w(\eta_1^2+\eta_2^2) - 2(\eta_1-\eta_2)^2\right]\ln\frac{(\xi_1\xi_2-1)^2 + w\xi_1\xi_2}{(\xi_1-\xi_2)^2 + w\xi_1\xi_2}$$
$$+F(\xi_1,\xi_2) - F\left(\xi_1,\frac{1}{\xi_2}\right) - F\left(\frac{1}{\xi_1},\xi_2\right) + F\left(\frac{1}{\xi_1},\frac{1}{\xi_2}\right), \tag{A1}$$

where

$$F(x_1,x_2) = \frac{s}{4}\left(\frac{\eta_1}{x_1}+\frac{\eta_2}{x_2}\right)\arctan\left(\frac{2(x_1x_2-1)+w}{s}\right)$$
$$+\frac{i}{8}s\mathrm{Li}_2\left(x_1x_2\frac{2-w-is}{2}\right)$$
$$-\frac{i}{8}s\mathrm{Li}_2\left(x_1x_2\frac{2-w+is}{2}\right).$$

Here $s=\sqrt{w(4-w)}$ and Li_2 represents Euler's dilogarithm. The analytical formula (A1) has been verified by comparison with a numerical evaluation of (17).

For numerical applications it is advantageous to use a manifestly real representation of (A1). As the imaginary contributions arising from the terms with the dilogarithms cancel each other, (A1) can be rewritten in terms of Clausen's integral [33], which can be evaluated more efficiently.

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