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DENSITY FUNCTIONAL APPROACH TO QHD

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A review of presently available applications of density functional concepts to nuclear systems characterised by QHD models is given. It is demonstrated that exchange-only Kohn-Sham results obtained with the local density approximation are essentially equivalent to Hartree-Fock results. In addition, the application of extended Thomas-Fermi models for cold and thermal nuclei is outlined.

Around 1980 the field theoretical model of quantum hadrodynamics (QHD) became a popular tool for the discussion of nuclear properties[1,2]. In this model, the strong interaction between nucleons is mediated by the exchange of mesons,

$$\begin{array}{lccccc} & \sigma, & \omega, & \rho, & \pi, & \dots \\ (J^\pi, T): & (0^+, 0) & (1^-, 0) & (1^-, 1) & (0^-, 1) & \dots \end{array} .$$

This model is not expected to be applicable in the regime of very high energies, where the quark substructure of the hadrons becomes apparent. It is expected to be of relevance as an effective field theory for questions of nuclear structure and for collisions up to intermediate energies. In this contribution we will address the question of calculating nuclear structure data on the basis of QHD, in particular the calculation of ground state properties.

Initially, applications of the QHD model were restricted to the Hartree approximation (or relativistic mean field approximation for the meson degrees of freedom). In the meantime, Hartree-Fock results have become available [3,4,5]. It is well known, though, that correlation effects are important in strongly interacting systems. These can be addressed eg. via a Dirac-Brueckner scheme. First results of this type are available for nuclear matter and an application of this scheme for finite nuclei has been given [5].

Another avenue to the discussion of the many body problem at hand is density functional theory [6] (DFT). In order to summarise this approach, we shall rely on the simplest QHD model, QHD-I — the linear σ-ω-model [7]. This model is characterised by the Lagrangian density

$$\begin{aligned} \hat{\mathcal{L}} &= \hat{\bar{\psi}}(x)[i\partial\!\!\!/ - M + g_s\hat{\phi}(x) - g_v\hat{V}\!\!\!/(x)]\hat{\psi}(x) + \delta\mathcal{L}_{CTC} \qquad (1) \\ &\quad + \frac{1}{2}[\partial_\mu\hat{\phi}(x)\partial^\mu\hat{\phi}(x) - m_s^2\hat{\phi}(x)^2] \\ &\quad - \frac{1}{4}[\partial^\mu\hat{V}^\nu(x) - \partial^\nu\hat{V}^\mu(x)][\partial_\mu\hat{V}_\nu(x) - \partial_\nu\hat{V}_\mu(x)] + \frac{1}{2}m_v^2\hat{V}_\mu(x)\hat{V}^\mu(x) . \end{aligned}$$

The nucleons, characterised by a single field $\hat{\psi}$, interact via exchange of massive scalar ($\hat{\phi}$) and vector ($\hat{V}_\nu$) mesons. The scalar σ-meson, which is responsible for the attractive part of the N-N interaction, couples to the scalar density

$$\hat{\rho_s}(x) = \hat{\bar{\psi}}(x)\hat{\psi}(x). \tag{2}$$

The ω-mesons, which generate the short range repulsion, couple to the fermion four current

$$\hat{j}^\mu(x) = \hat{\bar{\psi}}(x)\gamma^\mu\hat{\psi}(x). \tag{3}$$

The quantity $\delta\mathcal{L}_{\mathcal{CTC}}$ contains counterterms for purposes of renormalisation.

The basis statement of DFT is then: The ground state expectation value A_0 of any observable $\hat{A}$ for the many nucleon problem can be expressed rigorously as a functional of the ground state scalar density $\rho_s(\mathbf{x})$ and the ground state four current $j^\mu(\mathbf{x})$,

$$A_0[\rho_s, j^\mu] = < \Psi_0[\rho_s, j^\mu] \mid \hat{A} \mid \Psi_0[\rho_s, j^\mu] > \quad . \tag{4}$$

This extension of the Hohenberg-Kohn theorem of nonrelativistic DFT can be proven explicitly[8,9], provided the Ritz minimum principle is valid for interacting relativistic systems (after renormalisation).

The first task to be faced is the derivation of the functionals in questions, in particular for the ground state energy. We shall sidestep this problem for the moment and first ask the question: What options would be open if the functional for the ground state energy $E_0[\rho_s, j^\mu]$ (or a suitable approximation) would be available?

The Ritz principle leads directly to the variational equations

$$\frac{\delta E_0[\rho_s, j^\mu]}{\delta j^\lambda(\mathbf{x})} = \mu g_{\lambda 0} \qquad , \qquad \frac{\delta E_0[\rho_s, j^\mu]}{\delta \rho_s(\mathbf{x})} = 0. \tag{5}$$

These equations are the starting point for the application of extended Thomas-Fermi (ETF) models, in which the ground state energy is fully written as a functional of ρ_s and j^μ.

More accurate results are usually obtained with the Kohn-Sham (KS) scheme [9,10]. In this scheme one represents the density variables in terms of auxiliary spinor orbitals,

$$\rho_s(\mathbf{x}) = \rho_{s,vac}(\mathbf{x}) + \rho_{s,D}(\mathbf{x}) \quad , \tag{6}$$

with

$$\rho_{s,D}(\mathbf{x}) \quad = \quad \sum_{-M < \epsilon_k \leq \epsilon_F} \bar{\varphi}_k(\mathbf{x})\varphi_k(\mathbf{x})$$

$$\rho_{s,vac}(\mathbf{x}) \;=\; \frac{1}{2}\Bigg[\sum_{\epsilon_k \leq -M} \bar{\varphi}_k(\mathbf{x})\varphi_k(\mathbf{x}) - \sum_{\epsilon_k > -M} \bar{\varphi}_k(\mathbf{x})\varphi_k(\mathbf{x})\Bigg] \;,$$

and corresponding expressions for the components of the four current

$$j^\mu(\mathbf{x}) = j^\mu_{vac}(\mathbf{x}) + j^\mu_D(\mathbf{x}) \;. \tag{7}$$

One then rearranges the expression for the ground state energy by addition and subtraction of the noninteracting kinetic energy

$$T_s[j^\nu, \rho_s] \;=\; T_{s,vac}[j^\nu, \rho_s] + T_{s,D}[j^\nu, \rho_s] \tag{8}$$

with

$$T_{s,D} = \int d^3x \sum_{-M < \epsilon_k \leq \epsilon_F} \bar{\varphi_k}(\mathbf{x}) \; (-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + M) \; \varphi_k(\mathbf{x})$$

(and an analogous expression for $T_{s,vac}$) and the Hartree energy

$$\begin{aligned} E_H \;&=\; -\frac{g_s^2}{2}\int d^3x \; d^3y \; \frac{e^{-m_s|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} \; \rho_s(\mathbf{x}) \; \rho_s(\mathbf{y}) \\ &\quad + \frac{g_v^2}{2}\int d^3x \; d^3y \; \frac{e^{-m_v|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} \; j^\mu(\mathbf{x}) \; j_\mu(\mathbf{y}), \end{aligned} \tag{9}$$

so that

$$E_0[\rho_s, j^\mu] = T_s[\rho_s, j^\mu] + E_H[\rho_s, j^\mu] + E_{xc}[\rho_s, j^\mu]. \tag{10}$$

The exchange-correlation (xc) energy is the term, that remains after extraction of the dominant terms,

$$E_{xc} = T - T_s + W - E_H \;\;, \tag{11}$$

where W is the ground state expectation value of the complete N-N interaction energy. Exploitation of the variational principle (variation with respect to the spinor orbitals) leads to the selfconsistent Dirac-KS equations,

$$\Big\{ -i\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \beta\big[M - \phi_H - \phi_{xc} + \gamma_\mu(V_H^\mu + V_{xc}^\mu)\big]\Big\}\varphi_k = \epsilon_k\varphi_k \;, \tag{12}$$

with the standard Hartree potentials ϕ_H, V_H^μ and the xc-potentials

$$V_{\mu,xc}(\mathbf{x}) \;=\; \frac{\delta}{\delta j^\mu(\mathbf{x})} E_{xc}[\rho_s, j^\mu] \tag{13}$$

$$\phi_{xc}(\mathbf{x}) \;=\; -\frac{\delta}{\delta \rho_s(\mathbf{x})} E_{xc}[\rho_s, j^\mu] \;. \tag{14}$$

The following direct remarks apply: The solution of the Dirac KS problem including all vacuum corrections (as indicated above) would present a rather tremendous task, as negative energy and positive energy solutions have to be determined at each of the selfconsistency cycles. One of the standard approximations is therefore the no-sea approximation,

$$\rho_{s,vac}, \quad j^{\mu}_{s,vac}, \quad T_{s,vac}, \quad E_{xc,vac} \quad \longrightarrow \quad 0 \ .$$

If, in addition, all xc-effects are neglected, $E_{xc} \to 0$, one recovers the Hartree approximation. It is important to note, that xc-effects are represented in terms of local (i.e. multiplicative) potentials. This means for instance: Provided one can derive a reasonable functional for exchange (x) effects, then the KS approach will be much easier to handle than the (nonlocal) HF approach.

After setting the stage, we have to face the main task, the derivation of functionals. If one is interested in ETF applications one needs a representation of T_s in terms of the densities rather than orbitals $T_s = T_s[\rho_s, j^{\mu}]$. This can be obtained with gradient expansion techniques [11,9,12], which are not quite standard as renormalisation (emphasised by the counterterm implied above) is required. Results, to second order in the gradient terms (establishing the ETF2 model), are (for brevity $T^*_s = T_s - \int d^3r \rho_s \phi$ is shown)

$$\begin{aligned} T^*_s[k,M^*] &= T^*_{s,vac}[k,M^*] + T^*_{s,D}[k,M^*] \qquad (15) \\ T^*_{s,vac/D}[k,M^*] &= T^{*,[0]}_{s,vac/D}[k,M^*] + T^{*,[2]}_{s,vac/D}[k,M^*] \end{aligned}$$

with the kinetic energy densities

$$\begin{aligned} t^{*,[0]}_{s,vac}[k,M^*] &= -\frac{M^{*4}}{8\pi^2}\ln\left|\frac{M^*}{M}\right| + \frac{1}{32\pi^2}(M^{*4}-M^4) \\ &\quad + \frac{M^2}{4\pi^2}(M^*-M)^2 + \frac{5M}{12\pi^2}(M^*-M)^3 + \frac{11}{48\pi^2}(M^*-M)^4 \\ t^{*,[2]}_{s,vac}[k,M^*] &= \frac{1}{12\pi^2}\frac{k^2}{E^2}\ln\left|\frac{M^*}{M}\right|(\boldsymbol{\nabla}k)^2 + \frac{1}{6\pi^2}\frac{kM^*}{E^2}\ln\left|\frac{M^*}{M}\right|(\boldsymbol{\nabla}k\cdot\boldsymbol{\nabla}M^*) \\ &\quad - \frac{1}{24\pi^2}\left(1+2\frac{k^2}{E^2}\right)\ln\left|\frac{M^*}{M}\right|(\boldsymbol{\nabla}M^*)^2 \\ t^{*,[0]}_{s,D}[k,M^*] &= \frac{1}{8\pi^2}\left[kE^3 + k^3E - M^{*4}\mathrm{arcsinh}\left(\frac{k}{M^*}\right)\right] \\ t^{*,[2]}_{s,D}[k,M^*] &= \frac{1}{24\pi^2}\frac{k}{E}\left[1+2\frac{k}{E}\mathrm{arcsinh}\left(\frac{k}{M^*}\right)\right](\boldsymbol{\nabla}k)^2 \\ &\quad + \frac{1}{6\pi^2}\frac{kM^*}{E^2}\mathrm{arcsinh}\left(\frac{k}{M^*}\right)(\boldsymbol{\nabla}k\cdot\boldsymbol{\nabla}M^*) \end{aligned}$$

$$+\frac{1}{24\pi^2}\left[\frac{k}{E}-\left(1+2\frac{k^2}{E^2}\right)\mathrm{arcsinh}\left(\frac{k}{M^*}\right)\right](\boldsymbol{\nabla}M^*)^2 \quad ,$$

where $k(\mathbf{x}) = [3\pi^2 j^0(\mathbf{x})]^{\frac{1}{3}}$, $M^*(\mathbf{x}) = M - g_s\ \phi(\mathbf{x})$ and $E = \sqrt{M^{*\,2}+k^2}$. The no-sea approximation has not been evoked, so we explicitly see vacuum corrections. They are due to the scalar meson (they vanish for $\phi = 0$), vacuum corrections due to vector mesons only occur in the fourth order gradient terms.

The local density approximation (LDA) for exchange [10] is obtained by the evaluation of the nuclear matter exchange energy density e_x as a function of the Fermi momentum k_F (again renormalisation is involved) and the subsequent replacement $k_F \to [3\pi^2 j^0(\mathbf{x})]^{\frac{1}{3}}$. Results can actually be given analytically [10], although in terms of a messy expression finally involving Eulers dilogarithm,

$$e_{x,s}(\beta,M^*) = \frac{g_s^2(M^*)^4}{(2\pi)^4}\left\{\frac{1}{4}(\beta\eta-\ln\xi)^2+(1-\frac{w_s}{4})I(w_s,\xi,\xi)\right\} \quad (16)$$

$$e_{x,v}(\beta,M^*) = \frac{g_v^2(M^*)^4}{(2\pi)^4}\left\{\frac{1}{2}(\beta\eta-\ln\xi)^2-(1+\frac{w_v}{2})I(w_v,\xi,\xi)\right\}, \quad (17)$$

where $\beta = k_F/M^*$, $\eta = (1+\beta^2)^{1/2}$, $\xi = \beta+\eta$, $w_{s,v} = m_{s,v}^2/(M^*)^2$ and

$$\begin{aligned} I(w,\xi_1,\xi_2) &= \frac{w-2}{2}(\ln\xi_1\ln\xi_2-\beta_1\eta_1\ln\xi_2-\beta_2\eta_2\ln\xi_1)-\beta_1\beta_2 \quad (18)\\ &+\frac{1}{4}\Big[w(\eta_1^2+\eta_2^2)-2(\eta_1-\eta_2)^2\Big]\ln\frac{(\xi_1\xi_2-1)^2+w\xi_1\xi_2}{(\xi_1-\xi_2)^2+w\xi_1\xi_2}\\ &+F(\xi_1,\xi_2)-F\left(\xi_1,\frac{1}{\xi_2}\right)-F\left(\frac{1}{\xi_1},\xi_2\right)+F\left(\frac{1}{\xi_1},\frac{1}{\xi_2}\right), \end{aligned}$$

with

$$\begin{aligned} F(x_1,x_2) &= \frac{s}{4}\left(\frac{\eta_1}{x_1}+\frac{\eta_2}{x_2}\right)\arctan\left(\frac{2(x_1x_2-1)+w}{s}\right)\\ &+\frac{i}{8}s\mathrm{Li}_2\left(x_1x_2\frac{2-w-is}{2}\right)-\frac{i}{8}s\mathrm{Li}_2\left(x_1x_2\frac{2-w+is}{2}\right)\\ \mathrm{Li}_2(x) &= -\int_0^x\frac{\ln(1-z)}{z}dz \qquad ; \qquad s=\sqrt{w(4-w)}\ . \end{aligned}$$

In this case M^* has to be calculated from ρ_s via the standard nuclear matter relation [10]. Exchange corrections beyond the LDA are not known.

The situation with respect to correlation contributions is even more restricted: Two sets of nuclear matter results have been calculated.

1. The correlation contribution in the RPA limit [13] has been evaluated numerically for QHD-I in the no-sea approximation for the density range characterised by $0.6fm^{-1} \leq k_F \leq 1.8fm^{-1}$.

2. The correlation energy due to the sum of individual meson ladder contributions to the selfenergy has been evaluated [14] for the density range $1.0fm^{-1} \leq k_F \leq 1.8fm^{-1}$ in the no-pair approximation. In addition to contributions due to σ, ω, ρ and π mesons η and δ-meson contributions have been considered.

As a corollary I note that the DFT-approach can be extended to thermal systems [15,16]. For instance, in order to obtain an expression for the noninteracting free energy

$$F_s = T_s - TS_s$$

the starting point is the thermal Green's function

$$G(x,y) = \mathrm{Tr}\left\{ \frac{e^{-\beta(\hat{H}-\mu\hat{N})}}{\mathrm{Tr}(e^{-\beta(\hat{H}-\mu\hat{N})})} T_\tau \left[\hat{\psi}(x)\hat{\bar{\psi}}(y)\right] \right\} \tag{19}$$

where $x_0 = -i\tau_x$, $y = -i\tau_y$ and T_τ stands for "time ordering" of the real variables τ_x, τ_y. Again all quantities of interest can be extracted from $G(x,y)$. Questions of renormalisation arise, but do not differ from the situation at $T = 0$.

We finally present an indication of DFT results on the basis of the QHD model that have been obtained so far.

1. We begin with a comparison of HF and x-only LDA results for a QHD-I model. The model includes the exchange of photons, so that slight differences between proton and neutron data are observed. Fig.1 shows the proton densities obtained in the two approaches for ^{114}Sn, using the same set of model parameters. The closeness of the results is confirmed for neutron and baryon densities, for binding energies and mean radii of all spherical nuclei that have been considered [10].

   The conclusion, that one extracts from these results, is: The LDA for exchange (or, expressed differently, a multiplicative x-potential of rather simple extraction) is adequate in the case of short range interactions.

2. Quite similar statements can be made if one compares HF and LDA x-only results for QHD-II (involving the exchange of σ, ω, ρ and π-mesons as well as photons). This time the differences for the charge and baryon densities, obtained with the two approaches, are slightly larger. This is

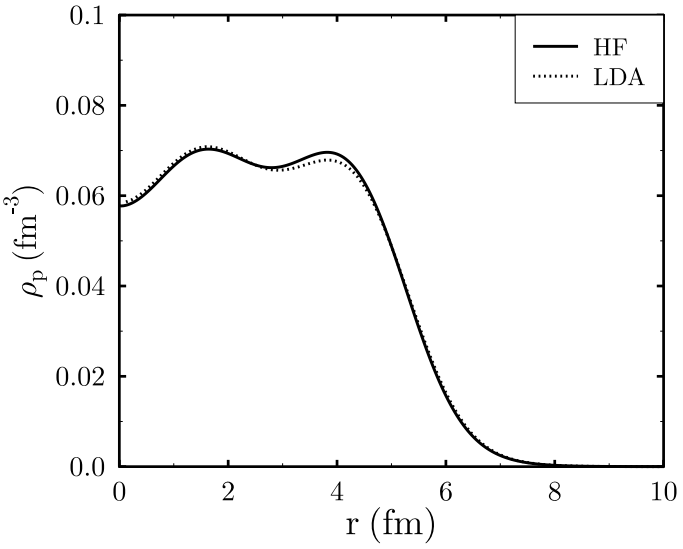

Figure 1: Proton point densities for ^{114}Sn from HF- [17] and LDA-calculations [10] (for the parameter set given in Ref. [3]).

a consequence of the contribution of the π-mesons, which is of longer range. On the other hand, results for binding energies and radii are still very close [18]. This is illustrated in Table 1, where results obtained with the parameter sets HF2 (without centre of mass corrections) and ZJO [4] (with cm corrections) are given.

3. If one compares Hartree results with the corresponding ETF results (available for the TF and ETF2 models [12,20]), one finds once more that these standard ETF functionals do not reproduce shell effects. The gradient corrected ETF2-functional yields, however, a more realistic surface structure for the nuclei.

4. Shell effects are known to be less important if one considers thermal systems. It can thus be expected that temperature dependent TF or ETF models provide reasonable results. A first investigation of various thermal nuclear systems (nuclear slabs, symmetric and asymmetric nuclei) addressing the questions of stability, appropriate equations of state etc. in terms of a thermal TF model for QHD-II (without photons) is available [16].

In summary we may then state that the application of DFT methods to

Table 1: Binding energies per nucleon (in MeV) and charge radii (in fm) from LDA-KS-calculations [18] for several spherical nuclei using two different parameters sets (HF2 [19] — without center of mass correction, ZJO [4] — including center of mass correction) in comparison with HF-calculations (using parameter set HF2 [19] — without center of mass correction) and experimental data (taken from Ref. [3]).

	$-E/A$				R_c			
	HF	LDA		EXP	HF	LDA		EXP
	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	

QHD systems looks quite promising. The obvious next step is the investigation of correlation contributions. First results for the nuclear matter problem indicate that they are quite large (as expected), so that their incorporation is essential. The hope is that nuclear matter correlation results can be used in the LDA form with the same success as the exchange contributions. If this is the case, a number of questions concerning the QHD model itself can be raised and answered, as eg.

- Can more involved models (with nonlinear terms and a larger number of mesons), that are applied with restrictive approximations, be replaced by simpler models, that are applied with full inclusion of correlations?

- Can one find one "realistic" parameter set, that is derived from nuclear structure data and applied to low/intermediate energy collision problems?

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