Extension of the relativistic Thomas-Fermi-Dirac-Weizsäcker model to arbitrary external fields

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We present an extension of the relativistic Thomas-Fermi-Dirac-Weizsäcker model to systems in arbitrary time-independent external four-potentials. We use a new gradient-expansion technique for the derivation of the ground-state energy and the ground-state four-current of relativistic fermions in the presence of electric as well as magnetic fields as functionals of the external four-potential. The ground-state energy functional of the four-current resulting from standard inversion of the semiclassical form is manifestly gauge invariant.

I. INTRODUCTION

Recently some interest has been focused on the density-functional theory of systems in arbitrary static magnetic fields.[1,2] We present in this contribution a generalization of the well-known Thomas-Fermi-Dirac-Weizsäcker (TFDW) model to such systems. As questions of gauge invariance arise (compare the comments on gauge invariance in Refs.1–5) in this connection, we first offer a comment on the uniqueness and the variational properties of the ground-state energy functional in the presence of external magnetic fields. In order to derive an explicit functional in a manifestly gauge-invariant fashion, we extend the previous consideration[6] of a relativistic TFDW model on the basis of a field-theoretical approach. The construction of the ground-state energy functional turns out to be more involved compared to the case of a system with a pure electrostatic external potential. For this reason it is more advantageous to generate the gradient expansion[7] envisaged with the aid of an approach based on Green's-function techniques.[5]

II. EXISTENCE THEOREM

In the discussion of existence theorems[8] for (nonrelativistic) systems in pure electrostatic potentials one has the statement that the ground-state density determines the corresponding potential only up to an additive constant and hence the ground state only up to a global phase factor. In a general situation, where a full four-potential is present, there exists only a unique relation between the ground-state four-current and a whole class of ground states which differ by phase factors due to gauge transformations.[3,4]

As a general gauge transformation in a static situation,

$$\Lambda(x)=cx^0+\lambda(\mathbf{x}) \quad \text{with } c=\text{const}, \quad \Delta\lambda(\mathbf{x})=0 \ ,$$

induces the transformation

$$\Psi'(x_1,\ldots,x_N) = \exp\left[-iNcx^0-i\sum_{n=1}^{N}\lambda(x_n)\right]\Psi(x_1,\ldots,x_N) \qquad (1)$$

of a many-particle wave function, one recognizes that expectation values are in general no longer gauge independent. Only those expectation values containing differentiation operators in the gauge-invariant form $i\nabla-\mathbf{V}(\mathbf{x})$ are uniquely determined by the physical four-current. A possibility for establishing a unique relation for all expectation values is the use of the paramagnetic current,[1,2] which is explicitly gauge dependent.

However, it seems to be natural to formulate the existence theorem of the general case[3,4] in terms of real physical quantities. To review very briefly the basic features let us assume a Hamiltonian of the form

$$H=H_{\text{internal}}+\int d^3x\, V^{\nu}_{\text{ext}}(\mathbf{x})j_{\nu}(\mathbf{x}) \ ,$$

where H_{internal} denotes the sum of the kinetic energy operator and the electron-electron interaction Hamiltonian of the electronic system (which might be relativistic) and V^{ν}_{ext} a classical external four-potential. The uniqueness of the relation between the class of ground states $\{|\Psi\rangle\}$ that contains all states that only differ by the phase shown in Eq. (1), the class of corresponding potentials $\{V^{\nu}_{\text{ext}}\}$, and the four-current can be demonstrated in the usual way. Assuming, e.g., two four-potentials V^{ν}_{ext} and V'^{ν}_{ext} that differ by more than a gauge transformation and denoting by $|\Psi\rangle$ and $|\Psi'\rangle$ arbitrary states of the corresponding ground-state classes which lead to the same four-current density j_{ν}, one obtains from the Ritz variational principle the inequality

$$E=\langle\Psi|H|\Psi\rangle<\langle\Psi'|H|\Psi'\rangle = E'+\int d^3x\, j_{\nu}(\mathbf{x})[V^{\nu}_{\text{ext}}(\mathbf{x})-V'^{\nu}_{\text{ext}}(\mathbf{x})] \ , \qquad (2)$$

for the ground-state energies E and E' of the two potentials. The ground-state energy is a gauge-invariant expectation value. If V^{μ}_{ext} and V'^{ν}_{ext} would differ only by a gauge transformation, the second term in the inequality (2) would vanish, due to current conservation. An analogous inequality can be derived by starting with E', and addition of both inequalities leads to the familiar contradiction

$$E+E'<E+E' \ .$$

The four-current density determines the class of potentials and therefore the class of ground states uniquely. Consequently, all gauge-invariant expectation values are uniquely given as functionals of the four-current:

$$O[j_\nu]=\langle\Psi[j_\nu]|O|\Psi[j_\nu]\rangle=\langle\Psi'[j_\nu]|O'|\Psi'[j_\nu]\rangle \ .$$

One now defines the functional

$$F[j_\nu]\equiv\langle\Psi[j_\nu]|H_{\text{internal}}|\Psi[j_\nu]\rangle \ ,$$

via an arbitrary representative state of the class of ground states corresponding to a given four-current j_ν. It is then straightforward to set up a minimum principle for the gauge-invariant functional

$$E[j'_\nu]=F[j'_\nu]+\int d^3x\, j'_\nu(\mathbf{x})V^\nu_{\text{ext}}(\mathbf{x}) \ , \tag{3}$$

by using the minimum principle for the class of ground states of H. The actual ground-state four-current j_ν corresponding to the four-potential V^ν_{ext} minimizes the functional (3),

$$E[j'_\nu]\geq E[j_\nu] \ . \tag{4}$$

Thus one finds the ground-state four-current by variation of $E[j_\nu]$,

$$\frac{\delta}{\delta j_\mu}E[j_\nu]=0 \ , \tag{5}$$

under the condition of charge and current conservation,

$$\int d^3x\, j^0(\mathbf{x})=N, \quad \nabla\cdot\mathbf{j}(\mathbf{x})=0 \ . \tag{6}$$

Of course, all the usual assumptions concerning v representability (and nondegeneracy) have to be made.

III. THE TFDW MODEL

In Ref. 6 we derived a relativistic density-functional representation of the kinetic energy and the exchange energy in the presence of an external electrostatic potential starting from the Hartree-Fock (HF) limit of QED. With the standard Kirzhnits[7] gradient-expansion technique the charge and energy densities can be expressed as functionals of the external potential. Elimination of the unknown potential by inversion of the representation of the charge density then leads to the desired energy expression in terms of the ground-state density. By analogy with the nonrelativistic TFDW model the kinetic energy functional was evaluated up to second-order gradient corrections, whereas the exchange energy was treated only to lowest order. We shall proceed in a similar way in this contribution.

Again the starting point is the Hartree-Fock approximated energy of the system,

$$\begin{aligned}E_{\text{HF}}=&\int d^3x \lim_{y\to x}{}_s\text{tr}\{[i\gamma\cdot\nabla_x-m-e\mathcal{V}_{\text{ext}}(\mathbf{x})]G_{\text{HF}}(x,y)\}\\&-\tfrac{1}{2}\int d^3x[\partial_k V_{\text{ext},0}(\mathbf{x})\partial^k V^0_{\text{ext}}(\mathbf{x})-\partial_k V_{\text{ext},l}(\mathbf{x})\partial^k V^l_{\text{ext}}(\mathbf{x})+\partial_k V_{\text{ext},l}(\mathbf{x})\partial^l V^k_{\text{ext}}(\mathbf{x})]\\&-i\frac{e^2}{2}\int d^3x\int d^4z\, D^{(0)}_{\rho\nu}(x-z)\{\lim_{u\to z}{}_s\text{tr}[\gamma^\nu G_{\text{HF}}(z,u)]\lim_{y\to x}{}_s\text{tr}[\gamma^\rho G_{\text{HF}}(x,y)]-\text{tr}[\gamma^\rho G_{\text{HF}}(x,z)\gamma^\nu G_{\text{HF}}(z,x)]\} \ ,\end{aligned} \tag{7}$$

where the abbreviations

$$\partial_k\equiv\frac{\partial}{\partial x^k}$$

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

and the sum convention have been used. To represent this energy approximately as a functional of the four-potential one needs a corresponding representation of the Hartree-Fock approximated Green's function G_{HF}. To this aim one first replaces G_{HF} by the propagator of an effective theory with the Lagrangian

$$\mathcal{L}_{\text{eff}}=\bar\psi(x)[i\partial\!\!\!/-m-e\mathcal{V}\!\!\!/_{\text{eff}}(\mathbf{x})]\psi(\mathbf{x})-\tfrac{1}{4}F^{\mu\nu}_{\text{eff}}(\mathbf{x})F_{\text{eff},\mu\nu}(\mathbf{x}) \ , \tag{8}$$

where $V^\nu_{\text{eff}}(\mathbf{x})$ represents an (unknown) classical potential. The corresponding Green's function is the propagator of a system of noninteracting particles in an arbitrary external four-potential. Thus the kinetic energy functional one derives from this approach is that of an equivalent system of noninteracting particles, i.e., the Kohn-Sham kinetic energy (analogous to the nonrelativistic case). The exchange energy obtained by replacing G_{HF} in Eq. (7) by the effective propagator corresponding to the Lagrangian (8) is evaluated only in lowest order in the fine-structure constant α.

The propagator of the effective theory can be given directly in its eigenfunction expansion, which is the starting point for a gradient expansion. However, the standard gradient-expansion scheme of Kirzhnits[7] is not adequate for systems in magnetic fields. An alternative gradient-expansion technique has been used to evaluate the Green's function up to second-order gradient contributions in a preceding paper.[5] Using this Green's function it is straightforward to derive the four-current and the energy density in terms of the external four-potential.

The four-current density,

$$j^\nu(x)=-\lim_{y\to x}{}_s\text{tr}[\gamma^\nu G(x,y)] \ ,$$

has to be renormalized in the standard fashion (for details see Ref. 6). For our purpose only the lowest-order counterterm is relevant, as $G_{\rm eff}$ does not contain any electron-electron interaction via exchange of photons,

$$j_R^\nu(\mathbf{x})=j_{\rm reg}^\nu(\mathbf{x})-\frac{Z_3^{(1)}}{e^2}\left[g^{\nu\mu}\partial_\rho\partial^\rho-\partial^\nu\partial^\mu\right]V_\mu(\mathbf{x}) , \quad (9)$$

where $Z_3^{(1)}$ represents the first-order contribution to the renormalization constant Z_3 and we set $V^\nu=eV_{\rm eff}^\nu$ for brevity. Note that the factor $1/e^2$ is due to our definitions of the current and the potential. Using, for example, dimensional regularization one finds

$$Z_3^{(1)}=-\frac{e^2}{12\pi^2}\Gamma\left[2-\frac{D}{2}\right] . \quad (10)$$

This counterterm cancels exactly the divergence occurring in $J_{\rm reg}^\nu$ with the result

$$\rho_R(\mathbf{x})=\frac{p(\mathbf{x})^3}{3\pi^2}+\frac{\Delta E(\mathbf{x})}{12\pi^2}\left[2\,\text{arcsinh}\left[\frac{p(\mathbf{x})}{m}\right]+\frac{E(\mathbf{x})}{p(\mathbf{x})}\right]+\frac{[\nabla E(\mathbf{x})]^2}{24\pi^2 p(\mathbf{x})}\left[3-\frac{E(\mathbf{x})^2}{p(\mathbf{x})^2}\right]+\frac{1}{24\pi^2 p(\mathbf{x})}F_{lk}(\mathbf{x})F^{lk}(\mathbf{x}) , \quad (11)$$

$$j_R^k(\mathbf{x})=\frac{1}{6\pi^2}\partial_l\left[F^{lk}(\mathbf{x})\,\text{arcsinh}\left[\frac{p(\mathbf{x})}{m}\right]\right] , \quad (12)$$

with

$$E(\mathbf{x})\equiv\varepsilon_F-V^0(\mathbf{x}) ,$$
$$p(\mathbf{x})\equiv(E(\mathbf{x})^2-m^2)^{1/2}\Theta(E(\mathbf{x})^2-m^2) ,$$

and the spatial components of the field tensor

$$F^{lk}(\mathbf{x})=\partial^l V^k(\mathbf{x})-\partial^k V^l(\mathbf{x}) .$$

ε_F represents the Fermi energy of the system. Note that $E(\mathbf{x})$ is a gauge-invariant quantity as a gauge transformation $V'^0=V^0+c$ has to be accompanied by a shift of the Fermi energy $\varepsilon_F'=\varepsilon_F+c$ in order to describe the same physical system after the gauge transformation. As one would have expected, the spatial components of the four-current vanish in lowest order. The $\hbar=0$ limit is equivalent to a homogeneous system where no current exists. Furthermore, one immediately recognizes that $\nabla\cdot j(\mathbf{x})$ vanishes due to the antisymmetry of F^{kl}, as demanded by current conservation for a static four-potential.

Besides the four-current the energy requires renormalization. The standard scheme leads to a counterterm due to the renormalization of the external field. Again, for the noninteracting limit (8) of the full Lagrangian of QED in an external potential only the lowest-order counterterm occurs:

$$\varepsilon_R(\mathbf{x})=\lim_{y\to x}{}_s\,\text{tr}\{[i\gamma\cdot\nabla_x-m-V(\mathbf{x})]G_{\rm eff}(x,y)\}+\frac{1+Z_3^{(1)}}{2e^2}[-\partial_l V_0(\mathbf{x})\partial^l V^0(\mathbf{x})+\partial_l V_k(\mathbf{x})\partial^l V^k(\mathbf{x})-\partial_l V_k(\mathbf{x})\partial^k V^l(\mathbf{x})] . \quad (13)$$

Subtracting the contribution of the negative-energy states one finds for the electronic part of the energy density corresponding to the expression (7), evaluated with the Green's function on the basis of the Lagrangian (8),

$$\begin{aligned}\varepsilon_{\rm kin,reg}(\mathbf{x})&=\lim_{y\to x}{}_s\,\text{tr}[(i\gamma\cdot\nabla_x-m)]G_{\rm eff}(x,y)]\\&=-\frac{1}{24\pi^2}\Gamma\left[2-\frac{D}{2}\right][\partial_l V_0(\mathbf{x})\partial^l V^0(\mathbf{x})-\partial_l V_k(\mathbf{x})\partial^l V^k(\mathbf{x})+\partial_l V_k(\mathbf{x})\partial^k V^l(\mathbf{x})]\\&\quad+\frac{1}{12\pi^2}\Gamma\left[2-\frac{D}{2}\right]V_k(\mathbf{x})\partial_l F^{lk}(\mathbf{x})+\frac{1}{4\pi^2}\left\{p(\mathbf{x})E(\mathbf{x})^3-\frac{m^2}{2}\left[p(\mathbf{x})E(\mathbf{x})+m^2\,\text{arcsinh}\left[\frac{p(\mathbf{x})}{m}\right]\right]\right\}\\&\quad+\frac{1}{12\pi^2}\left\{[\nabla E(\mathbf{x})]^2\left[-\frac{E(\mathbf{x})^3}{2p(\mathbf{x})^3}+\frac{E(\mathbf{x})}{p(\mathbf{x})}-\text{arcsinh}\left[\frac{p(\mathbf{x})}{m}\right]\right]+\Delta E(\mathbf{x})\left[\frac{E(\mathbf{x})^2}{p(\mathbf{x})}+p(\mathbf{x})\right]\right\}\\&\quad+\frac{1}{24\pi^2}F_{kl}(\mathbf{x})F^{kl}(\mathbf{x})\left[\frac{E(\mathbf{x})}{p(\mathbf{x})}-\text{arcsinh}\left[\frac{p(\mathbf{x})}{m}\right]\right]-\frac{1}{6\pi^2}V_k(\mathbf{x})\partial_l\left[F^{lk}(\mathbf{x})\,\text{arcsinh}\left[\frac{p(\mathbf{x})}{m}\right]\right] ,\end{aligned} \quad (14)$$

$$\begin{aligned}\varepsilon_{\rm pot,reg}(\mathbf{x})&=-\frac{1}{12\pi^2}\Gamma\left[2-\frac{D}{2}\right]V_k(\mathbf{x})\partial_l F^{lk}(\mathbf{x})\\&\quad+V^0(\mathbf{x})\left\{\frac{p(\mathbf{x})^3}{3\pi^2}+\frac{\Delta E(\mathbf{x})}{12\pi^2}\left[2\,\text{arcsinh}\left[\frac{p(\mathbf{x})}{m}\right]+\frac{E(\mathbf{x})}{p(\mathbf{x})}\right]+\frac{[\nabla E(\mathbf{x})]^2}{24\pi^2 p(\mathbf{x})}\left[3-\frac{E(\mathbf{x})^2}{p(\mathbf{x})^2}\right]\right\}\\&\quad+\frac{1}{6\pi^2}V_k(\mathbf{x})\partial_l\left[F^{lk}(\mathbf{x})\,\text{arcsinh}\left[\frac{p(\mathbf{x})}{m}\right]\right] .\end{aligned} \quad (15)$$

Both energy densities are not gauge invariant (although the corresponding energies are). Addition of both contributions and the counterterm of Eq. (13) leads to a finite and gauge-invariant total energy density. In order to define a renormalized kinetic energy density one subtracts the renormalized potential-energy density of the system,

$$\varepsilon_{\text{pot},R}(\mathbf{x})=\rho_R(\mathbf{x})V^0(\mathbf{x})-\mathbf{j}_R(\mathbf{x})\cdot\mathbf{V}(\mathbf{x})\ , \tag{16}$$

from the total energy density and obtains after partial integration,

$$\begin{aligned}\varepsilon_{\text{kin},R}(\mathbf{x})=&\frac{1}{4\pi^2}\left\{p(\mathbf{x})E(\mathbf{x})^3-\frac{m^2}{2}\left[p(\mathbf{x})E(\mathbf{x})+m^2\text{arcsinh}\left[\frac{p(\mathbf{x})}{m}\right]\right]\right\}\\&+\frac{1}{12\pi^2}\left\{[\nabla E(\mathbf{x})]^2\left[-\frac{E(\mathbf{x})^3}{2p(\mathbf{x})^3}+\frac{E(\mathbf{x})}{p(\mathbf{x})}-\text{arcsinh}\left[\frac{p(\mathbf{x})}{m}\right]\right]+\Delta E(\mathbf{x})\left[\frac{E(\mathbf{x})^2}{p(\mathbf{x})}+p(\mathbf{x})\right]\right\}\\&+\frac{1}{24\pi^2}F_{kl}(\mathbf{x})F^{kl}(\mathbf{x})\left[\frac{E(\mathbf{x})}{p(\mathbf{x})}+\text{arcsinh}\left[\frac{p(\mathbf{x})}{m}\right]\right]\ .\end{aligned} \tag{17}$$

One recognizes immediately that this expression is gauge invariant. In addition, the kinetic energy density as well as the four-current reduce to the expressions given in Ref. 6 for the case of a pure electrostatic potential.

The next step is the consistent inversion of the four-current functional up to second order. In order to construct a manifestly gauge-invariant inversion one represents E and the spatial components of the field tensor F^{kl} rather than V^ν as functionals of the four-current. The technical aspects do not differ greatly from the pure electrostatic case. The zeroth-order charge density only depends on $V^0(\mathbf{x})[p(\mathbf{x})]$,

$$\rho(\mathbf{x})=\rho^{[0]}(\mathbf{x})+\rho^{[2]}(\mathbf{x}),\quad \rho^{[0]}(\mathbf{x})=\frac{p(\mathbf{x})^3}{3\pi^2}$$

(the index $[n]$ denotes the order of $\hbar$) and the current contains no contributions of zeroth order. Thus one can replace $p(\mathbf{x})$,

$$\begin{aligned}p(\mathbf{x})&=\{3\pi^2[\rho(\mathbf{x})-\rho^{[2]}(\mathbf{x})-\cdots]\}^{1/3}\\&=[3\pi^2\rho(\mathbf{x})]^{1/3}-\frac{\pi^2\rho^{[2]}(\mathbf{x})}{[3\pi^2\rho(\mathbf{x})]^{2/3}}+\cdots\ ,\end{aligned} \tag{18}$$

by

$$q(\mathbf{x})\equiv[3\pi^2\rho(\mathbf{x})]^{1/3}\ , \tag{19}$$

in all terms which are of second order. In particular, one finds

$$\begin{aligned}\rho^{[2]}(\mathbf{x})=&\pi^2[\nabla\rho(\mathbf{x})]^2\left[\frac{1}{24q^3Q^2}-\frac{1}{8q^5}-\frac{q^2+Q^2}{6q^4Q^3}\text{arcsinh}\left[\frac{q}{m}\right]\right]\\&+[\Delta\rho(\mathbf{x})]\left[\frac{1}{12q^2}+\frac{1}{6qQ}\text{arcsinh}\left[\frac{q}{m}\right]\right]+\frac{1}{24\pi^2 q}F_{lk}(\mathbf{x})F^{lk}(\mathbf{x})\ ,\end{aligned} \tag{20a}$$

$$j^k(\mathbf{x})=\frac{1}{6\pi^2}\partial_l\left[\text{arcsinh}\left[\frac{q}{m}\right]F^{lk}(\mathbf{x})\right]\ , \tag{20b}$$

where the abbreviation

$$Q(\mathbf{x})\equiv(q(\mathbf{x})^2+m^2)^{1/2} \tag{21}$$

has been introduced . Equation (20b) is resolved by the nonlocal functional

$$F^{lk}(\mathbf{x})=\frac{3\pi}{2\text{arcsinh}(q/m)}\int d^3y\frac{1}{|\mathbf{x}-\mathbf{y}|}\left[\partial_y^l j^k(\mathbf{y})-\partial_y^k j^l(\mathbf{y})\right]\ . \tag{22}$$

This representation, together with Eqs. (18) and (20a), is the gauge-invariant version of the functional $V^\nu[j^\mu]$.

It remains to insert Eqs. (18), (20a), and (22) into the kinetic energy density, Eq. (17):

$$\begin{aligned}\varepsilon_{\text{kin},R}[\rho,j]=&\frac{1}{8\pi^2}\left[qQ^3+q^3Q-m^4\text{arcsinh}\left[\frac{q}{m}\right]\right]+\frac{1}{24\pi^2}\left[\nabla q\right]^2\frac{q}{Q}\left[1+2\frac{q}{Q}\text{arcsinh}\left[\frac{q}{m}\right]\right]\\&+\frac{3}{16\,\text{arcsinh}(q/m)}\int d^3y\int d^3z\left[\nabla_x\frac{1}{|\mathbf{x}-\mathbf{y}|}\right]\cdot\left[\nabla_x\frac{1}{|\mathbf{x}-\mathbf{z}|}\right]\mathbf{j}(\mathbf{y})\cdot\mathbf{j}(\mathbf{z})\\&-\frac{3}{16\,\text{arcsinh}(q/m)}\int d^3y\int d^3z\,\mathbf{j}(\mathbf{z})\cdot\left[\nabla_x\frac{1}{|\mathbf{x}-\mathbf{y}|}\right]\mathbf{j}(\mathbf{y})\cdot\left[\nabla_x\frac{1}{|\mathbf{x}-\mathbf{z}|}\right]\ .\end{aligned} \tag{23}$$

This is the (gauge-invariant) relativistic kinetic energy density of noninteracting particles in an arbitrary static four-potential. In contrast to the pure electrostatic case this functional is nonlocal.

To obtain the full extension of the relativistic TFDW model to systems in the presence of magnetic fields one has to add the potential energy of the interacting system to Eq. (23). Besides the potential energy due to the external potential,

$$\varepsilon_{\rm ext}(\mathbf{x}) = V^{\nu}(\mathbf{x}) j_{\nu}(\mathbf{x}) , \tag{24}$$

one has to take into account the direct potential energy,

$$\varepsilon_{\rm dir}(\mathbf{x}) = \frac{\alpha}{2} \int d^3y \frac{\rho(\mathbf{x})\rho(\mathbf{y}) - \mathbf{j}(\mathbf{x})\cdot\mathbf{j}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} , \tag{25}$$

and the exchange energy. As the TFDW model contains the exchange energy only to lowest orders of $\hbar$ as well as α, the presence of a magnetic field does not show up in $\varepsilon_x(\mathbf{x})$ in this approximation. Replacing $G_{\rm HF}$ in Eq. (7) by the lowest-order effective propagator one finds directly (see Ref. 6)

$$\varepsilon_{x,R}(\mathbf{x}) = \frac{\alpha}{8\pi^3} \left\{ 2m^2q^2 + q^2Q^2 - 6m^2 qQ \,\operatorname{arcsinh}\left[\frac{q}{m}\right] + 3m^4 \left[\operatorname{arcsinh}\left[\frac{q}{m}\right]\right]^2 \right\} . \tag{26}$$

It is straightforward to include more elaborate representations of the exchange energy as, e.g., given in Refs. 1 and 2.

Equations (23)–(26) constitute the extension of the relativistic TFDW model to systems in magnetic fields,

$$E_{eR\,\rm TFDW} = \int d^3x [\varepsilon_{{\rm kin},R}(\mathbf{x}) + \varepsilon_{\rm ext}(\mathbf{x}) + \varepsilon_{\rm dir}(\mathbf{x}) + \varepsilon_{x,R}(\mathbf{x})] . \tag{27}$$

The nonrelativistic limit of this functional is

$$\begin{aligned} \varepsilon_{e\rm TFDW}[\rho,\mathbf{j}] = {} & \frac{(3\pi^2\rho)^{5/3}}{10\pi^2 m} + \frac{(\nabla\rho)^2}{72 m\rho} + \frac{3m}{16(3\pi^2\rho)1/3} \int d^3y \int d^3z \left[\nabla_x \frac{1}{|\mathbf{x}-\mathbf{y}|}\right] \cdot \left[\nabla_x \frac{1}{|\mathbf{x}-\mathbf{z}|}\right] \mathbf{j}(\mathbf{y})\cdot\mathbf{j}(\mathbf{z}) \\ & - \frac{3m}{16(3\pi^2\rho)^{1/3}} \int d^3y \int d^3z\, \mathbf{j}(\mathbf{z})\cdot \left[\nabla_x \frac{1}{|\mathbf{x}-\mathbf{y}|}\right] \mathbf{j}(\mathbf{y})\cdot \left[\nabla_x \frac{1}{|\mathbf{x}-\mathbf{z}|}\right] \\ & + V^0\rho - \mathbf{V}\cdot\mathbf{j} + \frac{\alpha}{2}\int d^3y \frac{\rho(\mathbf{x})\rho(\mathbf{y}) - \mathbf{j}(\mathbf{x})\cdot\mathbf{j}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} - \frac{\alpha}{4\pi^3}(3\pi^2\rho)^{4/3} . \end{aligned} \tag{28}$$

Up to the contributions of the current it is identical with the well-known TFDW energy expression.

Introducing the interelectronic vector potential

$$\mathbf{W}(\mathbf{x}) \equiv \int d^3y \frac{\mathbf{j}(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|}$$

and the total electrostatic potential

$$U(\mathbf{x}) \equiv V_{\rm ext}(\mathbf{x}) + \frac{\alpha}{3\pi^2}\int d^3y \frac{p^3(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} ,$$

one can write the variational equations following from Eqs. (5) and (6) with (27) as (in the units $\hbar = c = m = 1$)

$$\begin{aligned} 0 = {} & 12qQ\left[Q + U + \mu - 1\right] + 6\frac{\alpha}{\pi} q[qQ - 3\,\operatorname{arcsinh}(q)] - \frac{9\pi^2}{4}\frac{(\nabla\times\mathbf{W})^2}{q\,\operatorname{arcsinh}^2(q)} - \frac{(\nabla q)^2}{2q}\left[1 + \frac{q^2}{Q^2} + 4\frac{q}{Q^3}\operatorname{arcsinh}(q)\right] \\ & - (\Delta q)\left[1 + 2\frac{q}{Q}\operatorname{arcsinh}(q)\right] , \end{aligned} \tag{29}$$

$$\Delta U = -4\pi\alpha\rho_{\rm ext} - \frac{4\alpha}{3\pi}q^3 , \tag{30}$$

$$\Delta \mathbf{W} = -4\pi\mathbf{j} , \tag{31}$$

$$\nabla\cdot\mathbf{W} = 0 , \tag{32}$$

$$\int d^3x\, q^3 = 3\pi^2 N , \tag{33}$$

where N is the electron number. Equation (32), together with Eq. (31), automatically guarantees $\nabla \cdot \mathbf{j}=0$.

It should be pointed out that the approximation used in the derivation of the functionals (27) and (28) is independent of the strength of the potential. It is an expansion around the homogeneous limit which has been used. Thus the model will be most adequate if the fields which are present do not vary too strongly. The strength of the potentials can be arbitrarily large. However, as the pure TFDW model has proved to be reasonably satisfactory, even for systems as inhomogeneous as atoms, one might hope for equivalent accuracy and regime of realiability in the extended case. A model calculation of atoms in magnetic fields is in progress.

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