Field-theoretical approach to a relativistic Thomas-Fermi-Dirac-Weizsäcker model

E. Engel and R. M. Dreizler
Institut für Theoretische Physik der Universität, Frankfurt am Main, Federal Republic of Germany
(Received 3 May 1986; revised manuscript received 26 August 1986)

We outline a systematic scheme for the derivation of relativistic energy density functionals on the basis of the Hartree-Fock limit of quantum electrodynamics. In particular, a relativistic analog of the nonrelativistic Thomas-Fermi-Dirac-Weizsäcker model is presented.

I. INTRODUCTION

Density-functional theory has been used with considerable success for the discussion of nonrelativistic many-particle systems.[1-4] The foundations of a relativistic density-functional theory were established by Rajagopal[5,6] and Vosko and MacDonald,[7] who demonstrated that the basic theorem of Hohenberg and Kohn[8] could be extended to the relativistic domain. Several attempts[9-11] followed to construct explicitly relativistic local density schemes, in particular, the form of the local relativistic exchange energy density being a point of interest and discussion since the seminal contributions of Salpeter[12] as well as Jancovici.[13]

The question of gradient corrections to a local scheme has been discussed previously[14] within the frame of a relativistic extension of the Thomas-Fermi-Dirac-Weizsäcker (TFDW) model on the basis of the Dirac equation. A number of problems, due to questions of renormalization and due to the discussion of vacuum contributions, have been pinpointed in turn.[15]

In the present contribution we shall discuss a systematic construction of the relativistic analog of the TFDW model on the basis of field theory (QED).[16-19] We define the starting point in Sec. II, review some basic relations for the four-current in Sec. III and describe the equivalent of the Hartree-Fock (HF) limit in QED in Sec. IV. The renormalization problem encountered is summarized in Sec. V. The details of the gradient expansion technique in the present situation and explicit final functionals are given in Sec. VI. The basic approximation involved is, in analogy and extension of the nonrelativistic limit, a representation of the full electron propagator by a Green's function of an effective field theory. We conclude the presentation by some remarks on the practical evaluation of the TFDW variational scheme in the relativistic case. We use the relativistic convention $\hbar = c = 1$ throughout.

II. THE GROUND STATE OF AN N-ELECTRON SYSTEM IN AN EXTERNAL POTENTIAL

Our starting point is the QED Lagrangian density augmented by external potential terms

$$\mathcal{L} = -\tfrac{1}{4}F_{\rho\nu}F^{\rho\nu} + \frac{\mu^2}{2}A_\nu A^\nu - \frac{\lambda}{2}(\partial_\nu A^\nu)^2 - \tfrac{1}{4}F_{\mathrm{ext},\rho\nu}F^{\rho\nu}_{\mathrm{ext}} + \tfrac{1}{4}\{[\bar{\psi},(i\vec{\partial} - m - e\boldsymbol{V}_{\mathrm{ext}})\psi] + [\bar{\psi}(-i\overleftarrow{\partial} - m - e\boldsymbol{V}_{\mathrm{ext}}),\psi]\} - \frac{e}{4}([\bar{\psi},\boldsymbol{A}\psi] + [\bar{\psi}\boldsymbol{A},\psi]) , \tag{2.1}$$

using the Feynman dagger notation,

$$\boldsymbol{A} = A_\nu \gamma^\nu ,$$

while the vector bars indicate in which direction the partial derivatives have to be taken. We work in the Gupta-Bleuler formalism[16] and use the convention $e = |e|$. The commutator representation of the Lagrangian ensures that the corresponding Hamiltonian is Hermitian and invariant under charge conjugation.[17] The photon mass μ is introduced to avoid infrared divergencies at intermediate steps and will have to be removed by taking the limit $\mu \to 0$ at the final stage. The importance of including the external field Lagrangian

$$-\tfrac{1}{4}F_{\mathrm{ext},\rho\nu}F^{\rho\nu}_{\mathrm{ext}}$$

will become apparent when renormalization is discussed in Sec. V. The external potential $V_{\mathrm{ext},\nu}$, which is assumed to be time independent, is treated classically. For the sake of simplicity, we eventually restrict ourselves to the case of a scalar (electrostatic) external potential,

$$\boldsymbol{V}_{\mathrm{ext}}(x^\nu) \to \gamma^0 V(\mathbf{x}) , \tag{2.2}$$

as we are primarily interested in atomic or molecular systems.

The Hamiltonian of the system under consideration is obtained via

$$H = \int d^3x\, \Theta^{00}(\mathbf{x}) \tag{2.3}$$

in the form

$$H=\int d^3x\left[\tfrac{1}{4}\{[\bar{\psi},(-i\gamma\cdot\vec{\nabla}+m+e\not{V}_{\rm ext})\psi]+[\bar{\psi}(i\gamma\cdot\overleftarrow{\nabla}+m+e\not{V}_{\rm ext}),\psi]\}+\frac{e}{8}([\bar{\psi},\not{A}\psi]+[\bar{\psi}\not{A},\psi])\right.$$
$$\left.+\frac{1}{2}\left[(\nabla V^0_{\rm ext})^2+\sum_k(\nabla V^k_{\rm ext})^2\right]+\tfrac{1}{2}[A^\nu(\partial^0)^2A_\nu-(\partial^0A_\nu)(\partial^0A^\nu)]\right] . \tag{2.4}$$

If we denote the (nondegenerate) ground state of the N-electron system, i.e., the state of lowest energy of the Fock-space sector with

$$\langle Q\rangle=-Ne ,$$

by $|g\rangle$ and the vacuum state of the problem, the state of lowest energy with

$$\langle Q\rangle=0 ,$$

by $|v\rangle$, we can write for the binding energy of the system

$$E_b=\langle g|H|g\rangle-\langle v|H|v\rangle$$
$$=E_g-E_v . \tag{2.5}$$

This construction leads to a finite energy value even if no normal-ordered representation of H is used, as all contributions to E_g and E_v from the "Fermi sea" cancel. The energy can be expressed in terms of the full interacting ground-state and vacuum electron propagators

$$G_g(x,y)=\langle g|T\psi_g(x)\bar{\psi}_g(y)|g\rangle , \tag{2.6a}$$
$$G_v(x,y)=\langle v|T\psi_v(x)\bar{\psi}_v(y)|v\rangle , \tag{2.6b}$$

and the reducible three-point functions

$$G^{(3)}_{g,\rho}(x,y|z)=\langle g|T\psi_g(x)\bar{\psi}_g(y)A_{g,\rho}(z)|g\rangle , \tag{2.6c}$$
$$G^{(3)}_{v,\rho}(x,y|z)=\langle v|T\psi_v(x)\bar{\psi}_v(y)A_{v,\rho}(z)|v\rangle , \tag{2.6d}$$

as

$$E_b=\int d^3x\lim_{y\to x}{}_s\,tr\{[i\gamma\cdot\nabla_x-m-e\not{V}_{\rm ext}(\mathbf{x})]\times[G_g(x,y)-G_v(x,y)]\}$$
$$-\frac{e}{2}\int d^3x\lim_{z\to x}\lim_{y\to z}{}_s\,{\rm tr}\{[G^{(3)}_{g,\rho}(x,y|z)-G^{(3)}_{v,\rho}(x,y|z)]\gamma^\rho\} . \tag{2.7}$$

The zero-point energy of the photon fields does not occur in view of the definition (2.5).[18] The limits indicated in Eq. (2.7) are defined as

$$\lim_{y-x}{}_s=\tfrac{1}{2}\Big(\lim_{y\to x,y^0>x^0}+\lim_{y\to x,y^0<x^0}\Big)\Big|_{(x-y)^2\geq 0} . \tag{2.8}$$

This structure is a consequence of the commutator form of the Lagrangian.

III. THE FOUR-CURRENT DENSITY

The four-current density of QED is defined as

$$j^\nu(x)=-e\lim_{y\to x}{}_s\,{\rm tr}[\gamma^\nu G(x,y)] . \tag{3.1}$$

The definition applies for both the ground state $|g\rangle$ and the vacuum state $|v\rangle$. As a large number of manipulations that follow are identical for the two states, we suppress the index except where needed for additional clarity. Using the fully reducible vacuum polarization insertion $\Pi^{\mu\nu}$, which is related to the full photon propagator $D^{\mu\nu}$ by

$$D_{\mu\nu}(x,y)=D^{(0)}_{\mu\nu}(x-y)+\int d^4z\,d^4u\,D^{(0)}_{\mu\lambda}(x-z)\times\Pi^{\lambda\rho}(z,u)D^{(0)}_{\rho\nu}(u-y) , \tag{3.2}$$

one can rewrite Eq. (3.1) as

$$j^\nu(x)=i\int d^4y\,\Pi^{\nu\mu}(x,y)V_{{\rm ext},\mu}(y) . \tag{3.3}$$

Now, as usual, one expresses the reducible function $\Pi^{\mu\nu}$ by the irreducible vacuum polarization $\omega^{\mu\nu}$. Working in momentum space,

$$\Pi^{\mu\nu}(x,y)=\int\frac{d^4p}{(2\pi)^4}\frac{d^4k}{(2\pi)^4}e^{-ipx+iky}\Pi^{\mu\nu}(p,k) , \tag{3.4}$$

this implies

$$\Pi^{\mu\nu}(p,k)=\omega^{\mu\nu}(p,k)+\int\frac{d^4q}{(2\pi)^4}\omega^{\mu\lambda}(p,q)D^{(0)}_{\lambda\rho}(q)\Pi^{\rho\nu}(q,k) . \tag{3.5}$$

In the presence of an external potential $\omega^{\mu\nu}(p,k)$ separates into two parts, the first containing all contributions to $\omega^{\mu\nu}$ without any connection to the external potential, the second containing the remainder. As a consequence of momentum conservation the first part has to vanish for $p\neq k$,

$$\omega^{\mu\nu}(p,k)=(2\pi)^4\delta^4(p-k)\omega^{\mu\nu}_1(p)+\omega^{\mu\nu}_2(p,k) . \tag{3.6}$$

The diagrammatic representation of $\omega^{\mu\nu}_1(p)$ and $\omega^{\mu\nu}_2(p,k)$ is indicated in Fig. 1.

If one separates $\Pi^{\mu\nu}(p,k)$ into a momentum-conserving part and a remainder similar as for $\omega^{\mu\nu}(p,k)$,

$$\Pi^{\mu\nu}(p,k)=(2\pi)^4\delta^4(p-k)\Pi^{\mu\nu}_1(p)+\Pi^{\mu\nu}_2(p,k) , \tag{3.7}$$

the connection of $\Pi^{\mu\nu}_1(p)$ with $\omega^{\mu\nu}_1(p)$ is simply established by inserting Eq. (3.6) into Eq. (3.5),

$$\Pi^{\mu\nu}_1(p)=\omega^{\mu\nu}_1(p)+\omega^{\mu\rho}_1(p)D^{(0)}_{\rho\lambda}(p)\omega^{\lambda\nu}_1(p)+\cdots . \tag{3.8}$$

This is exactly the reducible vacuum polarization of QED without external potential terms. Using current conservation,

$$\omega^{\mu\nu}_1(p)=-i(p^2g^{\mu\nu}-p^\mu p^\nu)\omega_1(p^2) , \tag{3.9}$$

the series in Eq. (3.8) can easily be summed to

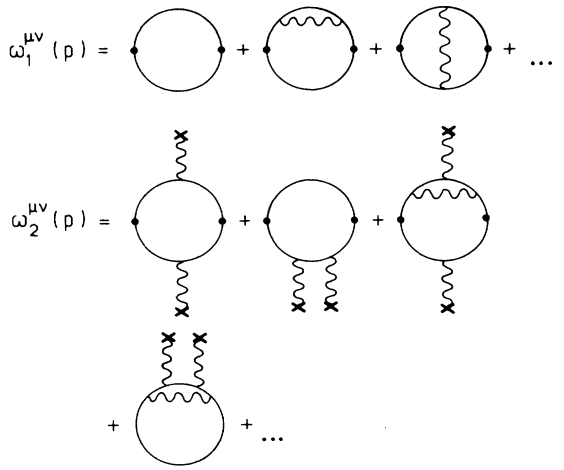

FIG. 1. Low-order contributions to the irreducible vacuum polarization.

$$\Pi_1^{\mu\nu}(p)=i(p^2g^{\mu\nu}-p^\mu p^\nu)\left[\frac{1}{1+\omega_1(p^2)}-1\right], \tag{3.10}$$

where Landau gauge has been used.

We thus finally obtain the equation

$$j^\mu(p)=-(p^2g^{\mu\nu}-p^\mu p^\nu)\left[\frac{1}{1+\omega_1(p^2)}-1\right]V_{\text{ext},\nu}(p)$$
$$+i\int\frac{d^4q}{(2\pi)^4}\Pi_2^{\mu\nu}(p,q)V_{\text{ext},\nu}(q) \tag{3.11}$$

for the exact electron current.

IV. THE HARTREE-FOCK APPROXIMATION

In order to extract an approximation similar to the HF limit of nonrelativistic many-particle physics,[20] we consider the irreducible three-point function $\Gamma^{(3)}$ (further denoted by Γ)

$$\Gamma_\rho(x,y\,|\,z)=\Gamma_\rho^{(0)}(x,y\,|\,z)$$
$$+(-ie)^3\langle s\,|\,T\bar\psi(z)\gamma_\rho\psi(z)$$
$$\times A(x)\psi(x)\bar\psi(y)A(y)\,|\,s\rangle_{c,\text{irred}}\,, \tag{4.1a}$$

where the reference state $|s\rangle$ represents either $|g\rangle$ or $|v\rangle$ and the subscripts indicate that only connected, one-particle irreducible graphs contribute to Γ. The lowest-order (in α) term is a simple vertex.

$$\Gamma_\rho^{(0)}(x,y\,|\,z)=-ie\gamma_\rho\delta^{(4)}(x-y)\delta^{(4)}(y-z)\,. \tag{4.1b}$$

The relation between Γ and $G^{(3)}$ reads

$$G_\rho^{(3)}(x,y\,|\,z)=G_{c,\rho}^{(3)}(x,y\,|\,z)$$
$$+ie\int d^4u\,D_{\rho\nu}^{(0)}(z-u)G(x,y)$$
$$\times\lim_{v\to u}{}_s\,tr[\gamma^\nu G(u,v)]\,, \tag{4.2a}$$

where the connected part $G_c^{(3)}$ of $G^{(3)}$ is given by

$$G_{c,\rho}^{(3)}(x,y\,|\,z)=\int d^4u_1d^4u_2d^4u_3D_{\nu\rho}(u_1,z)G(x,u_2)$$
$$\times\Gamma^\nu(u_2,u_3\,|\,u_1)G(u_3,y)\,. \tag{4.2b}$$

If we approximate Γ by its lowest order and if we use the free photon propagator $D_{\nu\rho}^{(0)}$ instead of $D_{\nu\rho}$ in Eq. (4.2b), we obtain, as shown in Ref. 21, a set of equations for the electron propagator, which is analogous to the Hartree-Fock limit of the nonrelativistic theory.

This approximation corresponds to the summation of selected subdiagrams in all orders of α and can be shown to amount to the standard factorization of the two-particle density matrix in terms of one-particle density matrices.

With the approximation indicated the energy E of either $|g\rangle$ or $|v\rangle$ can be written as

$$E=\int d^3x\,\varepsilon(\mathbf{x})$$
$$=\int d^3x\lim_{y\to x}{}_s\,tr\left[[i\gamma\cdot\nabla_x-m-eA(\mathbf{x})]G_{\text{HF}}(x,y)+\frac{1}{2}\left[[\nabla V_{\text{ext}}^0(\mathbf{x})]^2+\sum_k[\nabla V_{\text{ext}}^k(\mathbf{x})]^2\right]\right]$$
$$-i\frac{e^2}{2}\int d^3x\int d^4z\,D_{\rho\nu}^{(0)}(x-z)\{\lim_{u\to z}{}_s\,tr[\gamma^\nu G_{\text{HF}}(z,u)]\lim_{y\to x}{}_s\,\text{tr}[\gamma^\rho G_{\text{HF}}(x,y)]-\text{tr}[\gamma^\rho G_{\text{HF}}(x,z)\gamma^\nu G_{\text{HF}}(z,x)]\}\,, \tag{4.3}$$

with G_{HF} being either $G_{g,\text{HF}}$ or $G_{v,\text{HF}}$. One readily identifies the kinetic energy, external potential energy, and external field energy as well as the direct and exchange energy densities

$$\varepsilon(\mathbf{x})=\varepsilon_{\text{kin}}(\mathbf{x})+\varepsilon_{\text{ext}}(\mathbf{x})+\varepsilon_{\text{field}}(\mathbf{x})+\varepsilon_{\text{dir}}(\mathbf{x})+\varepsilon_{\text{ex}}(\mathbf{x})\,.$$

We shall use (4.3) as the starting point for the discussion of our relativistic energy density functional.

V. RENORMALIZATION

A look at the four-current or the exchange energy, represented by the diagram shown in Fig. 2, indicates that renormalization is necessary. We thus should have started with the renormalized Lagrangian

$$\mathscr{L}_R = Z_3\left[-\tfrac{1}{4}F_{R,\rho\nu}F_R^{\rho\nu}+\frac{\mu_R^2}{2}A_{R,\nu}A_R^\nu-\frac{\lambda_R}{2}(\partial_\nu A_R^\nu)^2-\tfrac{1}{4}F_{\mathrm{ext},R,\rho\nu}F_{\mathrm{ext},R}^{\rho\nu}\right]$$
$$+\frac{Z_2}{4}\{[\bar\psi_R,(i\overleftarrow{\partial}-m_R+\delta m-e_R\not{V}_{\mathrm{ext},R})\psi_R]+[\bar\psi_R(-i\overleftarrow{\partial}-m_R+\delta m-e_R\not{V}_{\mathrm{ext},R}),\psi_R]\}$$
$$-\frac{Z_1}{4}e_R([\bar\psi_R,\not{A}_R\psi_R]+[\bar\psi_R\not{A}_R,\psi_R]) \tag{5.1}$$

rather than (2.1). The quantities $Z_1=Z_2$, Z_3, and δm are the standard renormalization constants.

The renormalization procedure directly modifies the momentum-conserving parts of the vacuum polarization, the electron self-energy, and the irreducible three-point function. All diagrams with more than three external lines are overall convergent—only divergent subgraphs are renormalized due to the modification of the three functions above. Thus, for example, the Lagrangian (5.1) leads to the renormalized form of $\Pi_{1,R}^{\mu\nu}(p)$,

$$\Pi_{1,R}^{\mu\nu}(p)=i(p^2g^{\mu\nu}-p^\mu p^\nu)\left[\frac{1}{Z_3+\omega_1^{\mathrm{reg}}(p^2)}-1\right], \tag{5.2}$$

with

$$Z_3=1-\omega_1^{\mathrm{reg}}(p^2=0)\,, \tag{5.3}$$

where the constant Z_3 is expressed in terms of the renormalized (or physical) parameters e_R and m_R. We will, however, not display the index R for these parameters as well as for the renormalized fields A_R, ψ_R, and $V_{\mathrm{ext},R}$ with the understanding that only renormalized quantities occur in the following discussion. With the usual definition

$$\omega_{1,R}(p^2)=\omega_1^{\mathrm{reg}}(p^2)-\omega_1^{\mathrm{reg}}(p^2=0)\,, \tag{5.4}$$

one obtains finite expressions for $\Pi_{1,R}^{\mu\nu}(p)$,

$$\Pi_{1,R}^{\mu\nu}(p)=i(p^2g^{\mu\nu}-p^\mu p^\nu)\left[\frac{1}{1+\omega_{1,R}(p^2)}-1\right], \tag{5.5}$$

and the current

$$j_R^\mu(p)=-(p^2g^{\mu\nu}-p^\mu p^\nu)\left[\frac{1}{1+\omega_{1,R}(p^2)}-1\right]V_{\mathrm{ext},\nu}(p)$$
$$+i\int\frac{d^4q}{(2\pi)^4}\Pi_{2,R}^{\mu\nu}(p,q)V_{\mathrm{ext},\nu}(q)\,. \tag{5.6}$$

In the lowest order of α one finds

$$j_R^{(0),\mu}(p)=(p^2g^{\mu\nu}-p^\mu p^\nu)\omega_{1,R}^{(0)}(p^2)V_{\mathrm{ext},\nu}(p)$$
$$+i\int\frac{d^4q}{(2\pi)^4}\omega_2^{(0),\mu\nu}(p,q)V_{\mathrm{ext},\nu}(q)\,, \tag{5.7}$$

which is indicated by the series of Fig. 3. Here $\omega_2^{(0),\mu\nu}(p,q)$ is not changed by renormalization and $\omega_{1,R}^{(0)}(p^2)$ is given by

$$\omega_{1,R}^{(0)}(p^2)=\omega_1^{(0),\mathrm{reg}}(p^2)-\frac{e^2}{12\pi^2}\Gamma\left[2-\frac{D}{2}\right],$$

if dimensional regularization[22] is used. Finally, $j_R^{(0),\nu}$ is given in x space by

$$j_R^{(0),\nu}(x)=-\int d^4y\,\omega_{1,R}^{(0)}(x-y)(g^{\nu\mu}\partial_{y,\rho}\partial_y^\rho-\partial_y^\nu\partial_y^\mu)V_{\mathrm{ext},\mu}(y)$$
$$=j_{\mathrm{reg}}^{(0),\nu}(x)+\frac{e^2}{12\pi^2}\Gamma\left[2-\frac{D}{2}\right](g^{\nu\mu}\partial_{x,\rho}\partial_x^\rho-\partial_x^\nu\partial_x^\mu)V_{\mathrm{ext},\mu}(x)\,. \tag{5.8}$$

Concerning the exchange energy, it is sufficient (for our purpose) to consider the lowest-order contribution $\varepsilon_{\mathrm{ex}}^{(0)}$, obtained by replacing G_{HF} in Fig. 2 by $G^{(0)}$. This diagram is modified by three counterterms[23] corresponding to the divergent subgraphs shown in Fig. 4. The term resulting from the last diagram vanishes. The remaining two insertions into the free-electron propagator represent (as indicated in the figure) exactly the counterterms for the lowest-order self-energy $\Sigma^{(0)}$. If we express the exchange energy in terms of divergent, unrenormalized self-energy,

$$\varepsilon_{\mathrm{ex,reg}}^{(0)}(\mathbf{x})=-\tfrac{1}{2}\int d^4y\,tr[\Sigma_{\mathrm{reg}}^{(0)}(x,y)G^{(0)}(y,x)]\,, \tag{5.9}$$

it is obvious, in which fashion the renormalization of Σ,

$$\Sigma_R^{(0)}(x,y)=\Sigma_{\mathrm{reg}}^{(0)}(x,y)-\delta m\delta^4(x-y)-i(1-Z_2^{-1})[G_v^{(0)}(x,y)]^{-1}\,, \tag{5.10}$$

changes $\epsilon_{\mathrm{ex}}(0)$. In the context of Eq. (5.10), δm and Z_2 are understood to represent the lowest-order contributions of these quantities, which again can be made explicit by the dimensional regularization technique. Of course the ground state and the vacuum self-energy have to be renormalized by the same counterterms leading to the use of the inverse vacuum Green's function when renormalizing the ground-state self-energy. The resulting renormalized exchange energy density is (compare Ref. 24)

$$\varepsilon_{\mathrm{ex},R}^{(0)}(\mathbf{x})=-\tfrac{1}{2}\int d^4y[-ie^2D_{\rho\nu}^{(0)}(x-y)tr[\gamma^\rho G^{(0)}(x,y)\gamma^\nu G^{(0)}(y,x)]$$
$$-2\,tr(\{\delta m\delta^2(x-y)+i(1-Z_2^{-1})[G_v^{(0)}(x,y)]^{-1}\}G^{(0)}(y,x))]\,. \tag{5.11}$$

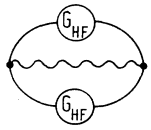

FIG. 2. The exchange energy graph in the HF approximation.

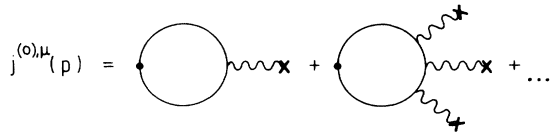

FIG. 3. The four-current density in lowest order of α.

Finally we write down the renormalized Hamiltonian computed from $\mathscr{L}_R$, Eq. (5.1),

$$\mathscr{H}_R=\frac{Z_2}{4}\{[\bar{\psi},(-i\boldsymbol{\gamma}\cdot\vec{\nabla}+m-\delta m+e\not{V}_{\text{ext}})\psi] +[\bar{\psi}(i\boldsymbol{\gamma}\cdot\overleftarrow{\nabla}+m-\delta m+e\not{V}_{\text{ext}}),\psi]\} +\frac{Z_1}{8}e([\bar{\psi},\not{A}\psi]+[\bar{\psi}\not{A},\psi]) +\frac{Z_3}{2}\left[(\nabla V^0_{\text{ext}})^2+\sum_k(\nabla V^k_{\text{ext}})^2\right] . \tag{5.12}$$

Note that the energy of the external field contains a term

$$-\frac{e^2}{2}\omega_1^{\text{reg}}(0)\left[(\nabla V^0_{\text{ext}})^2+\sum_k(\nabla V^k_{\text{ext}})^2\right] \tag{5.13}$$

which will compensate a divergence in the kinetic energy of the electrons as will be demonstrated in Sec. VI.

VI. THE GRADIENT EXPANSION

The main idea, which we use in order to make the transition to a density-functional representation, is the approximation of the full interacting propagators G_g as well as G_v by Green's functions of effective field theories, where the external potential and the interaction of the electrons via photons are represented in terms of an effective classical potential. As the ground state and the vacuum differ essentially, one can not expect to compute both G_g and G_v from one effective potential. So again the following discussion has to be carried through separately for the two cases.

The Lagrangian of an effective system,

$$\mathscr{L}_{\text{eff}}=\bar{\psi}(i\partial\!\!\!/-m-e\not{V}_{\text{eff}})\psi-\tfrac{1}{4}F^{\mu\nu}_{\text{eff}}F_{\text{eff},\mu\nu} , \tag{6.1}$$

as well as the corresponding field (Dirac) equation,

$$[-i\boldsymbol{\alpha}\cdot\nabla+\beta m+e\beta\not{V}_{\text{eff}}(\mathbf{x})]\Phi_n(\mathbf{x})=E_n\Phi_n(\mathbf{x}) , \tag{6.2}$$

and the Green's function,

$$G_s(x,y)=\Theta(x^0-y^0)\sum_{E_n>S}\Phi_n(\mathbf{x})\bar{\Phi}_n(\mathbf{y})e^{-iE_n(x^0-y^0)} -\Theta(y^0-x^0)\sum_{E_n\le S}\Phi_n(\mathbf{x})\bar{\Phi}_n(\mathbf{y})e^{-iE_n(x^0-y^0)} , \tag{6.3}$$

can be specified directly. The energy value S in Eq. (6.3) divides the one-particle spectrum of Eq. (6.2) into occupied electron states (or unoccupied positron states) with $E_n<S$ and unoccupied electron states with $E_n>S$. With respect to the ground state of the system, S equals the Fermi energy ε_F, for the vacuum state S is chosen to be $-m$.

It is obvious that the Green's function of the effective (local) theory cannot reproduce all properties of the full propagator. Nonetheless, we expect, in analogy to the nonrelativistic case, that the approximation suggested will yield a reasonable energy density functional.

In order to express the energy density as a functional of the charge density

$$\rho_s(\mathbf{x})=j_s^0(\mathbf{x}) ,$$

we need a representation of the electron propagator in terms of the charge density. This connection can be established by the gradient expansion technique.[25–27] Using the definition (6.3) of G_s and the Dirac-equation (6.2) one can write

$$\begin{aligned}G_s(x,y)&=\Theta(x^0-y^0)\Theta(\hat{H}_x-S)\sum_n\Phi_n(\mathbf{x})\bar{\Phi}_n(\mathbf{y})e^{-iE_n(x^0-y^0)}-\Theta(y^0-x^0)\Theta(S-\hat{H}_x)\sum_n\Phi_n(\mathbf{x})\bar{\Phi}_n(\mathbf{y})e^{-iE_n(x^0-y^0)}\\&=[\Theta(x^0-y^0)\Theta(\hat{H}_x-S)-\Theta(y^0-x^0)\Theta(S-\hat{H}_x)]e^{-i(x^0-y^0)\hat{H}_x}\sum_n\bar{\Phi}_n(\mathbf{x})\bar{\Phi}_n(\mathbf{y})\\&=[\Theta(x^0-y^0)-\Theta(S-\hat{H}_x)]e^{-i(x^0-y^0)\hat{H}_x}\sum_n\Phi_n(\mathbf{x})\bar{\Phi}_n(\mathbf{y}) .\end{aligned} \tag{6.4}$$

The index of $\hat{H}_x$ indicates that the Hamiltonian

$$\begin{aligned}\hat{H}_x&=-i\boldsymbol{\alpha}\cdot\nabla+\beta m+eV^0_{\text{eff}}(\mathbf{x})\\&=\hat{t}_x+\hat{v}_{\text{eff}}(\mathbf{x}) ,\end{aligned} \tag{6.5}$$

where the effective potential is assumed to be purely electrostatic (thus neglecting all magnetic field effects), acts on the coordinate $\mathbf{x}$. Introducing the effective local Fermi energy

$$\hat{E}_s(\mathbf{x})=S-\hat{v}_{\text{eff}}(\mathbf{x}) \tag{6.6}$$

and using the completeness of the solutions Φ_n of the Dirac equation (6.2), one finds

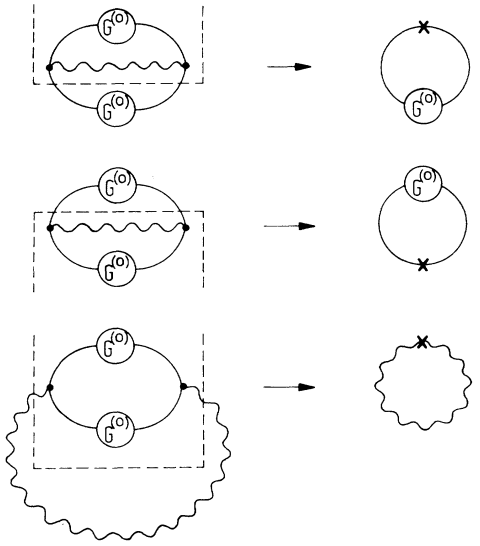

FIG. 4. Counterterms for the exchange graph.

$$G_s(x,y)=e^{i(x^0-y^0)S}\{\Theta(x^0-y^0)-\Theta[\hat{E}_s(\mathbf{x})-\hat{t}_x]\}$$

$$\times e^{i(x^0-y^0)[\hat{E}_s(\mathbf{x})-\hat{t}_x]}\delta^{(3)}(\mathbf{x}-\mathbf{y})\gamma^0 . \quad (6.7)$$

The Green's function of Eq. (6.7) can be represented in terms of Dirac plane waves, constituting a complete set of eigenfunctions of the kinetic energy operator $\hat{t}_x$,

$$\delta^{(3)}(\mathbf{x}-\mathbf{y})=\sum_{r=1}^{2}\int\frac{d^3p}{(2\pi)^3}e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}[u^r(p)\bar{u}^r(p)$$

$$-v^r(p)\bar{v}^r(p)] , \quad (6.8)$$

where $u^{1,2}(p),v^{1,2}(p)$ are the standard spinors (in the definition of Ref. 16).

The technical problem indicated in Eqs. (6.7) and (6.8) is the evaluation of the action of a function of two noncommutating operators (explicitly stressed by using the operator sign $\hat{}$) on eigenfunctions of one of the operators,

$$f(\hat{a}+\hat{b})\,|\,a\rangle=? \quad (6.9)$$

with

$$\hat{a}\,|\,a\rangle=a\,|\,a\rangle$$

and

$$[\hat{a},\hat{b}]\neq 0 .$$

The answer can be given (for details see Ref. 14) in the form of a gradient expansion

$$f(\hat{a}+\hat{b})\,|\,a\rangle=\sum_{n=0}^{\infty}f^{(n)}(a+\hat{b})\hat{O}_n\,|\,a\rangle . \quad (6.10)$$

$f^{(n)}$ is the nth derivative of the function f with respect to the complete argument and the operators $\hat{O}_n$ are determined by the multiple commutators of $\hat{a}$ an $\hat{b}$, as, e.g.,

$$[\hat{E}_s(\mathbf{x}),\hat{t}_x]=i\boldsymbol{\alpha}\cdot\nabla v_{\mathrm{eff}}(\mathbf{x}) ,$$

$$[[\hat{E}_s(\mathbf{x}),\hat{t}_x],\hat{t}_x]=-2[i\boldsymbol{\alpha}\cdot\nabla v_{\mathrm{eff}}(\mathbf{x})](\boldsymbol{\alpha}\cdot\nabla-\beta m)$$

$$-2[\nabla v_{\mathrm{eff}}(\mathbf{x})]\cdot\nabla-\Delta v_{\mathrm{eff}}(\mathbf{x}) .$$

Neglecting all contributions with derivatives of $v_{\mathrm{eff}}(\mathbf{x})$ beyond second order (and hence referring to a smooth potential), the result is a functional

$$G_s[E_s(\mathbf{x}),\partial_i E_s(\mathbf{x}),\partial_i\partial_j E_s(\mathbf{x})] . \quad (6.11)$$

We note that this approximation of G_s is not perturbative in the coupling constant, all orders of the nuclear charge $Z\alpha$ are included. From the functional (6.11) one readily obtains a four current

$$j_s^{\nu}(\mathbf{x})=g^{0\nu}\rho_s[E_s(\mathbf{x}),[\nabla E_s(\mathbf{x})]^2,\Delta E_s(\mathbf{x})] ,$$

which can be inverted order by order in the gradient expansion to yield

$$E_s=E_s[\rho_s,(\nabla\rho_s)^2,\Delta\rho_s]$$

and therefore the desired functionals

$$G_s[\rho_s,(\nabla\rho_s)^2,\Delta\rho_s]$$

and

$$\varepsilon_s[\rho_s,(\nabla\rho_s)^2,\Delta\rho_s] .$$

The details of the program outlined are discussed in Secs. VI A–VI E.

A. The electronic propagator in gradient expansion

Following the arguments starting from Eq. (6.7) one obtains, after some manipulations, an effective Green's function that separates into a "free" part and a "bound" part

$$G_s(x,y)=G_f(x,y)+G_{s,b}(x,y) . \quad (6.12)$$

The free part does not depend on S [note that $E_s(\mathbf{x})-S=-v_{\mathrm{eff}}(\mathbf{x})$ and $\partial_k E_s(\mathbf{x})=-\partial_k v_{\mathrm{eff}}(\mathbf{x})$] and is given to second order in the derivatives of $E_s(\mathbf{x})$ as

$$
\begin{aligned}
G_f^{[2]}(x,y)&=ie^{i(x^0-y^0)[E_s(\mathbf{x})-S]}\int\frac{d^4p}{(2\pi)^4}e^{-ip(x-y)}[1+K_1(p,\mathbf{x})+K_2(p,\mathbf{x})]\frac{(\not p+m)}{p^2-m^2+i\varepsilon}\ ,\\
K_1(p,\mathbf{x})&=i[\partial_j E_s(\mathbf{x})][\gamma^0\gamma^j(p^2-m^2)+4p^0p^j-2\gamma^0p^j(\not p-m)]\frac{1}{(p^2-m^2+i\varepsilon)^2}\ ,\\
K_2(p,\mathbf{x})&=\{[\partial_j\partial_k E_s(\mathbf{x})]K_{21}^{jk}(p,\mathbf{x})+[\partial_j E_s(\mathbf{x})][\partial_k E_s(\mathbf{x})]K_{22}^{jk}(p,\mathbf{x})\}\frac{1}{(p^2-m^2+i\varepsilon)^2}\ ,\\
K_{21}^{jk}(p,\mathbf{x})&=-2p^0g^{jk}+2p^j\gamma^0\gamma^k+8\frac{p^0p^jp^k}{p^2-m^2+i\varepsilon}+\gamma^0g^{jk}(\not p-m)-4\frac{\gamma^0p^jp^k}{p^2-m^2+i\varepsilon}(\not p-m)\ ,\\
K_{22}^{jk}(p,\mathbf{x})&=-g^{jk}+8\frac{(p^0)^2g^{jk}}{p^2-m^2+i\varepsilon}-12\frac{p^0p^j\gamma^0\gamma^k}{p^2-m^2+i\varepsilon}+8\frac{p^jp^k}{p^2-m^2+i\varepsilon}\\
&\quad-48\frac{(p^0)^2p^jp^k}{(p^2-m^2+i\varepsilon)^2}-4\frac{p^0\gamma^0g^{jk}}{p^2-m^2+i\varepsilon}(\not p-m)-4\frac{p^j\gamma^k}{p^2-m^2+i\varepsilon}(\not p-m)+24\frac{\gamma^0p^0p^jp^k}{(p^2-m^2+i\varepsilon)^2}(\not p-m)\ .
\end{aligned}
\tag{6.13}
$$

We denote the order of the gradient expansion by $[n]$ in contrast to (n) for the order of α. G_f can be viewed as the contribution of the Fermi sea. The lowest-order term of G_f in the gradient expansion $G_f^{[0]}$ differs from the standard free propagator only by a phase due to the presence of the potential.

The bound part represents the contribution of all discrete states with an energy smaller than ε_F. It has the form

$$
G_{s,b}^{[2]}(x,y)=e^{i(x^0-y^0)(E_s(\mathbf{x})-S)}\int\frac{d^4p}{(2\pi)^3}\frac{e^{-ip(x-y)}}{2E}\sum_{l=0}^{8}O^l(p,\mathbf{x})[c_l(\not p+m)-2E\gamma^0\bar{c}_l]
\tag{6.14}
$$

with

$$E=(\mathbf{p}^2+m^2)^{1/2}\ .$$

Explicit expressions for the factors $O^l(p,\mathbf{x})$, c_l, and $\bar{c}_l$ are given in the Appendix. Looking at the lowest-order contributions to $G_{s,b}$ (in the gradient expansion),

$$
G_{s,b}^{[0]}(x,y)=-e^{i(x^0-y^0)[E_s(\mathbf{x})-S]}\int\frac{d^4p}{(2\pi)^3}\frac{e^{-ip(x-y)}}{2E}\delta(p^0-E)\Theta[E_s(\mathbf{x})-E](\not p+m)\ ,
\tag{6.15}
$$

we note directly that it describes the density of free electrons filling all levels up to $E_s(\mathbf{x})$, again with a phase modulation due to the effective potential.

B. The four-current density in gradient expansion

Using dimensional regularization and Eqs. (3.1), (6.13), and (6.14) as a starting point we can calculate the four current as

$$
\begin{aligned}
j^{\nu}_{\mathrm{reg},s}(\mathbf{x})&=-\frac{e}{12\pi^2}g^{0\nu}\Gamma\left[2-\frac{D}{2}\right](m^2)^{(D/2-2)}\Delta E_s(\mathbf{x})+\frac{e}{3\pi^2}g^{0\nu}p_s(\mathbf{x})^3\\
&\quad+\frac{e}{12\pi^2}g^{0\nu}\left\{\Delta E_s(\mathbf{x})\left[2\,\mathrm{arcsinh}\left[\frac{p_s(\mathbf{x})}{m}\right]+\frac{E_s(\mathbf{x})}{p_s(\mathbf{x})}\right]+[\nabla E_s(\mathbf{x})]^2\left[\frac{3}{2p_s(\mathbf{x})}-\frac{E_s(\mathbf{x})^2}{2p_s(\mathbf{x})^3}\right]\right\}
\end{aligned}
\tag{6.16}
$$

with

$$
\begin{aligned}
p_s(\mathbf{x})&=[E_s(\mathbf{x})^2-m^2]^{1/2}\ \text{ where }\ E_s(x)^2\geq m^2\\
&=0\ \text{ elsewhere}\ .
\end{aligned}
$$

As expected the space components of $j^{\nu}_{\mathrm{reg},s}$ vanish for the specific choice (6.5). We recognize the divergent constant (as D is the dimension of our Minkowski space) times the Laplacian of the potential. Following the renormalization procedure of Sec. III for the special case of an effective Lagrangian, which means that the four current is given by the series of Fig. 3 and thus $j^{\nu}_{R,s}$ has to be computed via Eq. (5.8), we extract the renormalized four current [note that $\Delta E_s(\mathbf{x})=-e\Delta V(\mathbf{x})$]

$$
j^{\nu}_{R,s}(\mathbf{x})=\frac{e}{12\pi^2}g^{0\nu}\left\{4p_s(\mathbf{x})^3+\Delta E_s(\mathbf{x})\left[2\,\mathrm{arcsinh}\left[\frac{p_s(\mathbf{x})}{m}\right]+\frac{E_s(\mathbf{x})}{p_s(\mathbf{x})}\right]+[\nabla E_s(\mathbf{x})]^2\left[\frac{3}{2p_s(\mathbf{x})}-\frac{E_s(\mathbf{x})^2}{2p_s(\mathbf{x})^3}\right]\right\}\ .
\tag{6.17}
$$

C. The energy densities in gradient expansion

With the effective approximation to the Green's function given in (6.13) and (6.14) we are able to calculate the dependence of the energy densities on the local Fermi energy $E_s(\mathbf{x})$ and its derivatives. For the kinetic energy density we obtain

$$\begin{aligned}\varepsilon_{\mathrm{kin},s}(\mathbf{x})&=\lim_{y\to x}{}_s\,\mathrm{tr}[(i\gamma\cdot\nabla_x-m)G_s(x,y)]\\&=\frac{m^D}{4\pi^2}\Gamma\left[2-\frac{D}{2}\right]\frac{2}{D}\left[\frac{3-D}{2-D}\right]+\frac{1}{24\pi^2}\Gamma\left[2-\frac{D}{2}\right][\nabla E_s(\mathbf{x})]^2\\&\quad+\frac{1}{4\pi^2}\left\{p_s(\mathbf{x})E_s(\mathbf{x})^3-\frac{m^2}{2}\left[p_s(\mathbf{x})E_s(\mathbf{x})+m^2\,\mathrm{arcsinh}\left[\frac{p_s(\mathbf{x})}{m}\right]\right]\right\}\\&\quad+\frac{1}{12\pi^2}\left\{[\nabla E_s(\mathbf{x})]^2\left[-\frac{E_s(\mathbf{x})^3}{2p_s(\mathbf{x})^3}+\frac{E_s(\mathbf{x})}{p_s(\mathbf{x})}-\mathrm{arcsinh}\left[\frac{p_s(\mathbf{x})}{m}\right]\right]+\Delta E_s(\mathbf{x})\left[\frac{E_s(\mathbf{x})^2}{p_s(\mathbf{x})}+p_s(\mathbf{x})\right]\right\}.\end{aligned}\tag{6.18}$$

We discover exactly the predicted divergent part proportional to

$$e^2\frac{\omega_1^{\mathrm{reg}}(0)}{2}[\nabla V(\mathbf{x})]^2$$

which compensates the divergence in the external field energy. The second divergent term

$$\frac{m^D}{4\pi^2}\Gamma\left[2-\frac{D}{2}\right]\frac{2}{D}\left[\frac{3-D}{2-D}\right]$$

is due to the Fermi sea. This contribution which is independent of $E_s(\mathbf{x})$ cancels when the vacuum energy is subtracted from the ground-state energy.

The renormalized kinetic energy density thus reads

$$\begin{aligned}\varepsilon_{\mathrm{kin},R,s}(\mathbf{x})&=\frac{1}{4\pi^2}\left\{p_s(\mathbf{x})E_s(\mathbf{x})^3-\frac{m^2}{2}\left[p_s(\mathbf{x})E_s(\mathbf{x})+m^2\mathrm{arcsinh}\left[\frac{p_s(\mathbf{x})}{m}\right]\right]\right\}\\&\quad+\frac{1}{12\pi^2}\left\{[\nabla E_s(\mathbf{x})]^2\left[-\frac{E_s(\mathbf{x})^3}{2p_s(\mathbf{x})^3}+\frac{E_s(\mathbf{x})}{p_s(\mathbf{x})}-\mathrm{arcsinh}\left[\frac{p_s(\mathbf{x})}{m}\right]\right]+\Delta E_s(\mathbf{x})\left[\frac{E_s(\mathbf{x})^2}{p_s(\mathbf{x})}+p_s(\mathbf{x})\right]\right\}.\end{aligned}\tag{6.19}$$

The direct and external potential-energy densities are given in terms of the charge densities as

$$\varepsilon_{\mathrm{ext},R,s}(\mathbf{x})=V(\mathbf{x})_{\mathrm{ext}}j^0_{R,s}(\mathbf{x})\,,\tag{6.20}$$

$$\begin{aligned}\varepsilon_{\mathrm{dir},R,s}(\mathbf{x})&=-\frac{i}{2}\int d^4y D^{(0)}_{00}(x-y)j^0_{R,s}(\mathbf{x})j^0_{R,s}(\mathbf{y})\\&=\frac{1}{8\pi}\int d^3y\frac{1}{|\mathbf{x}-\mathbf{y}|}j^0_{R,s}(\mathbf{x})j^0_{R,s}(\mathbf{y})\,.\end{aligned}\tag{6.21}$$

The most involved energy density term is the exchange contribution. We shall restrict the consideration in analogy to the nonrelativistic TFDW model to the local density limit, neglecting gradient corrections. It is obvious that we have to invoke renormalization in the same fashion as in the case of the exchange energy $\varepsilon_{\mathrm{ex}}^{(0)}$, Eq. (5.9), in standard QED. From Eq. (5.11) we derive

$$\begin{aligned}\varepsilon_{\mathrm{ex},R,s}(\mathbf{x})=-\tfrac{1}{2}\int d^4y[&-ie^2D^{(0)}_{\rho\nu}(x-y)\mathrm{tr}[\gamma^\rho G^{[0]}_f(x,y)\gamma^\nu G^{[0]}_f(y,x)]\\&-2\,\mathrm{tr}(\{\delta m\,\delta^{(4)}(x-y)+i(1-Z^{-1})[G^{[0]}_v(x,y)]^{-1}\}G^{[0]}_f(y,x))]\\-\int d^4y\,\mathrm{tr}[\Sigma^{[0]}_{f,R}(x,y)G^{[0]}_{s,b}(y,x)]&+i\frac{e^2}{2}\int d^4y\,D^{(0)}_{\rho\nu}(x-y)\mathrm{tr}[\gamma^\rho G^{[0]}_{s,b}(x,y)\gamma^\nu G^{[0]}_{s,b}(y,x)]\,,\end{aligned}\tag{6.22}$$

where separation of G_s into G_f and $G_{s,b}$, Eq. (6.12), has been used. $\Sigma^{[0]}_{f,R}(x,y)$ is defined as

$$\Sigma^{[0]}_{f,R}(x,y)=-ie^2D^{(0)}_{\rho\nu}(x-y)\gamma^\rho G^{[0]}_f(x,y)\gamma^\nu-\delta m\,\delta^{(4)}(x-y)-i(1-Z_2^{-1})[G^{[0]}_v(x,y)]^{-1}\,.\tag{6.23}$$

In order to use Eq. (6.22) we need both $[G_v^{[0]}(x,y)]^{-1}$ and $\Sigma_{f,k}^{[0]}(x,y)$. $[G_v(x,y)]^{-1}$ can readily be given in momentum space

$$[G_v(p,k)]^{-1}=(2\pi)^4\delta^{(4)}(p-k)(-i)(\not p-m)+ie\not V_{\rm eff}(p-k)\ . \tag{6.24}$$

Fourier transformation yields

$$\begin{aligned}[G_v(x,y)]^{-1}&=-i\int\frac{d^4k}{(2\pi)^4}e^{-ik(x-y)}[\not k-m-e\not V_{\rm eff}(\mathbf{x})]\\&=-ie^{-ieV^v_{\rm eff}(\mathbf{x})(x_v-y_v)}\int\frac{d^4p}{(2\pi)^4}e^{-ip(x-y)}(\not p-m)\ ,\end{aligned} \tag{6.25}$$

reducing to

$$[G_v(x,y)]^{-1}=-ie^{-iv_{\rm eff}(\mathbf{x})(x_0-y_0)}\int\frac{d^4p}{(2\pi)^4}e^{-ip(x-y)}(\not p-m)$$

in our case of a scalar potential. As no gradient terms occur, $[G_v(x,y)]^{-1}$ equals $[G_v^{[0]}(x,y)]^{-1}$,

$$[G_v(x,y)]^{-1}=[G_v^{[0]}(x,y)]^{-1}\ . \tag{6.26}$$

$\Sigma_{f,k}^{[0]}(x,y)$ is, up to a phase factor, identical with the standard self-energy expression. The explicit form, Eq. (6.23), leads to the lowest-order renormalized self-energy of QED without external potential contributions modified by the phase factor

$$\Sigma_{f,k}^{[0]}(x,y)=e^{-iv_{\rm eff}(\mathbf{x})(x_0-y_0)}\int\frac{d^4p}{(2\pi)^4}e^{-ip(x-y)}\Sigma_{f,R}^{(0)}(p)\ , \tag{6.27}$$

$$\Sigma_{f,R}^{(0)}(p)=\frac{e^2}{8\pi^2}\left\{2m\left[\frac{5}{8}+\frac{m^2-p^2}{p^2}\ln\left|1-\frac{p^2}{m^2}\right|\right]+(\not p-m)\left[\tfrac{9}{4}+\ln\left|\frac{\mu^2}{m^2}\right|\right]-\frac{\not p}{2}\left[\frac{3}{2}+\frac{m^2}{p^2}+\frac{m^4-p^4}{p^4}\ln\left|1-\frac{p^2}{m^2}\right|\right]\right\}$$

with

$$\Sigma_{f,R}^{(0)}(p^2=m^2)=\frac{e^2}{8\pi^2}(\not p-m)\left[1-\ln\left|\frac{\mu^2}{m^2}\right|\right]\ .$$

The first term of Eq. (6.22), the Fermi sea contribution, cancels when the vacuum energy is subtracted from the ground-state energy. Considering

$$\begin{aligned}G_{s,b}^{[0]}(y,x)&=-e^{iv_{\rm eff}(\mathbf{x})(x_0-y_0)}\int\frac{d^4p}{(2\pi)^3}e^{ip(x-y)}\frac{\delta(p^0-E)}{2E}(\not p+m)\Theta[E_s(\mathbf{x})-E]\\&=-e^{iv_{\rm eff}(\mathbf{x})(x_0-y_0)}\int\frac{d^4p}{(2\pi)^3}e^{ip(x-y)}\delta(p^2-m^2)\Theta(p^0)(\not p+m)\Theta[E_s(\mathbf{x})-E]\ ,\end{aligned} \tag{6.28}$$

one shows directly that the self-energy contribution to $\varepsilon_{{\rm ex},R,s}(\mathbf{x})$ vanishes:

$$\begin{aligned}\int d^4y\,{\rm tr}[\Sigma_{f,k}^{[0]}(x,y)G_{s,b}^{[0]}(y,x)]&=-\frac{e^2}{8\pi^2}\int\frac{d^4p}{(2\pi)^3}\delta(p^2-m^2)\Theta(p^0)\Theta[E_s(\mathbf{x})-E](p^2-m^2)\left[1-\ln\left|\frac{\mu^2}{m^2}\right|\right]\\&=0\ .\end{aligned}$$

The remaining part can be computed with the aid of Eq. (6.15),

$$\varepsilon_{{\rm ex},R,s}(\mathbf{x})=\frac{e^2}{32\pi^4}\left\{2m^2p_s(\mathbf{x})^2+E_s(\mathbf{x})^2p_s(\mathbf{x})^2-6m^2p_s(\mathbf{x})E_s(\mathbf{x})\,{\rm arcsinh}\left[\frac{p_s(\mathbf{x})}{m}\right]+3m^4\left[{\rm arcsinh}\left[\frac{p_s(\mathbf{x})}{m}\right]\right]^2\right\}\ . \tag{6.29}$$

This expression represents the fully "retarded" exchange energy density: It has been derived with the time-dependent (free) photon propagator as a kernel rather than the static Coulomb interaction. It is identical with the result obtained by Jancovici[13] who used the Coulomb gauge rather than the Lorentz gauge employed here.

D. The relativistic TFDW energy density functional

The energy densities given in Sec. VI C are sufficient to establish the relativistic analogue of the nonrelativistic TFDW model. They are, however, not in the final form desired. It remains to invert the functional $j_{R,s}^0[E_s(\mathbf{x})]$, Eq. (6.17), in or-

der to exhibit the explicit dependence of the energy densities on the charge density itself.

The first step (writing ρ_s instead of $j^0_{R,s}$ for brevity) is simply accomplished order by order in the gradient terms. Separating ρ_s as

$$\rho_s(\mathbf{x})=\rho^{[0]}(\mathbf{x})+\rho^{[2]}(\mathbf{x}) ,$$

where the index indicates the order of the gradient terms, we have directly

$$\rho^{[0]}(\mathbf{x})=\frac{e}{3\pi^2}p_s(\mathbf{x})^3 ,$$

$$\rho^{[2]}(\mathbf{x})=\frac{e}{\pi^2}\left\{\Delta E_s(\mathbf{x})\left[\tfrac{1}{6}\operatorname{arcsinh}\left[\frac{p_s(\mathbf{x})}{m}\right]+\frac{E_s(\mathbf{x})}{12p_s(\mathbf{x})}\right]+[\nabla E_s(\mathbf{x})]^2\left[\frac{1}{8p_s(\mathbf{x})}-\frac{E_s(\mathbf{x})^2}{24p_s(\mathbf{x})^3}\right]\right\}, \tag{6.30}$$

as well as

$$p_s(\mathbf{x})=\left[\frac{3\pi^2}{e}[\rho_s(\mathbf{x})-\rho^{[2]}(\mathbf{x})]\right]^{1/3} , \tag{6.31a}$$

$$E_s(\mathbf{x})=\left[m^2+\left[\frac{3\pi^2}{e}[\rho_s(\mathbf{x})-\rho^{[2]}(\mathbf{x})]\right]^{2/3}\right]^{1/2} . \tag{6.31b}$$

Taking account the fact that $\rho^{[2]}(\mathbf{x})$ itself is of second order, one obtains

$$[\nabla E_s(\mathbf{x})]^2=\frac{\pi^4}{e^2}\left[m^2+\left[\frac{3\pi^2}{e}\rho_s(\mathbf{x})\right]^{2/3}\right]^{-1}\left[\frac{3\pi^2}{e}\rho_s(\mathbf{x})\right]^{-2/3}[\nabla\rho_s(\mathbf{x})]^2 , \tag{6.32a}$$

$$\begin{aligned}\Delta E_s(\mathbf{x})=&\frac{\pi^2}{e}\left[m^2+\left[\frac{3\pi^2}{e}\rho_s(\mathbf{x})\right]^{2/3}\right]^{-1/2}\left[\frac{3\pi^2}{e}\rho_s(\mathbf{x})\right]^{-1/3}\Delta\rho_s(\mathbf{x})\\&-\frac{\pi^4}{e^2}\left[m^2+\left[\frac{3\pi^2}{e}\rho_s(\mathbf{x})\right]^{2/3}\right]^{-1/2}\left[\frac{3\pi^2}{e}\rho_s(\mathbf{x})\right]^{-4/3}[\nabla\rho_s(\mathbf{x})]^2\\&-\frac{\pi^4}{e^2}\left[m^2+\left[\frac{3\pi^2}{e}\rho_s(\mathbf{x})\right]^{2/3}\right]^{-3/2}\left[\frac{3\pi^2}{e}\rho_s(\mathbf{x})\right]^{-2/3}[\nabla\rho_s(\mathbf{x})]^2 .\end{aligned} \tag{6.32b}$$

Reinsertion of Eqs. (6.32a) and (6.32b) into a consistent expansion of (6.31a) and (6.31b) to second order in gradient terms thus leads to the statements

$$E_s(\mathbf{x})=\beta_s(\mathbf{x})-\frac{\gamma_s(\mathbf{x})}{\alpha_s(\mathbf{x})\beta_s(\mathbf{x})} , \tag{6.33a}$$

$$p_s(\mathbf{x})=\alpha_s(\mathbf{x})-\frac{\gamma_s(\mathbf{x})}{\alpha_s^2(\mathbf{x})} , \tag{6.33b}$$

where the abbreviations

$$\alpha_s(\mathbf{x})=\left[\frac{3\pi^2}{e}\rho_s(\mathbf{x})\right]^{1/3} , \tag{6.33c}$$

$$\beta_s(\mathbf{x})=[m^2+\alpha_s^2(\mathbf{x})]^{1/2} , \tag{6.33d}$$

$$\begin{aligned}\gamma_s(\mathbf{x})=&\frac{\pi^2}{e}\Delta\rho_s(\mathbf{x})\left[\frac{1}{6\alpha_s(\mathbf{x})\beta_s(\mathbf{x})}\operatorname{arcsinh}\left[\frac{\alpha_s(\mathbf{x})}{m}\right]+\frac{1}{12\alpha_s^2(\mathbf{x})}\right]\\&+\frac{\pi^4}{e^2}[\nabla\rho_s(\mathbf{x})]^2\left[-\frac{\alpha_s^2(\mathbf{x})+\beta_s^2(\mathbf{x})}{6\alpha_s^4(\mathbf{x})\beta_s^3(\mathbf{x})}\operatorname{arcsinh}\left[\frac{\alpha_s(\mathbf{x})}{m}\right]-\frac{1}{8\alpha_s^5(\mathbf{x})}+\frac{1}{24\alpha_s^3(\mathbf{x})\beta_s^2(\mathbf{x})}\right]\end{aligned} \tag{6.33e}$$

have been used. These results again apply for both the ground state and the vacuum state. Insertion of the functionals $E_s[\rho_s(\mathbf{x})]$ and $p_s[\rho_s(\mathbf{x})]$ into the expressions for the energy functionals, Eqs. (6.19) and (6.29), yields the final form of the energy density

$$\varepsilon_{R,s}(\mathbf{x})=\frac{1}{8\pi^2}\left[\alpha_s(\mathbf{x})\beta_s^3(\mathbf{x})+\alpha_s^3(\mathbf{x})\beta_s(\mathbf{x})-m^4\operatorname{arcsinh}\left[\frac{\alpha_s(\mathbf{x})}{m}\right]\right]$$
$$+\frac{\pi^2}{24e^2}[\nabla\rho_s(\mathbf{x})]^2\left[\frac{1}{\alpha_s^3(\mathbf{x})\beta_s(\mathbf{x})}+\frac{2}{\alpha_s^2(\mathbf{x})\beta_s^2(\mathbf{x})}\operatorname{arcsinh}\left[\frac{\alpha_s(\mathbf{x})}{m}\right]\right]+V(\mathbf{x})_{\text{ext}}\rho_s(\mathbf{x})+\frac{1}{8\pi}\int d^3y\frac{\rho_s(\mathbf{x})\rho_s(y)}{|\mathbf{x}-\mathbf{y}|}$$
$$+\frac{e^2}{32\pi^4}\left\{2m^2\alpha_s^2(\mathbf{x})+\alpha_s^2(\mathbf{x})\beta_s^2(\mathbf{x})-6m^2\alpha_s(\mathbf{x})\beta_s(\mathbf{x})\operatorname{arcsinh}\left[\frac{\alpha_s(\mathbf{x})}{m}\right]+3m^4\left[\operatorname{arcsinh}\left[\frac{\alpha_s(\mathbf{x})}{m}\right]\right]^2\right\}, \tag{6.34}$$

once again valid for the ground state and the vacuum state.

In the nonrelativistic limit the functional goes over into the standard TFDW functional given in the literature.

E. The calculation of the electronic binding energy

The total binding energy is defined as a difference of two expressions, Eq. (2.5), such that all infinite Fermi sea contributions cancel. After renormalization the remaining parts are finite and satisfy a minimum principle:

$$\frac{\delta}{\delta\rho_g}(\langle g\,|\,H_R\,|\,g\rangle-E_{\text{FS}})=0\,, \tag{6.35a}$$

$$\frac{\delta}{\delta\rho_v}(\langle v\,|\,H_R\,|\,v\rangle-E_{\text{FS}})=0 \tag{6.35b}$$

(where E_{FS} represents the Fermi sea contributions).

This suggests a straightforward variational procedure for the determination of the binding energy: Minimize both E_g and E_v (under suitable constraints for total charge, etc.) and subtract them afterwards.

The existence of vacuum contributions to the energy (and the necessity to evaluate them) thus does not lead to a definite complication of the density-functional scheme in comparison to the nonrelativistic case. They constitute, however, an integral part of a consistent relativistic density-functional theory not fully covered by a theory on the basis of the Dirac equation.

VII. FINAL REMARKS

The relativistic density-functional formalism developed above on the basis of a field theoretical background is the equivalent of the TFDW formalism in nonrelativistic physics. In contrast to previous attempts on the basis of the Dirac equation[14] it is free of conceptual problems encountered in the former case. It can be considered as a sequel to first attempts to recognize and to deal with the renormalization problem and the vacuum contribution.[15] The not insubstantial, numerical work involved in carrying through the scheme indicated in Sec. VI E for atomic systems, together with an attempt to isolate dominant terms in the rather lengthy expressions, will be published separately.

The TFDW model can be viewed as an approximation to the Hartree-Fock limit, in particular the "retarded" exchange energy density ought to be relevant for a Slater-like relativistic Kohn-Sham scheme. We have not addressed the question of the correlation energy, although this is, at least in principle and in low order of α, possible. In addition, the structure of a fully gauge-invariant density functional, if an effective four potential rather than its scalar part is used, and the problem of gradient corrections to the exchange-correlation energy density remain open questions and will have to be tackled in the future.

ACKNOWLEDGMENTS

We thank P. Malzacher for helpful discussions. One of the authors (E.E.) gratefully acknowledges support by the Studienstiftung des deutschen Volkes.

APPENDIX

In this Appendix we collect explicit expressions for the abbreviations used in Sec. VI A

$$O^0=1\,,$$
$$O^1=i\boldsymbol{\alpha}\cdot\nabla E_s(\mathbf{x})\,,$$
$$O^2=-2i\mathbf{p}\cdot\nabla E_s(\mathbf{x})\,,$$
$$O^3=-\Delta E_s(\mathbf{x})\,,$$
$$O^4=-[\nabla E_s(\mathbf{x})]^2\,,$$
$$O^5=2\{(\mathbf{p}\cdot\nabla)[\boldsymbol{\alpha}\cdot\nabla E_s(\mathbf{x})]\}\,,$$
$$O^6=-4\{(\mathbf{p}\cdot\nabla)[\mathbf{p}\cdot\nabla E_s(\mathbf{x})]\}\,,$$
$$O^7=\{[\boldsymbol{\alpha}\cdot\nabla E_s(\mathbf{x})][\mathbf{p}\cdot\nabla E_s(\mathbf{x})]\}\,,$$
$$O^8=-2[\mathbf{p}\cdot\nabla E_s(\mathbf{x})]^2\,.$$

Defining

$$d=-\frac{d}{dE}\,,$$

one has for c_l and $\bar{c}_l$:

$$c_0=-\Theta(E_s(\mathbf{x})-E)\delta(p^0-E)\,,$$
$$c_1=-\left[\frac{1}{2E^2}+\frac{1}{2E}d\right]c_0\,,$$
$$c_2=c_3=-\left[\frac{1}{4E^2}d+\frac{1}{4E}d^2\right]c_0\,,$$

$$c_4=\left[\frac{1}{8E^4}+\frac{1}{8E^3}d-\frac{1}{8E^2}d^2-\frac{1}{6E}d^3\right]c_0\ ,$$

$$c_5=\left[\frac{3}{8E^4}+\frac{3}{8E^3}d+\frac{1}{8E^2}d^2\right]c_0\ ,$$

$$c_6=\left[\frac{1}{8E_4}d+\frac{1}{8E^3}d^2+\frac{1}{24E^2}d^3\right]c_0\ ,$$

$$c_7=\left[\frac{3}{4E^4}d+\frac{3}{4E^3}d^2+\frac{1}{4E^2}d^3\right]c_0\ ,$$

$$c_8=\left[\frac{5}{16E_6}+\frac{5}{16E^5}d+\frac{5}{16E^4}d^2+\frac{5}{24E^3}d^3+\frac{1}{16E^2}d^4\right]c_0\ ,$$

$$\bar{c}_0=0\ ,$$

$$\bar{c}_1=\left[-\frac{1}{4E^2}\right]c_0\ ,$$

$$\bar{c}_2=\bar{c}_3=\left[\frac{1}{8E^3}\right]c_0\ ,$$

$$\bar{c}_4=\left[\frac{1}{16E^4}+\frac{1}{8E^3}d\right]c_0\ ,$$

$$\bar{c}_5=\left[\frac{3}{16E^4}+\frac{1}{8E^3}d\right]c_0\ ,$$

$$\bar{c}_6=\left[-\frac{1}{8E^5}-\frac{1}{16E^4}d\right]c_0\ ,$$

$$\bar{c}_7=\left[-\frac{3}{8E^5}+\frac{1}{8E^3}d^2\right]c_0\ ,$$

$$\bar{c}_s=\left[\frac{5}{32E^6}-\frac{1}{16E^5}d-\frac{1}{16E^4}d^2\right]c_0\ .$$

[1] *Density Functional Methods in Physics,* Vol. 123 of *NATO ASI Series B,* edited by R. M. Dreizler and J. da Providencia (Plenum, New York, 1985).

[2] *Local Density Approximations in Quantum Chemistry and Solid State Physics,* edited by J. P. Dahl and J. Avery (Plenum, New York, 1984).

[3] *Density Functional Theory,* Vol. 187 of *Lecture Notes in Physics,* edited by J. Keller and J. L. Gázquez (Springer, Berlin, 1987).

[4] *Theory of the Inhomogeneous Electron Gas,* edited by S. Lundqvist and N. H. March (Plenum, New York, 1983).

[5] A. K. Rajagopal and J. Callaway, Phys. Rev. B **7**, 1912 (1973).

[6] A. K. Rajagopal, J. Phys. C **11**, 943 (1978).

[7] A. H. MacDonald and S. H. Vosko, J. Phys. C **12**, 2977 (1979).

[8] P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964).

[9] D. E. Ellis, J. Phys. B **10**, 1 (1977).

[10] R. M. Dreizler and E. K. U. Gross, in *Quantum Electrodynamics of Strong Fields,* Vol. 80 of *NATO ASI Series B* (Plenum, New York, 1983).

[11] M. V. Ramana and A. K. Rajagopal, Adv. Chem. Phys. **54**, 231 (1983).

[12] E. E. Salpeter, Astrophys. J. **134**, 669 (1961).

[13] B. Jancovici, Nuovo Cimento **25**, 428 (1962).

[14] E. K. U. Gross and R. M. Dreizler, Ref. 1, pp. 81—140.

[15] P. Malzacher and R. M. Dreizler, Z. Phys. D **2**, 37 (1986).

[16] C. Itzykson and J. B. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, 1980).

[17] G. Källen, *Quantum Electrodynamics* (Springer, Berlin, 1972).

[18] J. D. Bjorken and S. D. Drell, *Relativistic Quantum Fields* (McGraw-Hill, New York, 1965), Chap. 15.5.

[19] W. Greiner, B. Müller, and J. Rafelski, *Quantum Electrodynamics of Strong Fields* (Springer, Berlin, 1985).

[20] A. L. Fetter and J. D. Walecka, *Quantum Theory of Many Particle Systems* (McGraw-Hill, New York, 1971).

[21] P. G. Reinhard, W. Greiner and H. Arenhövel, Nucl. Phys. **A166**, 173 (1971).

[22] G. t'Hooft and M. Veltman, Nucl. Phys. **B44**, 189 (1972).

[23] See Ref. 16, Chap. 8—2.

[24] S. A. Chin, Ann. Phys. (N.Y.) **108**, 301 (1977).

[25] E. Wigner, Phys. Rev. **40**, 749 (1932).

[26] J. G. Kirkwood, Phys. Rev. **44**, 31 (1933).

[27] D. A. Kirznits, *Field Theoretical Methods in Many Body Systems* (Pergamon, New York, 1967).