Fourth-order gradient corrections to the relativistic Thomas-Fermi-Weizsäcker model

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We present a calculation of the fourth-order gradient corrections to the noninteracting kinetic energy of a relativistic system of electrons and positrons. The basis of the calculation is a recently published algorithm for the generation of the gradient expansion of the Green's function of a field-theoretical system characterized by a Lagrangian with an effective external potential.

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I. INTRODUCTION

The Thomas-Fermi model for relativistic many electron systems has been established quite early [1, 2] and has since been used for the discussion of a variety of problems [3]. The derivation of (second-order) gradient corrections [4] to this model could only be carried through after the realization that the problem had to be approached on the level of a field-theoretical formulation in order to handle questions of renormalization in a consistent manner [5]. A fully covariant formulation could in turn be obtained [6] on the basis of a recently published algorithm for the generation of the semiclassical expansion of the Green's function [7] in an effective field theory.

Numerical investigation of the relativistic Thomas-Fermi-Dirac-Weizsäcker model [8] yielded the expected improvements over the simpler version, however, the establishment of higher-order gradient corrections seems to be desirable.

In this paper we present the fourth-order gradient corrections to the (noninteracting) kinetic energy of a relativistic system of electrons and positrons on the basis of the expansion of the Green's function indicated above. In view of the relative complexity encountered in the standard steps of semiclassical expansion and inversion we used the readily available program package REDUCE [9] to handle technical details.

II. THE SEMICLASSICAL GRADIENT EXPANSION

Assume that a system of relativistic fermions can be described by the Lagrangian [we use the metric $g^{\mu\nu} = \mathrm{diag}(1,-1,-1,-1)$ and units with $\hbar = c = 1$]

$$\mathcal{L} = \overline{\psi}(x)[i\partial\!\!\!/ - m - V\!\!\!/(x)]\psi(x),$$

where $V_\nu(x)$ is an effective external four-potential in the framework of a Kohn-Sham formulation. Following [7] we expand the corresponding one-particle propagator in the form

$$G(x,y) = \sum_{n=0}^{\infty} G^{[n]}(x,y),$$

where $G^{[n]}(x,y)$ denotes the nth-order gradient contribution to $G(x,y)$. Introducing the partial Fourier transforms $g^{[n]}(p,x)$ by

$$G^{[n]}(x,y) = e^{-i(x-y)\cdot V(x)} \frac{1}{(2\pi)^4} \int d^4p\, e^{-ip\cdot(x-y)} g^{[n]}(p,x)$$

one readily establishes the recursion relation

$$(p\!\!\!/ - m) g^{[n]}(p,x) = i\left(\partial\!\!\!/ V_\nu(x) \frac{\partial}{\partial p_\nu} - \partial\!\!\!/\right) g^{[n-1]}(p,x)$$

which can be resolved (formally) in the form

$$g^{[n]}(p,x) = \left[\frac{i}{p\!\!\!/ - m}\left(\partial\!\!\!/ V_\nu(x)\frac{\partial}{\partial p_\nu} - \partial\!\!\!/\right)\right]^n g^{[0]}(p,x). \quad (1)$$

The quantity $g^{[0]}(p,x)$ is the local-density approximation of the Green's function of a homogenous relativistic electron gas in a constant four potential

$$g^{[0]}(p,x) = i(p\!\!\!/ + m)\left(\frac{1}{p^2 - m^2 + i\epsilon} + 2\pi i\,\Theta(E_s - p^0)\Theta(p^0)\delta(p^2 - m^2)\right) \quad (2)$$

with the local Fermi energy

$$E_s \equiv S - V^0(x).$$

The first part in (2) constitutes the contribution of the fermion vacuum, the second part is the contribution of free electrons with energy between $-m$ and S. Hence, one-particle states with energy below S are occupied, the others are unoccupied. As $g^{[n]}(p,x)$ is a linear function of $g^{[0]}(p,x)$, the separation into vacuum and free-electron contribution (denoted by the subscript "vac" and "el") applies in any order of the gradient expansion.

In the vacuum part of (1) it is reasonable to require that the pole structure is the same in every order. In order to facilitate the evaluation of the electron part of (1) the following remarks are pertinent: One may obtain the electron part $g^{[n]}_{\mathrm{el}}(p,x)$ from the vacuum part $g^{[n]}_{\mathrm{vac}}(p,x)$

by the replacement

$$\frac{1}{(p^2-m^2+i\epsilon)^{n+1}} \longmapsto 2\pi i\,\Theta(E_s-p^0)\frac{(-1)^n}{n!}\Theta(p^0)\delta^{(n)}(p^2-m^2), \quad (3)$$

where $\delta^{(n)}$ denotes the nth derivative of Dirac's δ function.

This can be demonstrated as follows: First one establishes that

$$\left(\not{\partial}V_\nu(x)\frac{\partial}{\partial p_\nu}-\not{\partial}\right)[\Theta(E_s-p^0)\Theta(p^0)]=0.$$

As a consequence one has to replace

$$\frac{d^s}{dz^s}\frac{1}{z+i\epsilon} \longmapsto 2\pi i\,\delta^{(s)}(z) \quad (4)$$

with $z\equiv p^2-m^2$. Second, terms of the form

$$T(z)=\frac{1}{z^r}\delta^{(s)}(z)$$

are treated by solving the equation

$$z^rT(z)=\delta^{(s)}(z)$$

for $T(z)$. The solution

$$T(z)=(-1)^r\frac{s!}{(r+s)!}\delta^{(r+s)}(z)$$

in combination with (4) and (1) readily proves the assertion (3).

Further simplification can be achieved with the relation

$$\Theta(p^0)\,\delta^{(n)}(p^2-m^2)=\frac{\delta^{(n)}(p^0-E)}{(p^0+E)^{n+1}},$$

where $E=\sqrt{\mathbf{p}^2+m^2}$, which can be demonstrated by induction.

The explicit evaluation of (1) to second order can still be done by hand, even when dealing with a full electromagnetic potential [6]. The evaluation of higher-order functions $g^{[n]}(p,x)$ becomes, however, extremely tedious, even if one restricts oneself to the case that the effective potential is purely electrostatic. For this reason the evaluation was done by developing a program in REDUCE for the case that

$$V_0(x)=V(\mathbf{x}) \quad \text{and} \quad V_i(x)=0 \quad \text{for} \quad i=1,2,3.$$

Once $g^{[n]}(p,x)$ is obtained the electron density (actually the charge density of the system divided by the elementary charge) and the total energy density of the system of noninteracting particles in an external field in nth order can be calculated as

$$\begin{aligned}\rho^{[n]}(x)&=-\lim_{\substack{s\\ y\to x}}\operatorname{tr}[\gamma^0G^{[n]}(x,y)]\\ &=-\frac{1}{(2\pi)^4}\int d^4p\,\operatorname{tr}[\gamma^0g^{[n]}(p,x)],\\ \varepsilon^{[n]}(x)&=-\lim_{\substack{s\\ y\to x}}\operatorname{tr}\left(i\gamma^0\frac{\partial}{\partial x^0}G^{[n]}(x,y)\right)\\ &=V^0(x)\rho^{[n]}(x)-\frac{1}{(2\pi)^4}\int d^4p\,\operatorname{tr}[p^0\gamma^0g^{[n]}(p,x)]\\ &=\varepsilon^{[n]}_{\text{ext}}(x)+\tau^{[n]}(x).\end{aligned}$$

The energy density decomposes directly into an electrostatic and a kinetic-energy density (including the rest mass contribution). The symmetric limit indicated stands for

$$\lim_{\substack{s\\ y\to x}}=\frac{1}{2}\left(\lim_{\substack{y\to x\\ y^0>x^0}}+\lim_{\substack{y\to x\\ y^0<x^0}}\right)\Bigg|_{(x-y)^2\geq 0}.$$

Again the explicit evaluation of the trace of $\gamma^0g^{[n]}(p,x)$ and the final integration is carried through with REDUCE. For the integration we note the following.

(1) Integrals occuring in the vacuum part of $G^{[n]}(x,y)$ are divergent and have to be handled by dimensional regularization [10]. The relevant formula to be used is

$$\begin{aligned}&\frac{1}{(2\pi)^D}\int d^Dp\frac{p^{\mu_1}\cdots p^{\mu_{2n}}}{(p^2-m^2+i\epsilon)^\alpha}\\ &\quad=(m^2)^{D/2-\alpha+n}(g^{\mu_1\mu_2}\cdots g^{\mu_{2n-1}\mu_{2n}}+\cdots)\\ &\qquad\times\frac{i}{(4\pi)^{D/2}}\frac{(-1)^{\alpha+n}}{2^n}\frac{\Gamma(\alpha-D/2-n)}{\Gamma(\alpha)},\end{aligned}$$

where $+\cdots$ stands for the sum over all distinct terms obtained by permutation of the indices $\mu_1\cdots\mu_{2n}$. For the case of a pure electrostatic potential some momenta are timelike (p^0), while the others are spacelike (p^i). In this case one has

$$\begin{aligned}&\frac{1}{(2\pi)^D}\int d^Dp\frac{(p^0)^{2\ell}p^{i_1}\cdots p^{i_{2n}}}{(p^2-m^2+i\epsilon)^\alpha}\\ &\quad=(m^2)^{D/2-\alpha+n+\ell}(2\ell-1)!!\,(g^{i_1i_2}\cdots g^{i_{2n-1}i_{2n}}+\cdots)\\ &\qquad\times\frac{i}{(4\pi)^{D/2}}\frac{(-1)^{\alpha+n+\ell}}{2^{n+\ell}}\frac{\Gamma(\alpha-D/2-n-\ell)}{\Gamma(\alpha)}\end{aligned}$$

with the convention $(-1)!!\equiv 1$.

(2) Integrals in the electron part of $G^{[n]}_{\text{el}}(x,y)$ are of the form

$$\begin{aligned}\int d^4p\,(p^0)^\ell p^{i_1}\cdots p^{i_{2n}}\frac{\delta^{(r)}(p^0-E)}{(p^0+E)^{r+1}}\Theta(E_s-p^0)&=(-1)^n\frac{2\pi}{(2n+1)!!}(g^{i_1i_2}\cdots g^{i_{2n-1}i_{2n}}+\cdots)\\ &\times\sum_{\substack{r_1+r_2+r_3=r\\ r_2\leq\ell}}\frac{(-1)^{r_2}(r+r_3)!}{r_1!\,r_2!\,r_3!}\frac{\ell!}{(\ell-r_2)!}\frac{1}{2^{r+r_3}}\\ &\times\left(\frac{d}{dE_s}\right)^{r_1-1}(p_s^{2n+1}E_s^{\ell-2r+r_1}),\end{aligned}$$

where the notation

$$\left(\frac{d}{dE_s}\right)^{-1} f(E_s) \equiv \int_m^{E_s} f(E)\,dE$$

has been used and p_s denotes the relativistic local Fermi momentum

$$p_s \equiv \begin{cases} \sqrt{E_s^2 - m^2} \text{ if } E_s \geq m \\ 0 \text{ otherwise.} \end{cases}$$

The results obtained with REDUCE for the fourth-order gradient contributions to the semiclassical expansion of the density and the kinetic-energy density, including the rest mass term, are (from now on we use units with $m = 1$)

$$\rho_{\rm vac}^{[4]} = \frac{1}{180\pi^2}[3\Delta^2 V + 2\Delta V(\nabla V)^2 + 2\nabla V\cdot\nabla(\nabla V)^2], \tag{5a}$$

$$\begin{aligned}\rho_{\rm el}^{[4]} = -\frac{1}{5760\pi^2}\Bigg(& 24\Delta^2 V\frac{E_s}{p_s^3}(4p_s^2-1) + 4(\Delta V)^2\frac{1}{p_s^5}(11p_s^2-15) + 2\Delta(\nabla V)^2\frac{1}{p_s^5}(7p_s^2-12) \\ & +4\nabla V\cdot\nabla\Delta V\frac{1}{p_s^5}(17p_s^2-24) + 4\Delta V(\nabla V)^2\frac{E_s}{p_s^7}(16p_s^6-8p_s^4+36p_s^2-75) \\ & +4\nabla V\cdot\nabla(\nabla V)^2\frac{E_s}{p_s^7}(16p_s^6-8p_s^4+21p_s^2-45) + 3(\nabla V)^4\frac{1}{p_s^9}(32p_s^4-80p_s^2-175)\Bigg),\end{aligned} \tag{5b}$$

$$\tau_{\rm vac}^{[4]} = \frac{1}{960\pi^2}[14(\Delta V)^2 + 22\nabla V\cdot\nabla\Delta V + 5\Delta(\nabla V)^2 + 8(\nabla V)^4], \tag{6a}$$

$$\begin{aligned}\tau_{\rm el}^{[4]} = -\frac{1}{5760\pi^2}\Bigg(& 24\Delta^2 V\frac{1}{p_s^3}(2p_s^2-1) + 12(\Delta V)^2\frac{E_s^3}{p_s^5}(7p_s^2-5) + 6\Delta(\nabla V)^2\frac{E_s^3}{p_s^5}(5p_s^2-4) \\ & +12\nabla V\cdot\nabla\Delta V\frac{E_s^3}{p_s^5}(11p_s^2-8) + 4\Delta V(\nabla V)^2\frac{1}{p_s^7}(40p_s^4-54p_s^2-75) \\ & +4\nabla V\cdot\nabla(\nabla V)^2\frac{1}{p_s^7}(20p_s^4-33p_s^2-45) + 3(\nabla V)^4\frac{E_s^3}{p_s^9}(16p_s^6-24p_s^4+70p_s^2-175)\Bigg).\end{aligned} \tag{6b}$$

Since the vacuum contributions are finite, further renormalization is not necessary in fourth order. The result for the vacuum part of the density can be interpreted in a direct fashion. The first term constitutes the Uehling term [11], the last two terms arise from variation of the Euler-Heisenberg-Lagrangian [12–14] with respect to $V_\mu(x)$

$$-\frac{\delta}{\delta V_\mu(x)}\frac{1}{360\pi^2}\int d^4x'[\tfrac{1}{4}(F_{\alpha\beta}F^{\alpha\beta})^2 + \tfrac{7}{16}(F_{\alpha\beta}{}^*F^{\alpha\beta})^2]$$

$$= \frac{1}{360\pi^2}\partial_\sigma(2F_{\alpha\beta}F^{\alpha\beta}F^{\sigma\mu} + \tfrac{7}{2}F_{\alpha\beta}{}^*F^{\alpha\beta}{}^*F^{\sigma\mu})$$

and restriction to the case of an electrostatic field and $\mu = 0$ [15]. Here the field-strength tensor and its dual form are defined by

$$F_{\mu\nu} = \partial_\mu V_\nu - \partial_\nu V_\mu \quad \text{and} \quad {}^*F_{\mu\nu} = \tfrac{1}{2}\epsilon_{\mu\nu\alpha\beta}F^{\alpha\beta}.$$

The program also reproduced the known results in zeroth and second order, and the fact, that odd orders vanish. After renormalization one finds

$$\rho^{[0]} = \frac{p_s^3}{3\pi^2}, \tag{7}$$

$$\rho^{[2]} = -\frac{1}{24\pi^2}\Bigg(2\Delta V\frac{1}{p_s}(2p_s\,\text{arcsinh}\,p_s + E_s) - (\nabla V)^2\frac{1}{p_s^3}(2p_s^2-1)\Bigg), \tag{8}$$

$$\tau^{[0]} = \frac{1}{8\pi^2}(E_s^3 p_s + E_s p_s^3 - \text{arcsinh}\,p_s), \tag{9}$$

$$\tau^{[2]} = -\frac{1}{24\pi^2}\Bigg(2\Delta V\frac{1}{p_s}(E_s^2+p_s^2) + (\nabla V)^2\frac{1}{p_s^3}[2p_s^3\,\text{arcsinh}\,p_s - E_s(p_s^2-1)]\Bigg), \tag{10}$$

where $\rho^{[n]}$ and $\tau^{[n]}$ denote (as usual) the sum of the vacuum and electron parts.

In the nonrelativistic limit ($p_s \ll m$) the fourth-order contributions $\rho_{\rm el}^{[4]}$ and $\tau_{\rm el}^{[4]}$ reduce to the results correctly established by Hodges [16] on the basis of the Kirzhnits formalism [17]. In the ultrarelativistic limit ($p_s \gg m$) Eqs. (5b) and (6b) are just the negative of (5a) and (6a), indicating a strong correlation in the high-density regime at the semiclassical level.

III. THE DENSITY GRADIENT EXPANSION

In order to obtain the noninteracting kinetic energy as a functional of the density one has to invert the semiclassical gradient expansion for the density and eliminate the effective potential from the semiclassical expansion of the energy. For this purpose one writes the density $\rho = \rho_{\rm vac} + \rho_{\rm el}$ in the form

$$\rho \underset{[4]}{=} \frac{p_s^3}{3\pi^2} + \rho^{[2]} + \rho^{[4]}, \tag{11}$$

where the second term is given by (8) and the last one denotes the sum of (5a) and (5b). The notation $\underset{[n]}{=}$ means "is equal in nth order." One obtains p_s as a function of ρ and its gradients by noting that (11) can be inverted consistently with the steps

$$p_s \underset{[0]}{=} (3\pi^2\rho)^{1/3} \equiv k,$$

$$p_s \underset{[2]}{=} k\left(1 - \frac{1}{3\rho}\rho^{[2]}(p_s^{[0]}, \nabla^2 E_s)\right) \tag{12}$$
$$\underset{[2]}{=} p_s^{[0]} + p_s^{[2]},$$

$$p_s \underset{[4]}{=} k\left(1 - \frac{1}{3\rho}\rho^{[2]}(p_s^{[0]} + p_s^{[2]}, \nabla^2 E_s) - \frac{1}{3\rho}\rho^{[4]}(p_s^{[0]}, \nabla^4 E_s) - \frac{1}{9\rho^2}\rho^{[2]}(p_s^{[0]}, \nabla^2 E_s)^2\right). \tag{13}$$

In this process the various derivatives of E_s ($\nabla E_s = -\nabla V$), which occur in (12) and (13), have to be expressed in terms of derivatives of the density. Second- and fourth-order derivatives can be generated consistently, by using

$$E_s = \sqrt{p_s^2 + 1}$$
$$\underset{[2]}{=} \epsilon - \frac{\pi^2}{k\epsilon}\rho^{[2]}$$
$$\underset{[2]}{=} \epsilon - \frac{1}{24}\left[2\Delta k\left(\frac{2}{\epsilon^2}\operatorname{arcsinh} k + \frac{1}{k\epsilon}\right) + (\nabla k)^2\left(\frac{4}{k\epsilon^4}\operatorname{arcsinh} k + \frac{k^2+\epsilon^2}{k^2\epsilon^3}\right)\right] \tag{14}$$

with $\epsilon = \sqrt{k^2+1}$. In order to execute the steps indicated, we again relied on a program in REDUCE. The program was checked by inserting the inverted form into Eq. (11) yielding the expected result

$$\rho \underset{[4]}{=} \frac{k^3}{3\pi^2}. \tag{15}$$

Finally p_s is inserted into the kinetic-energy expression

$$T \underset{[4]}{=} \int d^3x\,(\tau^{[0]} + \tau^{[2]} + \tau^{[4]}),$$

where $\tau^{[n]}$ includes the vacuum and electronic contribution [using Eqs. (9), (10), (6a), and (6b)]. This insertion was done again using the REDUCE language. The final result for the kinetic energy (including zeroth and second order for completeness) is

$$T^{[0]} = \int \frac{d^3x}{8\pi^2}[-\operatorname{arcsinh} k + k\epsilon(k^2+\epsilon^2)],$$

$$T^{[2]} = \int \frac{d^3x}{24\pi^2}\left[(\nabla k)^2\left(\frac{2k^2}{\epsilon^2}\operatorname{arcsinh} k + \frac{k}{\epsilon}\right)\right],$$

$$T^{[4]} = \int \frac{d^3x}{5760\pi^2}\left[16(\Delta k)^2\left(\frac{5k}{\epsilon^3}\operatorname{arcsinh}^2 k + \frac{5}{\epsilon^2}\operatorname{arcsinh} k - \frac{3k^2-2}{k\epsilon} + \frac{3k^2}{\epsilon^2}\right) + 2\Delta k(\nabla k)^2\left(\frac{80}{\epsilon^5}\operatorname{arcsinh}^2 k + \frac{20(2\epsilon^2+1)}{k\epsilon^4}\operatorname{arcsinh} k - \frac{21k^2-10}{k^2\epsilon^3} + \frac{48k}{\epsilon^4}\right) + (\nabla k)^4\left(\frac{80}{k\epsilon^7}\operatorname{arcsinh}^2 k + \frac{40(k^2+\epsilon^2)}{k^2\epsilon^6}\operatorname{arcsinh} k + \frac{16k^8+8k^6+12k^4+k^2+8}{k^3\epsilon^5} - \frac{16}{\epsilon^6}(k^4\epsilon^2 - 3)\right)\right].$$

In order to obtain the result in this minimal form suitable partial integrations with the assumption that $\rho(\mathbf{x})$ vanishes on the surface of a large sphere have to be performed. The nonrelativistic limit of $T^{[4]}$ coincides with the result given by Hodges [16].

IV. CONCLUSION

The results presented are relevant for the formulation of extended Thomas-Fermi models, as, e.g., the extended Thomas-Fermi-Dirac-Weizsäcker (TFDW4) model, of relativistic many-electron systems. They could, with some modifications, be extended to the discussion of a (global) density-functional description of other field theoretical systems, as, for instance, quantum hadrodynamics. In the relativistic TFDW4 model one has to consider the variational equations

$$\frac{\delta}{\delta k(\mathbf{x})}(T^{[0]} + T^{[2]} + T^{[4]} + E_{\text{ext}} + E_H + E_x^{[0]} - \mu N) = 0$$

including the Hartree term E_H for the direct interaction energy of the electrons and the local-density approximation for the relativistic exchange contribution [3]. The ensuing variational equations are reasonably involved, but

should, in analogy to the nonrelativistic case [18], be tractable. As inclusion of fourth-order gradient corrections did provide an improved description of ground-state properties for nonrelativistic atomic and nuclear systems, this effort is considered to be worthwhile. Work in this direction is in progress.

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