RELATIVISTIC BRUECKNER–HARTREE–FOCK THEORY: AN AB INITIO APPROACH FOR FINITE NUCLEI*

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Attempts are discussed to derive covariant density functionals *ab initio*, *i.e.* from the bare nucleon–nucleon forces. They are based on the Relativistic Brueckner–Hartree–Fock (RBHF) theory which, in most cases, has been applied for nuclear matter. For semi-microscopic functionals, such calculations are used to derive the density dependence of the parameters. In this way, only very few phenomenological parameters are left for the fine tuning. The RBHF calculations in finite nuclear systems are used to obtain additional formation as, for instance, the strength of effective tensor forces, which are difficult to obtain in a phenomenological way from the data.

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1. Introduction

Considerable progress has been achieved in recent years in *ab initio* derivations of nuclear properties from bare nucleon–nucleon forces. Nowadays, it is possible to solve the exact nuclear many-body problem for light nuclei on the computer. For heavier nuclei, approximate methods have been applied successfully. The investigation of nuclear properties for the majority of nuclear systems, however, is left to density functional methods. Non-relativistic [1, 2] and relativistic [3–7] versions allow an effective description of the nuclear many-body problem not only for ground-state properties, but also for excitations such as collective rotations and giant resonances and, by going beyond mean field, for sophisticated low-lying spectra in transitional nuclei [8, 9] and the coupling to complicated configurations [10]. 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 [11, 12], a goal which has been reached since many years in Coulombic systems. This functional should be

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able to explain as many data as possible within the same parameter set and to provide reliable predictions for 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, such attempts 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 sufficiently precise to achieve the required accuracy.

Symmetries play an essential role in the derivation of energy density functionals. One of the underlying symmetries of QCD is the Lorentz invariance and, therefore, covariant density functionals are of particular interest in nuclear physics. This symmetry not only allows to describe, in a consistent way, the spin–orbit coupling, which has an essential influence on the underlying shell structure, 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. It is true that the velocities of nucleons in the Fermi sea are relatively small. As sumrule approximations of QCD predict [13], there are large scalar and vector fields of opposite sign in the nuclear medium. Since the fifties, one knows [14] that they cancel in the average field, but they add up in the velocity-dependent spin–orbit term, such that even small velocities lead to large effects, which cannot be treated by perturbation theory. Of course, a non-relativistic expansion is possible, but it leads to various large correction terms at the cost of additional phenomenological parameters as the spin–orbit term in non-relativistic density functionals. Therefore, we restrict ourselves in the following to the Covariant Density Functionals Theory (CDFT).

2. Semi-microscopic density functionals

In Coulombic systems, 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 $E_\infty[\rho]$, 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 [15]. Of course, at present, there are no exact solutions for homogeneous nuclear matter available. One has to rely on approximate solutions, such as sophisticated variational calculations [16] or modern Brueckner–Hartree–Fock methods [17, 18]. The point coupling functional DD-PC1 of the Munich–Zagreb group [19] used this microscopic input together with experimental masses of 64 heavy deformed nuclei in order to adjust 10 phenomenological parameters, the four coupling constants α_S, α_V, α_{ST}, δ_S at saturation and six further parameters to describe the density dependence. The result is a semi-microscopic functional with an EoS nearly

identical to the microscopic EoS of the Illinois group [16] which can be used at higher densities in neutron stars with much more confidence than the extrapolations of phenomenological functionals adjusted only at saturation density and below. To reduce the number of phenomenological parameters, in analogy to the non-relativistic considerations of the Catania group [20], we went a step further and derived a semi-phenomenological relativistic functional DD-MEδ [21]. In contrast to the phenomenological covariant density functionals, where the isospin dependence is completely determined by the vector ρ-meson, microscopic Dirac–Brueckner–Hartree–Fock (DBHF) calculations [18] show clearly that there is also an isospin dependence in the scalar channel described by the isovector δ-meson (sometimes called a_0). We derived the four density-dependent parameters $g_\sigma(\rho)$, $g_\omega(\rho)$, $g_\rho(\rho)$, and $g_\delta(\rho)$ from *ab initio* calculations for nuclear matter (see Fig. 1). In addition, four

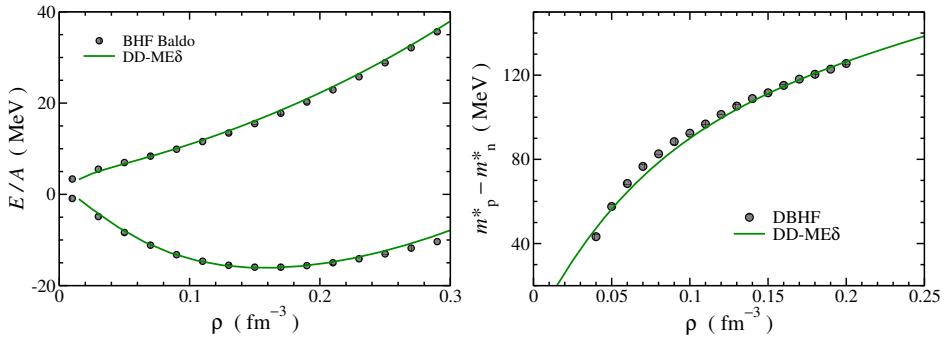

Fig. 1. (Color online) Binding energy per nucleon E/A for symmetric nuclear matter and for neutron matter (left panel), and proton–neutron effective mass difference as a function of the nucleon density in pure neutron matter (right panel). The dots represent the results of BHF [17] and RBHF [18, 22] calculations. The lines correspond to DD-MEδ. Figure taken from Ref. [21].

phenomenological parameters $g_\sigma(\rho_{\rm sat})$, $g_\omega(\rho_{\rm sat})$, $g_\rho(\rho_{\rm sat})$, and $\delta_{\rm S}$ where fitted to a set of spherical finite nuclei. This corresponds only to a fine-tuning of the values $g_\sigma(\rho)$, $g_\omega(\rho)$, $g_\rho(\rho)$. In fact, such a fine-tuning will always be necessary for microscopic nuclear energy density functionals, as we see in Table I, where the various contributions to the total energy of ^{208}Pb are given for the functionals DD-MEδ and DD-PC1. The scalar energy $E_{\rm S}$ of roughly 30 GeV is compensated to a large extent by the vector energy $E_{\rm V}$ and by the kinetic energy. The total binding energy $E_{\rm tot}$ of roughly 1.638 GeV represents only $\approx 5\%$ of the scalar energy. As a consequence, in order to reach an accuracy of 100 keV, as it is required for some astrophysical applications, one needs an accuracy of $0.1/30000 \approx 3 \times 10^{-6}$. This will never be reached in *ab initio* calculations.

TABLE I

Contributions to the total energy $E_{\rm tot}$ for ^{208}Pb in GeV, the scalar part $E_{\rm S}$, the vector part $E_{\rm V}$, the Coulomb energy $E_{\rm C}$, the kinetic energy $E_{\rm kin}$, and the center-of-mass correction $E_{\rm CM}$. Columns 3 and 6 give the percentages of these values in terms of $E_{\rm S}$, the 4$^{\rm th}$ and 7$^{\rm th}$ columns show the isovector contributions to $E_{\rm S}$ and $E_{\rm V}$.

^{208}Pb	DD-MEδ [21]			DD-PC1 [19]		
			$T=1$			$T=1$
$E_{\rm S}$	−30.014	100.00%	−0.173	−31.811	100.00%	0
$E_{\rm V}$	+24.642	82.10%	+0.275	+26.638	83.70%	+0.097
$E_{\rm C}$	+0.828	0.28%		+0.828	0.26%	
$E_{\rm kin}$	+2.916	9.71%		+2.710	8.52%	
$E_{\rm CM}$	−0.006			−0.006		
$E_{\rm tot}$	−1.633	5.44%		−1.641	5.16%	
ΔE	−0.004			−0.003		

A systematic investigation over the entire nuclear chart in Ref. [23] has shown that the semi-microscopic functional DD-MEδ has very similar properties as DD-MEδ. This is a remarkable result, because as compared to DD-ME2 with 8, DD-MEδ has only 4 phenomenological parameters. The rest is determined *ab initio*, *i.e.* by the bare nucleon–nucleon force through the relativistic and non-relativistic Brueckner–Hartree–Fock theory.

3. Microscopic density functionals for finite systems

The form of the semi-microscopic density functionals discussed in the last section is based on the Walecka model [24], where exchange terms are neglected. Therefore, these functionals do not contain tensor terms. On the other hand, it is well known that tensor terms play an important role in systems, which are not spin-saturated [25]. It is clearly seen that they have an influence on single-particle energies and on the spin–orbit splitting in such systems. In fact, pure mean field models, without tensor terms are not able to reproduce recent experimental data in Ref. [26] on the change of single-particle splittings along the Sb-isotopes. Using the Relativistic Hartree–Fock (RHF) theory, tensor forces can be included in CDFT-models based on the RHF theory [27–29]. However, it is very difficult to fit the corresponding parameters, because experimental single-particle energies are not only influenced by tensor forces, but also by correlations beyond mean field as, for instance, by the coupling to complex configurations [30, 31]. In addition, RHF calculations with finite range forces require tremendous numerical efforts and are, up to now, practically restricted to spherical or rather light axially deformed nuclei.

Therefore, to determine the strength of effective tensor forces in covariant density functionals, it has been proposed to carry out relativistic *ab initio* calculations in the framework of the relativistic Brueckner–Hartree–Fock theory [32]. The BHF theory is the mother of nuclear density functional theory in the early seventies. At that time, the non-relativistic BHF theory failed to reproduce the saturation properties of nuclear matter [33] due to the missing three-body forces. However, it turned out to be very successful to replace the microscopically determined G-matrix by a phenomenological density-dependent interaction [1]. In the eighties, it has been found that the saturation properties of nuclear matter can be reproduced by the RBHF theory [34–37]. An important part of the effective three-body forces in nuclear matter [38], the relativistic Z-diagram [39], is included in such calculations.

There are many approximate applications of the RBHF theory for finite nuclei [22, 40–43]. All of them are based on the solution of the RHBF equations in nuclear matter and the local density approximation. These results are used to adjust the parameters of relativistic Lagrangians, which are applied for calculations for finite nuclei in the framework of the relativistic Hartree (RH) or the relativistic Hartree–Fock (RHF) approximation. Since infinite nuclear matter is a spin-saturated system, none of these calculations allows to adjust the strength of effective tensor forces for applications in finite nuclei. This information can only be obtained by relativistic *ab initio* calculations in finite systems.

The RBHF equations for finite nuclear systems have the following form: using the Thompson choice, we start with the relativistic Bethe–Goldstone (RBG) equation

$$\langle a'b'|\bar{G}(W)|ab\rangle = \langle a'b'|\bar{V}|ab\rangle + \sum_{c<d} \langle a'b'|\bar{V}|cd\rangle \frac{Q(c,d)}{W - e_c - e_d} \langle cd|\bar{G}(W)|ab\rangle \tag{1}$$

for finite systems. Here, the quantum numbers $a, b, c, \ldots$ characterize single-particle states, which are the self-consistent solutions of the RHF equation (2)

$$(T + U)|k\rangle = e_k|k\rangle \,. \tag{2}$$

Q is defined as the Pauli operator: $Q(c,d) = 1$ for $e_c > e_\mathrm{F}$ and $e_d > e_\mathrm{F}$ and $Q(c,d) = 0$ for all other cases. The single-particle states $|k\rangle$ are Dirac spinors with large and small components. They are expanded in terms of a complete Dirac–Woods–Saxon basis [44] containing solutions with positive and negative energies. T is the kinetic energy and the RBHF potential U is given by

$$\langle a|U|b\rangle = \begin{cases} \frac{1}{2}\sum_{c=1}^{A}\langle ac|\bar{G}(e_a+e_c)+\bar{G}(e_b+e_c)|bc\rangle\,, & e_a,\ e_b \le e_{\rm F}\,, \\ \sum_{c=1}^{A}\langle ac|\bar{G}(e_a+e_c)|bc\rangle\,, & e_a \le e_{\rm F},\ e_b > e_{\rm F}\,, \\ \sum_{c=1}^{A}\langle ac|\bar{G}(e'+e_c)|bc\rangle\,, & e_a,\ e_b > e_{\rm F}\,, \end{cases} \tag{3}$$

where $e_{\rm F}$ is the Fermi energy. The choice of e' and further details are discussed in Refs. [45, 46]. This system of RBHF equations (1), (2) and (3) has to be solved iteratively.

The potential V in the BGE (1) is a relativistic bare nucleon–nucleon interaction. We use the Bonn potential [47]. The very repulsive character of the bare force at short distances causes a scattering of the occupied states up to very high momenta. This leads to the inversion of rather large matrices and to considerable computer time for the self-consistent solution of the system of RBHF equations. Therefore, at present, one is restricted to spherical nuclei with $A \le 48$. In Table II, we show the results for the nucleus ^{16}O and compare them with the experiment and with other calculations, *i.e.* with the phenomenological RHF models (DDRHF), where the parameters of the

TABLE II

Total energy, charge radius, matter radius, and $\pi 1p$ spin–orbit splitting of ^{16}O calculated by RBHF theory [45, 46] with the interactions Bonn A, B, and C, in comparison with experimental data [48–51]. The corresponding results from DDRHF with effective interactions PKO1 [52] and PKA1 [28], non-relativistic BHF [53] with $V_{\text{low-}k}$ derived from Argonne v_{18}, CC method [54], IM-SRG [55], NCSM [56], and SCGF method [57] with N^{3}LO, NLEFT [58] with N^{2}LO, and QMC method [59] with local chiral force N^{2}LO are also included.

	E [MeV]	r_c [fm]	r_m [fm]	$\Delta E^{ls}_{\pi 1p}$ [MeV]
Exp.	−127.6	2.70	2.54(2)	6.3
RBHF, Bonn A	−120.2	2.53	2.39	5.3
RBHF, Bonn B	−107.1	2.59	2.45	4.5
RBHF, Bonn C	−98.0	2.64	2.50	3.9
DDRHF, PKO1	−128.3	2.68	2.54	6.4
DDRHF, PKA1	−127.0	2.80	2.67	6.0
BHF, AV18	−134.2		1.95	13.0
CC, N^{3}LO	−120.9		2.30	
IM-SRG, N^{3}LO	−122.8			
NCSM, N^{3}LO	−119.7(6)			
SCGF, N^{3}LO	−122			
NLEFT, N^{2}LO	−121.4(5)			
QMC, N^{2}LO	−87	2.76		

Lagrangian have been adjusted, with non-relativistic BHF results, and with the results of various non-relativistic *ab initio* calculations. As compared to the experimental values, the RBHF results for the potential Bonn A show an underbinding of 5.8% and too small radii by roughly 5.9%. Of course, the results for the phenomenological models show perfect agreement, but the non-relativistic BHF calculations show an overbinding of 5.2% and too large radii by roughly 20%. For the other non-relativistic *ab initio* calculations, only binding energies are given in most cases and they are in rough agreement with the RBHF results, but it is known that the radii are usually 20% too small [60].

Neutron drops in an external field of oscillator shape have been investigated in Ref. [61] within the RHBF theory. It has been found that the tensor force produces a very specific pattern of the spin–orbit splitting for the various orbits in these systems. As expected, it is not reproduced by any of the usual CDFT functionals based on the relativistic Hartree approximation, but it is reproduced qualitatively by the RHF functional PKO1 which contains a tensor term. However, the strength of this term in PKO1 is somewhat too small. These investigations indicate that meta-data as the spin–orbit splittings in neutron drops can be used to adjust the strength of the tensor force in future functionals from *ab initio* calculations. Recently, this idea has been used in the non-relativistic case for the adjustment of the tensor force in the Skyrme functional Sami-T [62]. Investigations for relativistic density functionals are in progress.

4. Conclusions and outlook

We discussed recent attempts to derive covariant density functionals in a microscopic way from *ab initio* calculations. It is emphasized that, due to the large cancellation between the attractive scalar and repulsive vector components of the force, it will never be possible to reach in this way the required accuracy and a final fine tuning of a few parameters will always be necessary. On the other hand, the relativistic Brueckner–Hartree–Fock calculations in nuclear matter and in finite nuclei open new and very promising ways to determine the general structure and specific details of such functionals from the nucleon–nucleon scattering data. An example is the strength of tensor forces, which can be adjusted to the spin–orbit splittings in neutron droplets. Further examples could be the surface terms of such functionals, which, possibly could be determined by the RBFH calculations for half infinite nuclear matter.

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