Relativistic Brueckner–Hartree–Fock Theory for Finite Nuclei

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Starting with a bare nucleon-nucleon interaction, for the first time the full relativistic Brueckner–Hartree–Fock equations are solved for finite nuclei in a Dirac–Woods–Saxon basis. No free parameters are introduced to calculate the ground-state properties of finite nuclei. The nucleus $^{16}$O is investigated as an example. The resulting ground-state properties, such as binding energy and charge radius, are considerably improved as compared with the non-relativistic Brueckner–Hartree–Fock results and much closer to the experimental data. This opens the door for ab initio covariant investigations of heavy nuclei.

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Ab initio calculations, i.e., the proper description of finite nuclei with a bare nucleon-nucleon (NN) interaction adjusted only to the scattering data of free nucleons, form a central problem of theoretical nuclear physics since the middle of the last century. These realistic NN interactions are characterized by a repulsive core at short distances, a strong attraction in an intermediate range, and are dominated by one-pion exchange at large distances. Many methods have been proposed in the past to treat their singular behavior, such as Brueckner theory and variational methods. Recently, with the great progress of the high-precision NN interactions, such as Reid93, AV18, CD Bonn, and chiral potentials, and with increasing computer technology, more and more ab initio methods have been developed to study the nuclear many-body system, e.g., Green’s function Monte Carlo method, the self-consistent Green’s function method, the coupled-cluster method, the lattice chiral effective field theory, and the no-core shell model.

It has been found rather early that all the non-relativistic potentials systematically failed to reproduce the saturation properties of infinite nuclear matter in ab initio calculations. The saturation binding energies and the corresponding densities obtained with various forces are distributed on the so-called Coester line, which bypasses the experimental area considerably. Therefore, it has been concluded that the bare three-body force plays an essential role in the nuclear many-body problem, and all the modern non-relativistic investigations use such phenomenological terms. In this way, one was able to reproduce the saturation properties of nuclear matter and the ground-states and a few excited states of light nuclei. However, these calculations require extreme computational efforts and are very difficult to extend for heavy nuclei.

On the other side, it is known since more than 30 years that relativistic Brueckner–Hartree–Fock (RBHF) theory has no problems to reproduce empirical saturation data, even without three-body forces. This method is based on relativistic Hartree–Fock (RHF) calculations with an effective interaction, the $G$-matrix. It describes the scattering of two particles in the nuclear medium and is derived from the solution to the Bethe–Goldstone equation. It depends, in a self-consistent way, on the density and, therefore, in finite nuclei, on the position of the interacting particles. The non-relativistic BHF theory has been applied to study finite medium mass nuclei in the 1970s with different NN interactions. However, these applications have not been very successful because of the missing three-body interaction.

Inspired by the success of the RBHF theory in nuclear matter, it is a natural extension to study finite nuclei in the same framework. Nevertheless, in the 1980s, this was a formidable task and different approximations have been adopted. Mühler, Machleidt, and Brockmann applied the effective density approximation (EDA) where non-relativistic BHF

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expressed in the space of pair states. The Brueckner equation \( (3) \) is solved by matrix inversion in the space of pair states \( |ab\rangle \). These are pairs of Dirac-spinors with the full relativistic structure coupled to good angular momentum \( J \) (particle-particle \( (pp) \) coupling). The indices \( a \) and \( b \) run over all solutions of the Dirac equation (with positive and negative energies). The BG-equations are solved for each value of \( J \). This leads, for the various \( J \)-values, to a set of \( pp \)-coupled matrix elements of the \( G \)-matrix. The particle-hole \( (ph) \) coupled matrix elements of the \( G \)-matrix with \( I = 0 \) needed for the solution to the RHF equation \( (5) \) in the next step of the iteration are obtained by recoupling. The Pauli operator \( (4) \) and all its relativistic structure are here fully taken into account. In particular there is no angle averaging involved as it is the case in most Brueckner calculations in nuclear matter. Of course, in agreement with the \( no-sea approximation \), the sum of the intermediate states \( |mn\rangle \) in Eq. \( (3) \) does not include scattering to states in the Dirac sea.
In practice there are several problems. First, the $G$-matrix used in the RHF-equation (5) depends on the energy. As it turns out, this energy dependence is not uniquely defined. Several choices have been used in the literature.[42,43] We use here the so-called continuous choice for the evaluation of the mean potential as described in Eq. (1) of Ref. [43]. The BG equation (3) is solved for four different starting energies, and the $G$-matrix elements for the various starting energies required in this choice are obtained by interpolation.[43]

Second, the Pauli operator in Eq. (3) is obviously defined in the basis, in which the Dirac field of RHF equation (5) is diagonal. This requires, in each step of the iteration, a transformation of the basis and is connected with a considerable numerical effort. Therefore we adopt in this investigation a further approximation: assuming that the wave functions in the Pauli operator (4) are close to those of the original DWS basis, we evaluate the BG equation in this fixed basis. In the denominator of the BG equation (3), however, we have the starting energy $W$, i.e. the energy of the two incoming particle states before the scattering process and the energy $\varepsilon_m + \varepsilon_n$ of the particles afterwards. We use in all these cases the self-consistent single-particle energies of the corresponding RHF-potential with the same quantum numbers $(\ell j)$ and with the same number of radial nodes.

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. [2]. This is a relativistic two-body potential based on the exchange of the six mesons $\sigma$, $\omega$, $\rho$, $\pi$, $\eta$, and $\delta$, whose masses are less than 1 GeV with monopole form factors. The potential for the DWS basis is taken from Ref.[44]. In addition, the Coulomb exchange term is taken into account through the relativistic local density approximation of Ref.[45]. The microscopic center-of-mass correction $-P^2/2AM$ is included in the total energy and, as in the density functional STX6 of Ref.[46] it has been taken into account in the iterative solution to the RHF equation.

It is well known that the bare NN force contains a strong tensor part connecting the nucleons in the Fermi sea to states with high momenta in the continuum. In order to take this coupling fully into account one needs a relatively large basis and it is crucial to investigate the convergence of the RBHF calculation with the size of this basis. Therefore we show in Fig. 1 the resulting total energy and charge radius of $^{16}$O as functions of the cut-off energy $\varepsilon_{cut}$. The cut-off energy means that for each $(\ell j)$ value all the single-particle states with $\varepsilon_i \leq \varepsilon_{cut}$ are taken into account in the DWS basis. With increasing $\varepsilon_{cut}$ the energy and the charge radius of $^{16}$O decrease. We find satisfying convergence for $\varepsilon_{cut} = 1.1$ GeV with $E = -120.7$ MeV and $r_c = 2.52$ fm. Therefore, in the following, this value will be used.

| $E$ (MeV) | $r_c$ (fm) | $r_m$ (fm) | $\Delta E_{1p}$ (MeV) |
|-----------|-----------|-----------|-----------------|
| Exp.[47–49,53] | -127.6  | 2.70  | 2.54 | 6.3 |
| RBHF | -120.7  | 2.52  | 2.38 | 6.0 |
| BHF[28] | -105.0  | 2.29  | 7.5 |
| DDRHF[54] | -106.4  | 2.72  |  |
| DDRHF[54] | -142.6  | 2.62  | 4.5 |
| NCSM[51] | -119.7  |  |  |
| CC[52] | -121.0  | 2.30  |  |
| PKO1[38] | -128.3  | 2.68  | 2.54 | 6.4 |

The ground-state properties of $^{16}$O are listed in Table 1, including the total energy $E$, the charge radius $r_c$, the point matter radius $r_m$, and the proton spin-orbit splitting for the $1p$ shell. The results of our full RBHF calculation are compared with the corresponding experimental data[47–49] and with several other calculations: BHF is a non-relativistic Brueckner calculation[28] based on the interaction Bonn A. We also show the results obtained in the RHF calculations with the phenomenological effective interaction PKO1[38] 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 the RBHF theory are improved considerably as compared with the non-relativistic results. The deviations from the experimental values have been decreased from 18% to 6% in the case of the energy and from 16% to 7% in the case of the charge radius, which is consistent with the conclusions in the infinite nuclear matter.[50] This energy of $^{16}$O is also very close to the value of $E = -119.7$ MeV obtained within the non-core shell model (NCSM) using the chiral NN interaction N$^\infty$LO[51] and to the value of $E = -121.0$ MeV obtained within the coupled cluster (CC) method.[52] The spin-orbit splittings in the RBHF theory is only slightly smaller than the experimental data. For the $1p$ proton shell we have a deviation of about 5%. Of course, the results of the calculations with PKO1 which has been fitted to these data shows only a very small deviation of 0.5% for the energy, of 1.6% for the radius and the spin-orbit splitting.
Next in Fig. 2 we compare our self-consistent results in finite nuclei with those obtained in Ref. [54] by the two ab initio calculations based on the LDA. There the full RBHF equations are solved for nuclear matter at various densities and the corresponding scalar and vector self-energies are derived. Then density-dependent coupling strengths for the exchange of various mesons in the DDRH or DDRHF model have been adjusted to these results. In this case it is possible to investigate finite nuclei in an ab initio approach without any phenomenological parameters.

![Fig. 2](image)

**Fig. 2.** (Color online) Energy per particle and charge radius of $^{16}$O by (relativistic) BHF theories compared with the experimental data and other calculations. See text for details.

The results of these calculations based on the LDA are also listed in the 4th and the 5th rows of Table 1. The charge radii are rather well reproduced in these local density approaches. These values are considerably closer to the data than our calculations. There is, however, a considerable difference in the total energy between Hartree and Hartree–Fock results. DDRH shows 17% underbinding as compared with the experimental value. The Fock-term overshoots and shows a 12% overbinding. We have to keep in mind, however, that the methods connected with the LDA are always based on a mapping and there exist important uncertainties in this mapping, which deserve further investigations. The full solution to the RBHF equations in finite nuclei presented here is therefore very essential for comparisons in the future.

The single-particle energy levels of $^{16}$O for protons and neutrons obtained from the full RBHF calculation are plotted in Fig. 3. They are compared with the experimental data and the results of the non-relativistic BHF calculations. It is clearly seen that for protons and neutrons, the $p$-levels are slightly too low as compared with the data. This can possibly be understood by the fact that in all density-dependent mean-field calculations researchers find a too large gap in the single-particle spectrum at the Fermi surface. This seems to apply also for our results.

In the present method we sum up only ladder diagrams and neglect more complicated configurations in the intermediate states, which lead to energy-dependent self-energies and shifts of the single-particle spectrum in the neighborhood of the Fermi surface.[55]

In summary, the full relativistic Brueckner–Hartree–Fock (RBHF) equations have been solved for the first time for finite nuclei in a Dirac–Woods–Saxon (DWS) basis. In each step of the iteration the matrix elements of the $G$-matrix describing the scattering in the finite nuclear medium are determined by the solution to the Bethe–Goldstone equations in the DWS basis of sufficient size with the single-particle energies of the corresponding self-consistent relativistic potentials. 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 Born A adjusted to the scattering phase shifts in Ref. [2]. 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 three-body forces at this stage.

Modern non-relativistic BHF calculations in nuclear matter include three-body forces and are therefore able to reproduce the right saturation properties. An investigation of the microscopic origin of the various three-body terms showed that below and around nuclear saturation density, the three-body diagram with an NN-pair in the intermediate state that is coupled by $\sigma$-mesons to the other two nucleons (the so-called Z-diagram) is able to reproduce a large extent the total contribution of three-body forces. The other three-body diagrams cancel more or less in this density region. Therefore the successful description of nuclear saturation in the relativistic Brueckner theory is understandable because it includes automatically the Z-diagram. At the moment it is an open question to what extent one needs in a relativistic description additional bare three-body forces.

As an example we consider the nucleus $^{16}$O. We find convergence for a cutoff in the single-particle en-
ergy at $E_{cut} \approx 1.1$ GeV. The resulting binding energy is in good agreement with state-of-the-art parameter-free \textit{ab initio} calculations, but it still deviates by 6\% from the experimental data and the charge radius agrees with the experimental value up to 7\%. Also the spin-orbit splitting is well reproduced.

Despite the good agreement of these results, there is room for improvements. The RBHF theory presented here is no exact solution to 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. These effects have been taken into account in some approximation in non-relativistic calculations,[59] but for relativistic theories they are left for future investigations.

On the other side, 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.[37]

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References

[1] Jastrow R 1951 \textit{Phys. Rev.} \textbf{81} 165
[2] Machleidt R 1989 \textit{Adv. Nucl. Phys.} \textbf{19} 180
[3] Brueckner K A, Levinson C A and Mahmoud H M 1954 \textit{Phys. Rev.} \textbf{95} 217
[4] Day B D 1967 \textit{Rev. Mod. Phys.} \textbf{39} 719
[5] Jastrow 1955 \textit{Phys. Rev.} \textbf{98} 1479
[6] Day B D 1978 \textit{Rev. Mod. Phys.} \textbf{50} 495
[7] Stoks V G J, Kloepn R A M, Terheggen C P F and de Swart J J 1994 \textit{Phys. Rev. C} \textbf{49} 2950
[8] Wirtinga R B, Stoks V G and Schiavilla R 1995 \textit{Phys. Rev. C} \textbf{51} 58
[9] Machleidt R 2001 \textit{Phys. Rev. C} \textbf{63} 034001
[10] Epelbaum E, Hammer H W and Meissner U G 2009 \textit{Rev. Mod. Phys.} \textbf{81} 1773
[11] Machleidt R and Eistert D R 2011 \textit{Phys. Rep.} \textbf{503} 1
[12] Carlson J, Gandolfi S, Pedersen F, Pieper S c, Schiavilla R, Schmidt K E and Wirtinga R B 2015 \textit{Rev. Mod. Phys.} \textbf{87} 1067
[13] Dickhoff W H and Barbieri C 2004 \textit{Prog. Part. Nucl. Phys.} \textbf{52} 377
[14] Hagen G, Papenbrock T, Hjorth-Jensen M and Dean D J 2014 \textit{Rep. Prog. Phys.} \textbf{77} 066302
[15] Lee D 2009 \textit{Prog. Part. Nucl. Phys.} \textbf{63} 117
[16] Barrett B R, Narzval P and Vary J P 2013 \textit{Prog. Part. Nucl. Phys.} \textbf{69} 131
[17] Corner F, Cohen S, Day B and Vincent C M 1970 \textit{Phys. Rev. C} \textbf{1} 769
[18] Fujita J and Miyazawa H 1957 \textit{Prog. Theor. Phys.} \textbf{17} 360
[19] Brown G and Green A 1969 \textit{Nucl. Phys. A} \textbf{137} 1
[20] Song H Q, Baldo M, Giusfreda G and Lombardo U 1998 \textit{Phys. Rev. Lett.} \textbf{81} 1584
[21] Pieper S C and Wirtinga R B 2001 \textit{Annu. Rev. Nucl. Part. Sci.} \textbf{51} 53
[22] Anastasio M R, Celenza L S, Pong W S and Shakin C M 1983 \textit{Phys. Rev.} \textbf{100} 327
[23] Broennmann R and Machleidt R 1984 \textit{Phys. Lett. B} \textbf{149} 283
[24] ter Haar B and Malfliet R 1987 \textit{Phys. Rep.} \textbf{149} 207
[25] Bethe H A and Goldstone J 1957 \textit{Proc. R. Soc. A} \textbf{238} 551
[26] Becker R L, Davies K T R and Patterson M R 1974 \textit{Phys. Rev. C} \textbf{9} 1221
[27] Mithör R, Machleidt R and Broennmann R 1988 \textit{Phys. Lett. B} \textbf{202} 483
[28] Mithör R, Machleidt R and Broennmann R 1990 \textit{Phys. Rev. C} \textbf{42} 1981
[29] Broennmann R and Taki H 1992 \textit{Phys. Lett. B} \textbf{286} 408
[30] Fritz R, Mithör R and Machleidt R 1993 \textit{Phys. Rev. Lett.} \textbf{71} 46
[31] van Dalen E N E and Mithör R 2010 \textit{Int. J. Mod. Phys. E} \textbf{19} 2077
[32] van Gaai N, Carlson B V, Ma Z and Wolter H 2010 \textit{J. Phys. G} \textbf{37} 064043
[33] Zhou S G, Meng J and Ring P 2003 \textit{Phys. Rev. C} \textbf{68} 054323
[34] Ring P and Schuck P 1990 \textit{The Nuclear Many-Body Problem (Berlin: Springer-Verlag)}
[35] Bethe H A 1971 \textit{Ann. Rev. Nucl. Sci.} \textbf{21} 93
[36] Krenciglowa E M, Kund C L, Kuo T T S and Osmes E 1976 \textit{Ann. Phys. (N. Y.)} \textbf{101} 154
[37] Lalazissis G A, Karatzios S, Serna M, Otsuka T and Ring P 2000 \textit{Phys. Rev. C} \textbf{60} 041301
[38] Long W H, Van Gaai N and Meng J 2006 \textit{Phys. Lett. B} \textbf{640} 150
[39] Hafel M I and Tabakin F 1970 \textit{Nucl. Phys. A} \textbf{158} 1
[40] Schiller E, Mithör R and Czerwiński P 1999 \textit{Phys. Rev. C} \textbf{59} 2934
[41] Suzuki K, Okamoto R, Kohno M and Nagata S 2000 \textit{Nucl. Phys. A} \textbf{665} 92
[42] Rajamänt R and Bethe H A 1967 \textit{Rev. Mod. Phys.} \textbf{39} 745
[43] Davies K T R, Bäumler M, Tarrbout R M and Kuo T T S 1969 \textit{Phys. Rev. Lett.} \textbf{17} 1519
[44] Körpf W, Stärim M and Ring P 1991 \textit{Nucl. Phys. A} \textbf{533} 935
[45] Gu H Q, Liang H, Long W H, Gaai N V and Meng J 2013 \textit{Phys. Rev. C} \textbf{87} 041301
[46] Chalasniak E, Bönche P, Haensel P, Meyer J and Schaeffer R 1998 \textit{Nucl. Phys. A} \textbf{635} 331
[47] Wäng M, Audi G, Wapstra F, MacCormick M, Xu X and Pfeiffer B 2012 \textit{Chin. Phys. C} \textbf{36} 1003
[48] Angeles I and Marinova K 2013 \textit{At. Data Nucl. Data Tables} \textbf{99} 69
[49] Coraggio L, Itaco N, Covello D, Cangaro A and Kuo T T S 2003 \textit{Phys. Rev. C} \textbf{68} 034320
[50] Broennmann R and Machleidt R 1998 \textit{Phys. Rev. C} \textbf{42} 1860
[51] Roth R, Langhämmer J, Calac A, Binder S and Navratil P 2011 \textit{Phys. Rev. Lett.} \textbf{107} 072501
[52] Hagen G, Papenbrock T, Dean D J, Hjorth-Jensen M and Asokan B 2009 \textit{Phys. Rev. C} \textbf{80} 021306
[53] Ozawa A et al 2001 \textit{Nucl. Phys. A} \textbf{691} 590
[54] van Dalen E N E and Mithör R 2011 \textit{Phys. Rev. C} \textbf{84} 024320
[55] Livitina N and Ring P 2006 \textit{Phys. Rev. C} \textbf{73} 044320
[56] Baldo M, Bombaci I and Burgio G F 1997 \textit{Astron. Astrophys.} \textbf{328} 274
[57] Zuo W, Lejeune A, Lombardo U and Mathiot J 2002 \textit{Nucl. Phys. A} \textbf{706} 418
[58] Brown G E, Wèse W, Baym G and Speth J 1987 \textit{Commun. Nucl. Part. Phys.} \textbf{17} 39
[59] Neglée J 1982 \textit{Rev. Mod. Phys.} \textbf{54} 913