Ground-state properties of closed-shell nuclei with low-momentum realistic interactions

L. Coraggio,1 N. Itaco,1 A. Covello,1 A. Gargano,1 and T. T. S. Kuo2

1Dipartimento di Scienze Fisiche, Università di Napoli Federico II, and Istituto Nazionale di Fisica Nucleare, Complesso Universitario di Monte S. Angelo, Via Cintia - I-80126 Napoli, Italy
2Department of Physics, SUNY, Stony Brook, New York 11794

(Dated: October 29, 2018)

Ground-state properties of 16O and 40Ca are calculated with a low-momentum nucleon-nucleon potential, \( V_{\text{low-k}} \), derived from the chiral N3LO interaction recently constructed by Entem and Machleidt. The smooth \( V_{\text{low-k}} \) is used directly in a Hartree-Fock approach, avoiding the difficulties of the Brueckner-Hartree-Fock procedure. Corrections up to third order in the Goldstone expansion are evaluated, leading to results that are in very good agreement with experiment. Convergence properties of the expansion are examined.

PACS numbers: 21.30.Fe, 21.60.Jz, 21.10.Dr

I. INTRODUCTION

A fundamental problem in nuclear theory has long been the calculation of the bulk properties of closed–shell nuclei, such as their binding energy and charge radius, starting from realistic nucleon–nucleon (NN) potentials. Potentials like CD–Bonn [1], Nijmegen [2], Argonne v18 [3], and the new chiral potential of Ref. [4] reproduce the NN scattering data and the observed deuteron properties very accurately, but, because of their strong repulsion at short distances, none of them can be used directly in nuclear structure calculations.

A traditional approach to this problem is the Brueckner–Goldstone (BG) theory [5], where the Goldstone perturbative expansion is re-ordered summing to all orders a selected class of diagrams, the ladder diagrams. This implies replacing the bare interaction \( (V_{\text{NN}}) \) vertices by the reaction matrix \( (G) \) ones and omitting the ladder diagrams. Within this framework, one has the well known Brueckner–Hartree–Fock (BHF) theory when the self-consistent definition is adopted for the single–particle (SP) auxiliary potential and only the first–order contribution in the BG expansion is taken into account. The BHF approximation gives therefore a mean field description of the ground state of nuclei in terms of the \( G \) matrix, the latter taking into account the correlations between pairs of nucleons. However, owing to the energy dependence of \( G \), this procedure is not without difficulties. An important issue is the choice of the SP energies for states above the Fermi surface, which are not uniquely defined [6].

Calculations for finite nuclei within the BHF approach lead usually to insufficient binding energy as well as too small charge radii [7]. In this context, extensions of the conventional BHF approach have been proposed to account for long–range correlations [8]. It is worth mentioning that alternative approaches have been developed, as for instance the correlated basis function method [9] and the coupled cluster method [10], in both of which correlations are directly embedded into the wave functions. A comprehensive review of the various methods is given in Ref. [11], which also includes a discussion of calculations for nuclear matter as well as for finite nuclei. An other effort in this direction is the unitary model–operator approach of Suzuki and Okamoto [12].

Recently, a new technique to renormalize the short–range repulsion of a realistic NN potential by integrating out its high momentum components has been proposed [13, 14]. The resulting low–momentum potential, which we call \( V_{\text{low-k}} \), is a smooth potential that preserves the low–energy physics of \( V_{\text{NN}} \) and is therefore suitable for being used directly in nuclear structure calculations. We have employed \( V_{\text{low-k}} \) derived from modern NN potentials to calculate shell–model effective interactions by means of the \( Q \)-box plus folded diagram method. Within this framework, several nuclei with few valence particles have been studied [15, 16, 17], leading to the conclusion that \( V_{\text{low-k}} \) is a valid input for realistic shell-model calculations.

The main purpose of this paper is to show that this potential may also be profitably used for the calculation of ground state properties of doubly closed nuclei. To this end, we have employed the Goldstone expansion which, given the smooth behavior of \( V_{\text{low-k}} \), does not require any rearrangement. As a first step of our procedure, we solve the Hartree–Fock (HF) equations for \( V_{\text{low-k}} \). Then, using the obtained self–consistent field as auxiliary potential, we calculate the Goldstone expansion including diagrams up to third order in \( V_{\text{low-k}} \).

Here, we present the results obtained for 16O and 40Ca starting from the new realistic NN potential of Entem and Machleidt [4] based on chiral perturbation theory at the next-to-next-to-next-to-leading order (N3LO; fourth order). This potential is an improved version of the earlier chiral NN potential [13] (known as Idaho potential) constructed by the same authors, which includes two-pion exchange contributions only up to chiral order three. We have recently employed the latter potential in shell-model calculations for various two-particle valence nuclei.
The paper is organized as follows. In Sec. II we first describe the main features of the derivation of $V_{\text{low} - k}$, then outline the essentials of our calculation. In Sec. III we present our results and compare them with the experimental data. Some concluding remarks are given in Sec. IV.

II. METHOD OF CALCULATION

The first step in our approach is to integrate out the high-momentum components of $V_{NN}$. According to the general definition of a renormalization group transformation, the decimation must be such that the low-energy observables calculated in the full theory are preserved exactly by the effective theory. Once the relevant low-energy modes are identified, all remaining modes or states have to be integrated out.

For the nucleon-nucleon problem in vacuum, we require that the deuteron binding energy, low-energy phase shifts, and low-momentum half-on-shell $T$ matrix calculated from $V_{NN}$ must be reproduced by $V_{\text{low} - k}$.

The full-space Schrödinger equation may be written as

$$H\Psi_\mu = E_\mu \Psi_\mu; \quad H = H_0 + V_{NN},$$  \hspace{1cm} (1)

where $H_0$ is the unperturbed Hamiltonian, namely, the kinetic energy. The above equation can be reduced to a model-space one of the form

$$PH_{\text{eff}}P\Psi_\mu = E_\mu P\Psi_\mu; \quad H_{\text{eff}} = H_0 + V_{\text{low} - k},$$ \hspace{1cm} (2)

where $P$ denotes the model-space, which is defined by momentum $k \leq k_{\text{cut}} = \Lambda$, $k$ being the relative momentum and $k_{\text{cut}}$ a cut-off momentum.

The half-on-shell $T$ matrix of $V_{NN}$ is

$$T(k', k, k^2) = V_{NN}(k', k) +$$

$$+ \int_0^\infty q^2 dq V_{NN}(k', q) \frac{1}{k^2 - q^2 + i0^+} T(q, k, k^2),$$ \hspace{1cm} (3)

and the effective low-momentum $T$ matrix is defined by

$$T_{\text{low} - k}(p', p, p^2) = V_{\text{low} - k}(p', p) +$$

$$\int_0^\Lambda q^2 dq V_{\text{low} - k}(p', q) \frac{1}{p^2 - q^2 + i0^+} T_{\text{low} - k}(q, p, p^2).$$ \hspace{1cm} (4)

Note that for $T_{\text{low} - k}$ the intermediate states are integrated up to $\Lambda$.

It is required that, for $p$ and $p'$ both belonging to $P$ ($p, p' \leq \Lambda$), $T(p', p, p^2) = T_{\text{low} - k}(p', p, p^2)$. In Refs. [13, 14] it has been shown that the above requirements are satisfied when $V_{\text{low} - k}$ is given by the folded-diagram series

$$V_{\text{low} - k} = \hat{Q} - \hat{Q}' \int \hat{Q} + \hat{Q}' \int \hat{Q} - \hat{Q}' \int \hat{Q} \int \hat{Q} + \ldots,$$ \hspace{1cm} (5)

where $\hat{Q}$ is an irreducible vertex function, in the sense that its intermediate states must be outside the model space $P$. The integral sign represents a generalized folding operation [19], and $\hat{Q}'$ is obtained from $\hat{Q}$ by removing terms of first order in the interaction.

The above $V_{\text{low} - k}$ can be calculated by means of iterative techniques. We have used here an iteration method proposed in Ref. [20], which is particularly suitable for non-degenerate model spaces. This method, which we refer to as Andreozzi-Lee-Suzuki (ALS) method, is an iterative method of the Lee-Suzuki type, which converges to the lowest $d$ eigenvalues of $H$, $d$ being the dimension of the $P$ space. Since the $V_{\text{low} - k}$ obtained by this technique is non-hermitian, we have made use of the simple and numerically convenient hermitization procedure suggested in Ref. [20]. We have verified that the deuteron binding energy and the phase shifts up to the cut-off momentum $\Lambda$ are preserved by $V_{\text{low} - k}$.

An important question in our approach is what value one should use for the cut-off momentum. A discussion of this point as well as a criterion for the choice of $\Lambda$ can be found in Ref. [14]. According to this criterion, we have used here $\Lambda = 2.1$ fm$^{-1}$.

![FIG. 1: Behavior of $E_{HF}$ with $h\omega$ and $N$ for $^{16}$O.](image)

We have found it appropriate, however, to check on the sensitivity of our results to moderate changes in the value of $\Lambda$. It has turned out that they change very little when letting $\Lambda$ vary from 2.0 to 2.2 fm$^{-1}$. For instance, at the second order in the Goldstone expansion (see next section), the binding energy per nucleon for $^{16}$O is 7.29 and 7.12 MeV for $\Lambda = 2.0$ and $\Lambda = 2.2$ fm$^{-1}$, respectively.

As already mentioned in the Introduction, our starting point is the N$^3$LO potential [3]. From this potential we...
derive the corresponding $V_{\text{low-k}}$ and use it directly in a HF calculation. The HF equations are then solved for $^{16}\text{O}$ and $^{40}\text{Ca}$ making use of a harmonic-oscillator basis. We assume spherical symmetry, which implies that the HF SP states $|\alpha\rangle$ have good orbital and total angular momentum. Therefore, they can be expanded in terms of oscillator wave functions $|\mu\rangle$,

$$
|\alpha\rangle = \sum_{\mu} C_{\mu}^{\alpha} |\mu\rangle ,
$$

where the sum is over the principal quantum number only. The expansion coefficients $C_{\mu}^{\alpha}$ are determined by solving self-consistently the HF equations

$$
\sum_{\mu'} (\mu| t + U |\mu') C_{\mu'}^{\alpha} = \epsilon_{\alpha} C_{\mu}^{\alpha} ,
$$

where $t$ is the kinetic energy and the HF potential $U$ is defined as

$$
\langle \mu | U | \mu' \rangle = \sum_{\alpha_{h}} \langle \mu \alpha_{h} | V_{\text{low-k}} | \mu' \alpha_{h} \rangle ,
$$

with the index $\alpha_{h}$ referring to occupied states in the ground-state HF Slater determinant.

Once Eq. (7) has been solved, the ground-state properties of the nucleus can be calculated. In particular, the total energy has the well-known expression

$$
E_{HF} = \frac{1}{2} \sum_{\alpha_{h}} [\langle \alpha_{h} | t | \alpha_{h} \rangle + \epsilon_{\alpha_{h}}] .
$$

In our calculations the sum in the expansion (6) has been extended up to $N = 5$ terms. We have verified that this truncation is sufficient to ensure that the HF results do not significantly depend on the variation of the oscillator constant $h\omega$. This is illustrated in Figs. 1 and 2, where we show the behavior of the HF ground-state energy of $^{16}\text{O}$ and $^{40}\text{Ca}$ versus $h\omega$ for different values of $N$. The results for $N = 5$ are quite stable. In our calculations the values of $h\omega$ have been derived from the expression $h\omega = 45A^{-1/3} - 25A^{-2/3}$, which reproduces the rms radii in an independent-particle approximation with harmonic-oscillator wave functions. This expression gives $h\omega = 14$ and 11 MeV for $^{16}\text{O}$ and $^{40}\text{Ca}$, respectively. In solving Eq. (7), the Coulomb potential has been added to $V_{\text{low-k}}$ for protons.

![FIG. 2: Behavior of $E_{HF}$ with $h\omega$ and $N$ for $^{40}\text{Ca}$.
](https://example.com/fig2.jpg)

![FIG. 3: First-, second-, and third-order diagrams in the Goldstone expansion.
](https://example.com/fig3.jpg)

| nucleus | $B/A$ | $\langle r_c \rangle$ | Expt. |
|---------|-------|-----------------|------|
| $^{16}\text{O}$ | 3.23  | 2.30 | 7.52  | 7.98 |
| $^{40}\text{Ca}$ | 6.19  | 2.610 | 9.19  | 8.55 |

We use the HF basis to sum the Goldstone expansion including contributions up to third order in $V_{\text{low-k}}$. In Fig. 3 we report the first-, second-, and third-order diagrams. The intermediate states involved in the evaluation of these diagrams are those obtained from the lowest 10 and 11 h.o. major shells for $^{16}\text{O}$ and $^{40}\text{Ca}$, respectively. Our results show convergence for these large spaces: for example, the $^{16}\text{O}$ binding energy per nucleon in second order approximation is 7.03, 7.22, and 7.30 MeV when considering 9, 10, and 11 major shells, respectively. Similar diagrams have been used to calculate the corrections to the rms radius. As is well known, retaining only the first-order term in this expansion yields the HF results.

To conclude, it is worth stressing that using the Goldstone expansion in terms of $V_{\text{low-k}}$ one has to include also diagrams (b) and (c). This is not the case of the BG approach, where these diagrams are already contained in diagram (a) through the $G$ matrix.

| nucleus | $B/A$ | $\langle r_c \rangle$ | Expt. |
|---------|-------|-----------------|------|
| $^{16}\text{O}$ | 3.23  | 2.30 | 7.52  | 7.98 |
| $^{40}\text{Ca}$ | 6.19  | 2.610 | 9.19  | 8.55 |

Table I: Comparison of the calculated binding energy per nucleon (MeV/nucleon) and rms charge radius (fm) with the experimental data for $^{16}\text{O}$ and $^{40}\text{Ca}$.
III. RESULTS

In Table I, the calculated binding energy per nucleon and the rms charge radius for both $^{16}$O and $^{40}$Ca are compared with the experimental data [23, 24, 25]. This Table contains the HF results as well as the values obtained including second– and third–order contributions. We see that the renormalization of the short range repulsion through $V_{\text{low–}k}$ is sufficient to yield positive HF binding energies, albeit too small as compared to the experimental values. We also see that the HF approximation significantly underestimates the rms radii. This evidences the role of higher–order contributions in the Goldstone expansion to account for correlations beyond the mean field. The binding energies and radii calculated including diagrams up to third order are very satisfactory. In fact, the binding energies gain about 4 and 3 MeV for $^{16}$O and $^{40}$Ca, respectively, while the radii increase by about 0.4 and 0.8 fm coming quite close to the experimental values.

A discussion of the convergence properties of the perturbative series is now in order. To this end, the HF potential energy, the second–, and third–order corrections have to be compared. In $^{16}$O the HF potential energy per nucleon is $V^{(1)} = -23.5$ MeV, which is obtained by subtracting from the total HF energy the contribution of the kinetic term. Thus for the ratio of the second– to first–order term we obtain $V^{(2)}/V^{(1)} = 0.17$, while the ratio $V^{(3)}/V^{(2)}$ is 0.08. Similarly, for $^{40}$Ca we have $V^{(1)} = -33.7$ MeV, $V^{(2)}/V^{(1)} = 0.09$, and $V^{(3)}/V^{(2)} = 0.03$. On these grounds, we may conclude that the convergence of the series is fairly rapid and that higher–order contributions are negligible.

For the sake of completeness, in Tables II and III we report the HF single–hole energies as well as the energies of the low–lying particle states of $^{16}$O and $^{40}$Ca. In Tables IV and V the calculated occupation probabilities for states up to the Fermi level are reported.

### Table II: Calculated and experimental single–particle energies (MeV) for $^{16}$O. Experimental data are taken from [23, 24, 25].

| Orbital | Neutron Calc. | Neutron Expt. | Proton Calc. | Proton Expt. |
|---------|---------------|---------------|--------------|--------------|
| $s_{1/2}$ | -53.786 | -47 | -48.606 | -44 ± 7 |
| $p_{3/2}$ | -23.225 | -21.839 | -19.264 | -18.451 |
| $p_{1/2}$ | -15.649 | -15.663 | -11.841 | -12.127 |
| $d_{5/2}$ | -0.056 | -4.144 | 3.564 | -0.601 |
| $s_{1/2}$ | -0.481 | -3.273 | 2.651 | -0.106 |
| $d_{5/2}$ | 5.814 | 0.941 | 8.713 | 4.399 |

### Table III: Calculated and experimental single–particle energies (MeV) for $^{40}$Ca. Experimental data are taken from [23, 24, 25].

| Orbital | Neutron Calc. | Neutron Expt. | Proton Calc. | Proton Expt. |
|---------|---------------|---------------|--------------|--------------|
| $s_{1/2}$ | -97.944 | -87.501 | -49.1 ± 12 | 77 ± 14 |
| $p_{3/2}$ | -63.760 | -53.934 | -33.3 ± 6.5 | |
| $p_{1/2}$ | -54.959 | -45.269 | -32 ± 4 | |
| $d_{5/2}$ | -33.018 | -21.30 | -23.749 | -14.9 ± 2.5 |
| $s_{1/2}$ | -27.406 | -18.104 | -18.238 | -10.850 |
| $d_{3/2}$ | -19.595 | -15.641 | -10.663 | -8.328 |
| $f_{7/2}$ | -6.579 | -8.363 | 2.047 | -1.056 |
| $p_{3/2}$ | -4.325 | -6.420 | 3.293 | 0.631 |
| $p_{1/2}$ | -0.973 | 5.865 | |
| $f_{5/2}$ | 5.852 | 12.484 | |

### Table IV: Calculated occupation probabilities for $^{16}$O.

| Orbital | Proton | Neutron |
|---------|--------|---------|
| $s_{1/2}$ | 0.881 | 0.881 |
| $p_{3/2}$ | 0.822 | 0.818 |
| $p_{1/2}$ | 0.767 | 0.760 |

IV. CONCLUDING REMARKS

In this work, starting from the chiral N$^3$LO potential [4], we have performed calculations for the ground–state properties of the doubly closed nuclei $^{16}$O and $^{40}$Ca making use of the Goldstone expansion. This has been done within the framework of a new approach [13, 14] to the renormalization of the short–range repulsion of realistic NN potentials, wherein a low–momentum potential $V_{\text{low–}k}$ is constructed which preserves the low–energy physics of the original potential. We consider a main achievement of our study to have shown that $V_{\text{low–}k}$ is suitable for being used directly in the Goldstone expansion. Namely, unlike the traditional BHF approach, there is no need to first calculate the $G$ matrix. We have seen that taking into account higher–order contributions (essentially the second–order terms) of $V_{\text{low–}k}$ in the Goldstone expansion yields very good results for the binding energy and charge radius of $^{16}$O and $^{40}$Ca.
modern $N^3$LO potential come significantly closer to the experimental data. It should be noted that our results are quite good also when compared to those of recent BHF calculations, where different modern $NN$ potentials have been used and long-range correlations have been considered within the framework of the Green function approach.

In summary, we may conclude that the results of the present study, together with those of our recent shell-model calculations, show that the $V_{\text{low-k}}$ approach provides a simple and reliable way of "smoothing out" the repulsive core contained in the modern $NN$ potentials before using them in microscopic nuclear structure calculations.

**Acknowledgments**

This work was supported in part by the Italian Ministero dell'Istruzione, dell'Università e della Ricerca (MIUR) and by the U.S. DOE Grant No. DE-FG02-88ER40388. We would like to thank R. Machleidt for providing us with the matrix elements of the $N^3$LO potential.

---

**TABLE V: Calculated occupation probabilities for $^{40}$Ca.**

| Orbital | Proton | Neutron |
|---------|--------|---------|
| $s_{1/2}$ | 0.945 | 0.947 |
| $p_{3/2}$ | 0.931 | 0.932 |
| $p_{1/2}$ | 0.921 | 0.922 |
| $d_{5/2}$ | 0.885 | 0.884 |
| $s_{1/2}$ | 0.858 | 0.855 |
| $d_{3/2}$ | 0.811 | 0.807 |

---

[1] R. Machleidt, Phys. Rev. C **63**, 024001 (2001).
[2] V. G. J. Stoks, R. A. M. Klomp, C. P. F. Terheggen, and J. J. de Swart, Phys. Rev. C **49**, 2950 (1994).
[3] B. Wiringa, V. G. J. Stoks, and R. Schiavilla, Phys. Rev. C **51**, 38 (1995).
[4] D. R. Entem and R. Machleidt, nucl-th/0304018.
[5] See, for instance, B. D. Day, Rev. Mod. Phys. **39**, 719 (1967).
[6] I. S. Towner, *A Shell Model Description of Light Nuclei* (Clarendon Press, Oxford, 1977).
[7] K. W. Schmid, H. Mühler, and R. Machleidt, Nucl. Phys. A **530**, 14 (1991), and references therein.
[8] Kh. Gad and H. Mühler, Phys. Rev. C **66**, 044301 (2002).
[9] A. Fabrocini, F. Arias de Saavedra, and G. Có, Phys. Rev. C **61**, 044302 (2000), and references therein.
[10] Jochen H. Heisenberg and Bogdan Mihaila, Phys. Rev. C **59**, 1440 (1999), and references therein.
[11] H. Mühler and A. Polls, Prog. Part. Nucl. Phys. **45**, 243 (2000).
[12] K. Suzuki and R. Okamoto, Prog. Theor. Phys. **92**, 1045 (1994).
[13] S. Bogner, T. T. S. Kuo and L. Coraggio, Nucl. Phys. A **684**, 432c (2001).
[14] Scott Bogner, T. T. S. Kuo, L. Coraggio, A. Covello, and N. Itaco, Phys. Rev. C **65**, 051301(R) (2002).
[15] A. Covello, L. Coraggio, A. Gargano, N. Itaco, and T. T. S. Kuo, in *Challenges of Nuclear Structure*, Proceedings of the Seventh International Spring Seminar on Nuclear Physics, Maiori, Italy, 2001, edited by A. Covello (World Scientific, Singapore, 2002), p. 139.
[16] L. Coraggio, A. Covello, A. Gargano, N. Itaco, and T. T. S. Kuo, Phys. Rev. C **66**, 021303(R) (2002).
[17] L. Coraggio, A. Covello, A. Gargano, N. Itaco, and T. T. S. Kuo, Phys. Rev. C **66**, 064311 (2002).
[18] D. R. Entem and R. Machleidt, Phys. Lett. B **524**, 93 (2002); D. R. Entem, R. Machleidt, and H. Witala, Phys. Rev. C **65**, 064005 (2002).
[19] E. M. Kremciglwa and T. T. S. Kuo, Nucl. Phys. A **342**, 454 (1980).
[20] F. Andreozzi, Phys. Rev. C **54**, 684 (1996).
[21] J. Blomqvist and A. Molinari, Nucl. Phys. A **106**, 545 (1968).
[22] J. Goldstone, Proc. Roy. Soc. (London) A **239**, 267 (1957).
[23] G. Audi and A. H. Wapstra, Nucl. Phys. A **565**, 1 (1993).
[24] H. de Vries, C. W. de Jager, and C. de Vries, At. Data Nucl. Data Tables **36**, 495 (1987).
[25] E. G. Nadjakov, K. P. Marinova, and Yu. P. Gangrsky, At. Data Nucl. Data Tables **56**, 133 (1994).
[26] Data extracted using the NNDC On-Line Data Service from the ENSDF database, files revised as of December 5, 2001; M.R. Bhat, *Evaluated Nuclear Structure Data File (ENSDF), Nuclear Data for Science and Technology*, edited by S. M. Quaim (Springer-Verlag, Berlin, Germany, 1992), p. 817.
[27] M. A. K. Lodhi and B. T. Waak, Phys. Rev. Lett. **33**, 431 (1974).
[28] F. Tabakin, Ann. Phys. (N.Y.) **30**, 51 (1964); Phys. Rev. **174**, 1208 (1968).
[29] J. P. Elliott, A. D. Jackson, H. A. Mavromatis, E. A. Sanderson, and B. Singh, Nucl. Phys. A **121**, 241 (1968).
[30] A. K. Kerman, J. P. Svenne, and F. M. H. Villars, Phys. Rev. **147**, 710 (1966).
[31] A. K. Kerman and M. K. Pal, Phys. Rev. **162**, 970 (1967).
[32] W. H. Bassichis, A. K. Kerman, and J. P. Svenne, Phys. Rev. **160**, 746 (1967).