Non-Abelian density functional theory

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The density functional approach to a nuclear system with pi and rho coupling is framed. We also extend the Hohenberg-Kohn theorem and the self-consistent equations to the arbitrary gauge fields. Particularly, the binding energy of infinite nuclear matter within the nonlinear sigma model is calculated. [S0556-2813(98)01109-1]

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The relativistic density functional theory (DFT) for the last five years has become a successful tool for solving the nuclear many-body problem [1–9]. The main usefulness of this method is that it allows one (i) to take into account the correlation energy, (ii) to work with relatively simple one-particle equations, and (iii) to present the ground-state energy as a density functional. The last two points are especially important in comparison with relativistic Bruckner calculations [10] which include nonlocal equations. Moreover, the DFT methods make it possible to find separately the correlation energy, which we illustrate for calculations of the nonlinear sigma model.

DFT is based on the Hohenberg-Kohn (HK) theorem and Kohn-Sham (KS) equations. This nodal formalism, initially discussed in solid state physics, has been extended to quantum hadrodynamics with scalar σ and vector ω mesons (QHD-I) [3]. Though the power of the density functional in nuclear physics with pseudoscalar π and pseudovector ρ mesons (this version is called QHD-II) has been recently shown [9], the relevant fundamentals pertaining to the non-Abelian DFT have not been considered in detail. Below we try to perform this task, taking into account the interaction with an arbitrary gauge field, particularly QHD-II.

We start with the most general formulation of the HK theorem. It reads as follows. The stationary Schrödinger equation

$$\hat{H}_{\rm ren}|\Phi\rangle=[\hat{H}_{\rm int}+\hat{U}(A)]|\Phi\rangle=E|\Phi\rangle \tag{1}$$

for the ground state $|\Phi\rangle$ of an interacting many-fermion system gives the ground-state energy E. The renormalized Hamiltonian $\hat{H}_{\rm ren}=\hat{H}+CTC-VEV$ includes the term $\hat{U}(A)$ describing the interaction of the fermion quantum field $\hat{\psi}$ with the external classical static field $A(r)$, whereas the term $\hat{H}_{\rm int}$ corresponds to the interacting many-body system itself.

We say that two potentials A and A' belong to the same equivalence class when they differ by a gauge transform [3], while the two ground states $|\Phi\rangle$ and $|\Phi'\rangle$ are equivalent if $|\Phi'\rangle=e^{i\alpha}|\Phi\rangle$. (For a nondegenerate system the identical ground states correspond to the same energy and the same ground-state density.) Being constructed of these equivalence classes, the set of external potentials $P=\{A\}$ is mapped by a map $f:P\to G$ onto the set of all possible ground states $G=\{|\Phi\rangle\}$. The map is surjective, indeed: any ground state $|\Phi\rangle\in G$ has its original $A\in P$. The second map $s:G\to N$, being also surjective, maps the set G of the ground states onto the set of the ground-state densities $\{n\}=N$. The injectivity of the two maps implies that potentials differing by more than a gauge transform correspond to different ground states which give different ground-state densities. This entails the injectivity of the composition $s\circ f=h$ and the existence of the inverse map h^{-1}. Hence any ground state $|\Phi\rangle=|\Phi[n]\rangle$ can be presented as a unique functional of the ground-state density $n(r)$, as well as the ground-state density $E[n]=\langle\Phi[n]|\hat{H}|\Phi[n]\rangle$. Thus, establishing the injectivity of the two mappings f and s, the HK theorem justifies the possibility of using unique density functionals for the ground-state energy and other quantities.

The term $\hat{U}(A)$ reads as

$$\hat{U}(A)=\int d^3r\sum_i\{g_i\hat{Y}^iA_i\}$$

$$=\int d^3r[\hat{u}_\sigma+\hat{u}_\omega+\hat{u}_\pi+\hat{u}_\varrho],\quad \hat{Y}^i=\hat{\bar{\psi}}\Gamma^i\hat{\psi}, \tag{2}$$

where the first two terms in square brackets correspond to the interaction with external sigma- and omega-meson fields, respectively [11,12]

$$\hat{u}_\sigma=-g_s\hat{\bar{\psi}}\hat{\psi}\phi=-\hat{\varrho}_s\phi,\quad \hat{u}_\omega=g_\omega(\hat{\bar{\psi}}\gamma^\mu\hat{\psi})V_\mu=\hat{j}^\mu V_\mu, \tag{3}$$

while the interaction of fermions with pi- and rho-meson external potentials is given by

$$\hat{u}_\pi=ig_\pi(\hat{\bar{\psi}}\gamma_5\vec{\tau}\hat{\psi})\cdot\vec{\pi}=i\hat{\vec{\varrho}}_5\cdot\vec{\pi},$$

$$\hat{u}_\rho=\frac{1}{2}(g_\rho\hat{\bar{\psi}}\gamma^\mu\vec{\tau}\hat{\psi})\cdot\vec{b}_\mu=\frac{1}{2}\hat{\vec{w}}^\mu\cdot\vec{b}_\mu. \tag{4}$$

In the future we omit the coupling constants if they lead to confusion.

Let two potentials A, $A'\in P$, correspond to the identical ground states $|\Phi\rangle$, $|\Phi'\rangle\in G$. Then, inserting expressions (2)–(4) in Eq. (1), one obtains

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$$\int d^3r\Big[-\hat{\varrho}_s(\phi-\phi')+\hat{j}^\mu(V_\mu-V'_\mu)+i\hat{\vec{\varrho}}_5\cdot(\vec{\pi}-\vec{\pi}') + \frac{1}{2}\hat{\vec{w}}^\mu\cdot(\vec{b}_\mu-\vec{b}'_\mu)\Big]|\Phi\rangle=(E-E')|\Phi\rangle. \quad (5)$$

Contrary to the conserving baryon current $\hat{j}^\mu$, the quantity $\hat{\vec{w}}^\mu$, in general, does not coincide with the conserving isotopic current [11]

$$\hat{\vec{\mathbf{i}}}^0=\hat{\vec{w}}^0+\hat{\vec{b}}_\mu\times\hat{\vec{B}}^{0\mu}+\hat{\vec{\pi}}\times[\partial^0\hat{\vec{\pi}}+[\hat{\vec{\pi}}\times\hat{\vec{b}}^0]],$$

$$\vec{B}_{\mu\nu}=\partial_{[\mu}\vec{b}_{\nu]}-g_\rho[\vec{b}_\mu\times\vec{b}_\nu]. \quad (6)$$

However, in light of commuting the Hamiltonian $\hat{H}_{\rm ren}$ with the baryon and isotopic charge operators, $\hat{Q}$ and $\hat{\vec{I}}$, respectively, we state, that, if Eq. (5) has solutions, it will be written as

$$\int d^3r\Big[-c\hat{j}^0(r)+\frac{1}{2}\vec{c}\cdot\hat{\vec{w}}^0(r)\Big]|\Phi\rangle=\Big(-c\hat{Q}+\frac{1}{2}\vec{c}\cdot\hat{\vec{I}}\Big)|\Phi\rangle =(E-E')|\Phi\rangle, \quad (7)$$

with an arbitrary constant c and with an arbitrary constant vector $\vec{c}$, when

$$\hat{\vec{w}}^0(r)=\hat{\vec{\mathbf{i}}}^0(r). \quad (8)$$

If the equality (8) does not take place, then, inevitably, $\vec{c}=0$, and Eq. (7) reduces to the relevant QHD-I version [3], with no trouble concerning fulfillment of the theorem. Equation (6) reduces to Eq. (8) when only one component of the isotopic triplet is present, i.e., only neutral pions and rho mesons, and we come again to the QHD-I formulation. However, condition (8) takes place also in the case of the sigma, omega, and rho interactions as in [13] and at the approximation that the magnetic components of the rho-meson field are neglected, namely,

$$\hat{\vec{\pi}}(r)=0, \quad \hat{\vec{b}}_k(r)\simeq 0. \quad (9)$$

In the latter case we have to discover whether the potentials leading to Eq. (7) can be produced by a gauge transformation. The time-independent gauge transformations have the form

$$V'_\mu(r)=V_\mu(r)+\partial_\mu\Lambda(r,t), \quad \Lambda(r,t)=ct+\lambda(r), \quad (10)$$

$$\vec{b}'_0(r)=\vec{b}_0(r)+\vec{\theta}(r)\times\vec{b}_0(r)+\vec{q},$$

$$\vec{b}'_k(r)=\vec{b}_k(r)+\partial_k\vec{\theta}(r)+\vec{\theta}(r)\times\vec{b}_k(r), \quad (11)$$

where c is arbitrary, while $\vec{q}$ satisfies the constraint

$$\vec{q}\times\vec{b}_\mu(r)=0. \quad (12)$$

Inserting Eqs. (10) and (11) in Eq. (5), we come to Eq. (7) if

$$\partial_k\vec{\theta}(r)+\vec{\theta}(r)\times\vec{b}_k(r)=0, \quad \vec{q}+\vec{\theta}(r)\times\vec{b}_0(r)=\vec{c}. \quad (13)$$

For the approximation (9), Eqs. (12) and (13) yield

$$\vec{q}\times\vec{b}_0(r)=0, \quad \partial_k\vec{\theta}(r)=0, \quad \vec{q}+\vec{\theta}(r)\times\vec{b}_0(r)=\vec{c}, \quad (14)$$

which are satisfied for constant $\vec{b}_0$. For arbitrary $\vec{b}_0(r)$ the potentials in Eq. (7) differ by more than a gauge transformation (10) and (11), while the relevant ground states with energies E and E' are identical. Thus the DFT method cannot be applied to a model (9) with nucleons interacting through the pure electric rho-meson field.

Quite an analogous situation arises when we consider the interaction with the external gluon field incorporating the renormalized Hamiltonian [14] of quantum chromodynamics. The conserved color current $\hat{J}^{a\mu}=\hat{Y}^{a\mu}+f^{abc}\hat{F}^{b\mu\nu}\hat{A}^c_\mu$ coincides with $\hat{Y}^{a\mu}=\hat{\bar{\psi}}\gamma_\mu\lambda^a\hat{\psi}$ only in the case $\hat{A}^c_k=0$. The relevant analog of Eq. (7) will be a consequence of a time-independent gauge transformation

$$A^{a'}_\mu=A^a_\mu+\partial_\mu\varepsilon^a+f^{abc}\varepsilon_b A_{c\mu}, \quad \varepsilon^a=q^a t+\theta^a(r) \quad (15)$$

if

$$\partial_k\theta^a=0, \quad f^{abc}q_b A_{c0}(r)=0, \quad A'^a_0-A^a_0=q^a+f^{abc}\theta_b A_{c0}(r)=c^a. \quad (16)$$

For the gauge field, considered in [15], we can choose constant vectors q^a and θ^a satisfying the conditions (16). Yet for arbitrary $A^a_0(r)$ the potentials leading to the same ground state differ by more than a gauge transformation (16), but do correspond to the same ground state.

Now we shall prove the injectivity of the second map $s:G\to N$, mapping all the ground states $|\Phi\rangle\in G$ onto the ground-state densities $\{n\}=N$. The explicit expression of each element $n=(\rho_s,J^\mu,\vec{\varrho}_5,\vec{W}^\mu)$ of the set has the form $n^i=\langle\hat{Y}^i\rangle=\langle\Phi[n]|\hat{Y}^i|\Phi[n]\rangle_{\rm ren}$, namely,

$$\rho_s=\langle\hat{\varrho}_s\rangle, \quad J^\mu=\langle\hat{j}^\mu\rangle, \quad \vec{\varrho}_5=\langle\hat{\vec{\varrho}}_5\rangle, \quad \vec{W}^\mu=\langle\hat{\vec{w}}^\mu\rangle, \quad (17)$$

where the operators are defined by relations (3) and (4). If one suspects that the two distinct ground states $|\Phi\rangle$ and $|\Phi'\rangle$ lead to the same density $n^i=\langle\Phi|\hat{Y}^i|\Phi\rangle=\langle\Phi'|\hat{Y}^i|\Phi'\rangle$, a contradiction inevitably springs up: in light of Eqs. (2) and (17), one may write

$$E=\langle\Phi[n]|\hat{H}_{\rm ren}|\Phi[n]\rangle<\langle\Phi[n']|\hat{H}_{\rm ren}|\Phi[n']\rangle =\langle\Phi[n']|\hat{H}'_{\rm ren}|\Phi[n']\rangle+\langle\Phi[n']|\hat{U}(A)-\hat{U}(A')|\Phi[n']\rangle. \quad (18)$$

Then, interchanging the roles of primed and unprimed variables and writing the analogous formula, adding the latter to Eq. (18), we come to the incorrect statement $E+E'<E'+E$ that makes us recognize the injectivity of the second map.

Thus the HK theorem warrants the standard application of DFT to QHD-II. We can use the unique ground-state functional $E[n]=\langle\Phi[n]|\hat{H}_{\rm ren}|\Phi[n]\rangle$, which gives the exact

ground-state energy E and for all other densities $n' \neq n$ leads to a higher energy $\langle \Phi[n'] | \hat{H}_{\rm ren} | \Phi[n'] \rangle > E$.

It should be noted that the functional $F[n] = E[n] - U_A[n]$, where

$$U_A[n] = \langle \Phi[n] | \hat{U}(A) | \Phi[n] \rangle = \int d^3r \sum_i g_i n^i A_i , \tag{19}$$

does not depend on the external potentials at all. Setting external fields equal to zero, we treat $F[\varrho_s, \vec{\varrho}_5, J^\mu, \vec{W}^\mu]$ as the proper energy functional of the QHD-II system without external potentials. For a noninteracting system with the Hamiltonian $\hat{H}_0 = \hat{T} + \hat{U}(A)$, the kinetic energy functional T_0 reads

$$T_0[n] = \langle \Phi[n] | \hat{T} | \Phi[n] \rangle = \int d^3r \langle \Phi[n] | \overline{\psi} (i \gamma^k \partial_k + M) \psi | \Phi[n] \rangle \tag{20}$$

and coincides with $F[n]$ of the noninteracting system.

Let us consider the Hamiltonian

$$\hat{H}_{\rm ren}\{\xi\} = \hat{H} + (\xi - 1)\hat{H}_I + \hat{U}(A\{\xi\}),$$

$$\hat{H}_I = \int d^3r \sum_i [g_i \hat{Y}^i \hat{A}_i], \tag{21}$$

where the proper system in the external field A corresponds to $\xi = 1$, while $\xi = 0$ corresponds to the noninteracting system of Kohn-Sham particles moving in the self-consistent field $A^\# = A(\xi = 0)$ whose total energy is $E\{0\} = T_0 + U_{A^\#}$. It is clear that

$$\frac{d\hat{H}_{\rm ren}\{\xi\}}{d\xi} = \hat{H}_I + \int d^3r \sum_i \left[g_i \widehat{\overline{\psi}} \Gamma^i \hat{\psi} \frac{dA_i\{\xi\}}{d\xi} \right]. \tag{22}$$

In light of the Gellmann-Feynman theorem [6], the energy functional is presented in the form

$$E\{\zeta\} = E\{\zeta = 0\} + \int_0^\zeta d\xi \left\langle \Phi\{\xi\} \left| \frac{d\hat{H}_{\rm ren}\{\xi\}}{d\xi} \right| \Phi\{\xi\} \right\rangle . \tag{23}$$

Substituting Eq. (22), we then immediately obtain

$$E\{1\} = E[n] = T_0[n] + U_A[n] + R[n], \tag{24}$$

with the coupling term

$$R[n] = \int_0^1 d\xi \int d^3r \left\langle \Phi\{\xi\} \left| \sum_i g_i \widehat{\overline{\psi}} \Gamma^i \hat{\psi} \hat{A}_i \right| \Phi\{\xi\} \right\rangle . \tag{25}$$

The variational differentiation $\delta E[n] / \delta n^i = 0$ yields a set of single-particle equations

$$\left\{ -i\alpha \cdot \nabla + \beta \left[M - \phi^\# + \gamma^\mu V_\mu^\# + i \gamma_5 \vec{\tau} \cdot \vec{\pi}^\# + \frac{1}{2} \gamma^\mu \vec{\tau} \cdot \vec{b}_\mu \right] \right\} \varphi_m(r) = \epsilon_m \varphi_m(r), \tag{26}$$

$$\left\{ -i\alpha \cdot \nabla + \beta \left[M + \sum_i g_i \Gamma^i A_i^\# \right] \right\} \varphi_m(r) = \epsilon_m \varphi_m(r) \tag{27}$$

[where we have used the notation $\hat{\psi}(r) = \Sigma_m \varphi_m(r) \hat{a}_m^\dagger$ with index m related to the single-particle baryon densities], with self-consistent local potentials

$$A_i^\#(r) = A_i(r) + \frac{\delta R[n]}{\delta n^i(r)}, \tag{28}$$

provided that the noninteracting system of Kohn-Sham particles has the same ground-state energy as the real interacting system. Equations with the self-consistent potential $A^\#$ correspond to the equation for the self-consistent Green function of the Kohn-Sham particle, with the self-energy $\hat{\Sigma}$ replaced by the local potential (28). The Kohn-Sham equation (27) is solved self-consistently as in QHD-I [3]: substituting some approximate potentials in Eq. (27), we construct single-particle densities, then obtain new potentials, and so on, until the required accuracy is achieved. Equations (26) were solved in the frames of QHD-II with the exchange potentials [9]; they have the general form (27) for an arbitrary interaction of the current with the external field. The functional $R[n] = E_H[n] + E_x[n] + E_c[n]$ includes the Hartree term $E_H[n]$, the exchange (Fock) term $E_x[n]$, and the correlation energy $E_c[n]$. The Hartree and exchange contributions were discussed in detail by several authors [7–9]. The correlation energy, in spite of a thorough achievement within the σ-ω model [16], is rarely discussed in QHD-II.

The simplest method to evaluate the correlation energy is the random phase approximation (RPA) [17]. However, as was noted in [18], the QHD lattice calculations [19] showed that the RPA yields only 40% of the total correlation energy. Even if the vacuum effects are estimated [18], the correlation energy is not small with respect to the binding energy. Recently, a method [20], based on the density functional technique [6], for calculating the correlation energy with vacuum corrections has been achieved for the nonlinear sigma model. Nuclear matter calculations in the frames of that model are often applied to the equation of state [21]. On account of the extreme importance of the correlation energy [18], we appeal to the approximation [20] to carry out the present calculations for infinite matter.

Thus the total correlation energy is expressed as a sum of the sigma and pion contributions [20]:

$$E_c = -\frac{g^2}{2} \int_0^1 d\xi \int \frac{dq^4}{(2\pi)^4} V(q) \left[\frac{\chi_{\sigma 0}^2(q) R_{\sigma\xi}(q)}{1 - \chi_{\sigma 0}(q) R_{\sigma\xi}(q)} + 3 \frac{\chi_{\pi 0}^2(q) R_{\pi\xi}(q)}{1 - \chi_{\pi 0}(q) R_{\pi\xi}(q)} \right], \tag{29}$$

TABLE I. Binding and correlation energies vs Fermi momentum.

k_F (fm^{-1})	0.5	0.75	1.0	1.1	1.2	1.3	1.36	1.4	1.5	1.6	1.75	2
E_B (MeV)	−1.5	−4.5	−7.7	−9.0	−10.3	−11.8	−12.8	−12.3	−11.0	−6.2	4.6	36.6
E_σ (MeV)	−0.08	−0.17	−0.4	−0.7	−1.1	−1.7	−2.1	−2.3	−3.5	−4.4	−6.9	−16.7
E_π (MeV)	−0.09	−0.11	−0.3	−0.6	−.8	−1.6	−2.0	−2.2	−3.4	−4.2	−6.9	−16.9
$E_{\rm corr}$ (MeV)	−0.17	−0.28	−0.7	−1.3	−1.9	−3.3	−4.1	−4.5	−6.9	−8.6	−13.8	−33.6

where $\chi_{\sigma 0}$ and $\chi_{\pi 0}$ is the pion and sigma-meson noninteracting response functions, respectively; $R_{\sigma\xi}(q)$ and $R_{\pi\xi}$ are the pion and sigma-meson effective interactions. The potential

$$V(q) = -\frac{1}{\mu^2+\vec{q}^2-q_0^2} + \frac{2q_0^2}{(\mu^2+\vec{q}^2-q_0^2)^2} \tag{30}$$

and the interaction radius μ^{-1}, where

$$\frac{2M\mu^2}{g^2} = \rho_s - \frac{\mu^4}{\rho_s}\int \frac{dq^4}{(2\pi)^4}\frac{1}{\mu^2+\vec{q}^2-q_0^2}\left[\frac{\chi_{\sigma 0}^2(q)}{1-\chi_{\sigma 0}(q)R_\sigma(q)} + 3\frac{\chi_{\pi 0}^2(q)}{1-\chi_{\pi 0}(q)R_\pi(q)}\right], \tag{31}$$

are calculated self-consistently [20]. Substituting value of $g^2\rho_s/(2M)$ for μ^2, we, after several iterations, obtain with the required accuracy E_c, as well as E_H and E_x.

The coupling constant g was varied until the saturation density 0.17 fm^{-3} ($k_F = 1.36$ fm^{-3}) was achieved. This corresponds to $g^2/4\pi = 16.43$ and yields the compressibility $K = 314$ MeV. The equation of state for a wider range of k_F is shown in Table I.

At the saturation density the binding energy is $E_B = -12.8$ MeV per nucleon, while the correlation energy is $E_{\rm corr} = -4.2$ MeV, with a sigma and pion contribution of $E_\sigma = -2.1$ MeV and $E_\pi = -2.0$ MeV, respectively, not small, indeed, in comparison with E_B. More exact calculations beyond the approximation [20] will be performed in the future. Also, recent advances of the Thomas-Fermi approach to quantum chromodynamics [15] may inspire us to apply the density functional theory, considered above, at that range of parameters when the Thomas-Fermi model is not reliable.

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[1] M. Centelles, X. Viñas, M. Barranco, and P. Schuck, Nucl. Phys. **A519**, 73 (1990).
[2] D. Von-Eiff, S. Haddad, and M. K. Weigel, Phys. Rev. C **46**, 230 (1992).
[3] C. Speicher, R. M. Dreizler, and E. Engel, Ann. Phys. (N.Y.) **213**, 312 (1992).
[4] M. Centelles, X. Viñas, M. Barranco, and P. Schuck, Ann. Phys. (N.Y.) **221**, 165 (1993).
[5] H. Müller and R. M. Dreizler, Nucl. Phys. **A563**, 649 (1993).
[6] V. A. Khodel, V. R. Shaginyan, and V. V. Khodel, Phys. Rep. **249**, 1 (1994).
[7] X. Viñas, in *Response of Nuclear Systems on External Forces*, edited by J. Arias, M. Gallardo, and M. Losano (Springer, Berlin, 1995), p. 115.
[8] R. N. Schmid, E. Engel, and R. M. Dreizler, Phys. Rev. C **52**, 164 (1995).
[9] R. N. Schmid, E. Engel, and R. M. Dreizler, Phys. Rev. C **52**, 2804 (1995).
[10] S. Kinpara and T. Kohmura, Prog. Theor. Phys. **91**, 127 (1994).
[11] B. D. Serot and J. D. Walecka, Adv. Nucl. Phys. **16**, 1 (1986).
[12] R.-K. Su, T. Long, and Y.-J. Zhang, Phys. Rev. C **51**, 1265 (1995).
[13] M. Prakash, P. J. Ellis, E. K. Heide, and S. Rudaz, Nucl. Phys. **A575**, 583 (1994).
[14] X. Ji, Phys. Rev. D **52**, 271 (1995).
[15] D. D. Dixon, P. Kaus, and J. Wudka, Phys. Rev. D **55**, 6344 (1997).
[16] S. A. Chin, Ann. Phys. (N.Y.) **108**, 301 (1977).
[17] X. Ji, Phys. Lett. B **208**, 19 (1988).
[18] J. A. McNeil, C. E. Price, and J. R. Shepard, Phys. Rev. C **47**, 1534 (1993).
[19] R. Brockmann and J. Frank, Phys. Rev. Lett. **68**, 1830 (1992).
[20] B. L. Birbrair and A. B. Gridnev, Z. Phys. A **352**, 441 (1995).
[21] M. Prakash and T. L. Ainsworth, Phys. Rev. C **36**, 346 (1987).