Nuclear Pairing from Chiral Pion-Nucleon Dynamics:

Applications to Finite Nuclei

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Abstract

The $^1S_0$ pairing gap in isospin-symmetric nuclear matter and finite nuclei is investigated using the chiral nucleon-nucleon potential at the $\text{N}^3\text{LO}$ order in the two-body sector, and the $\text{N}^2\text{LO}$ order in the three-body sector. To include realistic nuclear forces in RHB (Relativistic Hartree Bolgoliubov) calculations we rely on a separable form of the pairing interaction adjusted to the bare nuclear force. The separable pairing force is applied to the analysis of pairing properties for several isotopic and isotonic chains of spherical nuclei.

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I. INTRODUCTION

Nuclear energy density functionals (EDF) provide a microscopic, globally accurate, and yet economic description of ground-state properties and collective excitations over the whole nuclide chart. Even though it originates in the effective interaction between nucleons, a generic density functional is not necessarily related to any given nucleon-nucleon (NN) potential and, in fact, some of the most successful modern functionals are entirely empirical [1]. Of course it is very much desirable to have a fully microscopic foundation for a universal density functional, and this is certainly one of the major challenges in low-energy nuclear structure physics [2].

The EDF approach to nuclear structure is analogous to Kohn-Sham density functional theory (DFT) and, because it includes correlations, goes beyond the Hartree-Fock approximation. Kohn-Sham DFT has the advantage of being a local scheme, but its usefulness crucially depends on our ability to construct accurate approximations for the most important part of the functional, that is, the universal exchange-correlation functional [3].

In a series of recent articles [4–6], concepts of effective field theory and density functional theory have been used to derive a microscopic relativistic EDF-based model of nuclear many-body dynamics constrained by in-medium QCD sum rules and chiral symmetry. The density dependence of the effective nucleon-nucleon couplings in this model (called FKVW in the following) is determined from the long- and intermediate-range interactions generated by one- and two-pion exchange processes. They are computed using in-medium chiral perturbation theory, explicitly including ∆(1232) degrees of freedom [7]. Divergent contributions to the nuclear matter energy density, calculated at three-loop level, are absorbed by few contact terms. These constants are understood to encode unresolved short-distance dynamics.

The relativistic FKVW model has successfully been employed in studies of ground-state properties of spherical and deformed nuclei using the Relativistic Hartree-Bogoliubov framework (RHB [8]). In the description of open-shell nuclei, in particular, a hybrid model has been used with the FKVW Kohn-Sham potential in the particle-hole (ph) channel and, like in most applications of RHB-based models, the pairing part of the empirical Gogny force [9] in the particle-particle (pp) channel.

Even though this approach has been very successful, it is not theoretically consistent because of the choice of the empirical effective interaction in the pp channel. Quite recently,
as part of a larger program to develop a framework of fully microscopic nuclear energy density functionals, much effort has been devoted to designing non-empirical pairing functionals \[10–14\].

The aim of this work is to formulate a consistent microscopic framework for open-shell nuclei, in which both the \(ph\) and the \(pp\) channels of the effective inter-nucleon interaction are determined by chiral pion-nucleon dynamics. Thus we consider a separable \(pp\) interaction based on a microscopic pairing interaction constrained by chiral dynamics (see Ref. \[15\] for previous calculations involving the \(N^2\)LO chiral potential), combine it with the FKVW functional in the \(ph\) channel and, employing the corresponding RHB model, present a study of pairing gaps in isotopic and isotonic chains of spherical open-shell nuclei.

We will use the realistic NN potential developed by the Idaho group at next-to-next-to-next-to-leading order (\(N^3\)LO) in the chiral expansion \[16\] (see also Ref. \[17\]), and a two-body density-dependent potential derived from the relevant diagrams at the \(N^2\)LO order in the three body sector \[18\] (see also Refs. \[14, 19–22\] for similar approaches and pertinent details).

The paper is organized as follows. In Sec. II we discuss results for the pairing gap of nuclear matter in the BCS approximation. Sec. III briefly reviews the method introduced by Y. Tian et al. \[23, 24\] to apply realistic pairing interactions to calculations of finite nuclei. In Sec. IV we analyze pairing gaps in spherical nuclei for several isotopic and isotonic chains. Sec. V summarizes the principal results.

II. PAIRING GAP IN A HOMOGENEOUS INFINITE SYSTEM

The momentum and density-dependent pairing field \(\Delta(k, k_F)\) in infinite matter is determined by the solution of the BCS gap equation

\[
\Delta(k, k_F) = -\frac{1}{4\pi^2} \int_0^\infty \frac{p^2 V(p, k) \Delta(p, k_F)}{\sqrt{\mathcal{E}(p, k_F) - \mathcal{E}(k_F, k_F)^2 + \Delta(p, k_F)^2}} \, dp ,
\]  

where \(V(p, k)\) represents the off-shell pairing potential in momentum space, \(\mathcal{E}(p, k_F)\) is the quasiparticle energy, and \(\mathcal{E}(k_F, k_F)\) is the Fermi energy.

The effective force in the pairing channel is, in principle, generated by the sum of all particle-particle irreducible Feynman diagrams \[25\]. In most application to nuclear and neutron matter, however, only the lowest-order term, that corresponds to the bare nucleon-nucleon interaction, is retained \[26\]. Terms of higher order in the effective pairing interaction
represent screening corrections to the bare force, caused by medium polarization effects (see Refs. \[27, 28\] and references therein). In the present analysis we only consider the bare interaction, while a study of polarization effects will be carried out in a forthcoming paper.

For the pairing potential \(V(p,k)\) we employ the simple ansatz:

\[
V(p,k) = V_2B(p,k) + V_{3B}(p,k,m) \simeq V_2B(p,k) + \tilde{V}_2B(k_F,p,k),
\]

where the three-body potential is approximated by an effective two-body density-dependent potential \(\tilde{V}_2B\) derived by Holt et al. in Ref. \[18\]. These authors showed that in the singlet channel (\(^1S_0\)) the overall effect of \(\tilde{V}_2B(k_F,p,k)\) is to reduce the strong S-wave attraction (cf. Fig. 6 of Ref. \[18\]). As suggested in Ref. \[18\], here we neglect a possible isotopic dependence that, in any case, is expected to be rather small for the nuclei considered in the present analysis (see also Ref. \[14\]). For both terms in Eq. (2) we follow standard procedures for the regulator functions, and refer the reader to the original papers for details.

For the single-particle spectrum that appears in the denominator of the gap equation (1) we employ the simple quadratic form

\[
E(p,k_F) - E(k_F,k_F) = \frac{p^2 - k_F^2}{2M^*(k_F)}.
\]

This approximation should suffice because the momenta \(p\) around \(k_F\) give the dominant contribution to the integral in Eq. (1). The effective nucleon mass \(M^*(k_F)\) was obtained in a very recent calculation (Fig. 9 of Ref. \[29\]), in which the nuclear energy density functional was derived to first order in the two- and three-nucleon interaction using a density matrix expansion.

Fig. 1 displays the pairing gap \(\Delta(k_F,k_F)\) in symmetric nuclear matter as function of the Fermi momentum \(k_F\). We plot results of the complete calculation that includes two and three-body forces (solid curve), and the pairing gap obtained with only the two-body NN potential at \(N^3\)LO (dashed curve). Our results are shown in comparison with those obtained in Ref. \[32\] using the \(V_{\text{lowk}}\) potential (with single particle energies computed in Brueckner-Hartree-Fock theory).

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1 In Ref. \[29\] the two-body interaction comprises long-range one- and two-pion exchange contributions and a set of contact terms contributing up to fourth power in momenta (\(N^3\)LOW potential developed lowering the cut-off scale to \(\Lambda = 414\) MeV). In addition, the authors employ the leading order chiral three-nucleon interaction with the corresponding parameters \(c_E, c_D\) and \(c_{1,3,4}\) adjusted in calculations of few-body systems. Even though the results are in good agreement with previous calculations \[30\], one should note that higher-order corrections could have non-negligible effects \[31\].
III. MAPPING PROCEDURE

To implement the chiral NN potential at N^3LO in the pairing channel of the RHB framework for finite nuclei, we adopt the approach of Refs. [23, 24] where a separable form of the pairing interaction was introduced, with parameters adjusted to reproduce the pairing properties of the Gogny force in nuclear matter. In nuclear matter the pairing force is separable in momentum space:

\[ \langle k | V^{1S0} | k' \rangle = -Gp(k)p(k') \] (4)

By assuming a simple Gaussian ansatz \( p(k) = e^{-a^2k^2} \), the two parameters \( G \) and \( a \) have been adjusted to reproduce the density dependence of the gap at the Fermi surface, calculated with a Gogny force. For the D1S parameterization of the Gogny force: \( G = 728 \text{ MeVfm}^3 \) and \( a = 0.644 \text{ fm} \). Here we apply the same procedure to the chiral NN potential at the N^3LO order. For finite nuclei, when the pairing force Eq. (4) is transformed from momentum to coordinate space, it takes the form:

\[ V(r_1, r_2, r'_1, r'_2) = G\delta(R - R')P(r)P(r')\frac{1}{2}(1 - P\sigma), \] (5)

where \( R = \frac{1}{2}(r_1 + r_2) \) and \( r = r_1 - r_2 \) denote the center-of-mass and the relative coordinates, \( P(r) \) is the Fourier transform of \( p(k) \):

\[ P(r) = \frac{1}{(4\pi a^2)^{3/2}}e^{-r^2/4a^2}, \] (6)

and the factor \( 1/2 (1 - P\sigma) \) projects on the \( 1S_0 \) channel. The pairing force has a finite range and, because of the presence of the factor \( \delta(R - R') \), it preserves translational invariance. Even though \( \delta(R - R') \) implies that this force is not completely separable in coordinate space, the corresponding anti-symmetrized \( pp \) matrix elements can be represented as a sum of a finite number of separable terms, using a method developed by Talmi and Moshinsky. When the nucleon wave functions are expanded in a harmonic oscillator basis, spherical or deformed, the sum converges relatively quickly. A relatively small number of separable terms reproduces with high accuracy the result of a calculation performed in the complete basis. We refer the reader to Ref. [23] for more details.

The parameters of the separable pairing force take the values: \( G = 892.0 \text{ MeVfm}^3 \) and \( a = 0.74 \text{ fm} \) for the N^3LO potential, and \( G = 1045.0 \text{ MeVfm}^3 \) and \( a = 0.86 \text{ fm} \) for the complete potential \( V(p,k) \). We note that recently a similar approach was employed in Refs.
where a low-rank separable representation was used to reproduce directly $V_{\text{low}k}$ and $V_{3N}$ in the $^1S_0$ channel (for $V_{3N}$ the density dependence was parametrized by a polynomial in the Fermi momentum).

IV. RESULTS FOR FINITE NUCLEI

Employing the RHB model with the FKVW functional in the $ph$ channel and the separable pairing force Eq. (5) in the $pp$ channel, we have calculated the self-consistent ground-state solutions for several sequences of isotopes (nickel, tin and lead) and isotones ($N = 28$, $N = 50$ and $N = 82$). The total binding energies and average pairing gaps are compared to available data in Figs. 2 and 3. The experimental masses are from Ref. 33, and the average proton and neutron gaps 

$$
\bar{\Delta} = \frac{\sum_k \Delta_k u_k v_k}{\sum_k v_k^2}
$$

are compared to empirical values determined using the 5-point formula 35 for even-even nuclei

$$
\Delta^{(5)}(N_0) = -\frac{1}{8} \left[ E(N_0 + 2) - 4E(N_0 + 1) + 6E(N_0) - 4E(N_0 - 1) + E(N_0 - 2) \right].
$$

$E(N_0)$ denotes the experimental binding energy of a nucleus with $N_0$ neutrons ($Z_0$ for protons). In Eq. (7) the sum is over proton or neutron canonical states, $\Delta_k$ is the diagonal matrix element of the pairing field in the canonical state $k$, and $v_k$ denotes the corresponding eigenvalue of the one-body density matrix (occupation factor).

The theoretical gaps shown in Figs. 2 and 3 have been calculated using the values of the parameters $G$ and $a$ that correspond to the nuclear matter pairing gaps in Fig. 1. The gaps calculated by including only the interaction $V_{2B}$ (blue diamonds) reproduce on a quantitative level the isotopic and isotopic trends of the empirical gaps. Including the three-nucleon interaction $V_{3B}$ induces a sizable reduction of the calculated gaps (green diamonds), and we note that similar conclusions were also reached in Ref. 14. The calculated gaps for the isotopic chains $Z = 28$, $Z = 50$ and $Z = 82$ indicate that missing contributions like, for instance particle-vibration coupling, could play an important role 36, 37. Fig. 3

In Refs. 12, 14 a somewhat different prescription was used for the pairing gaps. The theoretical gap

$\Delta_{\text{LCS}}$ (Lowest Canonical State) corresponds to the diagonal pairing matrix element $\Delta_i$ in the canonical single-particle state $\phi_i$ whose quasi-particle energy is the lowest, whereas experimental gaps are deduced from binding energies using three-point mass differences centered on odd-mass nuclei.
displays similar results for the proton pairing gaps of the isotonic chains $N = 28$, $N = 50$ and $N = 82$ (we note that here the contribution of the Coulomb interaction in the pairing channel is neglected). The subshell closures that appear at $N = 40$ in the nickel chain \[38\], and at $Z = 58$ in the $N = 82$ chain \[39\], lead to a strong reduction of pairing correlations in the corresponding calculated ground-states.

The influence of three-body forces on the total binding energy is much less pronounced, as shown in the lower panels of Figs.\[2\] and \[3\] where we display the absolute deviations of the calculated binding energies from the experimental values. On the one hand this is because pairing correlations contribute much less than the mean-field self-energies to the total binding. On the other hand this is a well known characteristic of a self-consistent calculation in that, for a given nucleus, a reduction of pairing results in an effective enhancement of the mean-field contribution to the total energy, and vice versa. In general, the combination of the FKVW $ph$ effective interaction and the separable pairing force Eq. \[5\] produces results for the total binding energies that are comparable to those obtained with the best empirical non-relativistic and relativistic energy density functionals. For the nickel isotopes the largest deviations are in the region $Z \approx N$, where one expects additional contributions from proton-neutron correlations that are not explicitly included in the FKVW functional. In the tin isotopes the calculated masses start deviating from data in neutron-rich nuclei beyond the major shell closure at $N = 82$, whereas for lead nuclei the deviations are most pronounced in the lightest, neutron-deficient isotopes that are characterized by soft potentials and shape coexistence.

V. CONCLUSIONS

A consistent microscopic approach to the structure of open-shell nuclei has been introduced, in which both the $ph$ and the $pp$ channels of the effective nuclear interaction are fully determined by chiral pion-nucleon dynamics. By employing an ansatz for the pairing force that is separable in momentum space, we have performed an efficient mapping of the chiral potential in the pairing channel (at the $N^3LO$ order and the $N^2LO$ in the two-body and three-body sectors, respectively) to an effective $pp$ interaction for finite nuclei. The two parameters of the separable pairing force are adjusted to reproduce the density dependence of the pairing gaps in symmetric nuclear matter. The resulting effective pairing interaction
thus enables, on the one hand, the treatment of pairing correlations in finite nuclei using pairing functionals constrained by chiral dynamics and, on the other hand, calculations in the $pp$ channel with a finite-range interaction. The significant advantage is that the computational cost is greatly reduced when compared to nonlocal finite-range forces like, for instance, the empirical Gogny force. A noteworthy result of the present investigation is that it confirms the important role of three-body forces in determining pairing gaps in finite nuclei.

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[1] M. Bender, P. H. Heenen and P. G. Reinhard, Rev. Mod. Phys. 75 (2003) 121.
[2] Focus Issue on Open Problems in Nuclear Structure Theory, J. Phys. G 37 (2010) Vol. 6.
[3] R. M. Dreizler and E. K. U. Gross, Density Functional Theory, Springer, Berlin (1990); E. Engel and R. M. Dreizler, Density Functional Theory: An Advanced Course, Springer, Berlin (2011).
[4] P. Finelli, N. Kaiser, D. Vretenar and W. Weise, Eur. Phys. J. A 17 (2003) 573.
[5] P. Finelli, N. Kaiser, D. Vretenar and W. Weise, Nucl. Phys. A 735 (2004) 449.
[6] P. Finelli, N. Kaiser, D. Vretenar and W. Weise, Nucl. Phys. A 770 (2006) 1.
[7] S. Fritsch, N. Kaiser and W. Weise, Nucl. Phys. A 750 (2005) 259.
[8] D. Vretenar, A. V. Afanasjev, G. A. Lalazissis and P. Ring, Phys. Rep. 409 (2005) 101.
[9] J. F. Berger, M. Girod and D. Gogny, Comput. Phys. Commun. 63 (1991) 365.
[10] T. Duguet and T. Lesinski, Eur. Phys. J. ST 156 (2008) 207.
[11] T. Lesinski, T. Duguet, K. Bennaceur and J. Meyer, Eur. Phys. J. A 40 (2009) 121.
[12] K. Hebeler, T. Duguet, T. Lesinski and A. Schwenk, Phys. Rev. C 80 (2009) 044321.
[13] T. Duguet, T. Lesinski, K. Hebeler and A. Schwenk, Mod. Phys. Lett. A 25 (2010) 1989.
[14] T. Lesinski, K. Hebeler, T. Duguet and A. Schwenk, arXiv:1104.2955 [nucl-th].
[15] N. Kaiser, T. Nikšić and D. Vretenar, Eur. Phys. J. A 25 (2005) 257.
[16] R. Machleidt and D. R. Entem, Phys. Rept. 503 (2011) 1.
[17] E. Epelbaum, H. -W. Hammer and U. -G. Meissner, Rev. Mod. Phys. 81 (2009) 1773.
[18] J. W. Holt, N. Kaiser and W. Weise, Phys. Rev. C 81 (2010) 024002.
[19] K. Hebeler and A. Schwenk, Phys. Rev. C 82 (2010) 014314.
[20] K. Hebeler, S. K. Bogner, R. J. Furnstahl, A. Nogga and A. Schwenk, Phys. Rev. C 83 (2011) 031301.
[21] S. Gandolfi, A. Yu. Illarionov, F. Pederiva, K. E. Schmidt and S. Fantoni, Phys. Rev. C 79 (2009) 054005.
[22] A. Lovato, O. Benhar, S. Fantoni, A. Y. Illarionov and K. E. Schmidt, Phys. Rev. C 83 (2011) 054003.
[23] Y. Tian, Z. Y. Ma and P. Ring, Phys. Lett. B 676 (2009) 44.
[24] Y. Tian, Z. Y. Ma and P. Ring, Phys. Rev. C 79 (2009) 064301.
[25] A.B. Migdal, *Theory of finite Fermi systems and applications to atomic nuclei*, Interscience, New York (1967).

[26] D.J. Dean and M. Hjorth-Jensen, Rev. Mod. Phys. **75** (2003) 607; and references therein.

[27] H.J. Schulze, J. Cugnon, A. Lejeune, M. Baldo and U. Lombardo, Phys. Lett. B **375**, (1996) 1.

[28] U. Lombardo, H. Schulze, C. -W. Shen and W. Zuo, Int. J. Mod. Phys. E **14** (2005) 513.

[29] J. W. Holt, N. Kaiser and W. Weise, arXiv:1107.5966 [nucl-th].

[30] S. Fritsch, N. Kaiser and W. Weise, Nucl. Phys. A **750** (2005) 259.

[31] J. W. Holt, N. Kaiser and W. Weise, arXiv:1106.5702 [nucl-th].

[32] A. Sedrakian, T. T. S. Kuo, H. Muther and P. Schuck, Phys. Lett. B **576** (2003) 68.

[33] G. Audi, A. H. Wapstra and C. Thibault, Nucl. Phys. A **729** (2003) 337.

[34] M. Bender, K. Rutz, P. G. Reinhard and J. A. Maruhn, Eur. Phys. J. A **8** (2000) 59.

[35] P. Moller and J. R. Nix, Nucl. Phys. A **536** (1992) 20.

[36] F. Barranco, P. F. Bortignon, R. A. Broglia, G. Colo, P. Schuck, E. Vigezzi and X. Vinas, Phys. Rev. C **72** (2005) 054314.

[37] G. Gori, F. Ramponi, F. Barranco, P. F. Bortignon, R. A. Broglia, G. Colo’ and E. Vigezzi, Phys. Rev. C **72** (2005) 011302.

[38] R. Broda, B. Fornal, W. Krolas, T. Pawlat, D. Bazzacco, S. Lunardi, C. Rossi-Alvarez, R. Menegazzo et al., Phys. Rev. Lett. **74** (1995) 868.

[39] W. H. Long, H. Sagawa, J. Meng and N. Van Giai, Europhys. Lett. **82** (2008) 12001.
FIG. 1. Pairing gaps in symmetric nuclear matter in the $^1S_0$ channel as functions of the Fermi momentum. The dashed curve is obtained by including only the two-body ($V_{2B}$) chiral interaction, whereas the solid curve also includes the contribution of three-body ($V_{3B}$) forces. The gaps are compared to those obtained in Ref. [32] using the $V_{\text{lowk}}$ potential.
FIG. 2. Theoretical average neutron pairing gaps \( \langle \Delta \rangle \) of the even-even isotopes of nickel \( Z = 28 \), tin \( Z = 50 \), and lead \( Z = 82 \), compared to the empirical values calculated from experimental masses using Eq. \( (5) \) (upper panel). Absolute deviations of the calculated binding energies from the experimental values \( [33] \) (lower panel).
FIG. 3. Same as described in the caption to Fig. 3 but for the chains of isotones $N = 28$, $N = 50$ and $N = 82$. 