On the way to a microscopic derivation of covariant density functionals in nuclei

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Abstract. Several methods are discussed to derive covariant density functionals from the microscopic input of bare nuclear forces. In a first step there are semi-microscopic functionals, which are fitted to ab-initio calculations of nuclear matter and depend in addition on very few phenomenological parameters. They are able to describe nuclear properties with the same precision as fully phenomenological functionals. In a second step we present first relativistic Brueckner-Hartree-Fock calculations in finite nuclei in order to study properties of such functionals, which cannot be obtained from nuclear matter calculations.

1. Introduction

At present, in spite of the important progress made recently in the ab-initio studies of nuclear properties, the majority of heavy nuclei are only accessible through nuclear density functional theory (DFT). Non-relativistic [1] and relativistic [2] 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, for complicated configurations [3] and for sophisticated low-lying spectra in transitional nuclei [4, 5].

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 [6, 7]. 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 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-inito functionals in nuclear physics, at least in foreseeable future will always depend on some phenomenological parameters for fine tuning.

Symmetries play an essential role in the construction of such functionals. 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 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 [2].
Of course, we do not need relativistic kinematics and therefore non-relativistic functionals are very successful too. However, this is only possible at the cost of additional phenomenological parameters connected with the relativistic corrections, as for instance the spin-orbit term. Because of the extremely large relativistic fields and because of the reduced effective mass in these systems such expansions in terms of the velocity do not reach the necessary precision required for such calculations.

2. Phenomenological covariant DFT’s
In contrast to non-relativistic functionals of Skyrme [8] or Gogny [9] type, which start from the beginning with roughly a dozen parameters and a simple power-law of $\sim \rho^3$ for the density dependence, relativistic functionals are based on the Walecka model [10] and start with only four parameters, the coupling constants for the three mesons $g_\sigma$, $g_\omega$, $g_\rho$, and the mass $m_\sigma$ of the $\sigma$-meson. These four parameters are clearly connected with basic properties of the effective nuclear force: medium range attraction ($g_\sigma$), short range repulsion ($g_\omega$), isospin dependence ($g_\rho$) and the range of the force ($m_\sigma$), which determines the surface properties, such as radii in finite nuclei. The details are, however more complicated. As Boguta and Bodmer [11] have pointed out already very early, this linear model fails to describe basic nuclear properties as for instance nuclear compressibility or nuclear deformations [12]. This was the birthday of covariant density functional theory and from that moment all the efforts have been devoted to a better description of the density dependence by additional phenomenological parameters. In a first step non-linear meson couplings have been proposed [11]. Examples are the parameter sets NL3[13] or FSUGold [14]. Modern versions, as for instance DD-ME2 [15] replace the non-linear meson couplings by density dependent coupling constants $g_\sigma(\rho)$, $g_\omega(\rho)$, and $g_\rho(\rho)$. Calculations with finite meson masses are still relatively complicated and therefore modern point-coupling functionals have been developed [16], which include zero-range forces and derivative terms. Again one has essentially only four parameters and their density dependence. All in all one has roughly 10 phenomenological parameters. This seems a similar number as in the non-relativistic case, but there is a difference: in the relativistic models most of the parameters (roughly 6) are used for a sophisticated description of the density dependence, while Skyrme or Gogny use only a power law $\rho^\alpha$, and even that $\alpha$ is most cases chosen as fixed $\alpha = \frac{1}{3}$ or $\alpha = 1$.

3. Semi-microscopic covariant DFTs
In Coulombic systems an essential input for the derivation of microscopic functionals [17] 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 [18, 19]. Of course, at present there are no exact solutions of the nuclear matter problem available. One has to rely on approximate solutions, such as sophisticated variational calculations [20] or modern Brueckner-Hartree-Fock methods [21].

The basic idea of microscopic covariant density functionals is therefore to start from RBHF-calculations in nuclear matter [22] of various densities and to map the results to a Walecka model with density dependent parameters [23, 24]. However, this mapping is not unique and therefore there are many open questions until today. In addition, none of these fully microscopic functionals is able reach the accuracy necessary for practical applications.

Much more successful are semi-microscopic functionals, which use microscopic calculations in nuclear matter in order to reduce the number of phenomenological parameters considerably. An example is the parameter set DD-ME2δ [25]. Here the density dependence of the corresponding meson-nucleon couplings is adjusted to microscopic calculations in nuclear matter and only four phenomenological parameters $g_\sigma(\rho_{\text{sat}})$, $g_\omega(\rho_{\text{sat}})$, $g_\rho(\rho_{\text{sat}})$ ($\rho_{\text{sat}}$ is the saturation density), and $m_\sigma$ are fine tuned by a fit to masses and radii of finite nuclei,
Extended applications of this functional on a global scale [26] have shown that the parameter set DD-MEδ is comparable with all the modern relativistic high precision functionals containing considerably more phenomenological parameters. The deviations between theoretical and experimental binding energies are well below 0.5%, with some exceptions for light nuclei. It should be emphasized that there are also successful non-relativistic semi-microscopic functionals based on the same concept [19].

We can conclude that, at present, we are able to derive very successful semi-microscopic covariant density functionals [25] from ab-initio results for nuclear matter and neutron matter that contain only few remaining parameters for a fine tuning.

4. The problem of tensor forces

We have to emphasize that all the microscopic input comes at this stage from ab-initio calculations in nuclear matter. On the other hand, there are problems in finite nuclei, where simple density functionals of this type consistently fail. An example are single-particle energies and their distribution. This has been found in an indirect way by global investigations in the area of transitional nuclei, which depend in some cases in a sensitive way on the single particle structure, but also in experimental observations of systematic shifts of single particle energies in isotopic chains. A famous case is the splitting of $1h_{11/2}$ and $1g_{7/2}$ proton configurations in the Sn-region [27], which show a very characteristic behavior as a function of the neutron number. None of the conventional density functionals can reproduce this behaviour on the Hartree level. Only relativistic Hartree-Fock calculations which contain tensor forces in the exchange terms can reproduce this behavior. However, the strength of the tensor has to be fitted in a phenomenological way [28]. Similar results have also been found in density dependent Relativistic Hartree-Fock (RHF) theory [29].

On the other hand, it is an open question whether these shifts in observed single particle energies are an indication of the necessity of effective tensor forces in relativistic density functionals. It is also known that present nuclear density functionals do not describe the exact solutions of the nuclear many-body problem. There are cases, which cannot be taken into account on the mean field level, and where one has to go beyond mean field. An example is particle vibrational coupling which has a considerable influence on the single particle energies. It can also be treated in covariant density functionals [30]. In fact, recently it has been shown by A. Afanasjev and E. Litvinova [31] that a large part of the shifts of $1h_{11/2}$ and $1g_{7/2}$ proton configurations in the Sn-region [27] can be described with the simple functional NL3* including quasiparticle-vibrational coupling.

5. Microscopic calculations in finite nuclei

The concept to derive density functionals from properties of infinite nuclear matter cannot teach us much when it comes to properties of the functionals, which do not show up in nuclear matter calculations as for instance the tensor term in spin non-saturated systems. Here one needs ab-initio calculations in finite nuclei. An obvious way to carry out such investigations is Brueckner theory, the mother of modern density functional theory in nuclei. The advantage of relativistic Brueckner theory is that one does not need three-body forces to get saturation in nuclear matter close to the experimental area. Therefore Relativistic Brueckner-Hartree-Fock (RBHF) theory has been used to describe also finite nuclei [23, 32, 33, 34]. In most of these applications the local density approximation (LDA) 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 for Walecka-type functionals are solved in finite nuclei with density dependent coupling constants adjusted to the results of nuclear matter calculations at the corresponding density. This provides a mapping of the microscopically obtained nuclear matter results onto RHF-models of Walecka type.
Although such calculations are successful, they cannot reach the accuracy of present day phenomenological covariant density functionals. In particular, the mapping is not unique and therefore the results of different groups deviate from each other considerably. Therefore we started a new project to solve the DBHF equations in large finite basis. First we started in an oscillator basis [35], but then we found we found a large Dirac-Woods-Saxon (DWS) basis more appropriate [36]. There are basis states with positive and negative energies and cut-off-parameters are introduced for the basis, such that convergence is achieved. For details see Ref. [37] 

Within relativistic Brueckner-Hartree-Fock (RBHF) theory [38, 39, 40] the relativistic Hartree-Fock (RHF) equations are solved with an effective interaction in the nuclear medium, the so-called G-matrix. Its matrix elements \( \langle ab | G(\omega) | cd \rangle \) are determined by the solution of the Bethe-Goldstone (BG) equation in the DWS basis

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

(1)

Here \( \bar{V}^N \) are the anti-symmetrized matrix elements of the relativistic bare force, \( H_0 \) are the self-consistent two-particle energies \( \epsilon_m + \epsilon_{m'} \) of the RHF-operator at each step of the iteration, and \( Q_F \) is the Pauli operator

\[
Q_F = \sum_{m < m'} |mm'\rangle \langle mm'|.
\]

(2)

summing over intermediate states \( m, m' \) above the Fermi surface. Since the single particle energies \( \epsilon_m \) and \( \epsilon_{m'} \) refer to the eigenvalues of the RHF-operator, Eq.(1) has to be transformed to the self-consistent relativistic Hartree-Fock basis during the iteration.

Table 1. Ground state properties of \(^{16}\text{O}\) obtained with RBHF theory are compared various other approximations and with experiment (from Ref. [41]).

|          | \( E \) (MeV) | \( r_c \) (fm) | \( r_m \) (fm) | \( \Delta E_{\pi p}^{ls} \) (MeV) |
|----------|----------------|---------------|---------------|-----------------------------|
| EXP      | -127.6         | 2.70          | 2.54(2)       | 6.3                         |
| RBHF, Bonn A | -113.5      | 2.56          | 2.42          | 5.4                         |
| RBHF (DWS) [37] | -120.7     | 2.52          | 2.38          | 6.0                         |
| DDRHF, PKO1 [29] | -128.3      | 2.68          | 2.54          | 6.4                         |
| DDRHF, PKA1 [42] | -127.0      | 2.80          | 2.67          | 6.0                         |
| BHF [43], Bonn A | -105.0     | 2.29          | 7.5           |                             |
| BHF [44], AV18  | -134.2      | 1.95          | 13.0          |                             |
| CC [45], N^3LO  | -120.9    | 2.30          |               |                             |
| NCSM [46], N^3LO | -119.7(6) | 2.30          |               |                             |
| NLEFT [47], N^2LO | -121.4(5) |               |               |                             |

As an application we consider the nucleus \(^{16}\text{O}\). We use the realistic NN interaction Bonn A which has been adjusted to the NN scattering data in Ref. [48]. The ground-state properties are listed in Table 1. The results of our full RBHF calculation are compared with the corresponding experimental data and with several other calculations: BHF are non-relativistic Brueckner calculations. We also show results obtained in RHF-calculations with the phenomenological effective interaction PKO1, which has been fitted to binding energies and charge radii of a set of spherical nuclei. It is seen that the ground-state properties in RBHF theory are improved considerably as compared with the non-relativistic results. Of course the results of the
calculations with PKO1 which has been fitted to these data shows only a very small deviation from the experimental values. At present our results show considerable underbinding. The origin for that is not clear and requires further investigations. It could have to do with the potential Bonn A, where the non-relativistic calculations show strong also underbinding, but it could be also caused by the fact, that Brueckner theory is only an approximation where 3-hole lines and higher configurations are neglected. Finally it could be an indication that we need three-body forces, even in the relativistic case.

In Fig. 1 we compare our results in a DWS-basis with non-relativistic BHF calculations [43] and with two versions of LDA [49]. The single-particle energy levels of $^{16}$O for protons and neutrons obtained from the full RBHF calculation are plotted in Fig. 2. They are compared with experimental data and (for the protons) with the results of non-relativistic BHF calculations.

![Figure 1. Energy per particle and charge radius of $^{16}$O by (relativistic) BHF theories compared with experimental data and other calculations. See text for details (from Ref. [37]).](image1)

![Figure 2. Single-particle spectra for protons and neutrons obtained from the solution of the RHF-equation are compared with experiment. (from Ref. [37]).](image2)

6. Conclusions
In summary, the full relativistic Brueckner-Hartree-Fock (RBHF) equations have been solved. The relativistic structure of the two-body matrix elements as well as of the Pauli operator is fully taken into account. The only input is the bare $NN$-interaction Bonn A adjusted to the scattering phase shifts in Ref. [48]. No other parameter is used. Since nuclear matter calculations within the same framework produce results far away from the Coester line and close to the experimental values of saturation, we neglect at this stage three-body forces.

Despite the good agreement of these results, there is room for improvements. The RBHF-theory presented here is no exact solution of the nuclear many-body problem. So far, rearrangement terms are not taken into account and higher order diagrams in the hole-line expansion are not included.

On the other hand, our method has the potential to investigate heavier nuclei, where exact solutions are impossible, in particular systems without spin saturation and with large neutron excess. In this case we hope to be able to gain a parameter-free, microscopic understanding of open questions in modern phenomenological density functional theories, such as their isospin dependence or the importance of the tensor terms.

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