Comparison of the relativistic Hartree-Fock approximation and its semiclassical expansion

D. Von-Eiff, S. Haddad, and M.K. Weigel
Sektion Physik, Ludwig-Maximilians-Universität München, Am Coulombwall 1, D-85748 Garching, Germany
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We present a comparison of a recent fully quantal relativistic Hartree-Fock approach with its semiclassical expansion. One obtains the same trends, i.e., a slight overbinding and smaller radii, as in similiar comparisons of (i) the nonrelativistic extended Thomas-Fermi method using Skyrme forces with the corresponding Hartree-Fock calculations and (ii) the relativistic semiclassical description with the relativistic Hartree theory.

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One of the main objectives of nuclear physics is the construction of a microscopic theory with a sufficient theoretical basis, which is capable of reproducing nuclear properties. Furthermore, such an approach should have enough predictive power for reliable extrapolations, for instance, for nuclear properties near the neutron-drip line, which are needed in astrophysical investigations. A further necessity is the limitation of the involved numerical effort in order to make the calculations feasible. In the nonrelativistic approach a big step towards this goal was achieved by treating the nuclei within the Hartree-Fock (HF) approximation with an effective Skyrme-force Hamiltonian. However, this method was still too complicated with respect to the computer time needed for a least-squares fit to all nuclei, which would lead to a nuclear mass formula of great sophistication. For that reason an extended Thomas-Fermi approximation (ETF) to the HF method has been developed, in which the problem is numerically tractable (for more details see, for instance, Refs. [1,2]).

In the relativistic approach, which has been applied successfully to a wide class of nuclear properties, the situation with respect to an overall description of nuclei is still in an infant stage in comparison with the nonrelativistic treatment. We will not repeat here all the merits and the advantages of the relativistic theory (for two excellent reviews see Refs. [3,4]), but mention only two important features: first, the natural explanation of the nuclear spin-orbit force having the right magnitude without extra parameters as in nonrelativistic Skyrme or Gogny forces. Second, it contains explicitly the mesonic degrees of freedom, which is advantageous in several respects (e.g., meson-exchange current contributions; see Refs. [3–5]). The drawbacks of the relativistic theory are the more complicated structures, which render the calculations rather cumbersome in comparison with their nonrelativistic counterparts. Therefore, relativistic treatments are dominantly done within the relativistic Hartree approximation (RHA), which reproduces the properties of spherical and axially symmetric deformed nuclei in a satisfactory manner [6–8]. However, the amount of fitted data is much less as in the nonrelativistic case. Relativistic Hartree-Fock (RHF) calculations are usually performed for some selected spherical nuclei [9–12], and attempts to perform a more general fit, as described above, are scarce [13]. The dynamics of the RHF treatment are governed by the standard one-boson-exchange (OBE) Lagrangian [4]

$$\mathcal{L} = \bar{\psi}\Big(i\gamma^\mu\partial_\mu - M + g_\sigma\sigma - g_\omega\gamma^\mu\omega_\mu - \frac{f_\pi}{m_\pi}\gamma_5\gamma^\mu\boldsymbol{\tau}\cdot\partial_\mu\boldsymbol{\pi} - g_\varrho\gamma^\mu\boldsymbol{\tau}\cdot\boldsymbol{\varrho}_\mu - \frac{f_\varrho}{4M}\sigma^{\mu\nu}\boldsymbol{\tau}\cdot\mathbf{G}_{\mu\nu}\Big)\psi + \frac{1}{2}\Big[\partial_\mu\sigma\partial^\mu\sigma - m_\sigma^2\sigma^2\Big] + \frac{1}{2}\Big[\partial_\mu\boldsymbol{\pi}\cdot\partial^\mu\boldsymbol{\pi} - m_\pi^2\boldsymbol{\pi}^2\Big] - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{1}{2}m_\omega^2\omega^\mu\omega_\mu - \frac{1}{4}\mathbf{G}^{\mu\nu}\cdot\mathbf{G}_{\mu\nu} + \frac{1}{2}m_\varrho^2\boldsymbol{\varrho}^\mu\cdot\boldsymbol{\varrho}_\mu, \quad (1)$$

with the field tensors

$$F_{\mu\nu} \equiv \partial_\mu\omega_\nu - \partial_\nu\omega_\mu \quad (2)$$

and

$$\mathbf{G}_{\mu\nu} \equiv \partial_\mu\boldsymbol{\varrho}_\nu - \partial_\nu\boldsymbol{\varrho}_\mu \quad , \quad (3)$$

where $\boldsymbol{\pi}$ and $\boldsymbol{\varrho}_\mu$ denote isovectors. The Lagrangian (1) includes the tensor ϱ-nucleon coupling which gives important contributions to nuclear properties (as, for instance, energy, incompressibility, etc. [4,11,14,15]). However, the neglect of this tensor coupling seems to simplify the RHF calculations (cf. Refs. [12,13]). The inclusion of σ self-interactions is possible in an approximate manner [12,15]. The Lagrangian (1) displays two additional advantages: First, it possesses a similiar structure as the free OBE potential; second, with density-dependent couplings it is possible to simulate the structure of the relativistic Brueckner-Hartree-Fock theory (RBHF) and apply the RBHF approach to finite systems [16]. The main difficulty concerning the RHF approximation seems to be the rather complicated numerical treatment [11,12]. That

TABLE I. RHF parameter set HF(δ) [12] and properties of symmetric nuclear matter. Physically fixed input parameters are M = 939 MeV, m_π = 138 MeV, m_ω = 783 MeV, m_ϱ = 770 MeV, $f_\pi^2/4\pi$ = 0.08, $g_\varrho^2/4\pi$ = 0.55, and f_ϱ/g_ϱ = 6.6. The effective Dirac mass M^* was calculated at the Fermi surface. J denotes the symmetry-energy parameter.

$g_\sigma^2/4\pi$	7.19
$g_\omega^2/4\pi$	8.22
m_σ (MeV)	525
E/A (MeV)	-15.75
ρ (fm^{-3})	0.1484
K (MeV)	399
M^*/M	0.60
J (MeV)	35.0

was one of the reasons that we studied in some former investigations relativistic semiclassical approaches with inclusion of Fock contributions, since such methods might offer the opportunity to simplify the calculation of finite nuclei [14,17–19]. Of course, it would be very interesting to compare such calculations with the outcome of a fully quantal RHF calculation. This opportunity is offered by a recent publication of Bernardos *et al.* [12] which gives the outcome of a RHF treatment with a Lagrangian of the structure given in Eq. (1). The corresponding parameters and nuclear matter results are given in Table I.

We have two different versions, denoted by RTFA-QC$_A$ and RTFA-QC$_B$, of the relativistic Thomas-Fermi approximation including quantum corrections, which are described in detail in Refs. [14,19]. They differ mainly in the treatment of the nuclear densities at the classical turning point. Furthermore, in RTFA-QC$_B$ the self-consistency problem of the tensor density is included and the momentum dependence of the Fock self-energies is treated in a more sophisticated manner. The comparison with the fully quantal results is shown in Table II. (A comparison for ^{208}Pb is not possible, since the numerical procedure in the RHF approximation does not converge [12], which emphasizes again the complexity of the relativistic approach.)

As expected, the semiclassical approximation with Wigner corrections overbinds in comparison with the RHF treatment and the rms charge radii are too small, since semiclassical treatments do not reproduce the quantal tail of a wave function approach in a satisfactory manner. These are known features from the nonrelativistic theory, which was the reason for the renormalization of the Skyrme-force parameters in the ETF approximation to the HF method [1]. Comparing the RHA with its semiclassical expansions the same effect for the binding energy is encountered (see Ref. [20] for ^{40}Ca and ^{208}Pb): One obtains energy changes of the same order (see Table II), namely, underbinding by neglecting the $\hbar^2$ terms and overbinding by their inclusion. One has to remark that the question of over- or underbinding for the zeroth-order semiclassical approximation to the RHA, TF$\hbar^0$, depends on the value of the effective Dirac mass. For higher values of M^*/M the authors of Ref. [20] obtain an overbinding

TABLE II. Comparison of the quantal RHF calculations [12], denoted by HF(δ), with the semiclassical approaches RTFA-QC$_A$ and RTFA-QC$_B$ for different nuclei (see text). RTFA-EX denotes the approximation where the $\hbar^2$-Wigner corrections are neglected. Given are the binding energy per particle E/A (MeV), the rms charge radii r_c (fm), and the proton spin-orbit splitting Δ_{LS} (MeV) for the $1p$ shell (^{16}O) and $1d$ shell (^{40}Ca and ^{48}Ca). The single-particle levels for the semiclassical approximations are calculated by solving the Dirac equation once, with the semiclassical self-energies as an input ("expectation value method"; not possible within the RTFA-QC$_A$ approach [14]). For the purpose of comparison we included also the results for the relativistic Hartree approach (RHA) and its semiclassical approximations, TF$\hbar^0$ and TF$\hbar^2$ (parameter set SRK3M5, M^*/M = 0.55; see Ref. [20]; the corresponding radii are the original proton rms radii).

			RTFA						
		HF(δ)	-EX$_A$	-QC$_A$	-EX$_B$	-QC$_B$	RHA[a]	TF$\hbar^0$[a]	TF$\hbar^2$[a]
^{16}O	E/A	6.36	5.70	6.36	6.22	7.48			
	r_c	2.74	2.69	2.68	2.69	2.62			
	Δ_{LS}	6.17	4.81		4.61	5.33			
^{40}Ca	E/A	7.73	7.42	8.52	7.34	7.84	7.62	7.31	7.97
	r_c	3.46	3.39	3.39	3.40	3.33	3.42	3.46	3.33
	Δ_{LS}	7.33	6.00		5.29	5.74			
^{48}Ca	E/A	7.96	7.72	8.75	7.54	8.33			
	r_c	3.47	3.47	3.43	3.47	3.39			
	Δ_{LS}	3.55	5.57		4.87	5.11			
^{90}Zr	E/A	8.34	8.25	9.26	8.06	8.77			
	r_c	4.24	4.21	4.20	4.22	4.18			
^{208}Pb	E/A		7.83	8.60	7.46	7.83	7.79	7.52	7.89
	r_c		5.41	5.39	5.43	5.40	5.47	5.60	5.51

[a] Ref. [20].

without $\hbar^2$ terms. Since the parameter set HF(δ) yields an effective Dirac mass $M^*/M = 0.60$, calculated at the Fermi surface, we have selected for comparison the results for $M^*/M = 0.55$ from Ref. [20]. Also with respect to the radii we obtain the same trend as in Ref. [20], i.e., a decrease of the radii by adding the $\hbar^2$ corrections.

As far as the differences of our two semiclassical treatments, RTFA-QC$_A$ and RTFA-QC$_B$, are concerned, one can pin down two different sources: First, one obtains different results due to different treatments of the Fock self-energies. Quantitatively this effect (around 0.4 MeV/A for ^{208}Pb) can be estimated by comparison of the results of the relativistic Thomas-Fermi approximation including exchange term corrections (RTFA-EX), where the $\hbar^2$-Wigner corrections are neglected. As they should, the charge radii are the same without Wigner corrections, since within both approaches they are solely determined by the relativistic Thomas-Fermi approximation [14,19] (the remaining differences are negligible and due to the different codes used). The second point concerns the different incorporation of the second-order density corrections. Since they are distributions in the mathematical sense resulting in well-defined integrals, they are used in RTFA-QC$_A$ for the evaluation of volume integrals only [14]. The treatment of RTFA-QC$_B$ [19] resembles more the procedure of Ref. [20], where one gets a stronger decrease in the radii.

In this work we have compared a fully quantal RHF calculation with two semiclassical approximations up to the order $\hbar^2$. The agreement of the semiclassical approaches with the RHF results is satisfactory. With respect to trends and sizes in the deviations the results are similiar to the nonrelativistic case and the relativistic mean field model.

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