

On the way to a microscopic derivation of covariant density functional theory

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Abstract. Several problems encountered on the way to a microscopic derivation of covariant density functionals are discussed. The starting point are semi-microscopic functionals adjusted to ab-initio calculations in nuclear matter. Since it is impossible to derive in this way the strength of tensor terms in such functionals we propose a solution of the relativistic Brueckner-Hartree-Fock equations in finite nuclei and show first results.

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1. Introduction

In recent years considerable progress has been achieved in ab-initio derivations of nuclear properties from bare nucleon-nucleon forces. For light nuclei it is possible to solve the exact nuclear many-body problem on the computer. For heavier nuclei approximate methods have been applied. The calculation of nuclear properties for the majority of nuclear systems, however, is left to density functional methods. Non-relativistic [1, 2] and relativistic [3, 4, 5, 6, 7] versions enable an effective description of the nuclear many-body problem not only for bulk properties, such as binding energies and radii, but also for collective excitations such as rotations and giant resonances, and, by going beyond mean field, complicated configurations [8, 9, 10, 11, 12] and sophisticated low-lying spectra in transitional nuclei [13, 14].

At present most of these functionals are purely phenomenological. Of course, one of the main goals in nuclear physics is to build a universal density functional theory based on microscopic calculations [15, 16]. This functional should be able to explain as many as possible measured data within the same parameter set and to provide reliable predictions for properties of nuclei far from stability not yet or never accessible to experiments in the laboratory. It should be derived in a fully microscopic way from the interactions between bare nucleons. At present, however, attempts to derive such a density functional provide only qualitative results for two reasons: first, the three-body term of the bare interaction is not known well enough and, second, the methods to derive such a functional are not precise enough to achieve the required accuracy. Note that a 1 per mille error in the binding energy per particle of symmetric nuclear matter leads to an error of several MeV in the binding energy of heavy nuclei, an error which is an order of magnitude larger than required by astrophysical applications. From such considerations it is evident, that successful ab-initio functionals in nuclear physics, at least in foreseeable future will always depend on a very small number phenomenological parameters for fine tuning. It is the number of final parameters which counts.

One of the underlying symmetries of QCD is Lorentz invariance and therefore covariant density functionals are of particular interest in nuclear physics. This symmetry not only allows



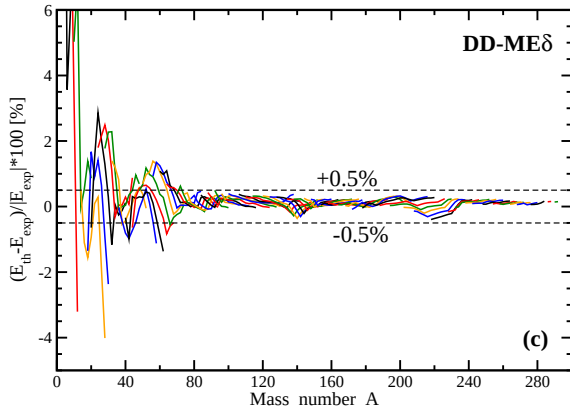


Figure 1. The relative difference between theoretical and experimental masses of 835 even-even nuclei investigated in relativistic Hartree Bogoliubov (RHB) calculations with the set DD-ME δ . If $E_{th} - E_{exp} < 0$, the nucleus is more bound in the calculations than in experiment. Dashed lines show the $\pm 0.5\%$ limit (from Ref. [17]).

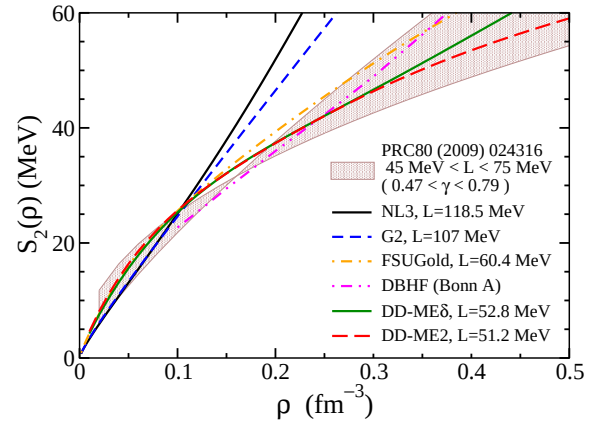


Figure 2. The symmetry energy as a function of the density. The results for DD-ME δ are compared with those of the density functionals NL3 [18], G2 [19], FSUGold [20], and microscopic DBHF calculations [21]. The shaded area represents the empirical region suggested by the available constraints on the L parameter (from Ref. [22]).

to describe the spin-orbit coupling, which has an essential influence on the underlying shell structure, in a consistent way, but it also puts stringent restrictions on the number of parameters in the corresponding functionals without reducing the quality of the agreement with experimental data. Therefore we restrict ourselves in the following to covariant density functionals.

2. Semi-microscopic functionals

In Coulombic system an essential input for the derivation of microscopic functionals is the exact numerical solution of the homogeneous electron gas at various densities. Starting from this energy functional $E[\rho]$ additional gradient terms and many other corrections have been added with great success. Therefore it seems to be reasonable to apply a similar concept in nuclear physics. Of course, at present there are no exact solutions of the nuclear matter problem available producing at least saturation at reasonable densities.

Therefore we followed the spirit of the Barcelona group [23], who used modern Brueckner-Hartree-Fock calculations in nuclear matter as a starting point for a semi-phenomenological non-relativistic potential, and derived in a similar way a relativistic functional DD-ME δ [22] with density dependent meson couplings. In contrast to the phenomenological density functionals with meson exchange such as NL3 [18] which contain usually only the σ -meson in the isoscalar scalar channel, the ω -meson in the isoscalar vector channel, and the ρ -meson in the isovector vector channel, microscopic Dirac-Brueckner-Hartree-Fock (DBHF) calculations show very clearly that there is also isospin-dependence in the scalar channel described by the δ -meson (a_0 -meson). The density dependence of the meson-nucleon coupling vertices in the new functional DD-ME δ [22] is derived from *ab-initio* DBHF calculations in nuclear matter. The starting point forms the Equation of State (EoS) of symmetric nuclear matter and of neutron matter derived by Baldo et al. [24] in a state-of-the-art non-relativistic Brueckner-Hartree-Fock calculation including relativistic corrections and three-body forces. In addition the isovector part of the effective Dirac mass $m_p^* - m_n^*$ derived by the Tübingen group [25] in DBHF theory determines the coupling constant of the δ -meson and its density dependence. Only four additional parameters,

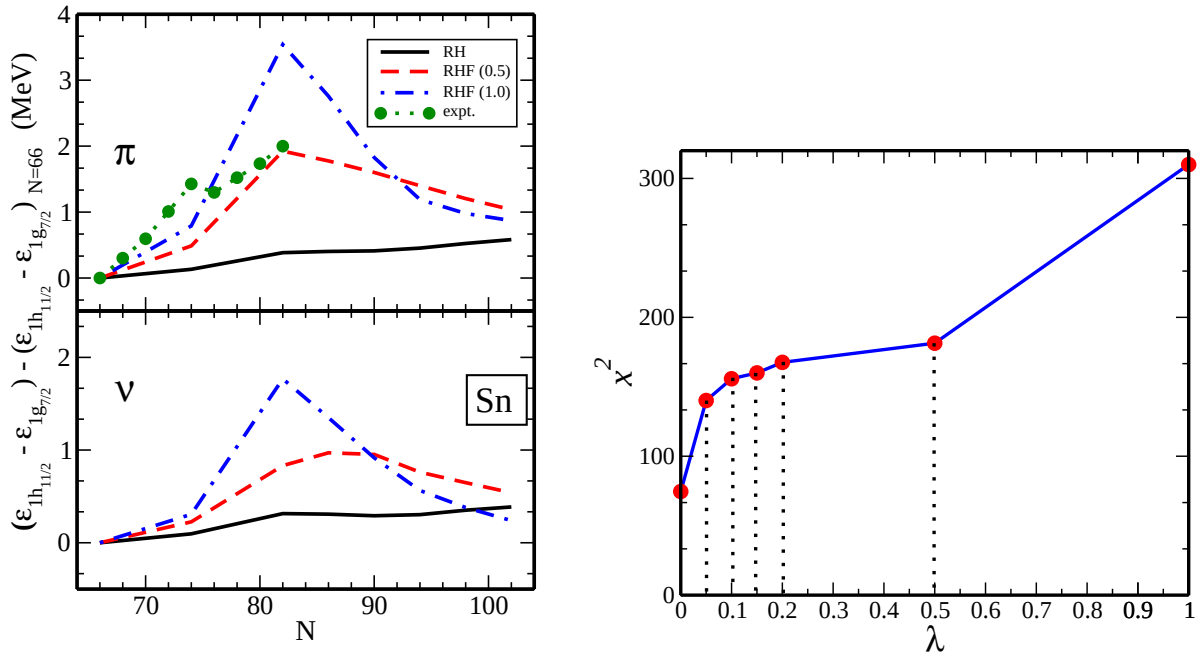


Figure 3. (left panel) The evolution of the $1h_{11/2}$ and $1g_{7/2}$ neutron and proton energy gap. The s.p levels of ^{116}Sn are taken as reference point. (right panel) χ^2 of the fit as function of the pion coupling constant in terms of the free pion coupling constant.(from Ref. [27]).

the coupling constants of the σ - the ω - and the ρ -meson at saturation density and the mass of the σ -meson are used for a fine-tuning of binding energies.

Extended applications of this functional on a global scale [17] have shown that it is comparable with all the modern relativistic high precision functionals containing considerably more phenomenological parameters. Fig. 1 shows that the deviations between theoretical and experimental binding energies are well below 0.5 %, with some exceptions for light nuclei. Since it is derived to a large extent from microscopic calculations, this functional contains a δ -meson. Its contributions in the iso-vector channel are not small. However, they are opposite in sign to those of the ρ -meson and for all the densities important in finite nuclei they are more or less compensated. The final iso-vector properties in this region are identical to high precision covariant density functionals without δ -meson. This is shown in Fig. 2 for the symmetry energy.

We can conclude that, at present, we are able to derive very successful semi-microscopic covariant density functionals [22, 26] from ab-initio results for nuclear matter and neutron matter, containing only few remaining parameters for a fine tuning.

3. Single particle energies and tensor terms

There are, however, additional problems, which cannot be treated with such simple Lagrangians. It is an open question, whether one needs further extensions. Famous examples are the tensor terms. In particular the momentum dependent tensor terms $\sim (\sigma_1 k_1)(\sigma_2 k_2)$ contained in the exchange terms of the σ - and ρ -meson. It leads to very specific properties of single particle energies, which cannot be reproduced in any of the simple mean field calculations. A famous case is the splitting of $1h_{11/2}$ and $1g_{7/2}$ proton configurations in the Sn-region. As it is shown in the left panel of Fig. 3, the experimental data can be reproduced by including the exchange term of a one-pion exchange using a strength parameter roughly one half of the experimental pion-nucleon coupling in the vacuum. The right panel of Fig. 3 shows that it is impossible to determine the size of this parameter by fitting to bulk properties, such a masses and radii, because the best fit is obtained without pion contributions. Similar results have also been found

in density dependent Relativistic Hartree-Fock (RHF) theory [28].

Of course, the results of the left panel of Fig. 3 would suggest to proceed on the phenomenological way and to fit to single particle energies. There are two reasons against such a procedure, first, according to the principle of the Kohn-Sham method in density functional theory, the single particle energies are only mathematical auxiliary objects and no measurable quantities, and second, there exists particle-vibrational coupling (PVC), which leads to a considerable fragmentation of the single particle levels. At present, it is not only conceptually, but also technically impossible to carry out such a fit. The experimental knowledge on the spectroscopic factors is mostly very limited and PVC calculations in deformed nuclei are extremely complicated. Most of the very few investigations with PVC are based on simple separable forces. In fact, recent investigations [29] show, that PVC plays also a considerable role in the Sn-isotopes shown in the left panel of Fig. 3.

4. Relativistic Brueckner-Hartree-Fock theory in finite nuclei

The concept to derive density functionals from properties of infinite nuclear matter, is very successful for general properties of these functionals. However, it cannot teach us too much when it comes to properties of the functionals, which do not show up in nuclear matter as for instance the tensor term in spin non-saturated systems. Nuclear matter is usually spin-saturated and therefore the contributions of the tensor term in first order are small. In order to study such effects from ab-initio calculations, we have to carry out microscopic calculations in finite nuclei, in particular also in heavy nuclei, which are not spin-saturated.

An obvious way to carry out such investigations is Brueckner theory, the mother of modern density functional theory in nuclei [30, 31]. The advantage of relativistic Brueckner theory is that one does not need three-body force to get saturation in nuclear matter. Therefore Dirac-Brueckner-Hartree-Fock (DBHF) theory has been used to describe also finite nuclei [32, 33, 34, 35]. To our knowledge in all these applications the local density approximation has been used, i.e. in a first step the self-energies are calculated in nuclear matter of various densities. In a second step the relativistic Hartree-Fock equations are solved in finite nuclei with density dependent coupling constants adjusted to the results of nuclear matter calculations at the corresponding density.

Although such calculations are successful, they cannot reach the accuracy of present day phenomenological covariant density functionals. It is also clear that this concept is relatively useless for a microscopic study of the influence of the tensor force in finite non spin-saturated nuclei, because, as discussed above, nuclear matter is spin-saturated.

By this reason we started a new project to solve the DBHF equations in finite systems. The relativistic Hartree-Fock equations will be solved in a large oscillator basis with N_f major shells [36, 27] by iteration. The interaction will be the G -matrix and its matrix elements $\langle ab|G(\omega)|cd\rangle$ will be determined, in each step of this iteration, by the solution of the Bethe-Goldstone (BG) equation

$$G(\omega) = \bar{V}^N + \bar{V}^N Q_F \frac{1}{\omega - H_0} Q_F G(\omega). \quad (1)$$

in the same relativistic oscillator basis (for details see Ref. [36]). Here $\bar{V}^N$ are the anti-symmetrized matrix elements the relativistic bare force *Bonn A* [37], H_0 are the self-consistent two-particle energies $\epsilon_m + \epsilon_{m'}$ of the RHF-operator at this step of the iteration, and Q_F is the Pauli operator

$$Q_F = \sum_{m < m'} |mm'\rangle \langle mm'|. \quad (2)$$

summing over intermediate states m, m' above the Fermi surface. Of course, since the single particle energies ϵ_m and $\epsilon_{m'}$ refer to the eigenvalues of the RHF-operator, the Pauli operator

(2) is defined in the corresponding relativistic Hartree-Fock basis. Therefore the full solution of this problem requires the transformation of the Pauli-operator from the RHF basis to the oscillator basis and this is the final goal of such calculations. In a first step we plan the so-called *oscillator* approximation for the Pauli operator, i.e. we use in Eq. (2) oscillator states for the wave functions $|mm'\rangle$. On the other hand self-consistent RHF-energies $\epsilon_m + \epsilon_{m'}$ with the same number of radial nodes will be used for H_0 . For light nuclei this seems to be a reasonable approximation.

The corresponding code has been developed and first preliminary results show the possibility of such a concept. However further tests are necessary and therefore we show here only first results in the local density approximation, where the mean field equations are solved for a density dependent interaction determined by the solution of the DBHF-equations in nuclear matter [38].

As an application we consider the nucleus ^{16}O . We use the realistic NN interaction Bonn A which has been adjusted to the NN scattering data in Ref. [37].

Table 1. Ground state properties of ^{16}O : total binding energy (MeV), charge radius (fm), and spin-orbit splitting (MeV) for the $1p$ proton shell. Experiments are compared with calculations discussed in the text. The theoretical values are given by their deviations from the experiment (in %). Negative (positive) values for the binding energies mean under- (over-) binding

	EXP. [39, 40]	PKO1 [28]	BHF [41]	DDBH	DDBHF	CC-NN [42]	CC-NNN [43]
E	-127.62	-0.6 %	-17.8 %	-15.8 %	-8.0 %	-5.3 %	+6.6 %
r_c	2.74	-1.6 %	-16.3 %	-4.9 %	-3.8 %	—	—
ΔE_{1p}^{ls}	6.3	+1.6 %	+19.0 %	-17.5 %	-23.8 %	—	—

The ground state properties, total binding energy, charge radius and the proton spin-orbit splitting for the $1p$ shell of ^{16}O are listed in Table 1. The experimental results are compared with a RHF calculation with the phenomenological set PKO1 [28], a non-relativistic Brueckner calculation BHF [41] with the potential *Bonn A*, two calculations using the local density approximations on the Hartree (DDBH) and on the Hartree-Fock (DDBHF) level. It is seen that the ground state properties in the Brueckner calculations in finite nuclei are improved considerably as compared to the non-relativistic results even in the local density approximation. The deviation from the experimental values have been decreased from 18% to 8% in the case of the energy and from 16 % to 4 % in the case of the charge radius, which is consistent with the conclusions in the infinite nuclear matter [44]. For the binding energy of ^{16}O the same quality is reached as in the coupled-cluster calculations based on chiral interactions at N^3L order using only two-body forces (CC-NN) [42] and in addition three-body forces (CC-NNN) [45].

In summary, a code has been developed for the solution of the Dirac-Brueckner-Hartree-Fock (DBHF) equations for finite nuclei in an oscillator basis. We hope that we can improve in this way the results of the local density approximation shown in Table 1. The only input is the bare NN-force Bonn A adjusted to the scattering phase shifts in Ref. [37]. No other parameter is used.

Of course there are many open problems: The oscillator approximation for the Pauli operator should be avoided. Heavier nuclei have to be investigated, in particular those with non spin-saturated configurations, as for instance ^{132}Sn or ^{208}Pb . This will give us information about the importance of the tensor term in finite nuclei. Pairing correlations and deformations should be included for the description of open shell nuclei.

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