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DENSITY FUNCTIONAL ASPECTS OF RELATIVISTIC FIELD THEORIES

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I INTRODUCTION

Given the tremendous success of density functional theory (DFT) for the description of nonrelativistic many particle systems the question for a relativistic extension arises quite naturally in view of the large number of problems in which relativistic effects play an important role. The most obvious area in which relativity can not be ignored is the physics and chemistry of heavy elements ($Z \geq 40$ — see e.g. [1]). Moreover, for an accurate description of high-Z atoms ($Z \geq 80$) and in particular for a discussion of collisions between such atoms (for a detailed account see [2]) or of exotic systems like superheavy elements ($Z \approx 114$ — see e.g. [2,3]) even radiative (i.e. quantumelectrodynamic) effects can no longer be neglected.

A brief look at the ground state of neutral Mercury may serve as an illustration of the importance of relativistic and radiative effects. The most drastic correction, of course, is introduced by relativistic kinematics which is directly reflected by the total ground state energy: Within the Hartree-Fock (HF) approximation this energy changes from its nonrelativistic value of $-18409.0a.u.$ [4] to $-19626.9a.u.$ [5]. Beyond the dominating role of kinetic effects one also finds substantial corrections for the exchange energy [5,6]: For Hg the relativistic Coulomb exchange energy is $-365.3a.u.$ which has to be compared to the nonrelativistic result of $-345.3a.u.$. Moreover, while the correlation energy is only slightly modified [7], radiative corrections reduce the binding energy of Hg by roughly $18.9a.u.$ [8] such that their contribution is much larger than the total correlation energy. However, not only global quantities are affected, also single particle orbitals undergo significant changes: While this is immediately clear for the innermost orbitals and the level splittings due to spin-orbit coupling, even the eigenvalue of the highest occupied ($6s_{1/2}$) orbital of Hg is 25% more attractive than its nonrelativistic counterpart reflecting the high ionisation potential of Hg [9]. As a consequence, the r-expectation value of this orbital is reduced by 15%. Quite generally, even the outermost $s_{1/2}$- and $p_{1/2}$-orbitals are contracted by relativistic kinematics, while d- and f-orbitals (and sometimes $p_{3/2}$-orbitals) are expanded due to the enhanced screening of the nuclear charge by the contracted s- and p-orbitals. These effects are particularly important e.g. for obtaining the correct ground states of negative ions (see e.g. [10]).

In accordance with the behaviour of atomic valence orbitals most bond lengths in molecules are also contracted. For instance the bond length of Au_2 is reduced from the nonrelativistic value of $5.48 a.u.$ to $4.61 a.u.$ [11], while its dissociation energy increases by about a factor of 2 [11]. On the other hand, there are also a few examples for substantial bond length expansion as e.g. Tl_2 for which the relativistic result of $7.1 a.u.$ has to be compared to the nonrelativistic value of $5.9 a.u.$ [12]. As a further manifestation of relativity in quantum chemistry we just mention the long-range form of the retarded van der Waals interaction (being proportional to R^{-7}) which is a direct consequence of the exchange of two transverse photons between the atoms (see e.g. [13]).

Also, it has been recognized quite early [14] that realistic band structures for high-Z metals can only be obtained taking into account relativistic kinematics. Moreover, a calculation for Pt [15] seems to indicate that the inclusion of relativistic corrections to the exchange energy further improves results for Fermi surfaces. In fact, even for valence levels the relativistic corrections to exchange are comparable to the total contributions of correlation [15].

The appropriate theory for the discussion of relativistic electronic systems is Quantumelectrodynamics (QED) (see e.g. [16–18]). While a truly covariant treatment would require to associate dynamic variables to both electrons and nuclei, the large nuclear mass in most situations allows to represent the nuclei as fixed external sources. Thus the relevant field theory is QED augmented by some static external four potential (we will not address time-dependent problems or exited states here). On this basis an extension of the Hohenberg-Kohn (HK) theorem [19] to the relativistic domain has first been formulated by Rajagopal and Callaway [20]. The corresponding Kohn-Sham (KS) equations [21] have been given by Rajagopal [22] and independently by MacDonald and Vosko [23]. As first application of the relativistic KS-scheme one could view the Dirac-Fock-Slater calculations by Liberman, Waber and Cromer [24]. By now many familiar DFT techniques are also available for the relativistic case and applications indicate that relativistic DFT methods join the strengths and deficiences of their nonrelativistic counterparts. Nevertheless, relativistic DFT is far from being as well developed as its nonrelativistic counterpart with respect to its foundations, the construction of explicit functionals and applications. In this contribution we will give an overview of the first two of these topics with specific emphasis on the field theoretical aspects of relativistic DFT, while no attempt is made to cover the area of applications (for an earlier review of this field see [25]). We also just mention that a time-dependent generalization of relativistic KS-equations has been suggested [26] and, using the time-dependent LDA for exchange and correlation, succesfully applied to the photoionization of Mercury [27] and Xe [26] as well as the evaluation of polarizabilities of heavy closed-shell atoms [28].

While the relativistic extension of DFT [20,22,23] was built on a field theoretical foundation, the additional features introduced by QED as compared to nonrelativistic many body theory were only partially taken into account. In addition to the relativistic kinematics of the electrons the finite speed of light introduces an important correction, i.e. the retardation of the instantaneous Coulomb interaction between the electrons. In the context of DFT this effect shows up in the exchange-correlation energy functional [22,23,29]. Furthermore, the existence of antiparticles (negative energy states) allows for the excitation of virtual electron-positron pairs which any consistent approach to relativistic systems necessarily has to include. As a consequence of any perturbative treatment of these radiative effects ultraviolett divergencies have to be dealt with, inevitably bringing up the question of renormalization. In fact, without renormalization any ground state energy obtained within QED is divergent! In an attempt to cope with this problem which obviously affects the proof of a relativistic HK-theorem we will devote a substantial part of this review of relativistic DFT to exposing its field theoretical background (Sections II-IV). In Section II the symmetries of QED (with external fields) are summarized in order to analyze the problem of ground states degeneracies and to exhibit a fundamental difference to the nonrelativistic situation concerning the electron spin. In this context also some properties of the relativistic homogeneous electron gas are discussed. After the definition of a suitable relativistic Schrödinger representation to be used for proving the HK-theorem the important issue of renormalization is addressed. It will be demonstrated that all counterterms required to keep ground state energies and ground state four currents finite are universal functionals of the external four potential. On this basis it will then be shown that the familiar scheme for proving the HK-theorem can be carried through if counterterms are included (in Section III). Some remarks are made on the nonrelativstic limit of relativistic DFT in order to make contact with nonrelativistic current-DFT [30,31] to the extent possible (in Section IV). Also, renormalized KS-equations will be set up (in Section V).

In the second part of this contribution we will review the techniques which have been used to obtain explicit functionals together with the corresponding results (Section VI) emphasizing the LDA for exchange and correlation as well as gradient corrections to the kinetic energy functional, i.e. extended Thomas-Fermi approximations. As in the nonrelativistic case the first manifestation of relativistic DFT was the formulation of a relativistic Thomas-Fermi (RTF) model by Vallarta and Rosen [32]. Applied to atoms, however, this RTF model leads to nonintegrable densities for point nuclei. While this problem can be overcome by using an extended nuclear charge distribution [33], it is nevertheless quite characteristic of the substantial complications introduced by any relativistic approach. The RTF model has e.g. been utilized for the inclusion of electronic screening effects in the description of supercritical atomic systems [34,35], in which nuclear charges beyond $Z = 137$ probe the structure of the QED vacuum, and the discussion [36] of nuclearites (extended systems with $10^2 < Z < 10^{18}$ and nuclear charge densities somewhat larger than that of usual nuclear matter). As in the nonrelativistic situation the RTF approximation has also been used to generate Z^{-1}-expansions for atomic properties [37] as well as to discuss atoms in extremely strong magnetic fields [38].

The derivation of gradient corrections [39–41] to the RTF model again exhibited the additional difficulties associated with the relativistic treatment of electronic systems: All divergencies inherent in the underlying quantum field theory, i.e. QED, show up in the construction of explicit functionals. Nevertheless, by now most ingredients of a relativistic extended Thomas-Fermi (RETF) approach are known. Both current contributions [42] and fourth order corrections [43] to the kinetic energy have been evaluated and the lowest order gradient correction has been extended to the temperature-dependent case [44]. Applications of these rather recent developments are limited — beyond tests for neutral atoms [45,46] only the discussion of atoms under compression [47,48] are found in the electronic case.

In contrast, semiclassical methods have been extensively used in the context of nuclear physics on the basis of the Skyrme model (for an overview see [49]). The phenomenological Skyrme interaction relies on the assumption of a static nucleon-nucleon potential and does neither take into account relativistic effects nor mesonic degrees of freedom. However, even for nuclear structure calculations for which the rather small total binding energy seems to indicate the legitimacy of a nonrelativistic treatment the drastic effects of spin-orbit coupling on the single particle spectrum call for a relativistic approach. Without doubt, relativistic effects become essential when one intends applications under extreme conditions, e.g. neutron stars or heavy ion collisions, where the nuclear density is much larger than the nuclear matter value. As a consequence inherently relativistic and thus field theoretical descriptions of strongly interacting systems have gained considerable attraction during recent years. While, as a matter of principle, Quantumchromodynamics (QCD) would provide the most appropriate basis in this context, a direct QCD description of nuclei does not yet seem to be possible. Thus at present one has to resort to effective field theories which should be understood as parametrizations of QCD. The most often used approach in this context is Quantumhadrodynamics (QHD) [50,51] in which the nucleon-nucleon interaction is represented in a phenomenological way by the exchange of various mesons thus treating the latter as dynamic degrees of freedom. Extensive calculations performed in the mean field approximation [52,53] demonstrate that the quality of the QHD description of ordinary nuclei is comparable to that achieved within the Skyrme model.

Encouraged by the success of DFT in the context of nonrelativistic nuclear physics it seems desirable to investigate its potential in the relativistic case. Recently, the foundations of a DFT approach to QHD have been established [54] by generalizing the HK-theorem and formulating the corresponding KS-equations. An extension to nonzero temperature [55] is also available. As in the electronic case the first DFT calculations in the context of QHD relied upon the TF approximation [56–58]. While to date applications of the QHD/KS-equations have not yet been reported, gradient corrections to the TF limit were derived by Centelles et al. [59] (and independently in Refs. [60,54] — for the temperature-dependent case see [61,55]). First results for finite nuclei and semiinfinite nuclear matter in the resulting ETF approximation [62–66] seem to indicate the usefulness of DFT concepts in the framework of relativistic nuclear physics. We will give a brief overview of the DFT approach to QHD in the third part of this contribution (Section VII), but content ourselves to DFT aspects (a more detailed account of the physics involved may be found in the contribution by M. Centelles in this volume).

II BASICS

II.1 Lagrangian

Field theoretical systems are characterized by specification of the Lagrangian density. In this section we consider QED, which is the appropriate quantum field theory for the description of relativistic atomic, molecular and condensed matter systems. However, as usual in this context, the nuclei will not be treated on a dynamical level but rather as fixed external sources. Thus the relevant Lagrangian reads

$$\begin{aligned}
\mathcal{L} &= \mathcal{L}_e + \mathcal{L}_\gamma + \mathcal{L}_{int} && (1)\\
\mathcal{L}_e(x) &= \frac{1}{4}\Big\{\Big[\hat{\overline{\psi}}(x), (i\overrightarrow{\not\partial} - m)\hat{\psi}(x)\Big] + \Big[\hat{\overline{\psi}}(x)(-i\overleftarrow{\not\partial} - m), \hat{\psi}(x)\Big]\Big\} && (2)\\
\mathcal{L}_\gamma(x) &= -\frac{1}{4}\hat{F}_{\mu\nu}(x)\hat{F}^{\mu\nu}(x) - \frac{\lambda}{2}(\partial_\nu \hat{A}^\nu(x))^2 && (3)\\
\mathcal{L}_{int}(x) &= -\,e\,\hat{j}^\nu(x)\,\Big(\hat{A}_\nu(x) + V_\nu(\boldsymbol{x})\Big) && (4)\\
\hat{F}_{\mu\nu}(x) &= \partial_\mu \hat{A}_\nu(x) - \partial_\nu \hat{A}_\mu(x) && (5)\\
\hat{j}^\nu(x) &= \frac{1}{2}\Big[\hat{\overline{\psi}}(x), \gamma^\nu \hat{\psi}(x)\Big] = \frac{1}{2}\sum_{a,b=1}^{4} \gamma^\nu_{ab}\Big[\hat{\overline{\psi}}_a(x), \hat{\psi}_b(x)\Big] && (6)
\end{aligned}$$

(our metric and notation are as in Ref. [18] — relativistic units $\hbar = c = 1$ are used). Here $\hat{\psi}(x)$ and $\hat{A}_\mu(x)$ denote the electron and photon field operators, respectively, while $V_\mu(\boldsymbol{x})$ represents the static C-number potential generated by the nuclei as well as additional time-independent electric or magnetic fields, if applied to the system. The vector bars on top of the partial derivatives indicate the direction in which the derivative has to be taken, i.e. in the second term of $\mathcal{L}_e$ the partial derivatives act on $\hat{\overline{\psi}}(x)$.

Note that due to the choice of a particular Lorentz frame in which the external sources are at rest the Lagrangian is no longer manifestly Lorentz invariant. Also the gauge invariance of the Lagrangian with respect to gauge transformations of the external potential has been partially broken: Only static gauge transformations are admitted within the rest frame of the nuclei. Of course, both symmetries would be restored if the external sources were treated as dynamical fields. With respect to the quantized electronic and photonic degrees of freedom, however, both the Lagrangian and the electronic four current $\hat{j}^\nu(x)$ have been written in a gauge and charge conjugation invariant form [16], i.e. under the charge conjugation $\hat{\mathcal{C}}$ the four current changes its sign,

$$\hat{\mathcal{C}}\, \hat{j}^\nu(x)\, \hat{\mathcal{C}}^+ = -\hat{j}^\nu(x) \quad ,$$

while in $\mathcal{L}$ the fermion charge manifests itself in the coupling to external sources,

$$\hat{\mathcal{C}}\, \mathcal{L}[V^\nu]\, \hat{\mathcal{C}}^+ = \mathcal{L}[-V^\nu] \quad .$$

For the photon fields we have chosen to work in the covariant gauge such that we had to introduce the gauge fixing term

$$-\frac{\lambda}{2}(\partial_\nu \hat{A}^\nu(x))^2$$

and to use the Gupta-Bleuler indefinite metric quantization. For most explicit considerations we will restrict ourselves to the so-called Feynman gauge, i.e. $\lambda = 1$. We also use a covariant gauge for the external potential which in the present situation reduces to $\partial_i V^i(\boldsymbol{x}) = \nabla \cdot \boldsymbol{V}(\boldsymbol{x}) = 0$.

II.2 Symmetries and conservation laws

In the framework of nonrelativistic DFT the question of degeneracy plays an important role for the basic statements of the HK-theorem (see e.g. [67]). In the nonrelativistic context the electron spin is the most obvious source for degeneracies. For relativistic systems, however, the intrinsic spin is no longer decoupled from orbital angular momentum. In order to examine under which circumstances the Lagrangian (1) can lead to degenerate ground states we consider its symmetries in some detail.

We first turn to continuous symmetries which in the field theoretical context are usually discussed on the basis of Noether's theorem (see e.g. [68,18]). The most obvious symmetry of the Lagrangian (1) is its gauge invariance which directly reflects current conservation,

$$\partial_\nu \hat{j}^\nu(x) = 0 \quad , \tag{7}$$

and thus the conservation of the total charge,

$$\hat{Q} = \int d^3x\; \hat{j}^0(x) = \frac{1}{2}\int d^3x\; \left[\hat{\psi}^+(x), \hat{\psi}(x)\right] \quad . \tag{8}$$

As a consequence any ground state resulting from (1) can be classified with respect to its charge.

Energy and momentum conservation can be directly deduced from the 'continuity' equation for the energy momentum tensor [68,16]. Here we base our considerations on the symmetric energy momentum tensor $\hat{T}^{\mu\nu}$ rather than the canonical $\hat{\Theta}^{\mu\nu}$. Both versions of the energy momentum tensor, of course, satisfy identical 'continuity' equations, i.e. all physical results are independent of this choice. For the $\hat{T}^{\mu\nu}$ resulting from (1) one finds

$$\begin{aligned}\hat{T}^{\mu\nu}(x) &= \frac{i}{8}\Big[\hat{\overline{\psi}}(x), \Big(\gamma^\mu \overrightarrow{\partial}^\nu + \gamma^\nu \overrightarrow{\partial}^\mu - \gamma^\mu \overleftarrow{\partial}^\nu - \gamma^\nu \overleftarrow{\partial}^\mu\Big)\hat{\psi}(x)\Big] \\ &\quad + \hat{F}^{\mu\rho}(x)\hat{F}_\rho{}^\nu(x) + \frac{1}{4}g^{\mu\nu}\hat{F}(x)^2 - \frac{\lambda}{2}g^{\mu\nu}\Big(\partial_\rho \hat{A}^\rho(x)\Big)^2 \\ &\quad -\lambda\Big(\partial_\rho\partial_\tau \hat{A}^\tau(x)\Big)\Big(g^{\mu\nu}\hat{A}^\rho(x) - g^{\mu\rho}\hat{A}^\nu(x) - g^{\nu\rho}\hat{A}^\mu(x)\Big) \\ &\quad -\frac{e}{2}\Big(\hat{j}^\mu(x)\hat{A}^\nu(x) + \hat{j}^\nu(x)\hat{A}^\mu(x)\Big) + \frac{e}{2}\Big(\hat{j}^\mu(x)V^\nu(\boldsymbol{x}) - \hat{j}^\nu(x)V^\mu(\boldsymbol{x})\Big) \quad .\end{aligned} \tag{9}$$

From the last line of Eq.(9) it is obvious that, as we are dealing with an open system, the source field breaks the symmetry of $\hat{T}_{\mu\nu}$. As an immediate consequence $\hat{T}_{\mu\nu}$ does not satisfy a homogeneous 'continuity' equation but rather the external potential acts as a source for momentum,

$$\partial_\mu \hat{T}^{\mu\nu}(x) = e\ \hat{j}_\mu(x)\ \partial^\nu V^\mu(\boldsymbol{x}) \quad . \tag{10}$$

Only the zeroth component of the total four momentum, i.e. the energy,

$$\hat{H} \equiv \int d^3x\ \hat{T}^{00}(x) \tag{11}$$

is conserved for time-independent external potentials: This implies that the system can be regarded as stationary in the rest frame of the sources. Note that the symmetry of $\hat{T}_{\mu\nu}$ could be restored by inclusion of the free electromagnetic Lagrangian corresponding to the sources,

$$\mathcal{L}_{ext}(x) = -\frac{1}{4}\Big[\partial_\mu V_\nu(x) - \partial_\nu V_\mu(x)\Big]\Big[\partial^\mu V^\nu(x) - \partial^\nu V^\mu(x)\Big] \quad ,$$

in the total Lagrangian (1), i.e. by inclusion of the energy and momentum of the sources in $\hat{T}_{\mu\nu}$.

The discussion of angular momentum conservation is based on the generalized angular momentum tensor,

$$\begin{aligned}\hat{J}^{\mu,\rho\lambda}(x) &= -\frac{1}{4}\Big[\hat{\overline{\psi}}(x), \Big(i\gamma^\mu\Big(x^\rho\overrightarrow{\partial}^\lambda - \overleftarrow{\partial}^\lambda x^\rho - x^\lambda\overrightarrow{\partial}^\rho + \overleftarrow{\partial}^\rho x^\lambda\Big) + \Big\{\gamma^\mu, \frac{\sigma^{\rho\lambda}}{2}\Big\}\Big)\hat{\psi}(x)\Big] \\ &\quad + \Big(\hat{F}^{\mu\nu}(x) + \lambda g^{\mu\nu}\Big(\partial\cdot\hat{A}(x)\Big)\Big) \\ &\qquad \times\Big(x^\rho\partial^\lambda\hat{A}_\nu(x) - x^\lambda\partial^\rho\hat{A}_\nu(x) + g^\rho{}_\nu\hat{A}^\lambda(x) - g^\lambda{}_\nu\hat{A}^\rho(x)\Big) \\ &\quad + \Big(g^{\mu\lambda}x^\rho - g^{\mu\rho}x^\lambda\Big)\mathcal{L}_\gamma(x) \quad ,\end{aligned} \tag{12}$$

which first of all demonstrates explicitly the coupling of spin and orbital angular momentum for both electrons and photons. In analogy to Eq.(10) the external potential acts as a source of angular momentum in the 'continuity' equation for $\hat{J}^{\mu,\rho\lambda}$,

$$\partial_\mu \hat{J}^{\mu,\rho\lambda}(x) = -\ e\ \hat{j}_\mu(x)\Big(x^\rho\partial^\lambda V^\mu(\boldsymbol{x}) - x^\lambda\partial^\rho V^\mu(\boldsymbol{x}) + g^{\rho\mu}V^\lambda(\boldsymbol{x}) - g^{\lambda\mu}V^\rho(\boldsymbol{x})\Big) \quad . \tag{13}$$

As for the linear momentum in general no component of the angular momentum is conserved. While for the conservation of a 'boost' momentum $\int d^3x\ \hat{J}^{0,0j}(x)$ both V^0 and V^j must vanish and the other two components of V^μ must not depend on x^j, the conservation of $\int d^3x\ \hat{J}^{0,ij}(x)$ requires specific spatial symmetries (if, for instance, all spatial components V^j vanish and V^0 only depends on $(x^1)^2 + (x^2)^2$, i.e. for axially symmetric electrostatic potentials, one finds as expected that the angular momentum with respect to the x^3-axis, $\int d^3x\ \hat{J}^{0,12}(x)$, is a conserved quantity).

So far only continuous symmetries have been considered. There are, however, also discrete symmetries which can lead to degeneracies:

- For parity to be a good quantum number some reflection symmetry of the potential is required.
- As for the Lagrangian, charge conjugation is no symmetry of the Hamiltonian,
$$\hat{\mathcal{C}}\ \hat{H}[V^\nu]\ \hat{\mathcal{C}}^+ = \hat{H}[-V^\nu] \quad ,$$
as long as the external potential does not vanish.
- Finally, time reversal leads to a twofold degeneracy only for purely electrostatic potentials $V^\mu = (V^0, \mathbf{0})$.

Thus one finds that for an external four potential which does not have any spatial symmetries most of the continuous and discrete symmetries of QED without external sources are broken and as a consequence the ground state of such a system is nondegenerate in general. In view of this fact there seems to be no need for introducing additional (artificial) coupling terms between the electrons and the external fields in order to lift possible degeneracies (as the coupling of the spin-density to a magnetic field for spin-dependent nonrelativistic systems).

II.3 Relativistic homogeneous electron gas

The Lagrangian of the relativistic homogeneous electron gas (RHEG) is obtained from the general $\mathcal{L}$, Eq.(1), by setting $V^\mu = 0$ which immediately leads to the conservation laws of closed systems. Thus both the complete four momentum,

$$\hat{P}^\mu \equiv \int d^3x\ \hat{T}^{0\mu}(x) \tag{14}$$

and all components of the (antisymmetric) angular momentum tensor,

$$\hat{M}^{\mu\nu} \equiv \int d^3x\ \hat{J}^{0,\mu\nu}(x) \tag{15}$$

are conserved. Also parity, charge conjugation and time-reversal invariances are manifest. As a consequence the ground state of the RHEG for a given energy density is at least fourfold degenerate. Thus in order to characterize a state completely one has to use a complete set of operators commuting with the Hamiltonian which splits up the total Fock space into subspaces with nondegenerate states of lowest energy (called the ground states of the subspaces in the following). The usual choice [17] for this complete set of operators is given by the three momentum $\boldsymbol{P}$, the charge $\hat{Q}$ as well as the square $\hat{W}^\mu \hat{W}_\mu$ and the third component of the Pauli-Lubanski vector,

$$\hat{W}_\mu \equiv -\frac{1}{2}\ \epsilon_{\mu\nu\rho\lambda}\ \hat{M}^{\nu\rho}\ \hat{P}^\lambda \quad . \tag{16}$$

Fortunately, for our purposes of examining ground states of purely electronic systems one can reduce the set of quantum numbers required for a complete characterization. On one hand, for a fixed Lorentz frame and a given sector of the Fock space defined by the quantum numbers $<\hat{Q}>$, $<\hat{W}^\mu \hat{W}_\mu>$ and $<\hat{W}^3>$ all states with nonvanishing three momentum (density) lead to a higher energy than that with $<\hat{\boldsymbol{P}}>= \mathbf{0}$,

$$\begin{aligned} &< \Psi(\boldsymbol{P}, Q, W^\mu W_\mu, W^3)|\hat{P}^0|\Psi(\boldsymbol{P}, Q, W^\mu W_\mu, W^3) >_{\boldsymbol{P}\neq\mathbf{0}} \\ > \quad &< \Psi(\mathbf{0}, Q, W^\mu W_\mu, W^3)|\hat{P}^0|\Psi(\mathbf{0}, Q, W^\mu W_\mu, W^3) > \quad , \end{aligned}$$

i.e. the energy of a RHEG is a minimum in its rest frame. Consequently one finds a nondegenerate ground state $|\Psi(Q, W^\mu W_\mu, W^3)>$ in each such subspace with arbitrary $<\hat{\boldsymbol{P}}>$.

Moreover, any real electron-positron pair present in a subspace with fixed Q and W^3 increases the total energy by about $2m$, the rest mass of the pair. Thus a restriction to the purely electronic sector of Fock space is appropriate for a description of atomic, molecular and condensed matter systems. In this sector the ground state is uniquely determined by Q and W^3, in other words, it is a unique functional of the corresponding densities j^0 and w^3, $|\Psi[j^0, w^3]>$, where $W^3 = \int d^3x\ w^3(\boldsymbol{x})$.

While the interpretation of the charge density as a basic variable for a DFT approach to the RHEG is obvious, w^3 requires some further consideration. Its physical content is most easily extracted for noninteracting single particle states. In this case an explicit evaluation of the eigenvalues of $\hat{W}^3$ is possible,

$$\hat{W}^3|k,\pm> = \pm\frac{\sqrt{m^2+\boldsymbol{k}^2}}{2}|k,\pm> \quad , \tag{17}$$

where $|k,\pm>$ denotes a one electron state with three momentum parallel to the 3-axis, $k^\mu = (\sqrt{m^2+\boldsymbol{k}^2}, 0, 0, |\boldsymbol{k}|)$ and spin $\pm 1/2$ in its rest frame. As a specific property of the RHEG the orbital angular momentum contribution to $\hat{W}^\mu$, Eq.(16), vanishes, suggesting to interpret W^3 as a relativistic extension of the usual spin and thus w^3 as a spin-density. Explicitly one obtains

$$\begin{aligned} &< \Psi(Q,W^3)|\hat{w}^3(\boldsymbol{x})|\Psi(Q,W^3)> \\ =\ & -\frac{1}{4}\,P^0\ <\Psi(Q,W^3)|\Big[\hat{\bar{\psi}}^+(x), \begin{pmatrix} \sigma^3 & 0 \\ 0 & \sigma^3 \end{pmatrix}\hat{\psi}(x)\Big]|\Psi(Q,W^3)> \quad , \end{aligned} \tag{18}$$

where $\hat{P}^\mu|\Psi(Q,W^3)> = g^{0\mu}P^0|\Psi(Q,W^3)>$ has been used. Eq.(18) exhibits clearly that w^3 is essentially identical to the usual spin-density. Thus one finds that in the interesting sector of Fock space the ground state of a RHEG is uniquely determined by the charge- and spin-densities. In general, however, spin and orbital angular momentum are intrinsically coupled such that the spin-density can not be used as a basic variable for a DFT approach to these systems. As a consequence the 'spin-polarized' RHEG is not an ideal basis for constructing fully relativistic energy functionals (for attempts to overcome this problem see e.g. [23,69,70]). Of course, this does not imply that the unpolarized RHEG does not form a reasonable starting point for deriving approximate functionals for applications in which current contributions are of minor importance.

As a further ingredient for the discussion of the RHEG which is required for many subsequent considerations we consider the noninteracting electron propagator. To this aim one first notes that w^3 combines spin and energy quantum numbers and thus is not Lorentz invariant. Consequently one often prefers to use a suitable combination of the components of $\hat{W}^\mu$ which does not show this deficiency. Again this combination is most easily constructed for noninteracting particles,

$$\frac{n\cdot\hat{W}}{m}|k,\pm> = \pm\frac{1}{2}|k,\pm> \quad , \tag{19}$$

where

$$n^\nu = \left(t^\nu - k^\nu\frac{t\cdot k}{m^2}\right)\frac{m}{|\boldsymbol{k}|} \qquad \text{with} \qquad n^2 = -1\ , \quad n\cdot k = 0\ , \quad t^\nu = (1,0,0,0)$$

has been chosen to make $n\cdot\hat{W}/m$ a Lorentz invariant polarization operator leading to the usual spin quantum numbers. Using $n\cdot\hat{W}/m$ it is now easy to construct projection operators on positive or negative polarization,

$$\Big(\frac{1}{2}\pm\frac{n\cdot\hat{W}}{m}\Big)|k,\pm> \;=\; \frac{1}{2}(1\pm\gamma_5\not{n})|k,\pm> \;=\; |k,\pm> \tag{20}$$

$$\Big(\frac{1}{2}\pm\frac{n\cdot\hat{W}}{m}\Big)|k,\mp> \;=\; \frac{1}{2}(1\pm\gamma_5\not{n})|k,\mp> \;=\; 0 \quad , \tag{21}$$

($\gamma_5 = i\gamma^0\gamma^1\gamma^2\gamma^3$). These projection operators allow for a direct evaluation of the electron propagator of a spin-polarized noninteracting RHEG,

$$\begin{aligned} G^0(k) &= G^0_V(k) + G^0_D(k) \\ G^0_V(k) &= i\frac{\not{k}+m}{k^2-m^2+i\epsilon} \\ G^0_D(k) &= -\pi\sum_{\eta=\pm}(1+\eta\gamma_5\not{n})(\not{k}+m)\frac{\delta(k^0-\sqrt{\boldsymbol{k}^2+m^2})}{2\sqrt{\boldsymbol{k}^2+m^2}}\Theta(k_F^\eta-|\boldsymbol{k}|) \quad . \end{aligned} \tag{22}$$

Here the complete propagator has been decomposed into the vacuum propagator G^0_V and the contribution G^0_D from the electrons with energies between m and $(k_F^2+m^2)^{1/2}$ and polarization $\eta/2$, i.e. the real electrons in the RHEG. The given form of $G^0_D(k)$ does not include the presence of real positrons in the gas (their propagator, however, would be completely analogous to G^0_D). While for strictly noninteracting particles the existence of a stable electron-positron gas is quite conceivable, dealing with short-lived interacting systems like positronium is beyond the scope of the present approach. Note, however, that the propagator (22), which will be used extensively in the following, does allow for the production of virtual electron-positron pairs such that evaluating e.g. energy contributions on its basis does include all relevant radiative corrections.

II.4 Gauge invariance and representations

The traditional proof of the HK theorem in the nonrelativistic domain is based on the Schrödinger picture. In a quantum field theory a manifestly covariant representation of the dynamics, incorporated in the field operators, requires the use of the Heisenberg picture. While at first glance the transition to the Schrödinger picture appears to be straightforward, a brief look at the usual discussion of gauge transformations demonstrates that this transition has to be handled with some care.

As already emphasized the Lagrangian (1) is gauge invariant with respect to gauge transformations of both the classical external and and the quantized interaction potential. Here only gauge transformations of the external potential are of interest,

$$V'_\mu(x) = V_\mu(x) + \partial_\mu\Lambda(x) \qquad , \qquad \partial_\mu\partial^\mu\Lambda(x) = 0 \quad . \tag{23}$$

where an explicitly time-dependent V^μ is introduced at this point in order to include the possibility of adiabatic switching of the potential. On the basis of (23) and the corresponding (unitary) gauge transformation of the spinor operators,

$$\hat{\psi}'(x) \;=\; \hat{U}(x^0)\;\hat{\psi}(x)\;\hat{U}^+(x^0) = e^{-ie\Lambda(x)}\;\hat{\psi}(x) \tag{24}$$

$$\hat{U}(x^0) \;=\; \exp\Big\{ie\int d^3x\;\hat{j}^0(x)\;\Lambda(x)\Big\} \tag{25}$$

one directly verifies form invariance of the Lagrangian, of the corresponding field equations and of the four current,

$$\mathcal{L}(\hat{\psi}',V'_\mu) \;=\; \mathcal{L}(\hat{\psi},V_\mu) \tag{26}$$

$$\Big(i\not{\partial}-m-e\hat{\not{A}}(x)-e\not{V}(x)\Big)\hat{\psi}(x) \;=\; 0 \tag{27}$$

$$\Big(i\not{\partial}-m-e\hat{\not{A}}(x)-e\not{V}'(x)\Big)\hat{\psi}'(x) \;=\; 0 \tag{28}$$

$$\hat{j}'_\mu(x) \;=\; \hat{j}_\mu(x) \quad , \tag{29}$$

as an expression of the gauge invariance of the theory.

If one considers the transformation (24) for the specific time $x^0 = t = 0$,

$$\hat{\psi}'(x^0 = 0, \boldsymbol{x}) = e^{-ie\Lambda(x^0=0,\boldsymbol{x})}\ \hat{\psi}(x^0 = 0, \boldsymbol{x}) \quad , \tag{30}$$

one realizes that the Heisenberg field operators $\hat{\psi}(x)$ at $x^0 = 0$ are not yet suitable to define a Schrödinger representation on which the proof of the relativistic HK-theorem could be based: The usual pattern of the proof requires identical field operators for different potentials, while (30) as the most simple example for the relation between field operators corresponding to different external potentials demonstrates that quite generally $\hat{\psi}'(x^0 = 0, \boldsymbol{x}) \neq \hat{\psi}(x^0 = 0, \boldsymbol{x})$.

This problem can be resolved by noting that the field equations for the Heisenberg operators (indexed with H for the moment for clarity) determine $\hat{\psi}_H$ only up to a *global* unitary transformation. The operator

$$\hat{\psi}_{\overline{H}}(x) = \hat{B}\hat{\psi}_H(x)\hat{B}^+$$

satisfies the same field equation as $\hat{\psi}_H(x)$,

$$\Big(i\partial\!\!\!/ - m - e\hat{A\!\!\!/}(x) - eV\!\!\!\!/(x)\Big)\hat{\psi}_{\overline{H}}(x) = \hat{B}\Big(i\partial\!\!\!/ - m - e\hat{A\!\!\!/}(x) - eV\!\!\!\!/(x)\Big)\hat{\psi}_H(x)\hat{B}^+ = 0 \quad , \tag{31}$$

as long as $\hat{B}$ commutes with $\hat{A\!\!\!/}(x)$ (and does not carry spinor indices). Eq.(31) emphasizes the fact that the Heisenberg representation is only determined uniquely if some additional boundary condition is applied. The usual choice of the boundary condition in the relativistic case is motivated by the concept of adiabatic switching which requires that any potential is switched off in the limit $x^0 \to -\infty$, leading to

$$\begin{array}{lcl} V_\nu(x) \underset{x^0\to-\infty}{\longrightarrow} 0 \\ V'_\nu(x) \underset{x^0\to-\infty}{\longrightarrow} 0 \end{array} \Longrightarrow \left.\begin{array}{l} \hat{\psi}_H(x) \\ \hat{\psi}'_H(x) \end{array}\right\} \underset{x^0\to-\infty}{\longrightarrow} \hat{\psi}_{H,0}(x) \ . \tag{32}$$

As a consequence the Heisenberg operators corresponding to different external potentials approach the free Heisenberg field operator $\hat{\psi}_{H,0}(x)$ in the limit $x^0 \to -\infty$. In nonrelativistic many body theory, on the other hand, one usually adjusts the Heisenberg representation so that it coincides with the Schrödinger representation at $t = 0$,

$$\hat{\psi}_{\overline{H}}(x^0 = 0, \boldsymbol{x}) = \hat{\psi}'_{\overline{H}}(x^0 = 0, \boldsymbol{x}) = \hat{\psi}_{H,0}(x^0 = 0, \boldsymbol{x}) = \hat{\psi}_S(\boldsymbol{x}) \ . \tag{33}$$

The latter boundary condition, of course, is more appropriate for proving a HK-theorem. The connection between the H-representation implied by (32) and the one defined by (33) can, however, be easily established using the time-evolution operator in the interaction representation,

$$\begin{aligned} \hat{\psi}_{\overline{H}}(x) &= \hat{T}_I^+(0,-\infty)\ \hat{\psi}_H(x)\ \hat{T}_I(0,-\infty) & (34)\\ \hat{T}_I(t,t') &= \mathbf{T}\exp\Big\{-ie\int_{t'}^{t} dx^0 \int d^3x\ \hat{j}^\nu_{H,0}(x)\ V_\nu(x)\Big\} \ , & (35) \end{aligned}$$

where $\hat{\psi}_{\overline{H}}(x)$ is the H-operator satisfying the nonrelativistic boundary condition (33),

$$\hat{j}^\nu_{H,0}(x) = \frac{1}{2}\Big[\hat{\overline{\psi}}_{H,0}(x), \gamma^\nu\hat{\psi}_{H,0}(x)\Big] \quad ,$$

and $\mathbf{T}$ denotes time-ordering. A relativistic S-representation suitable for our purposes can now be constructed from the transformed H-representation,

$$\begin{aligned} \hat{\psi}_S(\boldsymbol{x}) &= e^{-i\hat{H}x^0}\ \hat{\psi}_{\overline{H}}(x)\ e^{i\hat{H}x^0} & (36)\\ |\Psi_S(x^0)> &= e^{-i\hat{H}x^0}\ |\Psi_{\overline{H}}> & (37) \end{aligned}$$

It is this S-representation which will be referred to in the following (without, however, explicitly displaying any indices).

For completeness we list the resulting properties under the gauge transformation (23),

$$\hat{\psi}'_S(\boldsymbol{x}) = \hat{\psi}_S(\boldsymbol{x}) \tag{38}$$

$$\hat{\psi}'_H(x) = e^{-ie\Lambda(x)}\ \hat{\psi}_H(x) \tag{39}$$

$$\hat{\psi}'_{\overline{H}}(x) = e^{-ie\Lambda(x)}\ \hat{G}^+\hat{\psi}_{\overline{H}}(x)\hat{G} \tag{40}$$

$$\hat{G} = \exp\left\{ie\int d^3x\ \hat{j}^0_{\overline{H}}(0,\boldsymbol{x})\ \Lambda(0,\boldsymbol{x})\right\} \quad . \tag{41}$$

One explicitly verifies that $\hat{\psi}'_{\overline{H}}(0,\boldsymbol{x}) = \hat{\psi}_{\overline{H}}(0,\boldsymbol{x})$.

II.5 Renormalization

At this point one can write down the Hamiltonian corresponding to (1) in the S-representation discussed in the previous section (compare sections 7d,10g of Ref. [17]),

$$\hat{H}_S = \frac{1}{2}\int d^3x\ \Big\{\Big[\hat{\overline{\psi}}(\boldsymbol{x}), \Big(-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + m + e\hat{\not{A}}(\boldsymbol{x}) + e\not{V}(\boldsymbol{x})\Big)\hat{\psi}(\boldsymbol{x})\Big] \tag{42}$$

$$- \hat{\Pi}_\nu(\boldsymbol{x})\hat{\Pi}^\nu(\boldsymbol{x}) - \boldsymbol{\nabla}\hat{A}_\nu(\boldsymbol{x})\cdot\boldsymbol{\nabla}\hat{A}^\nu(\boldsymbol{x})\Big\}$$

$$\hat{\Pi}^\nu(\boldsymbol{x}) = e^{-i\hat{H}x^0}\ \partial_0\hat{A}^\nu_{\overline{H}}(x)\ e^{i\hat{H}x^0} \quad , \tag{43}$$

where we have chosen Feynman gauge. Unfortunately one is not yet in the position to prove a relativistic HK-theorem on the basis of the Hamiltonian (42) the reason being the well-known fact that a direct evaluation of the ground state expectation value $<\Psi|\hat{H}|\Psi>$ leads to various divergencies. To deal with this problem is the subject of renormalization. Thus before we are able to proceed to the HK-theorem we have to provide a renormalization procedure for the energy (and the four current) which is consistent with the scheme used for proving the HK-theorem.

To this aim one first has to distinguish the two basic types of divergencies which are found in $<\Psi|\hat{H}|\Psi>$:

- On one hand there is the divergent vacuum energy of noninteracting electrons and photons, i.e. the sum over the energy of all Fermi sea states in the electronic case and the zero point energy of the photons. These divergent energy contributions are usually removed by either normal ordering of the operators in the Hamiltonian or by explicit subtraction of the vacuum expectation value of the noninteracting Hamiltonian,

  $$\hat{H}_r = \hat{H} - <0|\hat{H}_{free}|0> \quad ,$$

  where

  $$\hat{H}_{free} = \frac{1}{2}\int d^3x\ \Big\{\Big[\hat{\overline{\psi}}(\boldsymbol{x}), \Big(-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + m\Big)\hat{\psi}(\boldsymbol{x})\Big] \tag{44}$$

  $$- \hat{\Pi}_\nu(\boldsymbol{x})\hat{\Pi}^\nu(\boldsymbol{x}) - \boldsymbol{\nabla}\hat{A}_\nu(\boldsymbol{x})\cdot\boldsymbol{\nabla}\hat{A}^\nu(\boldsymbol{x})\Big\} \quad ,$$

  such that $\hat{H}_r$ leads to a finite ground state energy for noninteracting homogeneous systems. Note that the renormalization constant $<0|\hat{H}_{free}|0>$ is independent of any external or interaction potential. Thus this type of divergency is of nonperturbative character and identical for all V^μ.

- In contrast the UV-divergencies of QED result from the interaction of electrons with photons and the external potential and are intrinsically related to the perturbative treatment of QFTs. They are absorbed by a redefinition of all coupling constants, masses and fields of the system. Thus one reinterprets the original Lagrangian as being written in terms of unrenormalized fields and parameters (denoted by an index 0) which differ from the physically relevant renormalized ones (without index) by renormalization constants,

$$\begin{aligned}
\mathcal{L}_R &= \frac{1}{4}\Big\{\Big[\hat{\overline{\psi}}_0(x), \big(i\overrightarrow{\partial\!\!\!/} - m_0 - e_0 V\!\!\!/_0(x) - e_0\hat{A\!\!\!/}_0(x)\big)\hat{\psi}_0(x)\Big] \\
&\qquad + \Big[\hat{\overline{\psi}}_0(x)\big(-i\overleftarrow{\partial\!\!\!/} - m_0 - e_0 V\!\!\!/_0(x) - e_0\hat{A\!\!\!/}_0(x)\big), \hat{\psi}_0(x)\Big]\Big\} \\
&\quad -\frac{1}{4}\hat{F}_{0,\mu\nu}(x)\hat{F}_0^{\mu\nu}(x) - \frac{1}{2}\big(\partial_\nu \hat{A}_0^\nu(x)\big)^2 \\
&= \frac{Z_2}{4}\Big\{\Big[\hat{\overline{\psi}}(x), \big(i\overrightarrow{\partial\!\!\!/} - m + \delta m - eV\!\!\!/(x) - e\hat{A\!\!\!/}(x)\big)\hat{\psi}(x)\Big] \\
&\qquad + \Big[\hat{\overline{\psi}}(x)\big(-i\overleftarrow{\partial\!\!\!/} - m + \delta m - eV\!\!\!/(x) - e\hat{A\!\!\!/}(x)\big), \hat{\psi}(x)\Big]\Big\} \\
&\quad -\frac{Z_3}{4}\hat{F}_{\mu\nu}(x)\hat{F}^{\mu\nu}(x) - \frac{Z_3}{2}\big(\partial_\nu \hat{A}^\nu(x)\big)^2 \quad ,
\end{aligned} \tag{45}$$

i.e.

$$\hat{\psi}_0(x) = \sqrt{Z_2}\hat{\psi}(x) \tag{46}$$

$$\hat{A}_0^\nu(x) = \sqrt{Z_3}\hat{A}^\nu(x) \tag{47}$$

$$V_0^\nu(x) = \sqrt{Z_3}V^\nu(x) \tag{48}$$

$$e_0 = \frac{Z_1}{Z_2\sqrt{Z_3}}\, e \tag{49}$$

$$m_0 = m - \delta m \quad . \tag{50}$$

The renormalization constants Z_1, Z_2, Z_3 and δm have to be understood as functions of the finite physical charge e and mass m of the electrons which can be constructed order by order in the perturbation series. It is important to notice that these constants are uniquely determined by vacuum QED without any external potential. Thus they do neither depend on the specific external potential present nor on the ground state corresponding to this potential. As a result of using the Lagrangian (45) all renormalized Greensfunctions of the theory (defined in terms of the renormalized fields) are finite, e.g. the electron propagator,

$$G_R(x,y) = <\Psi|\mathbf{T}\hat{\psi}(x)\hat{\overline{\psi}}(y)|\Psi> \quad . \tag{51}$$

Note that in contrast to Z_1, Z_2, Z_3 and δm themselves the actual counterterms constructed from these constants depend on V^μ (an example is given below).

For interacting systems, however, this standard renormalization scheme does not directly lead to finite ground state energies, but rather finite Greensfunctions. In fact, as will be shown below, keeping the ground state energy (and the four current) finite requires additional counterterms (which, however, are unambigously fixed by the procedure above — compare e.g. [71,72]). Moreover, it is by no means obvious whether the various counterterms introduced by this complex procedure are uniquely determined by the external potential V^μ only and do not also explicitly depend on the ground state $|\Psi>$ corresponding to V^μ. An explicit $|\Psi>$-dependence, however, would not allow to use the familiar scheme for proving the HK-theorem. In the following we will show that the counterterms fortunately can be understood as functionals of V^μ only.

One way of analyzing this problem is to write the ground state energy and four current in terms of the renormalized field operators and thus of the renormalized Greensfunctions,

$$
\begin{aligned}
E_{R,internal} &= <\Psi|\frac{1}{2}\int d^3x\ \left[\hat{\overline{\psi}}(x),\left(-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}+m+e\not{V}(\boldsymbol{x})\right)\hat{\psi}(x)\right]|\Psi> \qquad (52)\\
&\quad +E_{int,R,internal}+E_{\gamma,R,internal}\\
&= -\int d^3x\ \lim_{y\to x}{}_s\ tr\left[\left(-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}+m+e\not{V}(\boldsymbol{x})\right)G_R(x,y)\right]\\
&\quad +E_{int,R,internal}+E_{\gamma,R,internal}\\
j^\nu_{R,internal}(\boldsymbol{x}) &= <\Psi|\frac{1}{2}\left[\hat{\overline{\psi}}(x),\gamma^\nu\hat{\psi}(x)\right]|\Psi> \qquad (53)\\
&= -\lim_{y\to x}{}_s\ tr\left[G_R(x,y)\gamma^\nu\right] \quad ,
\end{aligned}
$$

where for brevity only the fermionic sector is shown explicitly in case of the energy and the symmetric limit is given by

$$
\lim_{y\to x}{}_s \equiv \frac{1}{2}\left(\lim_{y\to x,y^0>x^0}+\lim_{y\to x,y^0<x^0}\right)\Bigg|_{(x-y)^2\geq 0} \quad .
$$

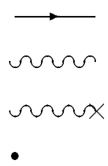
The energy and current defined by Eqs.(52,53) will be called *internally* renormalized as most of their initial divergencies are already eliminated by the standard scheme (i.e. inside the renormalized Greensfunctions). Moreover, Eqs.(52,53) explicitly demonstrate that the corresponding counterterms can be absorbed into a multiplicative, $|\Psi>$-independent renormalization of the fields. Thus using the Hamiltionian (42) with the renormalized fields appears to be a reasonable basis for a HK-theorem. Both $E_{R,internal}$ and $j^\mu_{R,internal}$, however, are still divergent and thus require additional counterterms.

This is most easily seen on the basis of an explicit example using perturbation theory whose elements, the electron propagator of the noninteracting RHEG, the noninteracting limit of the photon propagator,

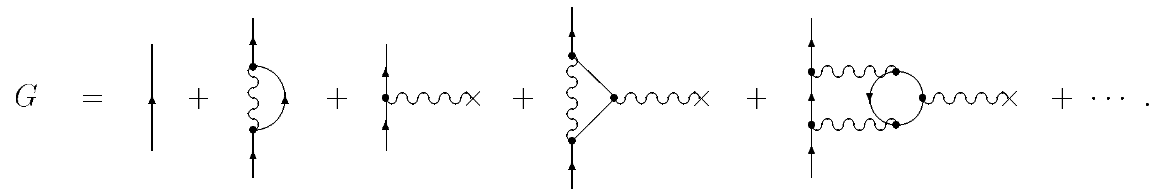
$$
D^{\mu\nu}_R(x,y) = <\Psi|\mathbf{T}\hat{A}^\mu(x)\hat{A}^\nu(y)|\Psi> \quad ,
$$

and the external potential, are represented diagrammatically by

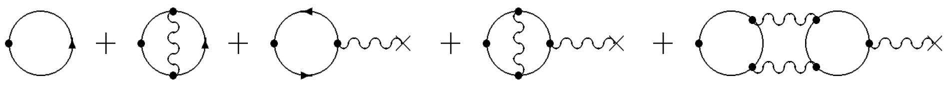
$G^0(p) =$
$D^0_{\rho\nu}(k) =$
$V_\rho(k) =$
$-ie\gamma^\mu =$.



To further simplify the discussion we restrict ourselves to the four current whose perturbation expansion can be obtained directly from the corresponding expansion of the electron propagator,



Applying the standard renormalization procedure all initially divergent loops in these diagrams are kept finite. The symmetric limit, however, which connects j^μ and G according to Eq.(53) introduces one further loop in the perturbative expansion of j^μ as compared to that of G. Thus the above diagrams for G lead to the following contributions to j^μ,

$-iej^\mu =$  $\cdots$. (54)

While after the standard renormalization procedure all those loops already present in the expansion of G are finite one immediately recognizes that the 'leftmost' loops which are due to the symmetric limit also lead to divergencies, the two types of divergent subgraphs generated being the noninteracting contribution to the photon 2-point function (as in the third diagram) and the first order (in e^2) vertex correction graph (as in the second and fourth diagram). All other leftmost subgraphs produced are finite (e.g. in the first and fifth diagram Furry's theorem for vacuum QED applies). To determine the structure of the counterterms required for the divergent subgraphs one expands j^μ in powers of V^μ,

$$j^\mu(\boldsymbol{x}) = j^\mu_{hom} + \sum_{n=1}^{\infty} \frac{e^n}{n!} \int d^4y_1 \ldots \int d^4y_n \; \chi^{(n+1),\mu\nu_1\ldots\nu_n}_{c,hom}(x, y_1, \ldots y_n) \; V_{\nu_1}(\boldsymbol{y}_1) \ldots V_{\nu_n}(\boldsymbol{y}_n) \, ,$$

where the $\chi^{(n),\mu\nu_1\ldots\nu_n}_{c,hom}$ represent the connected contributions to the time-ordered response functions of the RHEG (i.e. the reducible n-point functions) which are defined in analogy to the 2-point function,

$$\chi^{(2),\mu\nu}(x,y) \equiv \chi^{\mu\nu}(x,y) = -\, i\Big[< \Psi| \, \mathbf{T} \, \hat{j}^\mu(x) \, \hat{j}^\nu(y) \, |\Psi> \; - \, j^\mu(\boldsymbol{x}) \, j^\nu(\boldsymbol{y})\Big] \quad . \tag{55}$$

Thus the counterterms which keep j^μ finite are directly determined by the counterterms for the four current of the interacting RHEG and for the $\chi^{(n),\mu\nu_1\ldots\nu_n}_{c,hom}$. In the latter, however, only vacuum subgraphs diverge and thus the required counterterms can be obtained from the standard renormalization procedure. As an important consequence the counterterms for j^μ only depend on the density of the RHEG, i.e. the particle number, and on V^μ but not on the ground state corresponding to V^μ,

$$j^\nu_R(\boldsymbol{x}) = j^\nu_{R,internal}(\boldsymbol{x}) + \delta j^\nu[V^\nu] \quad . \tag{56}$$

The same arguments can be applied to the ground state energy. Again the additional counterterms required can be written as functionals of V^μ, but, in addition, one has to subtract the vacuum energy of the free systems (as discussed earlier),

$$E_R = E_{R,internal} - < 0|\hat{H}_{free}|0 > + \delta E[V^\nu] \quad . \tag{57}$$

Note that the decomposition of counterterms chosen here is somewhat arbitrary: One could also obtain E_R by first adding the counterterms which keep the energy of the interacting RHEG finite and subsequently all those counterterms which arise in addition for inhomogeneous systems,

$$E_R = E_{R,internal} + \delta E_{hom} + \delta E_{inhom}[V^\nu] \quad .$$

As an illustrative example for these statements we consider the most simple contributions to j^μ,

$$j^\mu(\boldsymbol{x}) = -tr\Big[\gamma^\mu G^0_{hom}(x-y=0)\Big] + e\int d^4y \; \Pi^{(0),\mu\nu}_{hom}(x,y) \; V_\nu(\boldsymbol{y}) + \ldots \; ,$$

i.e. the first and third diagram of Eq.(54). Here $\Pi^{(0),\mu\nu}_{hom}$ represents the relativistic Lindhard function, the noninteracting limit of the irreducible 2-point function,

$$\chi^{\mu\nu}(x,y) = \Pi^{\mu\nu}(x,y) - ie^2 \int d^4u \int d^4v \; \Pi^{\mu\rho}(x,u) \; D^0_{\rho\lambda}(u-v) \; \chi^{\lambda\nu}(v,y) \quad . \tag{58}$$

Using the decomposition of the electron propagator into a vacuum and an electron gas part, Eq.(22), one explicitly finds that the four current of the noninteracting RHEG is finite,

$$\begin{aligned} j^\mu_{0,hom} &= -tr\Big[\gamma^\mu\Big(G^0_V(x-y=0) + G^0_D(x-y=0)\Big)\Big] \\ &= -4\int \frac{d^4k}{(2\pi)^4}\left\{\frac{ik^\mu}{k^2-m^2+i\epsilon} - 2\pi k^\mu \frac{\delta(k^0-\sqrt{\boldsymbol{k}^2+m^2})}{2\sqrt{\boldsymbol{k}^2+m^2}}\Theta(k_F-|\boldsymbol{k}|)\right\} \\ &= g^{0\mu}\;\frac{k_F^3}{3\pi^2} \quad . \end{aligned} \tag{59}$$

Furthermore, using (22) all electron loops, as e.g. the most simple one constituting $\Pi^{(0),\mu\nu}_{hom}$, can be split into a vacuum contribution (obtained by using G^0_V for all propagators in the graph given) and a density dependent remainder,

$$\Pi^{(0),\mu\nu}_{hom}(x,y) = \Pi^{(0),\mu\nu}_V(x,y) + \Pi^{(0),\mu\nu}_D(x,y) \;, \tag{60}$$

such that

$$j^\mu(\boldsymbol{x}) = g^{0\mu}\;\frac{k_F^3}{3\pi^2} + e\int d^4y\;\Big\{\Pi^{(0),\mu\nu}_V(x,y) + \Pi^{(0),\mu\nu}_D(x,y)\Big\}V_\nu(\boldsymbol{y}) + \ldots \;.$$

For the case of $\Pi^{(0),\mu\nu}_{hom}$ only the pure vacuum contribution $\Pi^{(0),\mu\nu}_V$ diverges. The counterterm necessary to keep $\Pi^{(0),\mu\nu}_V$ finite is well known and leads to

$$\delta j^\mu(\boldsymbol{x}) = \frac{e}{12\pi^2}\Gamma\Big(2-\frac{D}{2}\Big)\partial_\rho\partial^\rho V^\mu(\boldsymbol{x}) \quad , \tag{61}$$

which explicitly exhibits the functional dependence of δj^μ on V^μ (here dimensional regularization has been used [73] — in the physical limit $D \to 4$ the Γ-function diverges like $2/(4-D)$). Note, however, that for more complex diagrams, e.g. those which consist of more than one electron loop, k_F also enters in the required counterterms. In complete analogy one obtains for the energy corresponding to the third diagram in Eq.(54),

$$\delta E_{inhom} = -\frac{e}{2}\int d^3x \; \delta j_\nu(\boldsymbol{x}) \; V^\nu(\boldsymbol{x}) \quad . \tag{62}$$

The counterterms (61,62) will be used subsequently to renormalize the gradient expansion for $T_s[n]$ (compare [41]).

III RELATIVISTIC HOHENBERG-KOHN THEOREM

A HK-theorem for relativistic systems has first been formulated by Rajagopal and Callaway [20] (see also Ref. [23,69]). While their discussion was based on QED, a number of questions which arise in the field theoretical context have not been really addressed, most noticably the problem of UV-divergencies. However, in particular for a proof relying on inequalities between energies it seems important to work with renormalized quantities. Thus in this section we will show explicitly that the scheme for proving a relativistic HK-theorem is not affected by the necessity to introduce counterterms.

The proof proceeds in two steps: First the map between external potentials and ground states is considered, followed by an analysis of the map between external potentials and ground state four currents. The starting point is the Hamiltonian (42) written in terms of the renormalized field operators to eliminate the majority of divergencies from the very outset. To construct a reductio ad absurdum we assume as usual that the two four potentials V^μ and V'^μ,

$$\hat{H}_R = \frac{1}{2}\int d^3x\ \Big[\hat{\overline{\psi}}(\boldsymbol{x}), \Big(-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + m + e\not{V}(\boldsymbol{x}) + e\hat{\not{A}}(\boldsymbol{x})\Big)\hat{\psi}(\boldsymbol{x})\Big] + \hat{H}_{R,\gamma} \tag{63}$$

$$\hat{H}'_R = \frac{1}{2}\int d^3x\ \Big[\hat{\overline{\psi}}(\boldsymbol{x}), \Big(-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + m + e\not{V}'(\boldsymbol{x}) + e\hat{\not{A}}(\boldsymbol{x})\Big)\hat{\psi}(\boldsymbol{x})\Big] + \hat{H}_{R,\gamma} \quad , \tag{64}$$

lead to the same ground state $\mid \Psi >$,

$$\hat{H}_R \mid \Psi > \ = \ E \mid \Psi > \tag{65}$$

$$\hat{H}'_R \mid \Psi > \ = \ E' \mid \Psi > \quad . \tag{66}$$

In Eqs.(65,66) the use of a suitable regularization has to be understood. A complete renormalization, however, is not necessary at this point as we are not aiming at a comparison of energies in this part of the proof. Subtracting both eigenvalue equations,

$$e\int d^3x\ \hat{j}^\nu_R(\boldsymbol{x})\Big[V_\nu(\boldsymbol{x}) - V'_\nu(\boldsymbol{x})\Big]|\Psi> = \Big[E - E'\Big]|\Psi> \quad , \tag{67}$$

one immediately recognizes that the desired contradiction originates from the lacking collinearity of the left and right hand sides in Eq.(67) for arbitrary V^μ and V'^μ: In general, $|\Psi>$ is not an eigenstate of

$$\int d^3x\ \hat{j}^\nu_R(\boldsymbol{x})\Big[V_\nu(\boldsymbol{x}) - V'_\nu(\boldsymbol{x})\Big]$$

as this operator does not commute with the Hamiltonians (63,64). The only exception is found by examining potentials which only differ by a gauge transformation,

$$V'_\nu(\boldsymbol{x}) = V_\nu(\boldsymbol{x}) + \partial_\nu\Lambda(t,\boldsymbol{x}) \tag{68}$$

$$\Lambda(t,\boldsymbol{x}) = ct + \lambda(\boldsymbol{x}) \tag{69}$$

$$\triangle\lambda(\boldsymbol{x}) = 0 \quad , \tag{70}$$

whose general form (23) has here been restricted to transformations connecting static V^μ and V'^μ. Inserting (68) into (67),

$$e\int d^3x\ \Big\{-c\hat{j}^0_R(\boldsymbol{x}) + \Big(\boldsymbol{\nabla}\cdot\hat{\boldsymbol{j}}_R(\boldsymbol{x})\Big)\lambda(\boldsymbol{x})\Big\}|\Psi> = \Big[E - E'\Big]|\Psi> \quad , \tag{71}$$

and using the fact that the total charge operator commutes with the Hamiltonian,

$$\int d^3x\ \hat{j}^0_R(\boldsymbol{x})|\Psi> = \hat{Q}|\Psi> = Q|\Psi> \quad , \tag{72}$$

one finds that four potentials which only differ by an additive constant in their electrostatic component produce identical ground states. As soon as $\nabla\lambda(\boldsymbol{x}) \neq 0$, however, the left hand side of (71) is no longer collinear with $|\Psi>$. In fact, using current conservation one can show that the state $|\Phi>$ generated by this component of (71),

$$\int d^3x\ \Big(\boldsymbol{\nabla}\cdot\hat{\boldsymbol{j}}_R(\boldsymbol{x})\Big)\lambda(\boldsymbol{x})|\Psi> = |\Phi> \neq 0 \quad ,$$

is orthogonal to $|\Psi>$, $<\Psi|\Phi> = 0$. Thus the result of this first part of the HK-proof is completely analogous to the nonrelativistic case: There exists a unique map between the set of four potentials (up to a global constant in V^0) and the set of ground states generated from these potentials.

In the second step one establishes a connection between the external potential and the corresponding four current. Again the proof proceeds by reductio ad absurdum. Assuming that V^μ and V'^μ lead to the same renormalized ground state four current one constructs a contradiction by comparing the renormalized ground state energy (57) of the unprimed and the primed system,

$$\begin{aligned} E_R &= <\Psi|\hat{H}_R|\Psi> + \delta E_{hom} + \delta E_{inhom}[V_\nu] \\ E'_R &= <\Psi|\hat{H}'_R|\Psi> + \delta E_{hom} + \delta E_{inhom}[V'_\nu] \quad . \end{aligned}$$

The basis for relating these quantities in the nonrelativistic context is provided by the Ritz variational principle. An analogous minimum property of the energy has also been used for relativistic systems [20]. While we are not aware of any rigorous minimum principle for renormalized energies of field theoretical systems, it nevertheless seems reasonable to assume its existence: On one hand, in the nonrelativistic limit the renormalized energies approach values which do satisfy the Ritz principle. On the other hand, real systems are stable (indicating that there exists a lower bound for energies) and QED has proven to be the most accurate theory available to date to describe these systems [74] (note that, as a matter of principle, one need not rely on perturbation theory to deal with QED-systems such that the asymptotic character of this expansion does not contradict this argument). On the basis of this physically motivated assumption one then obtains

$$E_R \; < \; <\Psi'|\hat{H}_R|\Psi'> + \delta E_{hom} + \delta E_{inhom}[V_\nu] \quad , \tag{73}$$

where the right hand side is finite due to the fact that $|\Psi>$ does not explicitly enter in $\delta E_{inhom}[V_\nu]$. Now one can add the terms required to generate E'_R on the right hand side,

$$\begin{aligned} E_R \; < \; & E'_R + e\int d^3x \; j^\nu_R \left[V_\nu - V'_\nu\right] \\ & + \delta E_{inhom}[V_\nu] - \delta E_{inhom}[V'_\nu] - e\int d^3x \; \left(\delta j^\nu[V_\nu] \; V_\nu - \delta j^\nu[V'_\nu] \; V'_\nu\right) \quad , \end{aligned}$$

where one has made use of the assumption $j^\mu_R = j'^\mu_R$ and added the counterterms required by (56). Interchanging the role of V^μ and V'^μ and combining both inequalities finally leads to the celebrated contradiction

$$E_R + E'_R < E_R + E'_R \quad .$$

Again potentials differing by gauge transformations represent an exception to this general statement: Clearly, for potentials which only differ by a constant in their electrostatic components the inequality (73) does not hold such that only gauge transformations of the spatial components remain to be discussed. In this case one obtains for the right hand side of (73),

$$<\Psi'|\hat{H}_R|\Psi'> + \delta E_{hom} + \delta E_{inhom}[V_\nu] = E'_R - e\int d^3x \; j^k_R(\boldsymbol{x}) \; \partial_k\lambda(\boldsymbol{x}) = E'_R \quad ,$$

where we have used current conservation. Moreover, all counterterms vanish as the $\chi^{(n),\mu\nu_1\ldots\nu_n}_{c,hom}$ are transverse with respect to their spatial components [72]. The latter argument, however, also implies that $E'_R = E_R$ as in the perturbation expansion of E' in powers of V'^μ all contributions from $\partial_k\lambda(\boldsymbol{x})$ drop out.

Thus we have found that the class of external potentials just differing by gauge transformations uniquely determines the ground state four current and vice versa,

$$\left\{V_\nu(\boldsymbol{x}) \middle| V_\nu(\boldsymbol{x}) + \partial_\nu\Lambda(t,\boldsymbol{x})\right\} \Longleftrightarrow j^\nu_R(\boldsymbol{x}) \quad .$$

Taking this statement together with the result of the first part of the proof one concludes that the class of physically equivalent ground states, i.e. those which result from four potentials just differing by $\partial_k \lambda(\boldsymbol{x})$, is uniquely determined by the four current. Choosing some arbitrary representative of this class, i.e. fixing the gauge, one ends up with the statement that all ground state observables are unique functionals of the four current,

$$O[j^\nu] = < \Psi[j_R^\nu] \mid \hat{O} \mid \Psi[j_R^\nu] > \quad .$$

Of course, DFT has to reflect an eventual gauge dependence of the operator $\hat{O}$ which is transferred into the corresponding functional $O[j^\nu]$.

The most important current functional is the ground state energy,

$$E_R[j_R^\nu] = < \Psi[j_R^\nu] \mid \hat{H}_R \mid \Psi[j_R^\nu] > + \delta E_{hom} + \delta E_{inhom}[V_\nu] \quad .$$

For $E_R[j^\nu]$ the minimum principle guarantees that the insertion of any four current different from the actual ground state four current j_R^ν leads to a higher energy. This then allows (neglecting the question of interacting v-representability) to obtain the exact j_R^ν by solution of a variational equation,

$$\frac{\delta}{\delta j_R^\nu(\boldsymbol{r})} \Big\{ E_R[j_R^\nu] - \mu \int d^3x \; j_R^0(\boldsymbol{x}) \Big\} = 0 \quad , \tag{74}$$

where charge conservation has been imposed.

Thus the final statements of the relativistic HK-theorem are rather similar to their nonrelativistic counterparts. Note, however, that this proof does not only include all relativistic but also all field theoretical, i.e. radiative, effects.

IV NONRELATIVISTIC LIMIT

Before proceeding with the discussion of relativistic DFT it seems appropriate at this point to make a few remarks on the nonrelativistic limit of the basic results obtained so far (see also the contribution by G. Vignale in this Volume). The weakly relativistic form of the Hamiltonian can either be derived from (9) using the Foldy-Wouthuysen transformation or by a direct weakly relativistic expansion,

$$\begin{aligned} \hat{H} \;=\; & \int d^3x \; \hat{\varphi}^+(\boldsymbol{x}) \Big\{ \frac{1}{2m} \Big[(-i\hbar \boldsymbol{\nabla})^2 + 2i\hbar \frac{e}{c} \boldsymbol{V}(\boldsymbol{x}) \cdot \boldsymbol{\nabla} + \frac{e^2}{c^2} \boldsymbol{V}(\boldsymbol{x})^2 \Big] \\ & - \frac{e\hbar}{2mc} \boldsymbol{\sigma} \cdot \Big(\boldsymbol{\nabla} \times \boldsymbol{V}(\boldsymbol{x}) \Big) + eV_0(\boldsymbol{x}) \Big\} \hat{\varphi}(\boldsymbol{x}) + \hat{H}_{ee} \quad . \end{aligned} \tag{75}$$

Here $\hat{\varphi}(\boldsymbol{x})$ denotes a two spinor field operator, $\boldsymbol{\sigma}$ are the usual Pauli matrices and we have not specified the structure of the electron-electron interaction $\hat{H}_{ee}$ which is irrelevant for the present purpose (in the strictly nonrelativistic limit it is just the standard Coulomb repulsion). Note that we have kept the gauge term $(e^2/c^2)\boldsymbol{V}^2$ although it is of the order $1/c^2$ and this order has not been included consistently. For the Hamiltonian (75) all arguments concerning symmetries and the resulting degeneracies given for its relativistic counterpart also apply. Consequently it seems questionable whether extensions of (75) including additional nonphysical couplings between the electrons and the external fields [31] are necessary in order to remove degeneracies.

The nonrelativistic limit of the four current is most conveniently written as a density $\hat{n}$ and a spatial current $\hat{\boldsymbol{j}}$,

$$\hat{j}^0(\boldsymbol{x}) \;=\; \hat{n}(\boldsymbol{x}) = \hat{\varphi}^+(\boldsymbol{x}) \, \hat{\varphi}(\boldsymbol{x}) \tag{76}$$

$$\hat{\boldsymbol{j}}(\boldsymbol{x}) = -\frac{i\hbar}{2m}\Big[\hat{\varphi}^+(\boldsymbol{x})\Big(\boldsymbol{\nabla}\hat{\varphi}(\boldsymbol{x})\Big) - \Big(\boldsymbol{\nabla}\hat{\varphi}^+(\boldsymbol{x})\Big)\hat{\varphi}(\boldsymbol{x})\Big] + \frac{\hbar}{2m}\,\boldsymbol{\nabla}\times\Big(\hat{\varphi}^+(\boldsymbol{x})\boldsymbol{\sigma}\hat{\varphi}(\boldsymbol{x})\Big) - \frac{e}{mc}\,\boldsymbol{V}(\boldsymbol{x})\hat{\varphi}^+(\boldsymbol{x})\hat{\varphi}(\boldsymbol{x}) = \hat{\boldsymbol{j}}_p(\boldsymbol{x}) - \frac{c}{e}\,\boldsymbol{\nabla}\times\hat{\boldsymbol{m}}(\boldsymbol{x}) - \frac{e}{mc}\,\boldsymbol{V}(\boldsymbol{x})\hat{n}(\boldsymbol{x}) \quad , \tag{77}$$

where it is been emphasized that $\hat{\boldsymbol{j}}$ consists of three contributions, the paramagnetic current $\hat{\boldsymbol{j}}_p$, the curl of the magnetization density $\hat{\boldsymbol{m}}$ and a gauge term. Both $\hat{H}$ and the physical current $\hat{\boldsymbol{j}}$ are gauge invariant,

$$\begin{aligned} \hat{\varphi}'(\boldsymbol{x}) &= e^{-ie\lambda(\boldsymbol{x})/\hbar}\,\hat{\varphi}(\boldsymbol{x}) \\ \boldsymbol{V}'(\boldsymbol{x}) &= \boldsymbol{V}(\boldsymbol{x}) - c\boldsymbol{\nabla}\lambda(\boldsymbol{x}) \end{aligned} \quad \Longrightarrow \quad \begin{aligned} H(\hat{\varphi}',\boldsymbol{V}') &= H(\hat{\varphi},\boldsymbol{V}) \\ \boldsymbol{j}(\hat{\varphi}',\boldsymbol{V}') &= \boldsymbol{j}(\hat{\varphi},\boldsymbol{V}) \end{aligned} \quad ,$$

in contrast to $\hat{\boldsymbol{j}}_p$.

For a DFT approach to this system one has to rewrite the Hamiltonian in terms of density/current operators in order to extract the quantities which couple to the external potentials,

$$\hat{H} = \int d^3x\,\Big\{\hat{\varphi}^+(\boldsymbol{x})\frac{(-i\hbar\boldsymbol{\nabla})^2}{2m}\hat{\varphi}(\boldsymbol{x}) + eV_0(\boldsymbol{x})\hat{n}(\boldsymbol{x})\Big\} + \hat{H}_{ee} - \int d^3x\,\frac{e}{c}\,\boldsymbol{V}(\boldsymbol{x})\cdot\Big\{\hat{\boldsymbol{j}}_p(\boldsymbol{x}) - \frac{c}{e}\,\boldsymbol{\nabla}\times\hat{\boldsymbol{m}}(\boldsymbol{x}) - \frac{e}{2mc}\,\boldsymbol{V}(\boldsymbol{x})\hat{n}(\boldsymbol{x})\Big\} \quad . \tag{78}$$

From (78) it is immediately clear that $\hat{\boldsymbol{j}}_p$ and $\hat{\boldsymbol{m}}$ only enter the Hamiltonian in the form

$$\hat{\boldsymbol{j}}_p(\boldsymbol{x}) - \frac{c}{e}\,\boldsymbol{\nabla}\times\hat{\boldsymbol{m}}(\boldsymbol{x})$$

such that only this combination can be used for proving a HK-theorem (but not both components individually). In addition one has to decide how to treat the gauge component of the current. In this respect two choices seem possible at first glance. On one hand one could use the physical current as the quantity coupling to $\boldsymbol{V}$,

$$\hat{H} = \hat{T} + \hat{H}_{ee} + \int d^3x\,\Big\{-\frac{e}{c}\,\boldsymbol{V}(\boldsymbol{x})\cdot\hat{\boldsymbol{j}}(\boldsymbol{x}) + \Big[eV_0(\boldsymbol{x}) - \frac{e^2}{2mc^2}\,\boldsymbol{V}^2(\boldsymbol{x})\Big]\hat{n}(\boldsymbol{x})\Big\} \quad , \tag{79}$$

which would suggest that n and $\boldsymbol{j}$ are the basic variables for a DFT approach (in analogy to the relativistic situation). Alternatively the form

$$\hat{H} = \hat{T} + \hat{H}_{ee} - \int d^3x\,\frac{e}{c}\,\boldsymbol{V}(\boldsymbol{x})\cdot\Big[\hat{\boldsymbol{j}}_p(\boldsymbol{x}) - \frac{c}{e}\,\boldsymbol{\nabla}\times\hat{\boldsymbol{m}}(\boldsymbol{x})\Big] + \int d^3x\,\Big[eV_0(\boldsymbol{x}) + \frac{e^2}{2mc^2}\,\boldsymbol{V}^2(\boldsymbol{x})\Big]\hat{n}(\boldsymbol{x}) \tag{80}$$

would identify n and $< \hat{\boldsymbol{j}}_p - (c/e)\boldsymbol{\nabla}\times\hat{\boldsymbol{m}} >$ as basic variables. However, while for the latter choice a HK-theorem can be proven [30] it seems impossible to do so for (79) the gauge term being the crucial problem. It appears that this problem is intrinsically related to the inconsistent expansion in powers of $1/c$ one is using in (75) as neglecting all contributions of the order $1/c^2$ also allows for proving a HK-theorem using $\boldsymbol{j}$ and n as basic variables.

V RELATIVISTIC KOHN-SHAM EQUATIONS

As for the nonrelativistic case one method to minimize the total energy functional is provided by the KS-equations [21]. Their relativistic extension has been introduced by Rajagopal [22] as well as MacDonald and Vosko [23] (see also [69]). As for the HK-theorem, however, the problem of radiative corrections has not been addressed in this context. Thus in the following we will formulate the KS-equations in a way which consistently includes vacuum corrections.

The starting point is a decomposition of the total energy functional into the kinetic energy functional of noninteracting particles $T_s[j^\mu]$, the external potential energy, a Hartree-like contribution $E_H[j^\mu]$ and the exchange-correlation energy functional $E_{xc}[j^\mu]$,

$$E[j^\nu] = T_s[j^\nu] + e\int d^3x\; j^\nu(\boldsymbol{x})V_\nu(\boldsymbol{x}) + E_H[j^\nu] + E_{xc}[j^\nu] \quad , \tag{81}$$

which essentially represents the definition of $E_{xc}[j^\mu]$. While the functional dependence of T_s on j^μ is not known explicitly, T_s can be expressed exactly in terms of the single particle four spinors $\varphi_n(\boldsymbol{x})$ resulting from a given local external potential (see e.g. [2]),

$$\begin{aligned} T_s[j^\nu] &= \frac{1}{2}\int d^3x \Big\{ \sum_{\epsilon_n\le\epsilon_F} \overline{\varphi}_n(\boldsymbol{x})\big[-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}+m\big]\varphi_n(\boldsymbol{x}) \\ &\qquad - \sum_{\epsilon_n>\epsilon_F} \overline{\varphi}_n(\boldsymbol{x})\big[-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}+m\big]\varphi_n(\boldsymbol{x})\Big\} - \delta T_s^{vac} \quad . \end{aligned}$$

Here the difference between the kinetic energies of occupied ($\epsilon_n \le \epsilon_F$) and unoccupied ($\epsilon_n > \epsilon_F$) single particle states is a consequence of the charge conjugation invariant form of the Hamiltonian, Eq.(9). The subtraction of δT_s^{vac} eliminates the (divergent) energy of the noninteracting free Fermi sea as discussed earlier. $T_s[j^\nu]$ can be decomposed into a vacuum contribution $T_{s,V}$ and the kinetic energy $T_{s,D}$ of the real electrons bound by the external potential (characterised by their eigenvalues between $-m$ and ϵ_F),

$$\begin{aligned} T_s[j^\nu] &= \frac{1}{2}\int d^3x \Big\{ \sum_{\epsilon_n\le -m} \overline{\varphi}_n(\boldsymbol{x})\big[-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}+m\big]\varphi_n(\boldsymbol{x}) \\ &\qquad - \sum_{\epsilon_n>-m} \overline{\varphi}_n(\boldsymbol{x})\big[-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}+m\big]\varphi_n(\boldsymbol{x})\Big\} - \delta T_s^{vac} \\ &\quad + \int d^3x \sum_{-m<\epsilon_n\le\epsilon_F} \overline{\varphi}_n(\boldsymbol{x})\big[-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}+m\big]\varphi_n(\boldsymbol{x}) \\ &= T_{s,V} + T_{s,D} \quad . \end{aligned} \tag{82}$$

The four current of noninteracting particles is obtained from the single particle spinors by

$$\begin{aligned} j^\nu(\boldsymbol{x}) &= \frac{1}{2}\Big\{ \sum_{\epsilon_n\le -m} \overline{\varphi}_n(\boldsymbol{x})\gamma^\nu\varphi_n(\boldsymbol{x}) - \sum_{\epsilon_n>-m} \overline{\varphi}_n(\boldsymbol{x})\gamma^\nu\varphi_n(\boldsymbol{x})\Big\} + \delta j^\nu_{vac}(\boldsymbol{x}) \\ &\quad + \sum_{-m<\epsilon_n\le\epsilon_F} \overline{\varphi}_n(\boldsymbol{x})\gamma^\nu\varphi_n(\boldsymbol{x}) \\ &= j^\nu_V(\boldsymbol{x}) + j^\nu_D(\boldsymbol{x}) \quad . \end{aligned} \tag{83}$$

Note that in order to treat the vacuum polarization current $j^\nu_V(\boldsymbol{x})$ and the corresponding vacuum correction to T_s consistently not only knowledge of all occupied states is required, but rather all continuum states must also be known which represents an enormous difficulty in real applications. For the direct electron-electron interaction energy

(Hartree term) it seems reasonable to choose the covariant form

$$E_H[j^\nu] = -i\frac{e^2}{2}\int d^3x \int d^4y \; j^\mu(\boldsymbol{x}) \; D^0_{\mu\nu}(x-y) \; j^\nu(\boldsymbol{y}) \tag{84}$$

rather than just its density-density contribution [23]. However, other choices are also possible and simply amount to a redefinition of $E_{xc}[j^\mu]$. In (85) $D^0_{\mu\nu}$ represents the free photon propagator,

$$D^0_{\mu\nu}(x-y) = -ig_{\mu\nu}\int \frac{d^4k}{(2\pi)^4}\,\frac{e^{-ik(x-y)}}{k^2+i\epsilon} \quad , \tag{85}$$

(Feynman gauge) such that E_H reduces to the familiar form

$$E_H[j^\nu] = \frac{e^2}{2}\int d^3x \int d^3y \; \frac{j^\nu(\boldsymbol{x})\; j_\nu(\boldsymbol{y})}{4\pi|\boldsymbol{x}-\boldsymbol{y}|} \quad .$$

Minimizing (81) with respect to auxilliary single particle spinors by which T_s and j^μ are constructed via (82,83) then leads to the relativistic KS-equations,

$$\gamma^0\Big\{ -i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla} + m + e\not{V}(\boldsymbol{x}) + \not{v}_H(\boldsymbol{x}) + \not{v}_{xc}(\boldsymbol{x})\Big\}\varphi_n(\boldsymbol{x}) = \epsilon_n\varphi_n(\boldsymbol{x}) \quad , \tag{86}$$

where

$$v^\nu_H(\boldsymbol{x}) \;=\; e^2\int d^3y \;\frac{j^\nu(\boldsymbol{y})}{4\pi|\boldsymbol{x}-\boldsymbol{y}|} \tag{87}$$

$$v^\nu_{xc}(\boldsymbol{x}) \;=\; \frac{\delta E_{xc}[j^\mu]}{\delta j_\nu(\boldsymbol{x})} \quad . \tag{88}$$

Assuming that the exact ground state four current of the interacting system is noninteracting v-representable this procedure generates the exact j^μ and the exact ground state energy,

$$\begin{aligned} E \;=\; & \frac{1}{2}\Big\{\sum_{\epsilon_n\le -m}\epsilon_n - \sum_{\epsilon_n>-m}\epsilon_n\Big\} - \delta T_s^{vac} \\ & + \sum_{-m<\epsilon_n\le\epsilon_F}\epsilon_n - E_H[j^\nu] + E_{xc}[j^\nu] - \int d^3x\; v^\nu_{xc}(\boldsymbol{x})\; j_\nu(\boldsymbol{x}) \quad . \end{aligned} \tag{89}$$

where the first line represents the so-called Casimir energy, i.e. the energy shift induced in the vacuum by the presence of the inhomogeneous KS potential. Note, however, that all other energy contributions in (89) also contain radiative corrections. Of course, in (89) $E_{xc}[j^\mu]$ is implicitly understood to be renormalized, i.e. renormalization has to be taken care of in the construction of any approximation for this functional.

It should be emphasized at this point that the complete KS-scheme simplifies considerably if all radiative corrections are neglected. As a matter of fact, we are not aware of any applications of the KS-equations in which vacuum corrections would have been included.

VI TECHNIQUES AND EXPLICIT FUNCTIONALS

In this section we will give an overview over the methods for constructing explicit relativistic functionals utilized so far. While most of the elaborate techniques available in the nonrelativistic case have been extended to the relativistic domain, their actual application turns out to be much more cumbersome. As a result the present knowledge about relativistic functionals is rather limited.

VI.1 Coupling constant integration approach to $E_{xc}[j^\nu]$

We start with a brief summary of the relativistic coupling constant integration method [75,76,29] and the approximations for $E_{xc}[j^\nu]$ obtained on its basis. Modifying the coupling strength between electrons and photons by a parameter λ,

$$\hat{H}_{ee} = \sqrt{\lambda}\; e \int d^3x\; \hat{j}^\nu(x)\; \hat{A}_\nu(x) \quad , \tag{90}$$

(where e has been scaled by $\sqrt{\lambda}$ to keep the analogy to the nonrelativistic case as close as possible) and adjusting the external four potential such that for all λ the same ground state four current is produced,

$$\hat{H}_{ext} = e \int d^3x\; \hat{j}^\nu(x)\; V_{\nu,\lambda}(\boldsymbol{x}) \quad , \tag{91}$$

the standard differentiation of the ground state energy with respect to λ leads to

$$\begin{aligned} E(\lambda = 1) \;&=\; E(\lambda=0) + \frac{e}{2}\int_0^1 \frac{d\lambda}{\sqrt{\lambda}} \int d^3x \;\; < \Psi_\lambda | \hat{j}^\nu(x) \hat{A}_\nu(x) | \Psi_\lambda > \\ &\quad + e \int d^3x\; j_\nu(\boldsymbol{x}) \left[V^\nu_{\lambda=1}(\boldsymbol{x}) - V^\nu_{\lambda=0}(\boldsymbol{x}) \right] \quad , \end{aligned} \tag{92}$$

where $|\Psi_\lambda>$ is the normalized ground state for given coupling strength. Now one can rewrite the kernel of the coupling constant integral in terms of the reducible current-current response function of the inhomogeneous system with coupling strength λ,

$$\begin{aligned} < \Psi_\lambda | \hat{j}^\nu(x) \hat{A}_\nu(x) | \Psi_\lambda > \;&=\; -ie\sqrt{\lambda} \int d^4y\; j^\mu(\boldsymbol{x})\; D^0_{\mu\nu}(x-y)\; j^\nu(\boldsymbol{y}) \\ &\quad + e\sqrt{\lambda} \int d^4y\; D^0_{\mu\nu}(x-y)\; \chi^{\mu\nu}_\lambda(x,y) \quad . \end{aligned} \tag{93}$$

Inserting (93) into (92) and comparing the result with (81) one finds a covariant representation for $E_{xc}[j^\nu]$,

$$E_{xc}[j^\nu] = \frac{e^2}{2}\int_0^1 d\lambda \int d^3x \int d^4y\; D^0_{\mu\nu}(x-y)\; \chi^{\mu\nu}_\lambda(x,y) \quad . \tag{94}$$

While this representation is formally exact, its usefulness is nevertheless limited by the enormous complexity of its main ingredient $\chi^{\mu\nu}_\lambda(x,y)$. Thus in practice (94) has only been utilized for deriving LDA functionals. The exchange-correlation energy density of the RHEG is given in terms of the corresponding response function as [75,76,29]

$$e^{LDA}_{xc}(n) = \frac{e^2}{2}\int_0^1 d\lambda \int d^4y\; D^0_{\mu\nu}(x-y)\; \chi^{\mu\nu}_{\lambda,hom}(x-y) \quad , \tag{95}$$

where we have restricted the discussion to unpolarized systems for simplicity. As there exists no spatial current in the unpolarized RHEG all energy contributions are functionals of the density n only. Eq.(95) has essentially been the basis for evaluating (i) the lowest order exchange contribution to the RHEG, and (ii) the RPA-contribution to the correlation energy density.

The exchange energy density of the RHEG has been calculated by a number of authors [75,77,76,22,23] (see [78–81] for the spin-polarized case). It is obtained from

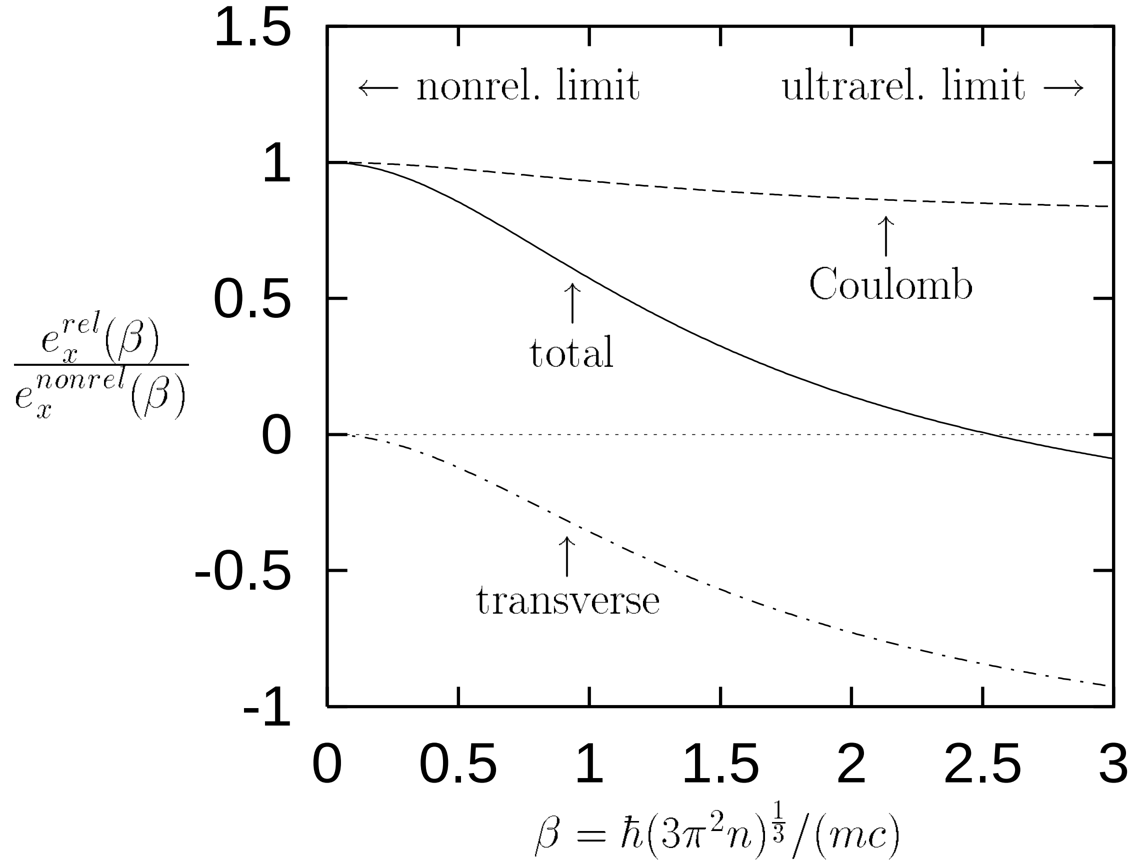


Figure 1: Relativistic corrections to the LDA exchange energy density: Total correction (97), Coulomb contribution (99) and transverse contribution (100).

(95) by replacing the complete $\chi^{\mu\nu}_{\lambda,hom}$ by its noninteracting limit, i.e. the relativistic Lindhard function $\Pi^{(0),\mu\nu}_{hom}$, Eq.(60),

$$e_x^{LDA}(n) = \frac{e^2}{2}\int d^4y \; D^0_{\mu\nu}(x-y)\; \Pi^{(0),\mu\nu}_{hom}(x-y) \quad . \tag{96}$$

The remaining loop integration can be performed analytically,

$$e_x^{LDA}(n) = c_{0x} n^{\frac{4}{3}} \left\{ 1 - \frac{3}{2}\left[\frac{\eta}{\beta} - \frac{1}{\beta^2} arsinh(\beta)\right]^2 \right\} \quad , \tag{97}$$

where β and η abbreviate the characteristic basic variables of relativistic functionals,

$$\beta = \frac{(3\pi^2 n)^{\frac{1}{3}}}{m} \qquad ; \qquad \eta = (1+\beta^2)^{\frac{1}{2}} \quad . \tag{98}$$

Note that while the inclusion of vacuum contributions in (96) requires renormalization [71,41], they do not contribute to e_x^{LDA}. In Eq.(97) e_x^{LDA} has been written as a product of its nonrelativistic limit $c_{0x} n^{\frac{4}{3}}$ and a relativistic correction factor. The latter is plotted in Fig.1 as a function of β. Also shown in Fig.1 is the standard decomposition of e_x^{LDA} into e_x^{Cou} representing the nonretarded density-density contribution and the remainder, called the transverse contribution,

$$\begin{aligned} e_x^{Cou} &= -\frac{e^2}{2}\int d^3y \; \frac{tr[\gamma^0 G(x,y)\gamma^0 G(y,x)]}{4\pi|\boldsymbol{x}-\boldsymbol{y}|}\Big|_{x^0=y^0} \qquad (99) \\ e_x^{tr} &= e_x^{total} - e_x^{Cou} \quad . \end{aligned}$$

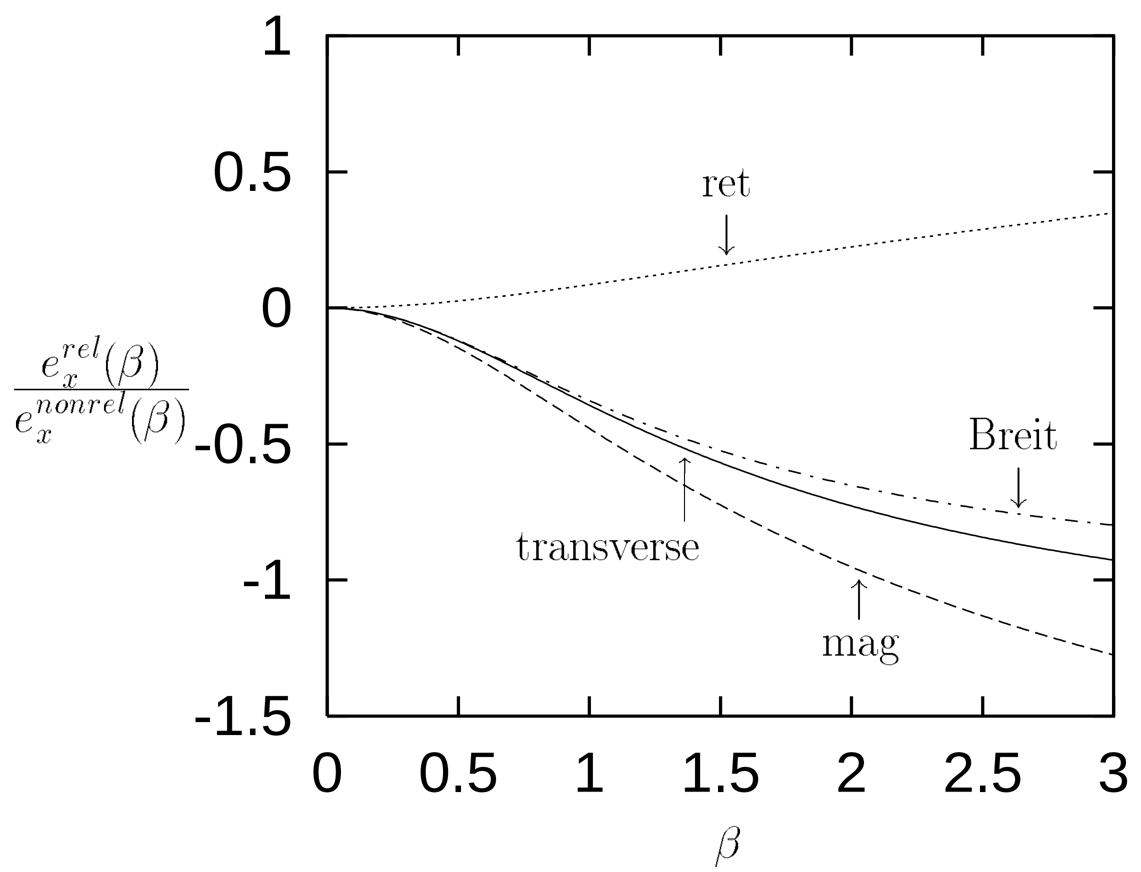


Figure 2: Relativistic corrections to the LDA exchange energy density: Magnetic, retardation and Breit contribution (e_x^{Breit} from Ref. [7] has been corrected for a typographical error).

Fig.1 demonstrates that in the nonrelativistic limit $\beta \to 0$ the Coulomb contribution dominates completely. However, while e_x^{Cou} is only weakly dependent on β, the tranverse part of e_x starts to increase rapidly with β and dominates in the ultrarelativistic limit in which e_x^{total} even changes its sign.

The origin of this high density behaviour can be traced somewhat further by a decomposition of the transverse contribution into a magnetic (current-current) and a retardation component,

$$\begin{aligned} e_x^{tr} &= e_x^{mag} + e_x^{ret} \qquad (100) \\ e_x^{mag} &= -\frac{e^2}{2}\int d^4y \int \frac{d^4k}{(2\pi)^4}\,\frac{e^{-ik(x-y)}}{k^2+i\epsilon}\; tr\Big[\gamma^j G(x,y)\gamma^j G(y,x)\Big] \\ e_x^{ret} &= \frac{e^2}{2}\int d^4y \int \frac{d^4k}{(2\pi)^4}\, e^{-ik(x-y)}\left[\frac{1}{k^2+i\epsilon}+\frac{1}{\boldsymbol{k}^2}\right] tr\Big[\gamma^0 G(x,y)\gamma^0 G(y,x)\Big] \quad , \end{aligned}$$

where (85) has been used to separate e_x^{Cou} from the total density-density contribution. Moreover, the first order term of the weakly relativistic expansion of e_x^{tr} represents the so-called Breit contribution [5],

$$\begin{aligned} e_x^{Breit} &= \frac{e^2}{2}\int d^3y\, \frac{tr[\gamma^j G(x,y)\gamma^j G(y,x)]}{4\pi|\boldsymbol{x}-\boldsymbol{y}|}\bigg|_{x^0=y^0} \\ &\quad -\frac{e^2}{2}\int d^4y \int \frac{d^4k}{(2\pi)^4}\, e^{-ik(x-y)}\,\frac{(k^0)^2}{\boldsymbol{k}^4}\; tr\Big[\gamma^0 G(x,y)\gamma^0 G(y,x)\Big] \quad . \end{aligned}$$

The corresponding LDA forms [7] are shown in Fig.2. While the retardation corrections

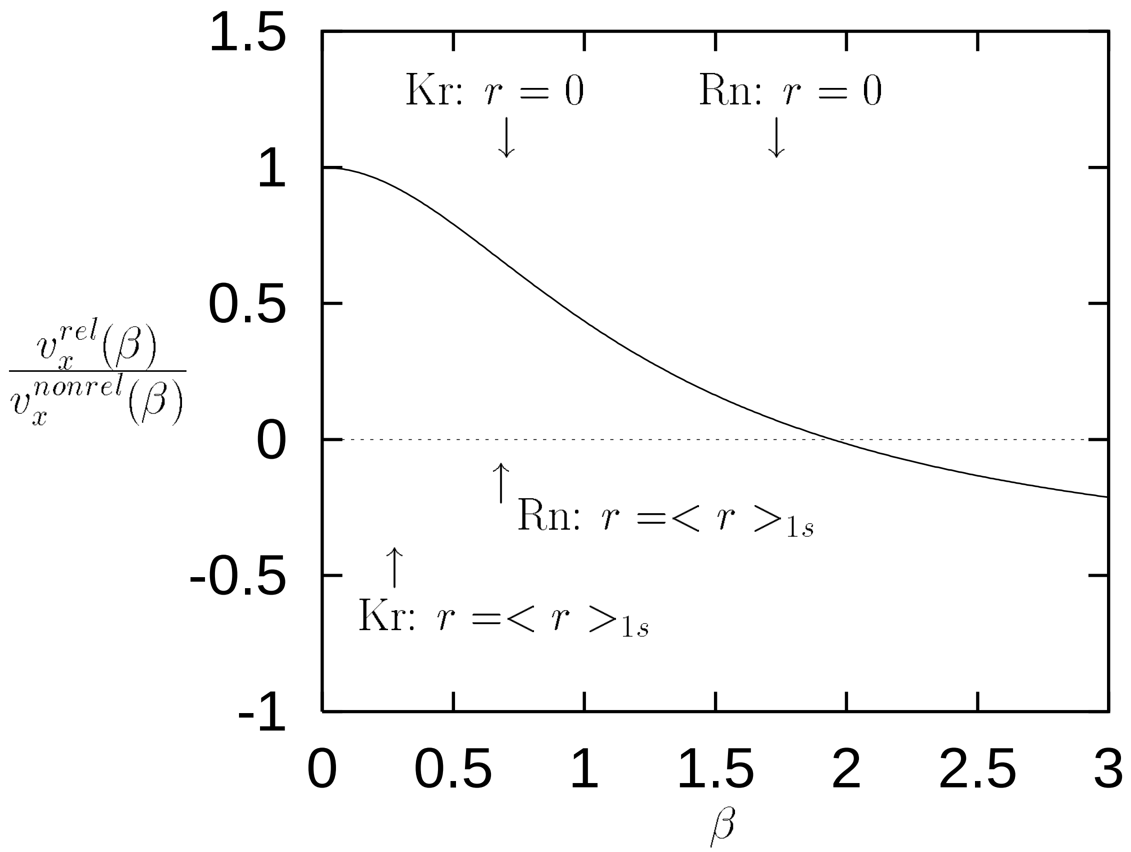


Figure 3: Relativistic correction to the total LDA exchange potential. The values of the densities of Kr and Rn at the origin ($r = 0$) and the r-expectation values of the $1s$-orbitals ($r =< r >_{1s}$) within nonrelativistic calculations are also indicated.

to e_x^{Cou} are comparably small and attractive, the dominating current-current component of e_x^{tr} is responsible for the sign change of e_x^{total}. This reflects the fact that the current-current contribution to E_H also has the opposite sign of the electrostatic component. Moreover, the nonretarded current-current contribution represents the major ingredient of e_x^{tr} as can be seen from the similarity of e_x^{tr} and e_x^{Breit} (compare [5]). In view of the dominating role of the current-current contribution, however, it seems questionable whether including e_x^{tr} is consistent with neglecting the spatial components of the Hartree potential.

The relativistic corrections are even more pronounced in the LDA exchange potential shown in Fig.3. Here we have also indicated the β-values at the origin and the r-expectation values of the $1s$-orbitals obtained by nonrelativistic calculations for Kr and Rn which give an idea to which extent these relativistic corrections actually affect the description of atomic systems. While from this comparison one would expect negligible corrections for atoms smaller than Kr, the difference between the nonrelativistic and relativistic forms of e_x^{LDA} should definitely be relevant for high Z atoms, in particular, taking into account that densities from relativistic calculations are even more concentrated around the origin.

Some numbers obtained for neutral Mercury may illustrate this point. As Table 1 shows the relativistic correction to the Coulomb exchange energy is larger than the difference between the nonrelativistic LDA result and the exact exchange-only energy ($-345.24 a.u.$ [83]), i.e. larger than the nonlocal correction to the nonrelativistic E_x. The total relativistic correction, on the other hand, is only about $2 a.u.$ as E_x^{tr} almost cancels with the relativistic correction to E_x^{Cou}. This result, however, should not be interpreted as an indication that relativistic effects are irrelevant for the exchange energy functional: When going from a nonrelativistic to a relativistic treatment the

	E_x	E_x^{Cou}	E_x^{tr}	E_x^{mag}	E_x^{ret}	E_x^{Breit}
NRHF	—	-345.30	—	—	—	—
NRLDA(NRLDA)	—	-331.88	—	—	—	—
NRLDA(LDA)	—	-353.55	—	—	—	—
HF	-343.11	-365.28	22.17	24.50	-2.33	22.66
LDA(HF)	-313.67	-347.93	34.25	42.47	-8.23	32.69
LDA(LDA)	-313.02	-347.02	34.00	42.16	-8.16	32.47
LDA(NRLDA)	-303.80	-327.31	23.51	28.83	-5.32	22.76

Table 1: Various contributions to the relativistic exchange energy of Hg: NRHF — nonrel. HF result [4], NRLDA(NRLDA) — nonrel. LDA functional with nonrel. LDA density, NRLDA(LDA) — nonrel. LDA functional with rel. LDA density, HF — rel. HF results [5,82], LDA(HF) — rel. LDA functionals with rel. HF density [7,82], LDA(LDA) — rel. LDA functionals with rel. LDA density [7], LDA(NRLDA) — rel. LDA functionals with nonrel. LDA density (all energies are in $a.u.$).

value of E_x on one hand changes due to the difference between the relativistic and the nonrelativistic density inserted in $E_x[n]$ and on the other hand due to the modified functional dependence of $E_x[n]$ on the density. In the LDA the former effect amounts to $-22a.u.$ (see the difference between E_x^{Cou} from NRLDA(LDA) and NRLDA(NRLDA) given in Table 1), while the latter contribution is of the order of $40a.u.$ (i.e. the difference between E_x^{Cou} from NRLDA(LDA) and E_x from LDA(LDA)). The sum of both contributions ($18a.u.$) very well reproduces the total relativistic correction found in the LDA which, however, completely misrepresents the HF result. As the form of the density is rather independent of the specific $E_x[n]$ used for its calculation one thus concludes that the relativistic modification of the functional dependence of $E_x^{LDA}[n]$ on n introduces an error of roughly 66%. This large error can be traced to the individual components. While the relativistic correction to E_x^{Cou} is underestimated by the LDA, the E_x^{tr} is overestimated. Inside E_x^{tr} the magnetic term E_x^{mag} dominates over E_x^{ret}, both components of E_x^{LDA} again being considerably different from their HF counterparts. Analyzing the relativistic corrections to the individual KS-orbitals [7] one finds that the major contribution to E_x^{tr} comes from the innermost $1s_{1/2}$-orbital, as is to be expected. In particular in the context of a relativistic calculation where the density close to the nucleus is rather inhomogeneous it is thus not surprising that the LDA gives rather inaccurate results for E_x^{tr} and its various components. In any case, both HF and LDA results show that E_x^{Breit} is a good approximation to the complete E_x^{tr}.

As far as the LDA for the correlation energy is concerned only the RPA is known to date [75,76,29]. It is obtained by approximating the complete $\chi^{\mu\nu}_{\lambda,hom}$ in (95) by its ring diagram form, i.e. using the Dyson equation (58) with the Lindhard function (60) as irreducible kernel. Utilizing the general tensor structure of the vacuum 2-point function,

$$\Pi_V^{\mu\nu}(q) = \Big(q^2 g^{\mu\nu} - q^\mu q^\nu\Big)\Pi_R(q^2) \quad , \tag{101}$$

and decomposing the density dependent part of $\Pi^{(0),\mu\nu}_{hom}$ somewhat further (according to (22),

$$\Pi_D^{(0),\mu\nu}(q) = \Pi_{VD}^{(0),\mu\nu}(q) + \Pi_{DV}^{(0),\mu\nu}(q) + \Pi_{DD}^{(0),\mu\nu}(q) \quad ,$$

one obtains for the exchange-correlation energy density [84],

$$e_{x,s}(n) \;=\; -i\frac{e^2}{2}\int \frac{d^4q}{(2\pi)^4}\,\frac{\Pi^{(0)}_{DD,\nu}{}^{\nu}(q)}{q^2[1+e^2\Pi_R^{(0)}(q^2)]+i\epsilon} \tag{102}$$

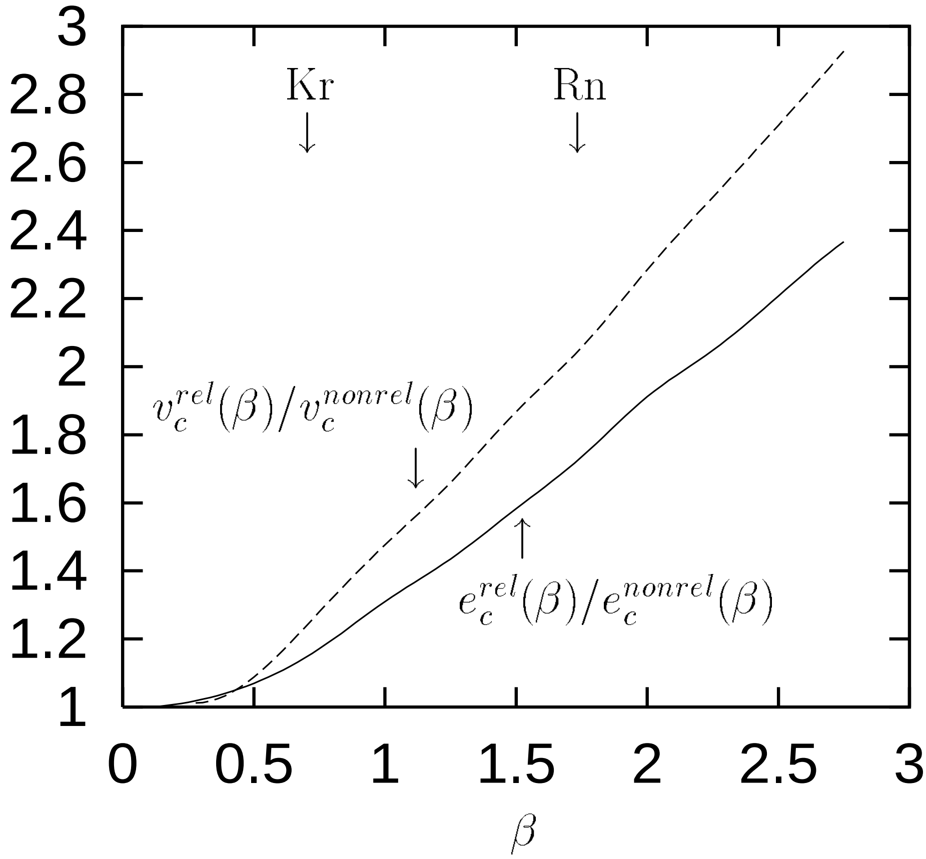


Figure 4: Relativistic corrections to the RPA correlation energy functional: $e_c^{rel}(\beta)/e_c^{nonrel}(\beta)$ — solid line, $v_c^{rel}(\beta)/v_c^{nonrel}(\beta)$ — dashed line (produced from data given in Ref. [29]). The values of the densities of Kr and Rn at the origin (from non-relativistic calculations) are also indicated.

$$e_{c,s}^{RPA}(n) \;=\; -\frac{i}{2}\int \frac{d^4q}{(2\pi)^4}\; Tr\Bigg\{ \ln\left[g_\mu{}^\nu + e^2 \frac{\Pi^{(0)}_{D,\mu}{}^{\nu}(q)}{q^2[1+e^2\Pi_R^{(0)}(q^2)]+i\epsilon}\right] - e^2 \frac{\Pi^{(0)}_{D,\mu}{}^{\nu}(q)}{q^2[1+e^2\Pi_R^{(0)}(q^2)]+i\epsilon}\Bigg\} \;. \qquad (103)$$

As to be expected the vacuum polarization $\Pi_R^{(0)}$ screenes the free electron-electron interaction which suggests the decomposition of the complete RPA exchange-correlation energy into a screened exchange contribution $e_{x,s}(n)$ (which, of course, is no longer linear in e^2 like (96)) and a screened correlation part $e_{c,s}^{RPA}(n)$. Neither $e_{x,s}(n)$ nor $e_{c,s}^{RPA}(n)$, however, have been evaluated so far. As for the case of exchange the RPA correlation energy (103) has only been calculated [29] for $\Pi_R^{(0)}(q) = 0$. The resulting $e_c^{RPA}(n)$ is plotted in Fig.4. As for $e_x^{LDA}(n)$ the relativistic correction to $e_c^{RPA}(n)$ is substantial, the correlation potential being somewhat more affected than the energy density. Note further, that the relativistic RPA functional approaches its nonrelativistic limit only for densities below those for which one expects the RPA to give realistic results (below $r_s \approx 0.01 a.u. \Rightarrow \beta \approx 1.4$). It is thus not clear whether knowledge of $e_c^{RPA}(n)$ is sufficient for extending electronic structure calculations to the relativistic domain as the relativistic corrections to correlation contributions beyond the RPA could be sizable. Moreover, as in the nonrelativistic case the LDA/RPA overestimates total atomic correlation energies considerably [7]. It remains to be examined how accurately the LDA/RPA reproduces the corresponding relativistic corrections. However, one would not expect the quality of the LDA/RPA for E_c in this respect to be very different from that of E_x^{LDA}. In any case the absolute size of the relativistic correction to E_c is rather small: Within the LDA for the RPA one obtains $E_c^{LDA} = -10.35a.u.$ [7] in the case of Hg which is only marginally larger than the corresponding nonrelativistic value of $-10.16a.u.$. This simply reflects the fact that the relativistic correction to E_c for the $1s_{1/2}$-orbital is rather small ($0.08a.u.$) [7].

VI.2 Linear response

Relativistic linear response corrections to the LDA have already been introduced in the seminal work on relativistic DFT by Rajagopal and Callaway [20]. Actual applications of this approach, however, are not known so far. In order to illustrate its general structure and to demonstrate the consistency of the various techniques for evaluating nonlocal corrections we here use the scheme to derive gradient corrections to $T_s[j^\mu]$.

We start with a brief outline of the method. Assuming V^μ to be a weak perturbation one obtains as induced density to first order in V^μ,

$$\begin{aligned} \delta j^\mu(\boldsymbol{x}) &= e\int d^4y\ \chi^{\mu\nu}_{hom}(x-y)\ V_\nu(\boldsymbol{y}) \\ &= e\int d^3y\ \chi^{\mu\nu}_{hom}(q^0=0,\boldsymbol{x}-\boldsymbol{y})\ V_\nu(\boldsymbol{y}) \quad . \end{aligned} \tag{104}$$

Charge conservation requires the induced charge distribution $\delta j^0(\boldsymbol{x})$ to integrate to zero,

$$j^0(\boldsymbol{x}) = n_0 + \delta j^0(\boldsymbol{x}) \qquad ; \qquad \int d^3x\ \delta j^0(\boldsymbol{x}) = 0 \quad , \tag{105}$$

while the spatial current $\boldsymbol{j}(\boldsymbol{x}) = \delta\boldsymbol{j}(\boldsymbol{x})$ (the current vanishes for the unperturbed system, the RHEG) has to satisfy current conservation, $\nabla\cdot\delta\boldsymbol{j}(\boldsymbol{x}) = 0$. Defining the inverse static response functions by

$$\begin{aligned} \chi^{\mu\nu}_{hom}(q^0=0,\boldsymbol{q})\ \chi^{-1,(0)}_{hom,\nu\rho}(q^0=0,\boldsymbol{q}) &= g^\mu{}_\rho + f(\boldsymbol{q}^2)g^{\mu i}q_i g_{\rho j}q^j \\ \Pi^{\mu\nu}_{hom}(q^0=0,\boldsymbol{q})\ \Pi^{-1,(0)}_{hom,\nu\rho}(q^0=0,\boldsymbol{q}) &= g^\mu{}_\rho + f(\boldsymbol{q}^2)g^{\mu i}q_i g_{\rho j}q^j \quad , \end{aligned}$$

(note that the transverse component $f(\boldsymbol{q}^2)q^iq_j$ is irrelevant in the following due to current conservation) one can evaluate the linear response contributions to T_s and E_{xc} [20] in complete analogy to the nonrelativistic case,

$$\begin{aligned} \delta T_s^{LR} &= -\frac{1}{2}\int\frac{d^3q}{(2\pi)^3}\ \delta j^\mu(\boldsymbol{q})\ \Pi^{-1,(0)}_{hom,\mu\nu}(q^0=0,\boldsymbol{q})\ \delta j^\nu(-\boldsymbol{q}) \\ \delta E_{xc}^{LR} &= \frac{1}{2}\int\frac{d^3q}{(2\pi)^3}\ \delta j^\mu(\boldsymbol{q})\Big[\Pi^{-1,(0)}_{hom,\mu\nu}(0,\boldsymbol{q}) - \Pi^{-1}_{hom,\mu\nu}(0,\boldsymbol{q})\Big]\delta j^\nu(-\boldsymbol{q}) \quad . \end{aligned}$$

Explicitly the tensor structure of the static response function is given by [85]

$$\Pi^{\mu\nu}_{hom}(q^0=0,\boldsymbol{q}) = \begin{pmatrix} \Pi_L(\boldsymbol{q}^2) & 0 \quad 0 \quad 0 \\ \begin{matrix}0\\0\\0\end{matrix} & \left(\delta_{ij} - \dfrac{q^iq^j}{\boldsymbol{q}^2}\right)\Pi_T(\boldsymbol{q}^2) \end{pmatrix} \tag{106}$$

and consequently the corresponding inverse reads

$$\Pi^{-1,\mu\nu}_{hom}(q^0=0,\boldsymbol{q}) = \begin{pmatrix} \dfrac{1}{\Pi_L(\boldsymbol{q}^2)} & 0 \quad 0 \quad 0 \\ \begin{matrix}0\\0\\0\end{matrix} & \left(\delta_{ij} - \dfrac{q^iq^j}{\boldsymbol{q}^2}\right)\dfrac{1}{\Pi_T(\boldsymbol{q}^2)} \end{pmatrix} \quad , \tag{107}$$

such that the δT_s^{LR} and δE_{xc}^{LR} are determined by the two scalar functions Π_L and Π_T,

$$\delta T_s^{LR} = -\frac{1}{2}\int\frac{d^3q}{(2\pi)^3}\left\{\frac{\delta n(\boldsymbol{q})\,\delta n(-\boldsymbol{q})}{\Pi_L^{(0)}(\boldsymbol{q}^2)} + \frac{\delta j^k(\boldsymbol{q})\,\delta j^l(-\boldsymbol{q})}{\Pi_T^{(0)}(\boldsymbol{q}^2)}\Big(\delta_{kl} - \frac{q^k q^l}{\boldsymbol{q}^2}\Big)\right\} \tag{108}$$

$$\begin{aligned}\delta E_{xc}^{LR} = \frac{1}{2}\int\frac{d^3q}{(2\pi)^3}\Big\{&\delta n(\boldsymbol{q})\Big[\frac{1}{\Pi_L^{(0)}(\boldsymbol{q}^2)} - \frac{1}{\Pi_L(\boldsymbol{q}^2)}\Big]\delta n(-\boldsymbol{q}) \\ &+ \delta j^k(\boldsymbol{q})\Big[\frac{1}{\Pi_T^{(0)}(\boldsymbol{q}^2)} - \frac{1}{\Pi_T(\boldsymbol{q}^2)}\Big]\delta j^l(-\boldsymbol{q})\Big(\delta_{kl} - \frac{q^k q^l}{\boldsymbol{q}^2}\Big)\Big\}\ .\end{aligned} \tag{109}$$

Unfortunately, only the noninteracting $\Pi_L^{(0)}$ and $\Pi_T^{(0)}$ are known [76] which prevents a direct application of (109) for the construction of nonlocal corrections to $E_{xc}[j^\mu]$. Moreover, we are not aware of any application of (108).

Eqs.(108,109) can also be used to evaluate gradient corrections. To this aim an expansion of Π_L and Π_T in powers of $\boldsymbol{q}^2$ is required. For their noninteracting limits one finds

$$\begin{aligned}\frac{1}{\Pi_L^{(0)}(\boldsymbol{q}^2)} &= -\frac{\pi^2}{k_F E_F}\Big\{1 + \frac{1}{12}\Big[1 + 2\frac{k_F}{E_F}arsinh\Big(\frac{k_F}{m}\Big)\Big]\frac{\boldsymbol{q}^2}{k_F^2} + \ldots\Big\} \\ \frac{1}{\Pi_T^{(0)}(\boldsymbol{q}^2)} &= -\frac{6\pi^2}{arsinh(k_F/m)\boldsymbol{q}^2} + \ldots\ .\end{aligned}$$

where $E_F = \sqrt{m^2 + k_F^2}$. Insertion into Eqs.(108,109) and subsequent Fourier transformation leads to

$$\begin{aligned}\delta T_s^{[2]}[j^\nu] = &\frac{1}{24\pi^2}\int d^3x\,\frac{1}{k_F^3 E_F}\Big[1 + 2\frac{k_F}{E_F}arsinh\Big(\frac{k_F}{m}\Big)\Big]\Big[\nabla\delta j^0(\boldsymbol{x})\Big]^2 \\ &+\frac{3}{16}\int d^3x\int d^3y\,\frac{1}{arsinh(k_F/m)}\,\frac{\delta\boldsymbol{j}(\boldsymbol{x})\cdot\delta\boldsymbol{j}(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}\ ,\end{aligned}$$

where again current conservation has been used. For the density component of $\delta T_s^{[2]}[j^\nu]$ (i.e. the first line) one now can simply replace $\nabla\delta j^0(\boldsymbol{x}) = \nabla j^0(\boldsymbol{x})$ and, correct to second order, $k_F = [3\pi^2 j^0(\boldsymbol{x})]^{\frac{1}{3}}$. While one can also utilize $\delta\boldsymbol{j}(\boldsymbol{x}) = \boldsymbol{j}(\boldsymbol{x})$, the density dependent prefactor $1/arsinh(k_F/m)$ of the current component can not be expressed unambigously in terms of $j^0(\boldsymbol{x})$ as now two spatial variables are available. Similar to the situation for the complete linear response corrections (108,109) one is left with a choice for this substitution. Abbreviating this (symmetric) function of $\boldsymbol{x}$ and $\boldsymbol{y}$ by $\bar\beta(\boldsymbol{x},\boldsymbol{y})$ one thus obtains

$$\begin{aligned}\delta T_s^{[2]}[j^\nu] = &\frac{m^2}{24\pi^2}\int d^3x\,(\boldsymbol{\nabla}\beta)^2\,\frac{\beta}{\eta}\Big[1 + 2\frac{\beta}{\eta}arsinh(\beta)\Big] \\ &+\frac{3}{16}\int d^3x\int d^3y\,\frac{1}{arsinh(\bar\beta(\boldsymbol{x},\boldsymbol{y}))}\frac{\boldsymbol{j}(\boldsymbol{x})\cdot\boldsymbol{j}(\boldsymbol{y})}{|\boldsymbol{x}-\boldsymbol{y}|}\ .\end{aligned} \tag{110}$$

It should be emphasized, however, that in contrast to this linear response approach a direct gradient expansion of $T_s[j^\mu]$ determines the current contribution to the second order gradient correction [42] completely.

It is interesting to analyze how the nonrelativistic limit of (110) is obtained by nonrelativistic linear response. While this is well known for the density contribution, the situation is less clear for the current-current response terms as a strictly nonrelativistic approach to current-DFT would be based on the paramagnetic current (defined in Eq.(77)) [30]. Nevertheless the nonrelativistic limit of (110) is a functional of n and the physical current $\boldsymbol{j}$. As will be shown in the following the crucial distinction between both basic variables of the energy functional is closely related to the definition of the external potential energy in the nonrelativistic case.

The density and current induced in a nonrelativistic homogeneous electron gas (HEG) by a perturbing four potential $(V_0, \boldsymbol{V})$ (on the basis of the Hamiltonian (80)) is given by

$$\begin{aligned}
\delta n(\boldsymbol{x}) &= \int d^3y\ \chi_{nn,hom}(q^0=0,\boldsymbol{x}-\boldsymbol{y})\ \Big[eV_0(\boldsymbol{y})+\frac{e^2}{2mc^2}\boldsymbol{V}(\boldsymbol{y})^2\Big] && (111)\\
\delta\boldsymbol{j}(\boldsymbol{x}) &= \delta\boldsymbol{j}_p(\boldsymbol{x})-\frac{c}{e}\ \boldsymbol{\nabla}\times\delta\boldsymbol{m}(\boldsymbol{x})-\frac{e}{mc}\ \boldsymbol{V}(\boldsymbol{x})\ n_0 && (112)\\
\delta j^k(\boldsymbol{x}) &= -\int d^3y\ \chi^{kl}_{jj,hom}(q^0=0,\boldsymbol{x}-\boldsymbol{y})\ \frac{e}{c}\ V^l(\boldsymbol{y}) && (113)\\
\delta m^k(\boldsymbol{x}) &= \int d^3y\ \chi^{kl}_{mm,hom}(q^0=0,\boldsymbol{x}-\boldsymbol{y})\ \epsilon_{lij}\ \partial^y_i V^j(\boldsymbol{y}) && (114)\\
&= \int d^3y\ \chi^{kl}_{mm,hom}(q^0=0,\boldsymbol{x}-\boldsymbol{y})\ B^l(\boldsymbol{y})\quad ,
\end{aligned}$$

where $\chi_{nn,hom}(q^0=0,\boldsymbol{x}-\boldsymbol{y})$, $\chi^{kl}_{jj,hom}(q^0=0,\boldsymbol{x}-\boldsymbol{y})$ and $\chi^{kl}_{mm,hom}(q^0=0,\boldsymbol{x}-\boldsymbol{y})$ denote the static density-density, paramagnetic current-current and spin-spin response functions of the nonrelativistic HEG,

$$\begin{aligned}
\chi_{nn}(x^0-y^0,\boldsymbol{x},\boldsymbol{y}) &= -i\Big[<\Psi|\ \mathbf{T}\ \hat n(x)\ \hat n(y)\ |\Psi> - n(\boldsymbol{x})\ n(\boldsymbol{y})\Big]\\
\chi^{kl}_{jj}(x^0-y^0,\boldsymbol{x},\boldsymbol{y}) &= -i\Big[<\Psi|\ \mathbf{T}\ \hat j^k_p(x)\ \hat j^l_p(y)\ |\Psi> - j^k_p(\boldsymbol{x})\ j^l_p(\boldsymbol{y})\Big]\\
\chi^{kl}_{mm}(x^0-y^0,\boldsymbol{x},\boldsymbol{y}) &= -i\Big[<\Psi|\ \mathbf{T}\ \hat m^k(x)\ \hat m^l(y)\ |\Psi> - m^k(\boldsymbol{x})\ m^l(\boldsymbol{y})\Big]\quad .
\end{aligned}$$

For an unpolarized HEG their tensor structure is given by

$$\begin{aligned}
\chi^{kl}_{jj,hom}(q^0=0,\boldsymbol{q}) &= -\frac{n_0}{m}\ \Big[\delta_{kl}+\Big(\delta_{kl}-\frac{q^kq^l}{\boldsymbol{q}^2}\Big)P(\boldsymbol{q}^2)\Big] && (115)\\
\chi^{kl}_{mm,hom}(q^0=0,\boldsymbol{q}) &= -\frac{n_0}{m}\ \frac{e^2}{c^2}\ \delta_{kl}\ \frac{Q(\boldsymbol{q}^2)}{\boldsymbol{q}^2}\quad , && (116)
\end{aligned}$$

which allows to invert (111-114),

$$\begin{aligned}
eV_0(\boldsymbol{q})+\frac{e^2}{2mc^2}\boldsymbol{V}^2(\boldsymbol{q}) &= \Big(\frac{1}{\Pi(\boldsymbol{q}^2)}-v(\boldsymbol{q})\Big)\delta n(\boldsymbol{q})\\
\frac{e}{c}\ V^k(\boldsymbol{q}) &= \frac{m}{n_0}\ \Big(\delta_{kl}-\frac{q^kq^l}{\boldsymbol{q}^2}\Big)\frac{1}{P(\boldsymbol{q}^2)+Q(\boldsymbol{q}^2)}\delta j^l(\boldsymbol{q})\quad ,
\end{aligned}$$

where $\boldsymbol{V}^2(\boldsymbol{q})$ represents the Fourier transform of $\boldsymbol{V}(\boldsymbol{x})^2$ (its internal structure is irrelevant in the following) and $\Pi(\boldsymbol{q}^2)$ is the static irreducible polarization insertion. Abbreviating

$$\boldsymbol{j}_s(\boldsymbol{r}) = -\frac{c}{e}\ \nabla\times\delta m(\boldsymbol{r})$$

the energy correction to second order in the perturbation is given by

$$\delta E^{LR} = \int d^3r\ \Big\{\Big[eV_0(\boldsymbol{r})+\frac{e^2}{2mc^2}\boldsymbol{V}(\boldsymbol{r})^2\Big]\Big[n_0+\frac{\delta n(\boldsymbol{r})}{2}\Big]-\frac{1}{2}\frac{e}{c}\ \boldsymbol{V}(\boldsymbol{r})\cdot\Big[\delta\boldsymbol{j}_p(\boldsymbol{r})+\delta\boldsymbol{j}_s(\boldsymbol{r})\Big]\Big\},$$

where the product of the gauge term and $\delta n(\boldsymbol{r})$ has been kept in spite of the fact that it is of third order. At this point one has to make a choice which energy contribution is understood as the external potential energy. In this respect basically two choices are possible. From the nonrelativistic Hamiltonian (80) one would conclude

$$E^{nonrel}_{ext} = \int d^3r\ \Big\{\Big[eV_0(\boldsymbol{r})+\frac{e^2}{2mc^2}\boldsymbol{V}(\boldsymbol{r})^2\Big]\ \Big[n_0+\delta n(\boldsymbol{r})\Big]-\frac{e}{c}\ \boldsymbol{V}(\boldsymbol{r})\cdot\Big[\delta\boldsymbol{j}_p(\boldsymbol{r})+\delta\boldsymbol{j}_s(\boldsymbol{r})\Big]\Big\}\quad ,$$

while the nonrelativistic limit of the standard relativistic external potential energy in (81) leads to

$$E_{ext}^{rel} = \int d^3r \left\{ eV_0(\boldsymbol{r}) \left[n_0 + \delta n(\boldsymbol{r}) \right] - \frac{e}{c} \boldsymbol{V}(\boldsymbol{r}) \cdot \delta \boldsymbol{j}(\boldsymbol{r}) \right\} \quad .$$

Depending on this choice one either finds

$$\begin{aligned} & \delta T_s^{nonrel} + \delta E_{xc}^{nonrel} \\ = \quad & -\frac{1}{2} \int \frac{d^3q}{(2\pi)^3} \left\{ \frac{\delta n(\boldsymbol{q})\ \delta n(-\boldsymbol{q})}{\Pi(\boldsymbol{q}^2)} \right. \\ & \qquad + \frac{m}{n_0} \frac{1}{\boldsymbol{q}^2} \Big[\boldsymbol{q} \times \Big(\delta \boldsymbol{j}_p(\boldsymbol{q}) + \delta \boldsymbol{j}_s(\boldsymbol{q}) \Big) \Big] \cdot \Big[\boldsymbol{q} \times \Big(\delta \boldsymbol{j}_p(-\boldsymbol{q}) + \delta \boldsymbol{j}_s(-\boldsymbol{q}) \Big) \Big] \\ & \qquad \left. \times \frac{P(\boldsymbol{q}^2) + Q(\boldsymbol{q}^2)}{1 + P(\boldsymbol{q}^2) + Q(\boldsymbol{q}^2)} \right\} \end{aligned} \tag{117}$$

on the basis of E_{ext}^{nonrel} or

$$\delta T_s^{rel} + \delta E_{rel}^{LR} = -\frac{1}{2} \int \frac{d^3q}{(2\pi)^3} \left\{ \frac{\delta n(\boldsymbol{q})\ \delta n(-\boldsymbol{q})}{\Pi(\boldsymbol{q}^2)} - \frac{m}{n_0} \frac{[\boldsymbol{q} \times \delta \boldsymbol{j}(\boldsymbol{q})] \cdot [\boldsymbol{q} \times \delta \boldsymbol{j}(-\boldsymbol{q})]}{\boldsymbol{q}^2 [P(\boldsymbol{q}^2) + Q(\boldsymbol{q}^2)]} \right\} \tag{118}$$

from E_{ext}^{rel}. Thus one can explicitly verify that the total energy can either be written as a functional of $\boldsymbol{j}_p + \boldsymbol{j}_s$ or $\boldsymbol{j}$ depending on the decomposition of the energy into its components. It must be emphasized, however, that the difference between both variants is of third order in the perturbation. Thus it is not surprising that the treatment of this energy component within linear response is not unambigous.

To complete the discussion we note the expansions of the noninteracting current-current and spin-spin response functions,

$$\frac{m}{n_0} \frac{1}{[P^{(0)}(\boldsymbol{q}^2) + Q^{(0)}(\boldsymbol{q}^2)]} = \left[-\frac{k_F}{12\pi^2 m} + \frac{k_F}{4\pi^2 m} \right]^{-1} \frac{1}{\boldsymbol{q}^2} + \dots \quad , \tag{119}$$

which reflect the well known Landau- and Pauli-susceptibilities. Inserting (119) into (118) one obtains the nonrelativistic limit of (110) (in momentum space),

$$\delta T_s^{rel,[2]}[n, \boldsymbol{j}] = \frac{3}{16} \int \frac{d^3q}{(2\pi)^3} \frac{m}{k_F} \left[\frac{(4\pi)^2}{\boldsymbol{q}^4} [\boldsymbol{q} \times \delta \boldsymbol{j}(\boldsymbol{q})] \cdot [\boldsymbol{q} \times \delta \boldsymbol{j}(-\boldsymbol{q})] \right] \quad . \tag{120}$$

VI.3 Gradient expansion

While in the preceding section gradient corrections have been obtained on the basis of the linear response approach, we here summarize the scheme and results of the direct gradient expansion (GE). In fact, on the basis of this first (historically) tool for deriving gradient terms a variety of functionals both for QED and QHD systems have been constructed and tested for simple model systems. Moreover, as already emphasized, the direct GE allows to determine current contributions uniquely which makes it particurlarly valuable for relativistic DFT. While this scheme has mainly been used for deriving the GE of $T_s[j^\mu]$, it is not restricted to this most simple current functional [86,87].

The first relativistic GE introduced by Gross and Dreizler [39] proceeds in complete analogy to the nonrelativistic commutator formalism of Kirzhnits [88]. It basically consists of four steps:

- The GE starts with an expansion of the electron propagator of noninteracting particles in some arbitrary local external potential V^μ (or, alternatively, the one-particle density matrix or the Wigner function) in powers of gradients of V^μ,

$$\begin{aligned} G(x,y) &= G^{[0]}(V_\mu(\boldsymbol{x}), x_\rho - y_\rho) + G^{[1]}(V_\mu(\boldsymbol{x}), \partial_k V_\mu(\boldsymbol{x}), x_\rho - y_\rho) \\ &\quad + G^{[2]}(V_\mu(\boldsymbol{x}), \partial_k\partial_l V_\mu(\boldsymbol{x}), \partial_k V_\mu(\boldsymbol{x})\partial_l V_\nu(\boldsymbol{x}), x_\rho - y_\rho) + \ldots \quad . \end{aligned} \tag{121}$$

  At this point no renormalization is required as $G(x,y)$ does not contain any loop contributions. The corresponding expansion of the propagator of the interacting system of actual interest can be generated by Dyson's equation, i.e. by a perturbation expansion with respect to $G(x,y)$.

- The 'semiclassical' expansion of $G(x,y)$, Eq.(121), then allows to evaluate the corresponding expansions of the four current of noninteracting particles,

$$j^\nu(\boldsymbol{x}) = \tilde{j}^{\nu,[0]}(V_0(\boldsymbol{x})) + \tilde{j}^{\nu,[2]}(V_0(\boldsymbol{x}), \partial_k\partial_l V_\mu(\boldsymbol{x}), \partial_k V_\mu(\boldsymbol{x})\partial_l V_\nu(\boldsymbol{x})) + \ldots \quad , \tag{122}$$

  and all energy functionals,

$$\begin{aligned} \tilde{T}_s[V^\mu] &= \int d^3x\ t_s(\boldsymbol{x}) \\ t_s(\boldsymbol{x}) &= \tilde{t}_s^{[0]}(V_0(\boldsymbol{x})) + \tilde{t}_s^{[2]}(V_0(\boldsymbol{x}), \partial_k\partial_l V_\mu(\boldsymbol{x}), \partial_k V_\mu(\boldsymbol{x})\partial_l V_\nu(\boldsymbol{x})) + \ldots \quad , \end{aligned} \tag{123}$$

  where for simplicity we here restrict ourselves to T_s. Note however, that, as a matter of principle, also energy components with a more complicated G-dependence can be dealt with (while for the exchange energy of electronic systems an incorrect gradient coefficient is obtained in the nonrelativistic case [86] and a divergent result for the relativistic case [87], these problems are not due to the direct GE but rather the vanishing photon mass — in a theory with massive bosons like QHD this difficulty would not arise). As in Eqs.(122,123) the symmetric limit introduces loop divergences both expansions require renormalization.

- In the next step the 'semiclassical' expansion of j^ν has to be inverted to the order in gradients one is interested in,

$$V_\mu[j^\nu] = V_\mu^{[0]}(j^0(\boldsymbol{x})) + V_\mu^{[2]}(j^0(\boldsymbol{x}), \partial_k\partial_l j^\nu(\boldsymbol{x}), \partial_k j^\nu(\boldsymbol{x})\partial_l j^\rho(\boldsymbol{x})) + \ldots \quad , \tag{124}$$

  thus yielding V_μ as a functional of j^ν.

- Finally one inserts $V_\mu[j^\nu]$ into the 'semiclassical' expansion of the energy to obtain the desired gradient expanded current functional,

$$T_s[j^\nu] = \int d^3x \left\{ t_s^{[0]}(j^0(\boldsymbol{x})) + t_s^{[2]}(j^0(\boldsymbol{x}), \partial_k\partial_l j^\nu(\boldsymbol{x}), \partial_k j^\nu(\boldsymbol{x})\partial_l j^\rho(\boldsymbol{x})) + \ldots \right\} \quad . \tag{125}$$

  Note that for finite systems the form of all gradient corrections can be simplified by subsequent partial integrations. In the case of $t_s^{[2]}$, for instance, a partial integration allows to eliminate the $\partial_k\partial_l j^\nu$-contribution.

While this procedure appears to be straightforward, the details of the relativistic 'semiclassical' expansion on the basis of Kirzhnits' commutator formalism are rather cumbersome (compare e.g. [41]). In the meantime, however, more efficient techniques for the 'semiclassical' expansion of $G(x,y)$ have been suggested [89,59,60,90] which substantially reduce the computational effort. Moreover, the method which we will briefly sketch here [89] as an addition consistently includes all vacuum contributions to $G(x,y)$.

The method is based on an iterative solution of the Dyson equation for $G(x,y)$,

$$\Big(i\partial\!\!\!/_x - m - V\!\!\!/(\boldsymbol{x})\Big)G(x,y) = i\delta^{(4)}(x-y) \quad , \tag{126}$$

whose solution is well known solution for $\boldsymbol{x}$-independent external potentials,

$$G^{[0]}(x,y) = e^{-i(x-y)\cdot V} \int \frac{d^4p}{(2\pi)^4}\, e^{-ip\cdot(x-y)} G^{[0]}(p_\mu, V_\nu) \tag{127}$$

$$G^{[0]}(p_\mu, V_\nu) = i\frac{p\!\!\!/ + m}{p^2 - m^2 + i\epsilon} - 2\pi(p\!\!\!/ + m)\frac{\delta(p^0 - E)}{2E}\Theta(\epsilon_F - V^0 - p^0) \ , \tag{128}$$

which explicitly demonstrates the inclusion of vacuum corrections. This solution for homogeneous systems motivates the general ansatz of $G(x,y)$ as a power series in gradients of V^μ,

$$G(x,y) = e^{-i(x-y)\cdot V(\boldsymbol{x})} \int \frac{d^4p}{(2\pi)^4}\, e^{-ip\cdot(x-y)} \sum_{n=0}^{\infty} G^{[n]}(p_\mu, V_\nu(\boldsymbol{x})) \quad , \tag{129}$$

where $[n]$ denotes the order of gradients. Insertion into (126) leads to a recursion relation for the $G^{[n]}$,

$$(p\!\!\!/ - m)G^{[n]}(p_\mu, V_\nu(\boldsymbol{x})) = \Big[\Big(i\partial\!\!\!/ V_\nu(\boldsymbol{x})\Big)\frac{\partial}{\partial p_\nu} - i\partial\!\!\!/\Big] G^{[n-1]}(p_\mu, V_\nu(\boldsymbol{x})) \quad , \tag{130}$$

which is solved by

$$G^{[n]}(p_\mu, V_\nu(\boldsymbol{x})) = \Big\{G^{[0]}(p_\mu, V_\nu)\Big[\Big(i\partial\!\!\!/ V_\nu(\boldsymbol{x})\Big)\frac{\partial}{\partial p_\nu} - i\partial\!\!\!/\Big]\Big\}^n G^{[0]}(p_\mu, V_\nu) \quad , \tag{131}$$

where the appropriate boundary conditions have been included. Note that this procedure can be extended to deal with the additional scalar potential arising in the context of nuclear physics [54].

It is instructive to go through the complete expansion scheme for a simple example, which is here chosen to be the second order GE of the kinetic energy functional for a purely electrostatic external potential $V = eV^0$. In this case the 'semiclassical' expansions of the density $n = j^0$ and t_s are given by

$$\begin{aligned}
\tilde{n}[V] &= \frac{p^3}{3\pi^2} + \frac{1}{12\pi^2}\Gamma\Big(2 - \frac{D}{2}\Big)(\boldsymbol{\nabla}^2 V) \\
&\quad -\frac{1}{12\pi^2}\Big\{\Big[\frac{E}{p} + 2arsinh\Big(\frac{p}{m}\Big)\Big](\boldsymbol{\nabla}^2 V) + \Big[\frac{E^2}{p^2} - 3\Big]\frac{(\boldsymbol{\nabla} V)^2}{2p}\Big\}
\end{aligned} \tag{132}$$

$$\begin{aligned}
\tilde{t}_s[V] &= \frac{m^4}{4\pi^2}\Gamma\Big(2 - \frac{D}{2}\Big) + \frac{1}{8\pi^2}\Big\{pE^3 + p^3E - arsinh\Big(\frac{p}{m}\Big)\Big\} \\
&\quad +\frac{1}{24\pi^2}\Gamma\Big(2 - \frac{D}{2}\Big)(\boldsymbol{\nabla} V)^2 \\
&\quad -\frac{1}{12\pi^2}\Big\{\Big[\frac{E^2}{p} + p\Big](\boldsymbol{\nabla}^2 V) + \Big[\frac{E^3}{2p^3} - \frac{E}{p} + arsinh\Big(\frac{p}{m}\Big)\Big](\boldsymbol{\nabla} V)^2\Big\} \quad ,
\end{aligned} \tag{133}$$

where

$$E = \epsilon_F - V(\boldsymbol{x}) \qquad ; \qquad p = \sqrt{E^2 - m^2}\ \Theta(E^2 - m^2) \tag{134}$$

and dimensional regularization has been used. One immediately recognizes the divergent kinetic energy of the Fermi sea, $m^4/(4\pi^2)\Gamma(2-D/2)$, and the UV-divergencies from the symmetric limit in both $\tilde{n}[V]$ and $\tilde{t}_s[V]$. The counterterms required to eliminate these divergencies have already been discussed earlier. While the former contribution is removed by subtraction of $< 0|\hat{H}_{free}|0 >$, the latter terms are due to the third diagram in Eq.(54). The corresponding counterterms are given in Eqs.(61,62). Adding these counterterms to (133,134) one ends up with finite 'semiclassical' expansions [41],

$$\tilde{n}_R[V] = \tilde{n}[V] - \frac{1}{12\pi^2}\Gamma\Big(2-\frac{D}{2}\Big)(\boldsymbol{\nabla}^2 V) \tag{135}$$

$$\tilde{t}_{s,R}[V] = \tilde{t}_s[V] - \frac{1}{24\pi^2}\Gamma\Big(2-\frac{D}{2}\Big)(\boldsymbol{\nabla} V)^2 \quad . \tag{136}$$

Now the third step of the GE-procedure, i.e. the inversion of $\tilde{n}_R[V]$, is straightforward and insertion into (133) leads to

$$T_s^{[0]}[n] = \frac{m^4}{8\pi^2}\int d^3x \, \Big[\beta\eta^3 + \beta^3\eta - arsinh(\beta)\Big] \tag{137}$$

$$T_s^{[2]}[n] = \frac{m^2}{24\pi^2}\int d^3x \, \frac{\beta}{\eta}\,\Big[1 + 2\frac{\beta}{\eta}arsinh(\beta)\Big]\,(\boldsymbol{\nabla}\beta)^2 \quad , \tag{138}$$

where the superscript $[n]$ again indicates the order of the contribution. One recognizes the kinetic energy of free electrons $T_s^{[0]}[n]$, i.e. the relativistic Thomas-Fermi energy, which has first been calculated by Vallarta and Rosen [32]. Furthermore, $T_s^{[2]}[n]$ agrees with the density contribution obtained with the linear response scheme, Eq.(110), demonstrating the consistency of these methods. Note that the only contributions of the vacuum part of the propagator (121) are the divergencies which have been eliminated by renormalization. In the nonrelativistic limit $T_s^{[2]}[n]$ approaches the Kirzhnits gradient correction [88]. The effect of the relativistic corrections are plotted in Fig.5. As for e_{xc} these corrections are noticable, in particular for $t_s^{[2]}$.

In contrast to $T_s^{[2]}$ the corresponding fourth order gradient corrections [43] contain a radiative contribution $T_{s,V}^{[4]}$,

$$T_s^{[4]}[n] = T_{s,V}^{[4]}[n] + T_{s,D}^{[4]}[n]$$

$$T_{s,V}^{[4]}[n] = \frac{1}{360\pi^2}\int d^3x \, \Big\{3\frac{\beta^2}{\eta^2}(\boldsymbol{\nabla}^2\beta)^2 + 6\frac{\beta}{\eta^4}(\boldsymbol{\nabla}^2\beta)(\boldsymbol{\nabla}\beta)^2 + \frac{3-\beta^4\eta^2}{\eta^6}(\boldsymbol{\nabla}\beta)^4\Big\} \tag{139}$$

$$\begin{aligned} T_{s,D}^{[4]}[n] = \frac{1}{5760\pi^2}\int d^3x \, \Big\{ & 4\frac{(\boldsymbol{\nabla}^2\beta)^2}{\beta\eta}\Big[3(1-4\beta^2) + 5\Big(1+2\frac{\beta}{\eta}arsinh(\beta)\Big)^2\Big] \\ & + 2\frac{(\boldsymbol{\nabla}^2\beta)(\boldsymbol{\nabla}\beta)^2}{\beta^2\eta^3}\Big[-41\beta^2 + 20\Big(1+2\frac{\beta}{\eta}arsinh(\beta)\Big) \\ & \qquad \times\Big(\frac{\beta^2+\eta^2}{2} + 2\frac{\beta}{\eta}arsinh(\beta)\Big)\Big] \\ & + \frac{(\boldsymbol{\nabla}\beta)^4}{\beta^3\eta^5}\Big[3 - 19\beta^2 - 8\beta^4 + 8\beta^6 + 16\beta^8 \\ & \qquad + 20\Big(\frac{\beta^2+\eta^2}{2} + 2\frac{\beta}{\eta}arsinh(\beta)\Big)^2\Big]\Big\} \quad . \end{aligned} \tag{140}$$

In $T_{s,V}^{[4]}$ the $(\nabla\beta)^4$-term corresponds to the so-called Euler-Heisenberg energy [18] (for purely electrostatic potentials). The nonrelativistic limit of $T_{s,D}^{[4]}$ reproduces the result of Hodges [91] and Jennings [92].

At this point it seems appropriate to illustrate the properties of these gradient corrected functionals by an application to spherical atoms. Adding the external potential energy, the Hartree term and $E_x^{LDA}[n]$ these functionals constitute extended Thomas-Fermi (ETF) models,

$$E^{ETF2N}[n] = \sum_{i=0}^{N} T_s^{2i}[n] + E_{ext}[n] + E_H[n] + E_x^{LDA} \quad ,$$

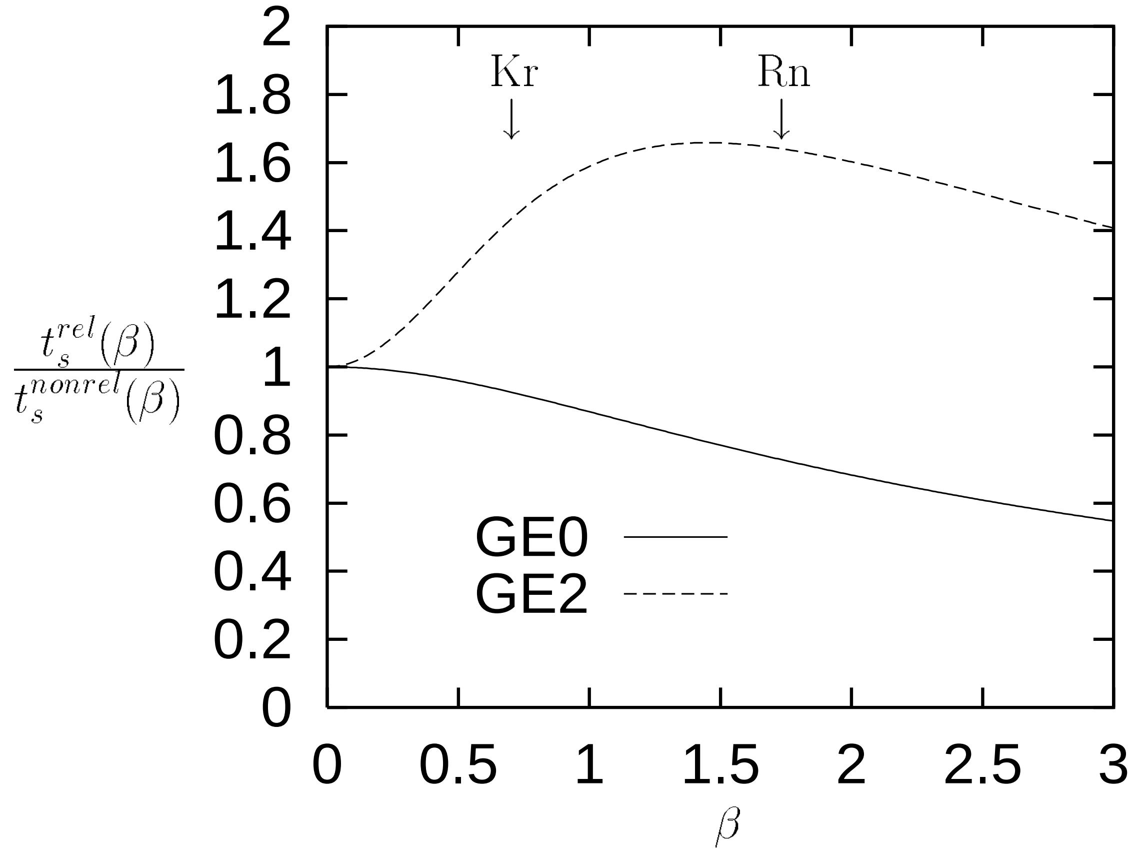


Figure 5: Relativistic corrections to kinetic energy densities. Eq.(137) — solid line (GE0), Eq.(138) — dashed line (GE2). Also the values of the densities of Kr and Rn at the origin (from nonrelativistic calculations) are indicated.

which allow for a direct energy minimization via the variational equation (74). The results of ETF-calculations reproduce the gross features of atoms, while missing their detailed quantum mechanical structure. The quality of the results is well characterized by the accuracy which is achieved for atomic ground state energies. In Fig.6 we compare the percentage deviation of relativistic ETF energies [45,46] from Dirac-Fock data with the corresponding nonrelativistic errors [94,93]. In case of the relativistic fourth order model (RETF4) vacuum contributions have not been included as the DF-energies used as reference standard also do not contain radiative corrections (Note that we have not been able to solve the RETF4 variational equations without radiative corrections beyond $Z = 69$ — at present. It is not clear whether this indicates a fundamental property of the RETF4-functional or is due to numerical difficulties). One first notes that the accuracy of the relativistic ETF energies is very similar to that of nonrelativistic results which they smoothly approach for small nuclear charge Z. Moreover, the errors of the second order expansion (of the order of 5%) are about twice as large as those of fourth order calculations indicating some convergence of the GE.

We just remark that for the complete RETF4 functional including $T_{s,V}^{[4]}$ the corresponding variational equations can be solved for the full range of Z [95]. However, due to the underlying physical concept the Euler-Heisenberg-like $T_{s,V}^{[4]}$ can not describe vacuum polarization effects in atoms adequately so that these results only demonstrate the feasibility of calculations in which vacuum corrections are included fully in a variational scheme.

The direct GE has also been applied to evaluate the current contribution to $T_s^{[2]}$

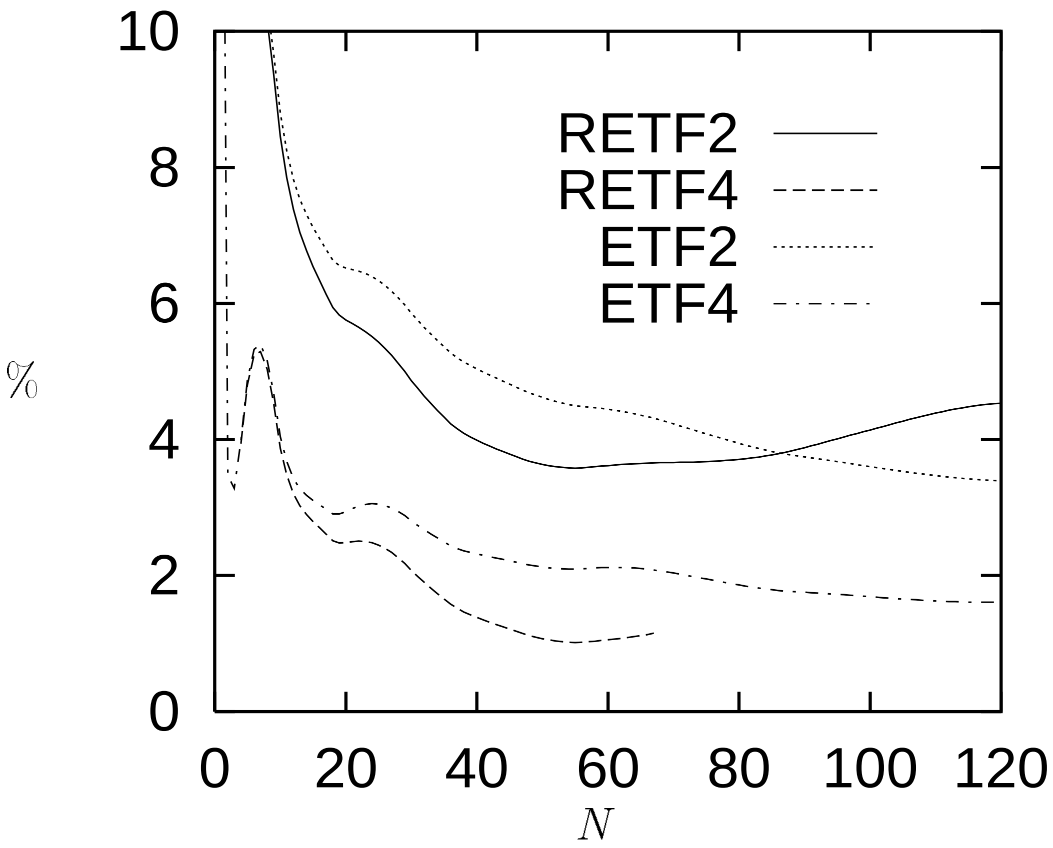


Figure 6: Percentage deviation of ground state energies for neutral spherical atoms obtained by solution of Eq.(74) from Hartree-Fock results (from Ref. [9]): Comparison of ETF2 and ETF4 for nonrelativistic and relativistic case — from Refs. [45,93,46].

[42],

$$T_s^{[2]}[\boldsymbol{j}] = \frac{3}{16}\int d^3x \, \frac{1}{arsinh(\beta(\boldsymbol{x}))} \times \int d^3y \int d^3z \sum_{k,l=1}^{3} \frac{\partial_k^y j^l(\boldsymbol{y})\partial_k^z j^l(\boldsymbol{z}) - \partial_k^y j^l(\boldsymbol{y})\partial_l^z j^k(\boldsymbol{z})}{|\boldsymbol{x}-\boldsymbol{y}| \; |\boldsymbol{x}-\boldsymbol{z}|} \quad , \tag{141}$$

and a temperature-dependent extension of (138) [44]. Note that the direct GE provides an unambigous result for $T_s^{[2]}[\boldsymbol{j}]$ in contrast to the linear response approach as here no expansion in powers of V^μ itself is involved. Neglecting the $\boldsymbol{x}$-dependence of β one can reduce (141) to (110). While (141) due to its complexity has not been utilized so far, we show some results from temperature-dependent ETF calculations [48]. In Fig.7 the density of Au obtained from RETF2-calculations (without exchange which is negligible for higher temperature) is plotted for various T and fixed compression (i.e. the complete electronic charge is kept within a Wigner-Seitz cell of radius $r_s = 3.01 a.u.$). As expected the density becomes smoother with increasing temperature reducing the importance of gradient corrections. Fig.8 shows the variation of pressure with T for various compressions (i.e. r_s), again for Au. Here the RETF2-results are compared to the predictions on the basis of the RHEG. One recognizes that for higher temperature and compression inhomogeneity corrections become less important.

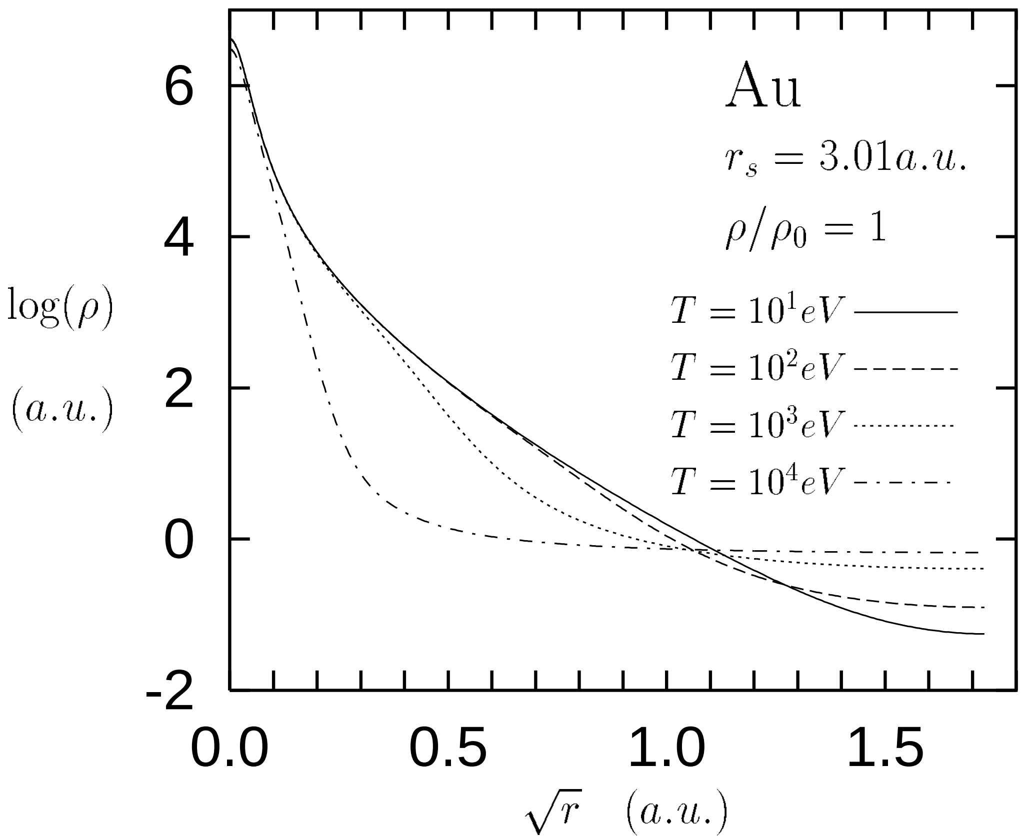


Figure 7: Density of Au for various temperatures (and fixed compression) from RETF2-calculations (from Ref. [48]).

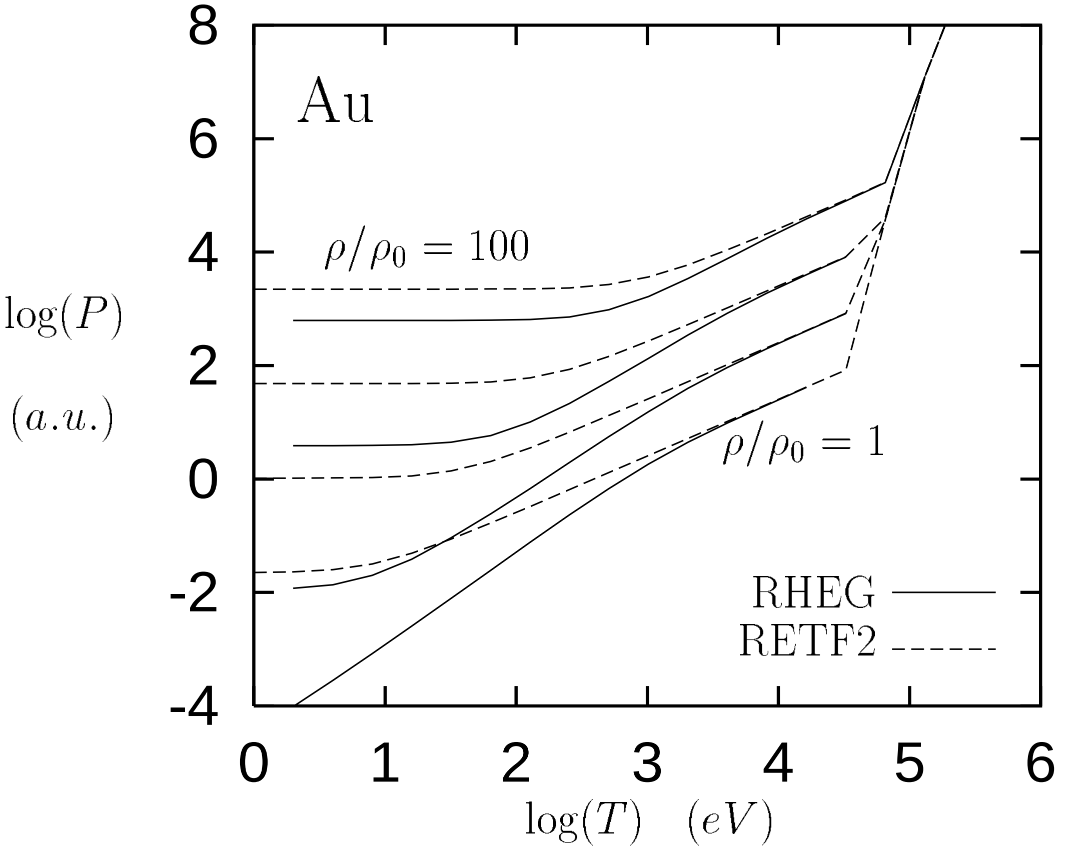


Figure 8: Variation of pressure with temperature for various compressions: Solid line — results from relativistic homogeneous electron gas, dashed lines — results from temperature dependent relativistic ETF2 model (from Ref. [48]).

VII DENSITY FUNCTIONAL APPROACH TO RELATIVISTIC NUCLEAR PHYSICS

While in a first step electronic systems have been approached by relativistic DFT methods, a DFT discussion of strongly interacting systems for which relativistic (and radiative) effects are much more important seems at least as interesting. In this section we summarize a DFT approach to Quantumhadrodynamics (QHD) [54,59] which represents an effective field theory for nuclear systems at low and intermediate energies. Thus its structure and most of its physical parameters (like meson masses and coupling constants) have to be understood as parametrizations of the underlying fundamental field theory (Quantumchromodynamics). Due to this effective nature several variants have been suggested for this theory differing in their degree of sophistication, their range of applicability and the values of the effective parameters. As a consequence the optimum form of such an effective theory is still a matter of current research. Here, however, we will completely focus on the density functional aspects of QHD without addressing its physical merits and failures (for a more detailed account of the physical implications of QHD see e.g. [96,52,97] — see also the contribution by M. Centelles in this volume). It is our understanding that these DFT concepts should be transferable to other field theories for nuclear systems.

The structure of QHD is most easily extracted from the Lagrangian of its most simple version (QHD-I — linear σ-ω model),

$$\begin{aligned}\hat{\mathcal{L}}_{QHD\text{-}I} &= \hat{\bar{\psi}}(x)\Big[i\not\partial - M + g_s\hat{\phi}(x) - g_v\hat{\not V}(x) + g_s\phi_{ext}(\boldsymbol{x}) - g_v\not V_{ext}(\boldsymbol{x})\Big]\hat{\psi}(x) \qquad (142)\\ &+\frac{1}{2}\Big[\partial_\mu\hat{\phi}(x)\partial^\mu\hat{\phi}(x) - m_s^2\hat{\phi}(x)^2\Big]\\ &-\frac{1}{4}\Big(\partial_\mu\hat{V}_\nu(x) - \partial_\nu\hat{V}_\mu(x)\Big)\Big(\partial^\mu\hat{V}^\nu(x) - \partial^\nu\hat{V}^\mu(x)\Big) + \frac{1}{2}m_v^2\hat{V}_\mu(x)\hat{V}^\mu(x) \quad .\end{aligned}$$

In this model the nucleons are characterized by a single field $\hat{\psi}$ of mass M (protons and neutrons are not distinguished) and interact via massive scalar ($\hat{\phi}$) and vector ($\hat{V}^\mu$) mesons. While the scalar σ-meson which is responsible for the attractive part of the nucleon-nucleon interaction couples to the scalar density

$$\hat{\rho}_s(x) = \hat{\bar{\psi}}(x)\hat{\psi}(x) \quad ,$$

the ω-mesons which generate the short range repulsion of nucleons couple to the fermion four current like photons in QED. In (142) we have in addition introduced auxilliary time-independent external potentials ϕ_{ext} and V^μ_{ext} which couple to the fermions like their quantized counterparts. Of course, in real nuclear systems no such ϕ_{ext} and V^μ_{ext} are present. Here these potentials only serve to identify the basic variables of DFT and to construct explicit functionals for the actual broken symmetry ground states (in analogy to the introduction of an external magnetic field for the discussion of spin-polarized systems in nonrelativistic DFT). Physically ϕ_{ext} and V^μ_{ext} could be interpreted as the mean fields generated by the mesons, such that the quantized fields $\hat{\phi}$ and $\hat{V}^\mu$ only represent deviations from these mean fields (compare [69]).

The statements of a HK-theorem for the system (142) and their proof [54] are completely analogous to those for QED systems with the only difference that the presence of the additional scalar potential ϕ_{ext} is reflected by the additional basic variable ρ_s. Here we just list the main results:

- The class of ground states resulting from external potentials which only differ by gauge transformations is a unique functional of the ground state four current j^ν and the ground state scalar density ρ_s,

$$|\Psi> = |\Psi[j^\nu,\rho_s]> \quad .$$

- All ground state observables thus become functionals of j^ν and ρ_s,

$$O[j^\nu, \rho_s] \equiv < \Psi[j^\nu, \rho_s]| \, \hat{O} \, |\Psi[j^\nu, \rho_s] > \quad .$$

- The minimum principle leads to the variational equations

$$\frac{\delta E[j^\nu, \rho_s]}{\delta j^\lambda(\boldsymbol{x})} = \mu \, g_{\lambda 0} \tag{143}$$

$$\frac{\delta E[j^\nu, \rho_s]}{\delta \rho_s(\boldsymbol{x})} = 0 \tag{144}$$

which now allow to determine both the exact j^ν and the exact ρ_s.

- Also KS-equations can be set up in which in addition to the exchange-correlation potential corresponding to the vector mesons,

$$v_{xc}^\nu(\boldsymbol{r}) = \frac{\delta E_{xc}[j^\mu, \rho_s]}{\delta j_\nu(\boldsymbol{r})} \quad ,$$

now a scalar exchange-correlation potential,

$$v_{xc}^s(\boldsymbol{r}) = \frac{\delta E_{xc}[j^\mu, \rho_s]}{\delta \rho_s(\boldsymbol{r})} \quad ,$$

has to be included in the selfconsistent procedure.

Note that the current standard treatment of QHD-systems within the mean field (or Hartree) approximation just represents the most simple form of the KS-approach in which all exchange-correlation effects are neglected, $E_{xc}[j^\mu, \rho_s] = 0$. We furthermore remark that the basic ingredient of a nontrivial KS-approach to QHD, i.e. the LDA for $E_{xc}[j^\mu, \rho_s]$, is available numerically [84,98,99].

In the following, however, we will not persue the KS-scheme any further but rather focus on ETF approximations to the mean field limit which have been extensively used in the context of nonrelativistic nuclear physics (on the basis of the Skyrme-model — see [49]). In particular in view of applications to astrophysical systems (see e.g. [100]) in which the nucleon density can be extremely high a relativistic extension of ETF methods allowing for the extraction of gross features seems desirable. Moreover, the TF approximation has been the basis for a number of successful applications of QHD (see e.g. [56–58]) and, as in the nonrelativistic case, the inclusion of gradient corrections is expected to improve results further.

The only part of the energy functional which has to be considered on the mean field level is the kinetic energy functional T_s. However, in order to allow for actual physical applications of the resulting ETF functional the discussion must be based on a more realistic version of QHD than (142). The present standard Lagrangian for the description of nuclei (QHD-II) is given by

$$\mathcal{L}_{QHD\text{-}II} = \mathcal{L}_{nuc} + \mathcal{L}_\sigma + \mathcal{L}_\omega + \mathcal{L}_\rho + \mathcal{L}_\gamma + \mathcal{L}_{int} \tag{145}$$

$$\mathcal{L}_{nuc} = \hat{\overline{\psi}}_p \Big(i\partial\!\!\!/ - M \Big) \hat{\psi}_p + \hat{\overline{\psi}}_n \Big(i\partial\!\!\!/ - M \Big) \hat{\psi}_n \tag{146}$$

$$\mathcal{L}_\sigma = \frac{1}{2} \Big[\partial_\mu \hat{\phi} \partial^\mu \hat{\phi} - m_s^2 \hat{\phi}^2 \Big] - \frac{b}{3} \hat{\phi}^3 - \frac{c}{4} \hat{\phi}^4 \tag{147}$$

$$\mathcal{L}_\omega = -\frac{1}{4} \Big(\partial_\mu \hat{V}_\nu - \partial_\nu \hat{V}_\mu \Big) \Big(\partial^\mu \hat{V}^\nu - \partial^\nu \hat{V}^\mu \Big) + \frac{1}{2} m_v^2 \hat{V}_\mu \hat{V}^\mu \tag{148}$$

$$\mathcal{L}_\rho = -\frac{1}{4} \Big(\partial_\mu \hat{\boldsymbol{b}}_\nu - \partial_\nu \hat{\boldsymbol{b}}_\mu - g_\rho \, \hat{\boldsymbol{b}}_\mu \times \hat{\boldsymbol{b}}_\nu \Big) \cdot \Big(\partial^\mu \hat{\boldsymbol{b}}^\nu - \partial^\nu \hat{\boldsymbol{b}}^\mu - g_\rho \, \hat{\boldsymbol{b}}^\mu \times \hat{\boldsymbol{b}}^\nu \Big) \tag{149}$$

$$+\frac{1}{2}m_\rho^2\hat{\boldsymbol{b}}_\mu\cdot\hat{\boldsymbol{b}}^\mu$$

$$\mathcal{L}_\gamma = -\frac{1}{4}\Big(\partial_\mu\hat{A}_\nu-\partial_\nu\hat{A}_\mu\Big)\Big(\partial^\mu\hat{A}^\nu-\partial^\nu\hat{A}^\mu\Big)-\frac{1}{2}\Big(\partial_\nu\hat{A}^\nu\Big)^2 \tag{150}$$

$$\mathcal{L}_{int} = g_s\hat{\phi}\Big[\hat{\overline{\psi}}_p\hat{\psi}_p+\hat{\overline{\psi}}_n\hat{\psi}_n\Big]-g_v\hat{V}_\mu\Big[\hat{\overline{\psi}}_p\gamma^\mu\hat{\psi}_p+\hat{\overline{\psi}}_n\gamma^\mu\hat{\psi}_n\Big] \tag{151}$$
$$-e\hat{A}_\mu\hat{\overline{\psi}}_p\gamma^\mu\hat{\psi}_p-\frac{g_\rho}{2}\hat{b}_\mu^{(3)}\Big[\hat{\overline{\psi}}_p\gamma^\mu\hat{\psi}_p-\hat{\overline{\psi}}_n\gamma^\mu\hat{\psi}_n\Big]+\ldots\quad,$$

where all auxilliary external potentials have been dropped from the very outset as we will not go through a HK existence theorem again. (145) extends (142) in two directions: On one hand the scalar meson Lagrangian has been modified to include a nonlinear self-interaction which allows to obtain a more realistic compression modulus for nuclear matter. Furthermore, by including two additional important interaction particles, the ρ-meson and the photon, protons and neutrons are now distinguished. Note that the coupling terms due to the other components of the isovector ρ-meson (not explicitly shown in (151)) which mix $\hat{\psi}_p$ and $\hat{\psi}_n$ are not relevant for the following.

In the mean field approximation (and including time reversal symmetry and charge conservation) the QHD-II Hamiltonian reduces to [53]

$$\hat{H}_{MF} = \int d^3x\,\Big\{\hat{\overline{\psi}}_p(x)\Big(-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}+M\Big)\hat{\psi}_p(x)+\hat{\overline{\psi}}_n(x)\Big(-i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}+M\Big)\hat{\psi}_n(x) \tag{152}$$
$$+\frac{1}{2}\Big[\Big(\boldsymbol{\nabla}\phi(\boldsymbol{x})\Big)^2+m_s^2\phi(\boldsymbol{x})^2\Big]+\frac{b}{3}\phi(\boldsymbol{x})^3+\frac{c}{4}\phi(\boldsymbol{x})^4$$
$$-\frac{1}{2}\Big[\Big(\boldsymbol{\nabla}V_0(\boldsymbol{x})\Big)^2+m_v^2V_0^2(\boldsymbol{x})\Big]-\frac{1}{2}\Big(\boldsymbol{\nabla}A_0(\boldsymbol{x})\Big)^2$$
$$-\frac{1}{2}\Big[\Big(\boldsymbol{\nabla}b_0^{(3)}(\boldsymbol{x})\Big)^2+m_\rho^2(b_0^{(3)})^2(\boldsymbol{x})\Big]$$
$$-g_s\phi(\boldsymbol{x})\hat{\rho}_s(x)+V_p(\boldsymbol{x})\hat{\rho}_p(x)+V_n(\boldsymbol{x})\hat{\rho}_n(x)\Big\}\quad,$$

where V_0, ϕ, A_0 and b_0^3 are the expectation values of the corresponding operators with respect to the mean field ground state and

$$\hat{\rho}_s(x) = \hat{\overline{\psi}}_p(x)\hat{\psi}_p(x)+\hat{\overline{\psi}}_n(x)\hat{\psi}_n(x) \tag{153}$$
$$\hat{\rho}_p(x) = \hat{\psi}_p^+(x)\hat{\psi}_p(x) \tag{154}$$
$$\hat{\rho}_n(x) = \hat{\psi}_n^+(x)\hat{\psi}_n(x) \tag{155}$$
$$V_p(\boldsymbol{x}) = g_vV_0+\frac{g_\rho}{2}b_0^{(3)}+eA_0 \tag{156}$$
$$V_n(\boldsymbol{x}) = g_vV_0-\frac{g_\rho}{2}b_0^{(3)}\quad. \tag{157}$$

V_n and V_p exhibit most clearly that protons and neutrons couple differently to ρ-mesons and photons. Of course, both proton and neutron numbers are conserved separatly,

$$N_p = \int d^3x\ <\hat{\rho}_p(x)> \tag{158}$$
$$N_n = \int d^3x\ <\hat{\rho}_n(x)>\quad. \tag{159}$$

The Hamiltonian (152) allows for a direct identification of ρ_s, ρ_p and ρ_n as basic DFT variables for this reduced variant of QHD-II which forms the standard starting point for applications of this theory (compare e.g. [101,52,53]).

Within the ETF approach one thus has to approximately evaluate the functional dependence of T_s on these densities. This is most easily done by the direct GE discussed in the previous section. For technical reasons, however, it is preferable in this case not to consider T_s itself but rather

$$T_s^*[\rho_p,\rho_n,\rho_s] \equiv T_s[\rho_p,\rho_n,\rho_s] - g_s \int d^3x\ \rho_s(\boldsymbol{x})\ \phi(\boldsymbol{x}) = T_s^*[k_p,M^*] + T_s^*[k_n,M^*] \quad (160)$$

and to use

$$\begin{aligned} k_p(\boldsymbol{x}) &= \Big(3\pi^2\rho_p(\boldsymbol{x})\Big)^{\frac{1}{3}} && (161)\\ k_n(\boldsymbol{x}) &= \Big(3\pi^2\rho_n(\boldsymbol{x})\Big)^{\frac{1}{3}} && (162)\\ M^*(\boldsymbol{x}) &= M - g_s\ \phi(\boldsymbol{x}) && (163)\end{aligned}$$

as independent variables (as a consequence the scalar density has to be understood as a functional of k_p, k_n and M^*, $\rho_s[k_p,k_n,M^*]$, which also can be evaluated in form of a GE). Moreover, in (160) the total $T_s^*[k_p,k_n,M^*]$ has already been decomposed into the individual contributions from protons and neutrons (with identical density dependence $T_s^*[k,M^*]$) reflecting the fact that T_s^* corresponds to noninteracting nucleons. To second order one obtains for $T_s^*[k,M^*]$ [54,59],

$$\begin{aligned} T_s^*[k,M^*] &= T_{s,V}^*[k,M^*] + T_{s,D}^*[k,M^*] && (164)\\ T_{s,V/D}^*[k,M^*] &= T_{s,V/D}^{*,[0]}[k,M^*] + T_{s,V/D}^{*,[2]}[k,M^*] && (165)\\ t_{s,V}^{*,[0]}[k,M^*] &= -\frac{M^{*4}}{8\pi^2}\ln\left|\frac{M^*}{M}\right| + \frac{1}{32\pi^2}(M^{*4}-M^4) && (166)\\ &\quad +\frac{M^2}{4\pi^2}(M^*-M)^2 + \frac{5M}{12\pi^2}(M^*-M)^3 + \frac{11}{48\pi^2}(M^*-M)^4 \\ t_{s,V}^{*,[2]}[k,M^*] &= \frac{1}{12\pi^2}\frac{k^2}{E^2}\ln\left|\frac{M^*}{M}\right|(\boldsymbol{\nabla}k)^2 + \frac{1}{6\pi^2}\frac{kM^*}{E^2}\ln\left|\frac{M^*}{M}\right|(\boldsymbol{\nabla}k\cdot\boldsymbol{\nabla}M^*) && (167)\\ &\quad -\frac{1}{24\pi^2}\Big(1+2\frac{k^2}{E^2}\Big)\ln\left|\frac{M^*}{M}\right|(\boldsymbol{\nabla}M^*)^2 \\ t_{s,D}^{*,[0]}[k,M^*] &= \frac{1}{8\pi^2}\Big[kE^3 + k^3E - M^{*4} arsinh\Big(\frac{k}{M^*}\Big)\Big] && (168)\\ t_{s,D}^{*,[2]}[k,M^*] &= \frac{1}{24\pi^2}\frac{k}{E}\Big[1+2\frac{k}{E} arsinh\Big(\frac{k}{M^*}\Big)\Big](\boldsymbol{\nabla}k)^2 && (169)\\ &\quad +\frac{1}{6\pi^2}\frac{kM^*}{E^2} arsinh\Big(\frac{k}{M^*}\Big)(\boldsymbol{\nabla}k\cdot\boldsymbol{\nabla}M^*) \\ &\quad +\frac{1}{24\pi^2}\Big[\frac{k}{E} - \Big(1+2\frac{k^2}{E^2}\Big) arsinh\Big(\frac{k}{M^*}\Big)\Big](\boldsymbol{\nabla}M^*)^2 \quad , \end{aligned}$$

where $E = \sqrt{M^{*2}+k^2}$. In contrast to the electronic case here vacuum corrections (which again require renormalization [54]) already contribute to the TF-limit of T_s^*. Of course, the GE in this respect reproduces the results of the direct field theoretical evaluation of vacuum contributions [102]. One furthermore recognizes that for $\phi = 0$ the GE of the electronic T_s, Eqs.(137,138), is obtained. Finally, one can check that (168,169) lead to the correct nonrelativistic limit (compare e.g. [103]).

It has been demonstrated [102,104] that vacuum corrections are much more important for a QHD-description of nuclei than they are for the ground state properties of atoms or molecules. Nevertheless, for most applications these contributions can be absorbed by a redefinition of the various parameters of QHD-II [105]. In fact, almost all parameter sets and applications of QHD-II in the literature are based on this so-called no-sea approximation such that for a first test of the ETF approach it seems appropriate to follow this standard. Thus our ETF2 energy functional reads

$$E^{ETF2}[k_p,k_n,M^*] = \sum_{i=0}^{1}\Big\{T_{s,D}^{[2i]}[k_p,M^*] + T_{s,D}^{[2i]}[k_n,M^*]\Big\} + E_H[k_p,k_n,M^*] \quad (170)$$

$$
\begin{aligned}
E_H[k_p,k_n,M^*] \;=\; & \frac{g_v^2}{2}\int d^3x \int d^3y\; [\rho_p(\boldsymbol{x})+\rho_n(\boldsymbol{x})]\;[\rho_p(\boldsymbol{y})+\rho_n(\boldsymbol{y})]\;\frac{e^{-m_v|\boldsymbol{x}-\boldsymbol{y}|}}{4\pi|\boldsymbol{x}-\boldsymbol{y}|}\\
& -\frac{g_s^2}{2}\int d^3x \int d^3y\; \rho_s(\boldsymbol{x})\;\rho_s(\boldsymbol{y})\;\frac{e^{-m_s|\boldsymbol{x}-\boldsymbol{y}|}}{4\pi|\boldsymbol{x}-\boldsymbol{y}|}\\
& +\frac{e^2}{2}\int d^3x \int d^3y\; \rho_p(\boldsymbol{x})\;\rho_p(\boldsymbol{y})\;\frac{1}{4\pi|\boldsymbol{x}-\boldsymbol{y}|}\\
& +\frac{g_\rho^2}{4}\int d^3x \int d^3y\; \Big[\rho_p(\boldsymbol{x})-\rho_n(\boldsymbol{x})\Big]\;\Big[\rho_p(\boldsymbol{y})-\rho_n(\boldsymbol{y})\Big]\;\frac{e^{-m_\rho|\boldsymbol{x}-\boldsymbol{y}|}}{4\pi|\boldsymbol{x}-\boldsymbol{y}|}\quad .
\end{aligned}
$$

The QHD-II variational equations are then solved for fixed proton and neutron number,

$$
\frac{\delta}{\delta k_p(\boldsymbol{r})}\Big\{E^{ETF2}[k_p,k_n,M^*]-\mu_p\int d^3x\;\frac{k_p(\boldsymbol{x})^3}{3\pi^2}\Big\} \;=\; 0 \tag{171}
$$

$$
\frac{\delta}{\delta k_n(\boldsymbol{r})}\Big\{E^{ETF2}[k_p,k_n,M^*]-\mu_n\int d^3x\;\frac{k_n(\boldsymbol{x})^3}{3\pi^2}\Big\} \;=\; 0 \tag{172}
$$

$$
\frac{\delta}{\delta M^*(\boldsymbol{r})}E^{ETF2}[k_p,k_n,M^*] \;=\; 0\quad , \tag{173}
$$

to obtain the corresponding ETF2 ground state densities and energies. As examples we show in Figs.9,10 the nucleon densities of ^{16}O and ^{208}Pb from TF and ETF2 calculations [106] in comparison with Hartree results [101] (which in the present context serve as exact reference standard). As in the case of atoms the TF/ETF2 solutions are not able to follow the detailed shell structure but rather average through the Hartree-density. One furthermore notes that in the physically most interesting surface region the ETF2 density is somewhat steeper and thus closer to the Hartree result than the TF solution.

The different description of surfaces is even more obvious from an application of the ETF2 approach to semiinfinite nuclear matter. The density profiles resulting from TF- and ETF2-calculations for the parametrization PW1 are compared in Fig.11. Unfortunately, one does not find ETF2-solutions for certain QHD-II parametrizations [62,65]. In fact, with decreasing effective mass $M_0^* = M - g_s\phi(z=-\infty)$ the surface steepness of the ETF2-solution increases such that eventually an exact solution of Eqs.(171-173) is no longer possible. The same effect is found for increasing m_s, while keeping all other parameters fixed [106]. This is most easily demonstrated for the surface profiles of semiinfinite nuclear matter which are obtained for various scalar meson masses m_s appoaching a critical value ($m_s \approx 515 MeV$). Fig.12 shows that with increasing m_s density oscillations build up which finally lead to a numerical instability. The origin of this problem is the Klein-Gordon equation for the scalar potential ϕ, Eq.(173), which explicitly reads

$$
(\boldsymbol{\nabla}^2 - m_s^2)\phi = -g_s\Big[\rho_s^{[0]}(k_p,k_n,M^*)+\rho_s^{[2]}[k_p,k_n,M^*]\Big]+b\phi^2+c\phi^3\quad . \tag{174}
$$

Note that the right hand side of (174) also contains $\boldsymbol{\nabla}^2\phi$ inside the gradient correction to the scalar density, $\rho_s^{[2]}$, making (174) a highly nonlinear differential equation. To allow for an application of the ETF2 approximation for those parameter sets for which (174) can not be solved exactly one decomposes ϕ and (174) in the spirit of the GE [65],

$$
\phi(\boldsymbol{r}) \;=\; \phi_0(\boldsymbol{r})+\phi_2(\boldsymbol{r}) \tag{175}
$$

$$
(\boldsymbol{\nabla}^2 - m_s^2)\phi_0 \;=\; -g_s\rho_s^{[0]}(k_p,k_n,M-g_s\phi_0)+b\phi_0^2+c\phi_0^3 \tag{176}
$$

$$
\begin{aligned}
(\boldsymbol{\nabla}^2 - m_s^2)\phi_2 \;=\; & -g_s\rho_s^{[2]}[k_p,k_n,M-g_s\phi_0]\\
& +\Big[2b\phi_0+3c\phi_0^2-g_s\frac{\partial\rho_s^{[0]}(k_p,k_n,M-g_s\phi_0)}{\partial\phi_0}\Big]\phi_2\quad ,
\end{aligned} \tag{177}
$$

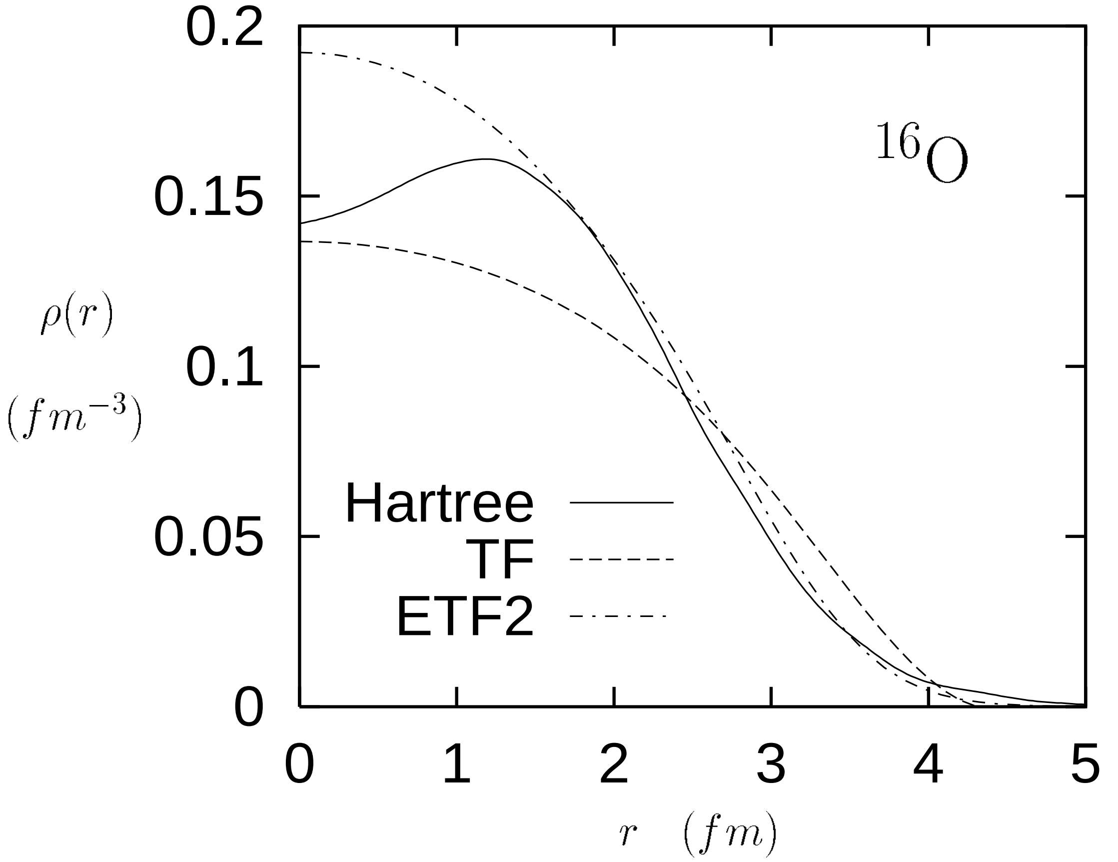


Figure 9: Density profiles for ^{16}O from TF and ETF2 calculations in comparison to Hartree result [101] (parameter set: NL1) — from Ref. [106].

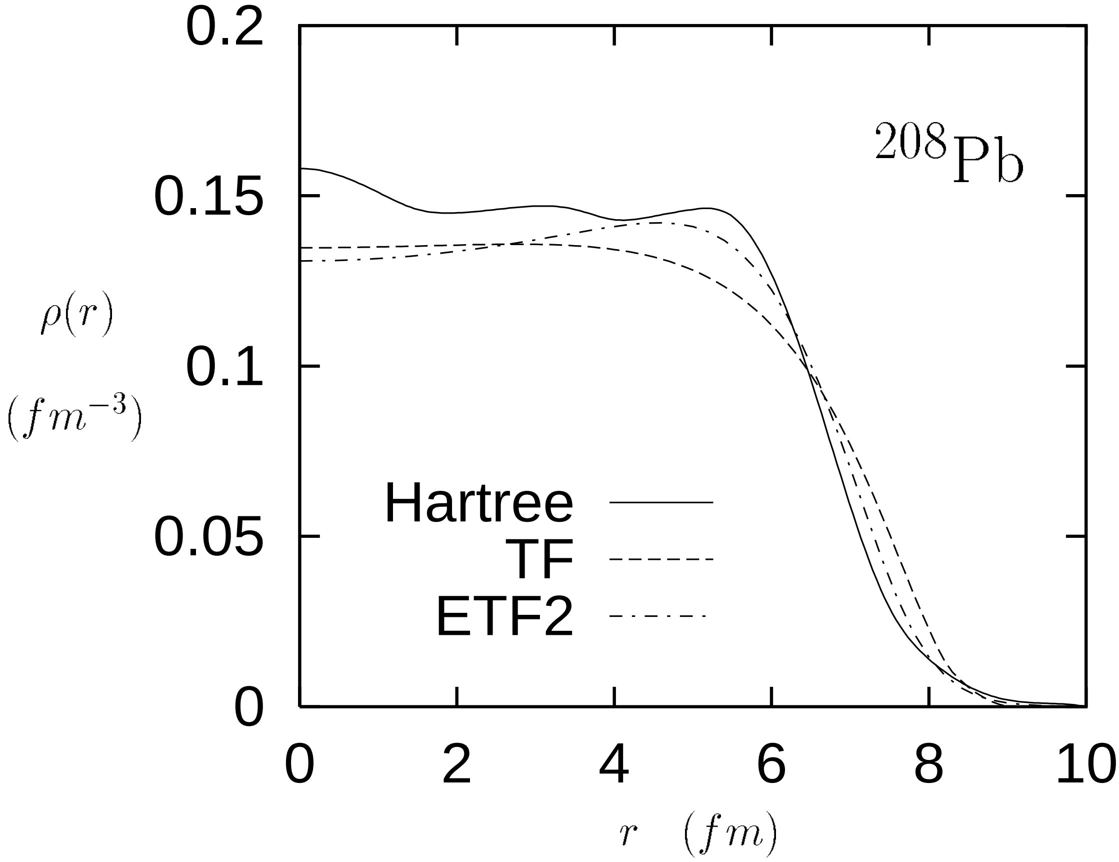


Figure 10: Same as Fig.9 for ^{208}Pb — from Ref. [106].

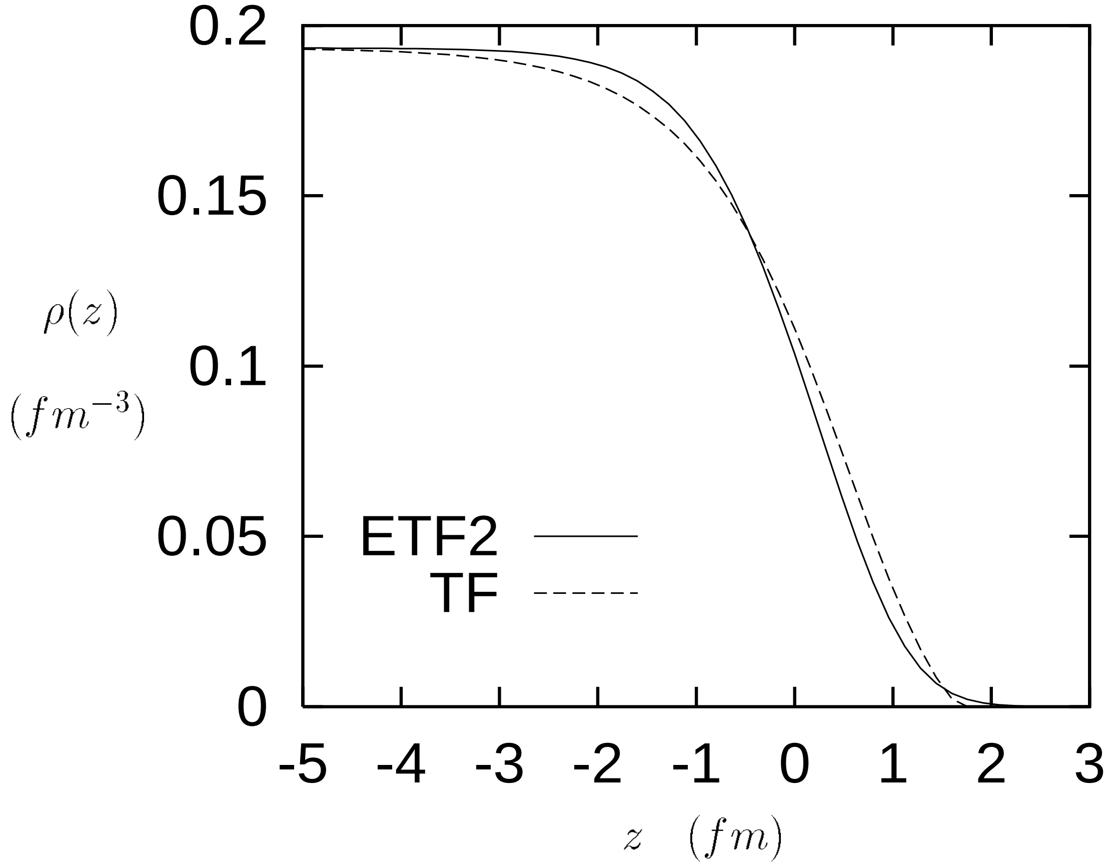


Figure 11: Density profiles for the surface of semiinfinite nuclear matter from TF and ETF2 calculations (parameter set: PW1) — from Ref. [106].

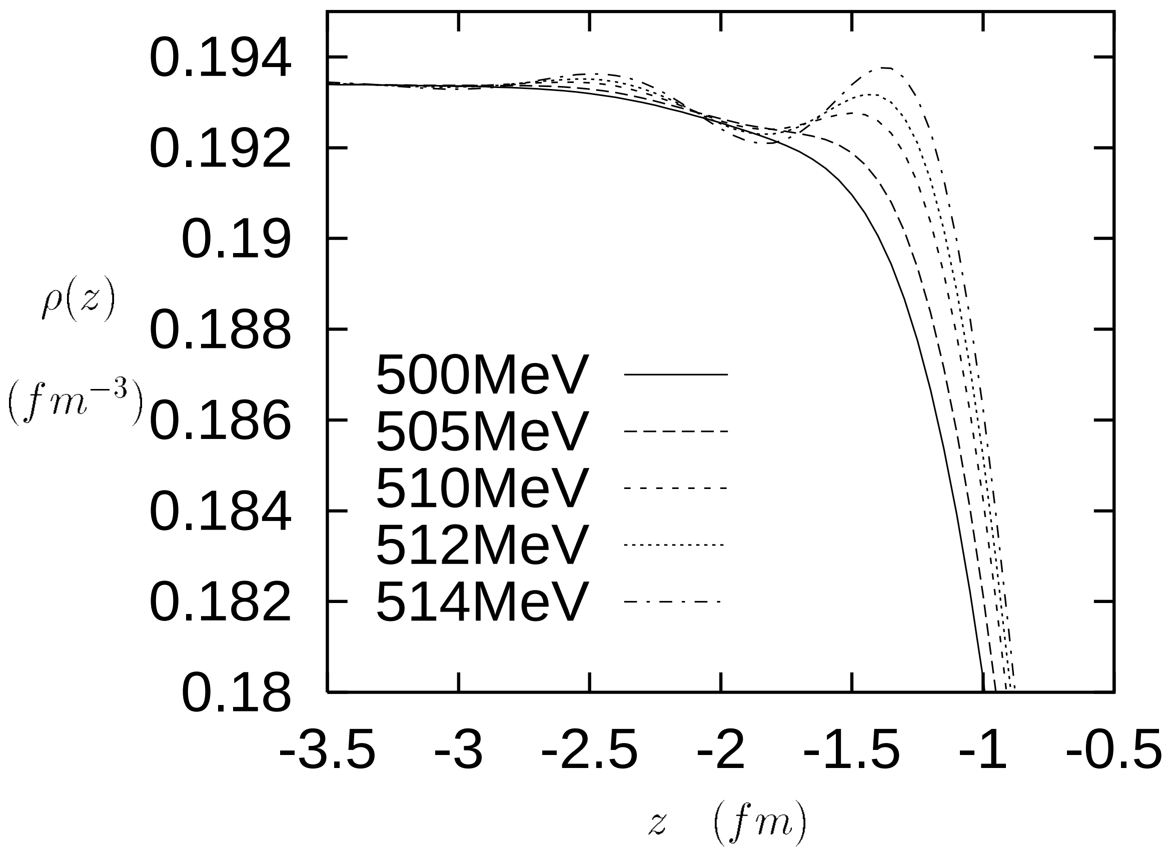


Figure 12: Density profiles for the surface of semiinfinite nuclear matter from ETF2 calculations for various almost critical scalar meson masses m_s — from Ref. [106].

	$E/A\ [MeV]$			$r_c\ [fm]$		
	H	ETF2	TF	H	ETF2	TF
^{16}O	-7.18	-7.49	-7.03	2.77	2.64	2.80
^{56}Ni	-8.47	-8.75	-8.31	3.70	3.73	3.89
^{90}Zr	-8.68	-8.92	-8.56	4.28	4.23	4.39
^{118}Sn	-8.57	-8.74	-8.42	4.64	4.60	4.75
^{136}Xe	-8.36	-8.51	-8.24	4.82	4.80	5.14
^{140}Ce	-8.39	-8.56	-8.27	4.90	4.86	5.00
^{208}Pb	-7.83	-7.97	-7.74	5.53	5.56	5.68

Table 2: Comparison of binding energies E (per nucleon) and r.m.s. charge radii r_c of spherical nuclei from TF and ETF2 calculations with Hartree results [53] (reduced by the center of mass correction $E_{cm} = -30.75A^{-1/3}MeV$) for the parametrisation NL1 [101].

	$E/A\ [MeV]$			$r_c\ [fm]$		
	H	ETF2	TF	H	ETF2	TF
^{16}O	-7.14	-7.41	-7.21	2.70	2.58	2.63
^{56}Ni	-8.36	-8.89	-8.68	3.76	3.69	3.74
^{90}Zr	-8.70	-9.08	-8.90	4.27	4.21	4.26
^{118}Sn	-8.61	-8.89	-8.72	4.62	4.58	4.62
^{136}Xe	-8.36	-8.60	-8.45	4.80	4.77	4.81
^{140}Ce	-8.46	-8.70	-8.55	4.88	4.84	4.87
^{208}Pb	-7.83	-8.08	-7.95	5.50	5.51	5.54

Table 3: Same as Table 2 for the parametrization NL2 [107].

and neglects all gradient contributions beyond second order for consistency. Combining (175-177) with the variational equations (171,172) solutions for all parametrizations suggested in the literature can be obtained. As an illustration in Fig.13 the density profile of semiinfinite nuclear matter obtained by this perturbative scheme for a parameter set whose scalar mass is almost critical (i.e. the most critical set of Fig.12) is compared to the exact solution. While the surface steepness is not affected substantially, the perturbative solution smoothly averages through the oscillations in the exact solution. In Fig.14 the corresponding scalar potential is shown (note the different scale of ϕ_0). As is obvious from this plot the exact ϕ exhibits higher gradients than the perturbative solution. In addition the onset of an oscillatory behaviour can already be recognized in ϕ. As in the case of the density the expanded scalar potential looks much smoother than the exact ϕ. We just remark that the differences between the ground state energies from exact and perturbative solutions are marginal. One can thus conclude that the perturbative scheme (175-177) forms a reliable basis for obtaining ETF2-solutions for those parameter sets for which an exact solution is not possible.

The 'semiclassical' nature of ETF2-densities is reflected by the accuracy of the corresponding ground state energies and charge radii. In Tabs.2,3 we list these quantities for a number of spherical nuclei and two different parametrizations (NL1 — [101]; NL2 — [107]). As the comparsion of TF/ETF2-solutions with Hartree results shows the overall accuracy of these approximations is of the order of 2-5% in close analogy to the corresponding nonrelativistic case and the situation for QED systems. Moreover, for the parametrizations NL2 one notes that the TF energies and radii are closer to Hartree

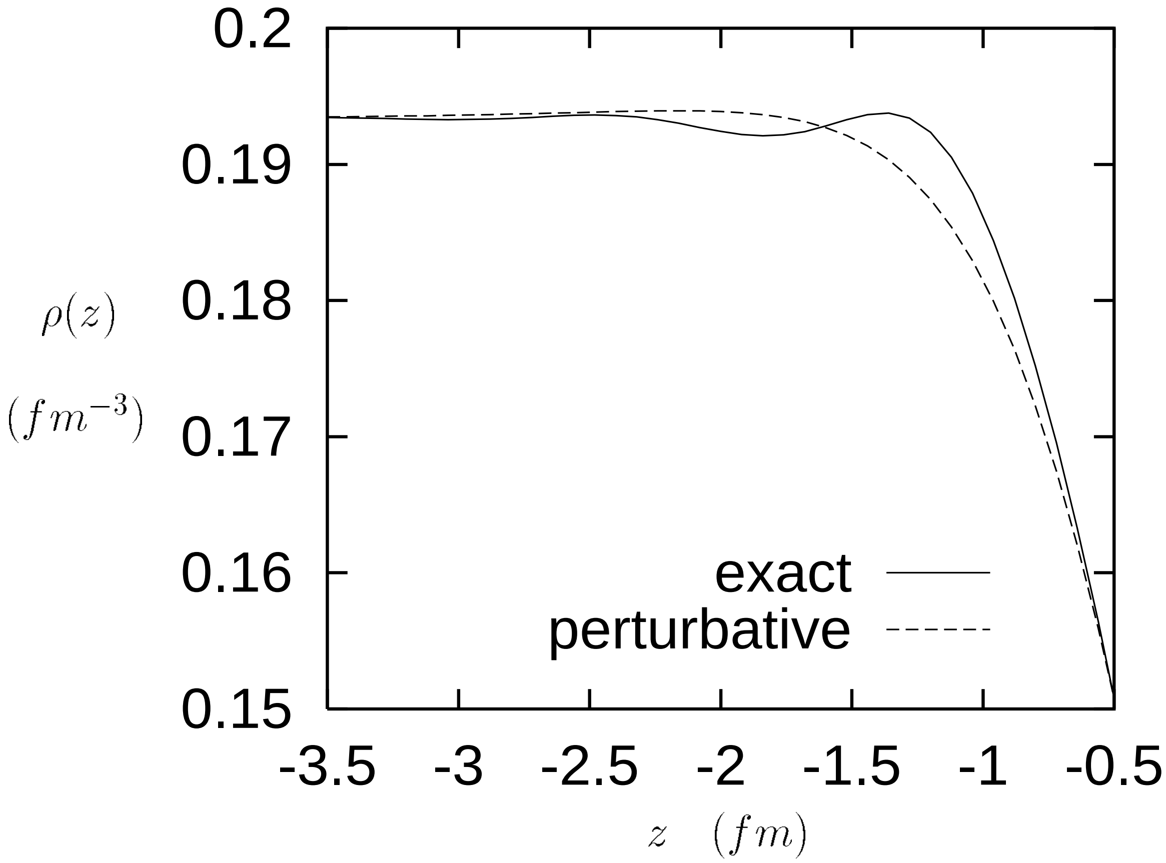


Figure 13: Density profiles for the surface of semiinfinite nuclear matter from exact and perturbative ETF2 calculations for $m_s = 514MeV$ — from Ref. [106].

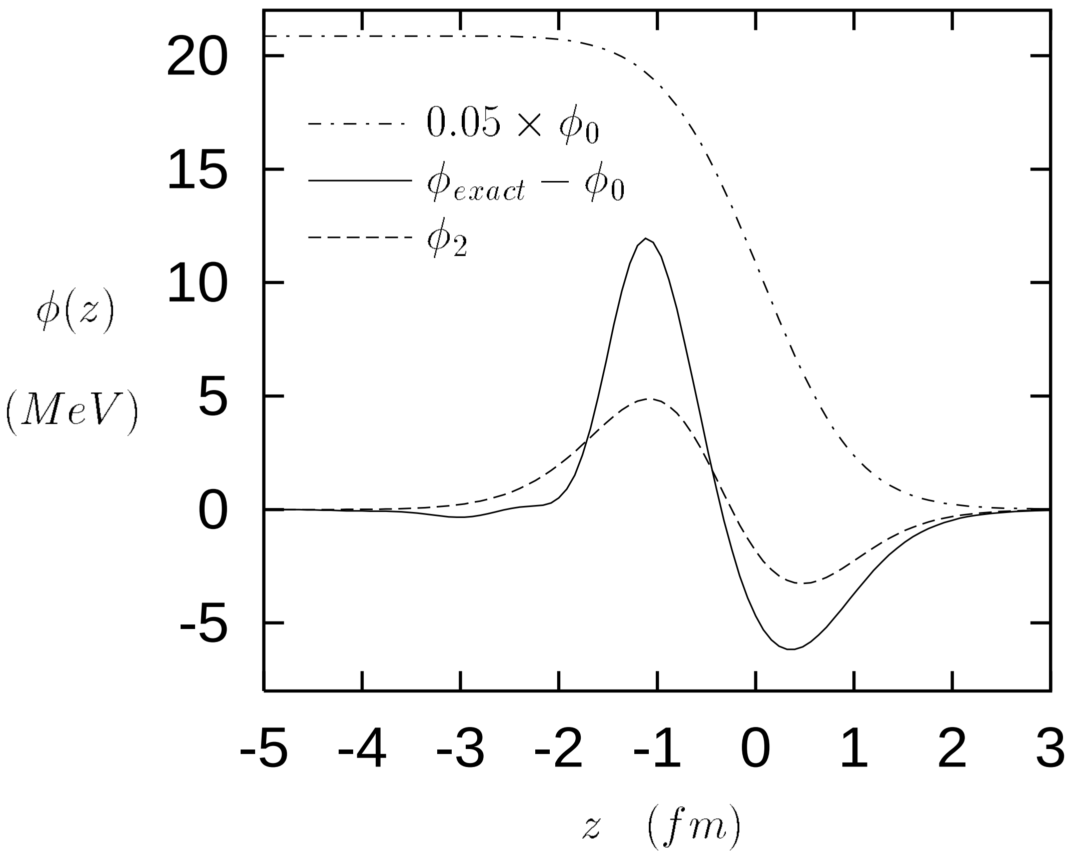


Figure 14: Components of scalar potential for the surface of semiinfinite nuclear matter from exact and perturbative ETF2 calculations for $m_s = 514MeV$ — from Ref. [106].

data than those from the ETF2-calculations thus questioning the concept of the GE. This result, however, must be regarded as fortuitous. This point is demonstrated in Figs.15,16 where the accuracies of the ground state energy and charge radius of ^{208}Pb from various parametrizations are shown (note that the ETF-approach should be most appropriate for large systems). The 8 parametrizations chosen enclose the physically relevant regime in the multidimensional parameter space of QHD. From this analysis it is clear that for most of the interesting parametrizations the ground state energies and in particular the charge radii from the ETF2 approach are more accurate than their TF counterparts. There are, however, certain types of parameter sets for which TF solutions accidentially come closer to Hartree results. Nevertheless, taking the improved surface profile of ETF2-densities together with this at least statistical improvement of global nuclear properties as compared to the often applied TF approximation the ETF2 scheme seems an adequate tool for the discussion of large hadronic systems. The importance of fourth order gradient corrections which turned out to be required for the successful ETF-description of nuclei within the nonrelativistic Skyrme-model remains to be analyzed.

We close this section with some brief remarks on the temperature-dependent extension [55] of the DFT-approach to QHD-systems. While the basic variables of DFT in this case are the same as for $T = 0$, i.e. j^ν and ρ_s, the role of the energy is now played by the thermodynamic potential,

$$\Omega[j_0^\nu, \rho_{s,0}] < \Omega[j^\nu, \rho_s] \qquad \text{for} \qquad j^\nu \neq j_0^\nu \qquad \text{or} \qquad \rho_s \neq \rho_{s,0} \quad , \tag{178}$$

where j_0^ν and $\rho_{s,0}$ are the equilibrium four current and scalar density, respectively. As a result these quantities can be obtained by minimizing the free energy functional,

$$F[j^\nu, \rho_s] = \Omega[j^\nu, \rho_s] + \mu \int d^3x \; j^0(\boldsymbol{x}) \quad , \tag{179}$$

with respect to the four current and the scalar density,

$$\frac{\delta F[j^\nu, \rho_s]}{\delta j^0(\boldsymbol{r})} = \mu \quad , \quad \frac{\delta F[j^\nu, \rho_s]}{\delta j^k(\boldsymbol{r})} = 0 \quad , \quad \frac{\delta F[j^\nu, \rho_s]}{\delta \rho_s(\boldsymbol{r})} = 0 \quad . \tag{180}$$

As for the zero temperature case this minimization can be performed via KS-equations.

As an example for the application of this scheme we show the density profiles of a ^{40}Ca nucleus embedded in a thermal nucleon bath for various temperatures in Fig.17 (obtained from temperature-dependent TF calculations [66]). With increasing temperature the nucleus becomes less localized until it finally dissolves in the bath. As a further illustration in Fig.18 the thermal excitation energy, i.e. the difference between the energy of the equilibrium configuration at temperature T and the ground state energy at $T = 0$, is plotted as a function of the size of the nucleus. Two parameter sets are shown demonstrating that for high temperature ΔE is rather sensitive to the parametrization chosen. For both parameter sets, however, ΔE scales linearly with the baryon number.

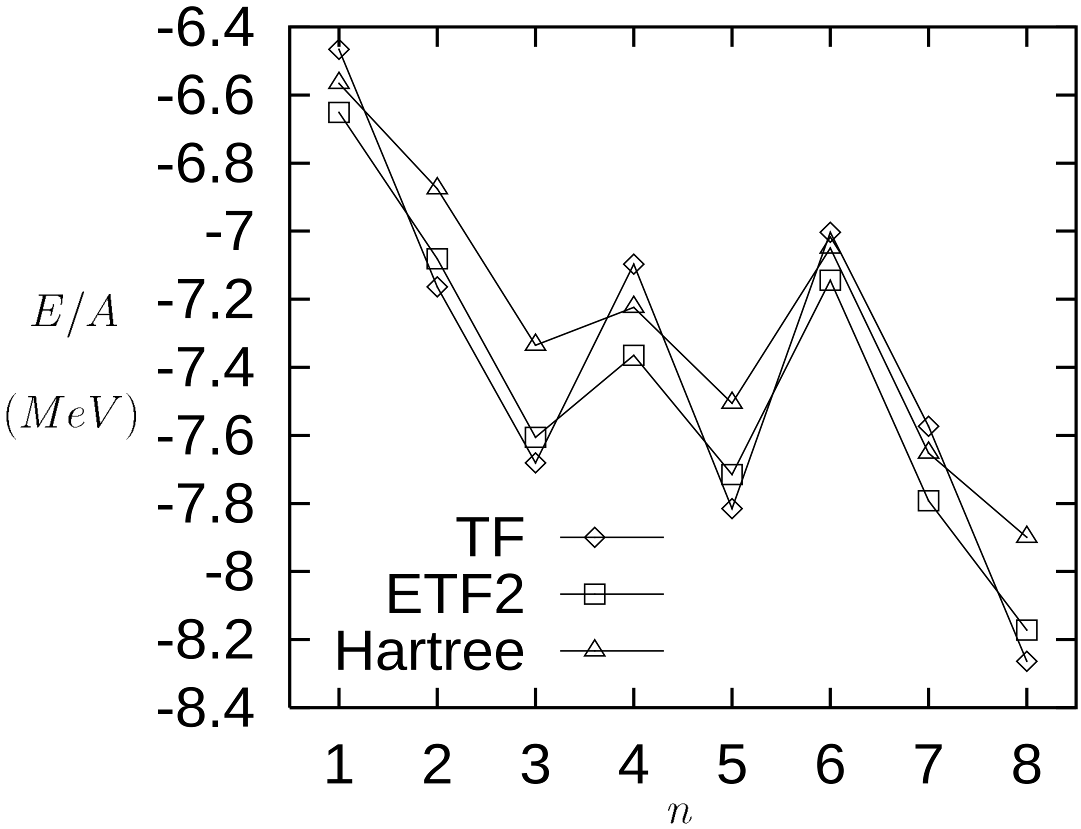


Figure 15: Binding energies (per nucleon) of ^{208}Pb from TF and ETF2 calculations in comparison to Hartree results for various parametrizations (connecting lines are only drawn to guide the eye) — from Ref. [65].

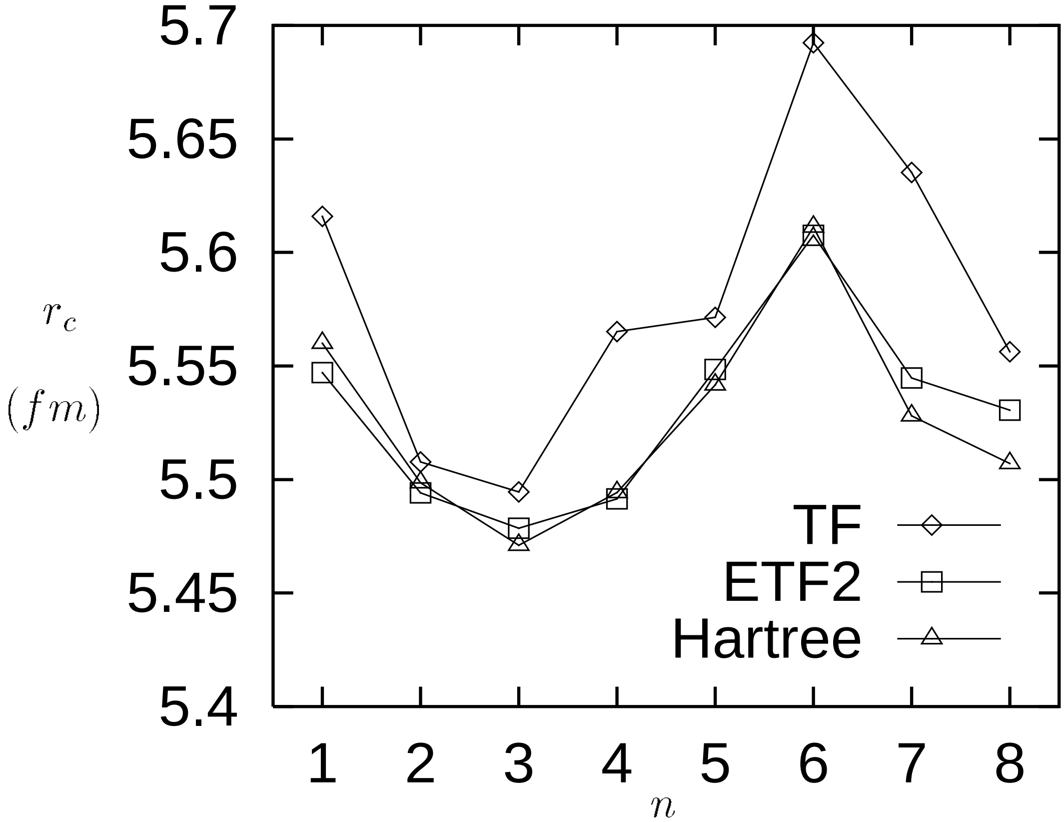


Figure 16: Charge radii of ^{208}Pb from TF and ETF2 calculations in comparison to Hartree results for various parametrizations (connecting lines are only drawn to guide the eye) — from Ref. [65].

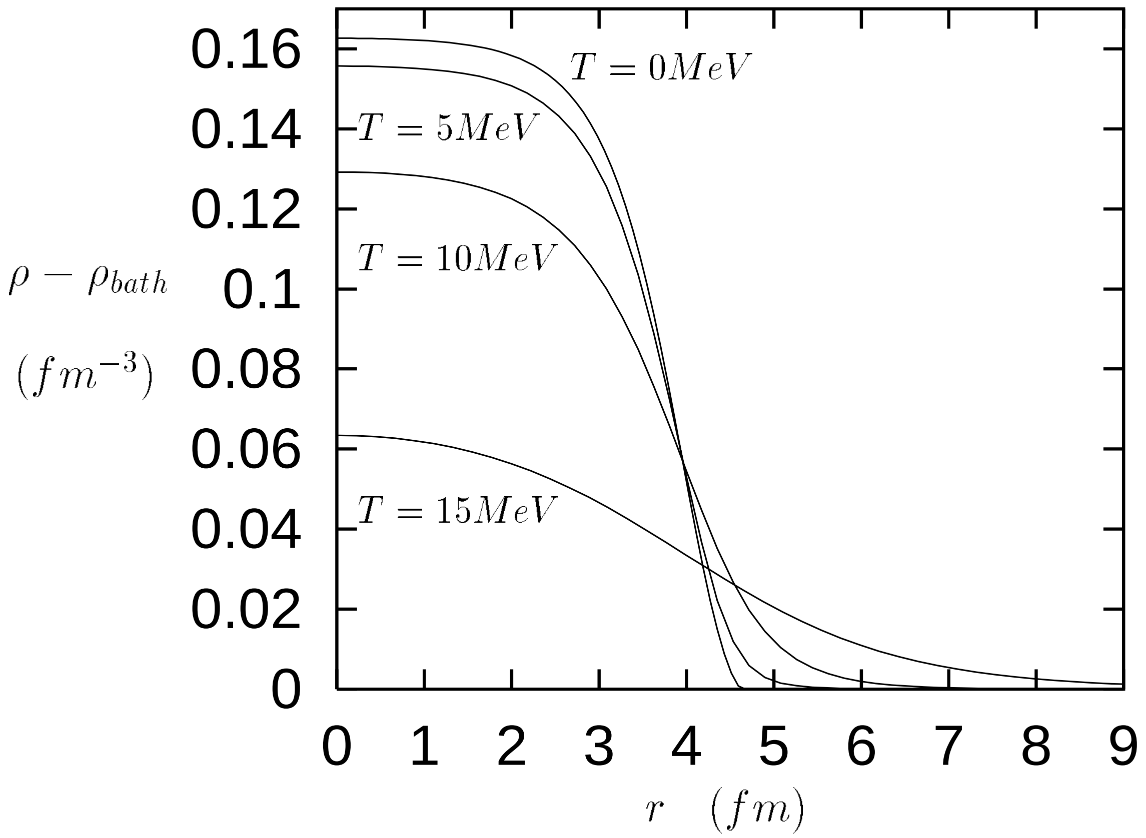


Figure 17: Density profiles for ^{40}Ca in thermal nucleon bath for various temperatures (parameter set: SRK3M7) — from Ref. [66].

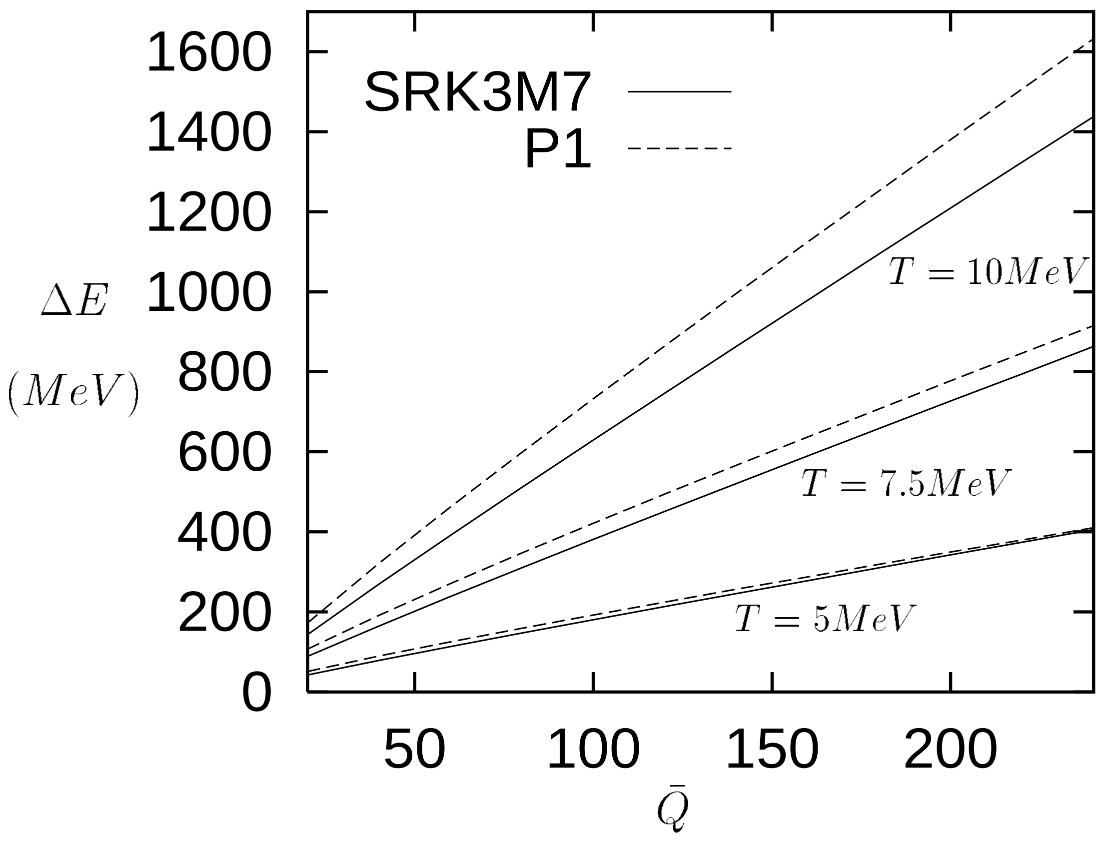


Figure 18: Thermal excitation energies $\Delta E = E(T) - E(T = 0)$ as a function of the baryon number $\bar{Q}$ for two different parameter sets — from Ref. [66].

VIII CONCLUDING REMARKS

We close by summarizing those points we wanted to emphasize in this overview of relativistic DFT:

- The standard renormalization procedure allows a consistent inclusion of radiative effects in relativistic DFT thus establishing a field theoretical extension of DFT.
- The complete variety of techniques successfully utilized in the nonrelativistic context can be extended to the relativistic domain. Their actual application, however, becomes much more involved.
- As a consequence only a few explicit functionals have been constructed and tested so far. In particular, little is known about nonlocal corrections to the exchange-correlation functional.
- We have not tried to review real applications of relativistic DFT. However, to summarize their present status it seems that although the applications reported in the literature were quite successful, relativistic DFT is far from being as well developed as its nonrelativistic counterpart.
- The complete DFT formalism can be transferred to relativistic nuclear physics which might become a new important domain of DFT. It is worth pointing out that the application of DFT concepts does not seem to be restricted to the level of an effective description of nuclear systems but could also be useful for a more fundamental treatment. However, at present only the most basic elements of this new field are available.

Let us finally express our hope that the present contribution will stimulate renewed interest and further progress in relativistic DFT such that one eventually will be able to solve those problems which remain open to date.

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