

Ab-initio Gorkov-Green's function calculations of open-shell nuclei

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(Dated: November 20, 2012)

We present results from a new *ab-initio* method that uses the self-consistent Gorkov-Green's function theory to address truly open-shell systems. The formalism has been recently worked out up to second order and is implemented here in nuclei for the first time on the basis of realistic nuclear forces. Benchmark calculations indicate that the method is in agreement with other *ab-initio* approaches in doubly-closed shell ^{40}Ca and ^{48}Ca . We find good convergence of the results with respect to the basis size in ^{44}Ca and ^{74}Ni and discuss quantities of experimental interest including ground-state energies, pairing gaps and particle addition/removal spectroscopy. These results demonstrate that the Gorkov method is a valid alternative to multireference approaches for tackling degenerate or near degenerate quantum systems. In particular, it increases the number of mid-mass nuclei accessible in an *ab-initio* fashion from a few tens to a few hundreds.

PACS numbers: 21.10.-k, 21.30.Fe, 21.60.De

Introduction. - The reach of *ab-initio* nuclear structure calculations has extended tremendously over the last decade. Methods such as coupled-cluster (CC) [1], in-medium similarity renormalization group (IMSRG) [2] or Dyson self-consistent Green's function [3] (Dyson-SCGF) have accessed medium-mass nuclei up to $A \sim 60$ on the basis of realistic two-nucleon (2N) and three-nucleon (3N) [4, 5] forces. In their current implementations, such methods are however limited to doubly closed (sub-)shell nuclei and their immediate neighbors [6, 7]. As one increases the nuclear mass, longer chains of truly open-shell nuclei connecting isolated doubly closed-shell ones emerge and cannot be accessed with existing approaches. Many-body techniques that could tackle genuine (at least) singly open-shell systems would immediately extend the reach of *ab-initio* studies from a few tens to several hundreds of mid-mass nuclei. It is the aim of the present Letter to propose one manageable way to fill this gap.

Typically, open-shell systems can be dealt with via multireference schemes such as, e.g., multireference CC [8, 9] or configuration interaction techniques [2, 10] that, however, become quickly unfeasible for large model spaces. Keeping the simplicity of a single reference method requires, in any of these approaches, to formulate the expansion scheme around a reference state that can tackle Cooper pair instabilities, e.g. to build the correlated state on top of a Bogoliubov vacuum that already incorporates static pairing correlations. A single reference can thus be retained at the price of breaking the symmetry associated with particle number conservation. The associated contamination of the results that arises in finite systems eventually calls for the restoration of the broken symmetry [11]. Recently, Bogoliubov-based many-body methods have been imported to quantum chemistry to deal with near-degeneracies and non-dynamical correlations and proven to be extremely powerful [12]. Further extension to calculate affinities and ionization energies would require an electron at-

tachment/removal formalism as the one employed here.

The present work discusses the first application of extending Dyson-SCGF theory to the Bogoliubov algebra [13], i.e. it carries out the *ab-initio* Gorkov-SCGF formalism [14] in finite nuclei for the first time. The results confirm that this approach is computationally feasible. Thus, the method is applicable to several isotopic and isotonic chains of interest—e.g. Oxygen, Calcium, Nickel, $N=20$ and $N=28$ —that include several isotopes previously not reachable by *ab-initio* approaches. Another specific benefit is to eventually provide a way to understand microscopically and quantitatively the processes responsible for the superfluid character of atomic nuclei [15]. The Gorkov-SCGF method could also be used to extend to harmonic confining potentials calculations of homogeneous ultracold Fermi gases throughout the BCS-BEC crossover [16]. In the present application normal and anomalous self-energies are calculated up to second-order and on the basis of 2N interactions only. This constitutes a Kadanoff-Baym Φ -derivable approximation [17]; as such, the method involves dressed propagators and is thus intrinsically non-perturbative. In the short-term future, the objectives are to incorporate 3N interactions into the framework and to generalize state-of-the-art n -th order Algebraic Diagrammatic Construction [ADC(n)] [18] and Faddeev random-phase approximation [19, 20] truncation schemes to the Gorkov context.

Below, we present proof-of-principle calculations of systems in the calcium isotopic chain and benchmark them to state-of-the-art CC and Dyson-SCGF methods for closed-shells. The open-shell ^{44}Ca and ^{74}Ni nuclei are then taken as specific examples to illustrate the binding energy convergence with respect to the size of the harmonic oscillator basis used to expand the many-body problem. Observables of experimental interest including radii and pairing gaps, as well as adjacent isotopes' spectroscopy are discussed. Eventually, the effective neutron shell structure [13, 21, 22] is displayed.

Method. - Results displayed in the present Letter strictly rely on the formalism and the numerical implementation detailed in Refs. [13] and [23], respectively. Given the intrinsic Hamiltonian $H_{\text{int}} \equiv T + V - T_{CM}$, Gorkov-SCGF theory targets the ground state $|\Psi_0\rangle$ of the grand-canonical-like potential $\Omega \equiv H_{\text{int}} - \mu A$, where μ is the chemical potential and A the particle-number operator, having the number $A = \langle \Psi_0 | A | \Psi_0 \rangle$ of particles on average¹. The complete one-body information contained in $|\Psi_0\rangle$ is embodied in a set of four Green's functions² $\mathbf{G}^{sg'}(\omega)$ known as Gorkov propagators [14]. Their matrix elements read in the Lehmann representation as

$$G_{ab}^{11}(\omega) = \sum_k \left\{ \frac{U_a^k U_b^{k*}}{\omega - \omega_k + i\eta} + \frac{\bar{V}_a^{k*} \bar{V}_b^k}{\omega + \omega_k - i\eta} \right\}, \quad (1a)$$

$$G_{ab}^{12}(\omega) = \sum_k \left\{ \frac{U_a^k V_b^{k*}}{\omega - \omega_k + i\eta} + \frac{\bar{V}_a^{k*} \bar{U}_b^k}{\omega + \omega_k - i\eta} \right\}, \quad (1b)$$

$$G_{ab}^{21}(\omega) = \sum_k \left\{ \frac{V_a^k U_b^{k*}}{\omega - \omega_k + i\eta} + \frac{\bar{U}_a^{k*} \bar{V}_b^k}{\omega + \omega_k - i\eta} \right\}, \quad (1c)$$

$$G_{ab}^{22}(\omega) = \sum_k \left\{ \frac{V_a^k V_b^{k*}}{\omega - \omega_k + i\eta} + \frac{\bar{U}_a^{k*} \bar{U}_b^k}{\omega + \omega_k - i\eta} \right\}. \quad (1d)$$

The poles of the propagators are given by $\omega_k \equiv \Omega_k - \Omega_0$, where the index k refers to normalized eigenstates of Ω that fulfil

$$\Omega |\Psi_k\rangle = \Omega_k |\Psi_k\rangle. \quad (2)$$

The residue of $\mathbf{G}^{sg'}(\omega)$ associated with pole ω_k relates to the probability amplitude \mathbf{U}_k (\mathbf{V}_k) to reach state $|\Psi_k\rangle$ by adding (removing) a nucleon to (from) $|\Psi_0\rangle$ on a single-particle state³.

Self-consistent, i.e. *dressed*, propagators are solutions of Gorkov's equation of motion

$$\begin{pmatrix} \mathbf{T} + \boldsymbol{\Sigma}^{11}(\omega) - \mu \mathbf{1} & \boldsymbol{\Sigma}^{12}(\omega) \\ \boldsymbol{\Sigma}^{21}(\omega) & -\mathbf{T} + \boldsymbol{\Sigma}^{22}(\omega) + \mu \mathbf{1} \end{pmatrix} \Big|_{\omega_k} \begin{pmatrix} \mathbf{U} \\ \mathbf{V} \end{pmatrix}_k = \omega_k \begin{pmatrix} \mathbf{U} \\ \mathbf{V} \end{pmatrix}_k, \quad (3)$$

whose output is the set of $(\mathbf{U}, \mathbf{V})_k$ and ω_k . Equation (3) reads as an eigenvalue problem in which the normal $[\boldsymbol{\Sigma}^{11}(\omega)$ and $\boldsymbol{\Sigma}^{22}(\omega)]$ and anomalous $[\boldsymbol{\Sigma}^{12}(\omega)$ and $\boldsymbol{\Sigma}^{21}(\omega)]$ irreducible self-energies act as *energy-dependent* potentials. Eventually, the total binding energy of the A-body system is computed via the Koltun-Galitskii sum rule [24]

$$E_0^A = \frac{1}{4\pi i} \int_{C\uparrow} d\omega \text{Tr}_{\mathcal{H}_1} \left[\mathbf{G}^{11}(\omega) [\mathbf{T} + (\mu + \omega) \mathbf{1}] \right]. \quad (4)$$

Separation energies between the A-body ground state and eigenstates of $A \pm 1$ systems are related to the poles ω_k through

$$E_k^\pm \equiv \mu \pm \omega_k = \pm [\langle \Psi_k | H_{\text{int}} | \Psi_k \rangle - \langle \Psi_0 | H_{\text{int}} | \Psi_0 \rangle] \mp \mu [\langle \Psi_k | A | \Psi_k \rangle - (A \pm 1)], \quad (5)$$

where the error associated with the difference between the average number of particles in state $|\Psi_k\rangle$ and the targeted particle number $A \pm 1$ is taken care of by the last term of Eq. (5). Spectroscopic factors associated with the *direct* addition and removal of a nucleon are defined as

$$S F_k^+ \equiv \text{Tr}_{\mathcal{H}_1} [\mathbf{U}_k \mathbf{U}_k^\dagger] \quad \text{and} \quad S F_k^- \equiv \text{Tr}_{\mathcal{H}_1} [\mathbf{V}_k^* \mathbf{V}_k^T]. \quad (6)$$

In open-shell nuclei, the odd-even staggering of nuclear masses is a fingerprint of pairing correlations and offers, through finite odd-even mass difference formulae, the possibility to extract the pairing gap. The most commonly used [25] three-point-mass difference formula $\Delta_n^{(3)}(A)$ equates the pairing gap with the Fermi gap in the one-nucleon addition/removal spectra E_k^\pm , e.g. $\Delta_n^{(3)}(A) \equiv (-1)^A [E_0^+ - E_0^-]/2$. One-body observables such as mass or charge radii can be easily computed from $\mathbf{G}^{11}(\omega)$ [13]. Moreover, effective single-particle energies (ESPE) introduced by Baranger as centroids e_a^{cent} of one-nucleon addition and removal spectra E_k^\pm can be naturally computed in the present context [13]. Last but not least, the normal self-energy $\boldsymbol{\Sigma}^{11}(\omega)$ is identified with the microscopic nucleon-nucleus optical potential [26, 27], allowing for the computation of scattering states [28].

Proceeding to actual Gorkov-SCGF calculations, we retain both first and second order diagrams in the expansion of the four self-energies $\boldsymbol{\Sigma}^{sg'}(\omega)$ [13]. At first order in vacuum interactions, Eq. (3) reduces to an ab-initio Hartree-Fock-Bogoliubov (HFB) problem with static, i.e. energy-independent, normal and anomalous self-energies accounting for Hartree-Fock and Bogoliubov diagrams, respectively. The HFB solution is used as a reference state to generate second order diagrams. In the present application, self-consistency is limited to the static part [29] $\boldsymbol{\Sigma}^{sg'}(\infty)$ of the self energy. This constitutes the so-called "sc0" approximation that grasps the dominant fraction of self-consistency effects at a tractable numerical cost [20]. All technical aspects will be reported in a forthcoming publication [23].

Results. - Figure 1 displays the binding energies of calcium isotopes and compares them to single-reference CC and Dyson-SCGF for closed-shell ^{40}Ca and ^{48}Ca . Calculations are performed in a fixed model space of eight harmonic oscillator shells, $N_{\text{max}} = 7$, and oscillator energy $\hbar\omega = 12$ MeV. A G-matrix [30] interaction based on the realistic Argonne AV18 [31] and fixed starting energy $\omega_{st} = -40$ MeV is used. Already at second-order in the self-energy, Gorkov-SCGF can provide comparable accuracy to CC singles and doubles (CCSD). Higher order corrections introduced by triples $[\Lambda\text{-CCSD(T)}]$ [9] are closely reproduced by Dyson-SCGF in the ADC(3) approximation [18] after including doubles corrections to its coupling amplitudes $[\text{ADC}(3)\text{-D}]$ [3]. Since the extension of Gorkov's formalism to ADC(3) schemes is within computational reach, this gives confidence that Gorkov-SCGF calculations can be improved to desired accuracy. Note that earlier calculations with second-order self-energies already gave quantitative results, although limited to small model spaces and closed-shell systems [32–34]. Findings shown in Fig. 1 demonstrate the feasibility of first-principle calculations

¹ Any consideration associated with $A=N+Z$ applies in fact separately to the number of protons Z and to the number of neutrons N .

² Vectors and matrices defined on the one-body Hilbert space \mathcal{H}_1 are denoted as bold quantities throughout the paper.

³ The component of vector \mathbf{U}_k associated with a single-particle state a is denoted by U_a^k . Correspondingly, the component associated with the time-reversed state \bar{a} (up to a phase η_a) is denoted by \bar{U}_a^k [13].

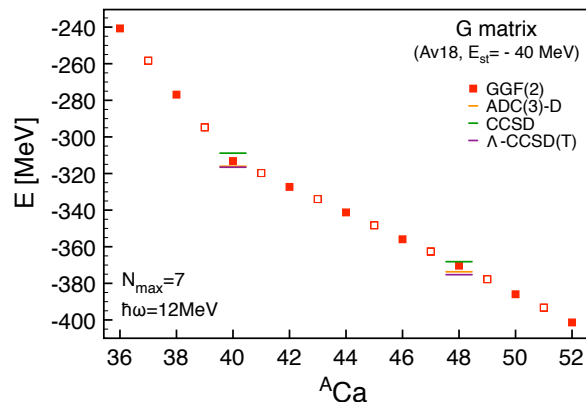


FIG. 1. (Color online) Binding energy of Ca isotopes from (sc0) second-order Gorkov-SCGF obtained in a fixed model space of eight shells. Gorkov propagators are calculated for even-A (filled symbols) while odd-A results (open symbols) are computed according to the prescription of Ref. [25].

along full isotopic chains and constitute the main result of the present work.

Let us now go to larger model spaces and discuss the two examples of mid-shell ^{44}Ca and ^{74}Ni . In the following, calculations are performed with a next-to-next-to-next-to-leading-order ($N^3\text{LO}$) 2N chiral interaction [35] complemented by the Coulomb force and evolved using free-space similarity renormalization group (SRG) [36] to $\lambda = 2.0 \text{ fm}^{-1}$. Figure 2 displays the binding energy of ^{74}Ni as a function of the harmonic oscillator spacing $\hbar\omega$ and for an increasing size $N_{max} \equiv \max(2n + l)$ of the single-particle model space. The convergence pattern obtained here on the basis of a soft 2N interaction is similar to those generated for doubly-closed shell nuclei with currently available ab-initio methods. Overall, convergence is well attained for $N_{max} = 13$. In ^{44}Ca , going

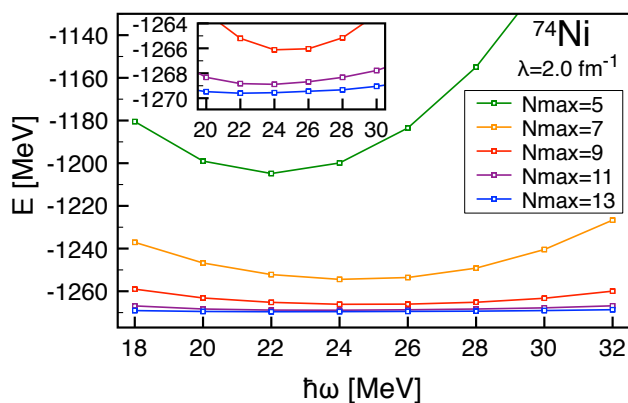


FIG. 2. (Color online) Binding energy ^{74}Ni as a function of the harmonic oscillator spacing $\hbar\omega$ and for an increasing size N_{max} of the single-particle model space. Results are from (sc0) second-order Gorkov-SCGF calculations. The insert show a zoom on the most converged results.

	E_0^A	$\Delta_n^{(3)}(\text{A})$	r_{rms}
^{44}Ca	-669.6(1)	1.16	2.48
^{74}Ni	-1269.7(2)	1.17(1)	2.75

TABLE I. Binding energy (MeV), neutron pairing gap (MeV) and matter root mean square radius (fm). Results are from second-order (sc0) Gorkov-SCGF calculations and are extrapolated to infinite oscillator basis size using the method of Ref. [37]. The extrapolation error is indicated only when it is bigger than the last digit shown.

from $N_{max} = 11$ to $N_{max} = 13$ lowers the minima by just a few keV. Also, the binding energy calculated for $N_{max} = 13$ varies by less than 200 keV over a wide range of $\hbar\omega$ values. In ^{74}Ni , going from $N_{max} = 11$ to $N_{max} = 13$ yields an additional 600 keV, while scanning a large range of oscillator frequencies only changes the binding energy by about 1 MeV.

Table I gives examples of observables of interest in the ground state of ^{44}Ca and ^{74}Ni . The values quoted are extrapolated to infinite oscillator basis size using the method proposed in Ref. [37]. Note that the present results nicely demonstrate the feasibility of Gorkov-SCGF in the medium mass region but are not expected to reproduce the experiment. Issues related to over binding of SRG-evolved 2N interactions are known to be cured by including 3N forces [4, 5, 38] and this is also confirmed by preliminary work in which 3N forces are approximately added to Gorkov-SCGF [39]. For example, 3N forces raise the radius of ^{44}Ca to 2.94 fm (closer to the experimental value of 3.52 fm) and the neutron $f_{7/2}-d_{3/2}$ shell gap is reduced to 7.2 MeV, in agreement with the data driven predictions of Ref. [40].

Figure 3 displays one-neutron addition and removal spectral strength distributions (SSD) in ^{44}Ca . Results are shown over a large range of final states in ^{43}Ca and ^{45}Ca characterized by spectroscopic factors as small as 0.2%. One observes a fragmentation of the spectroscopic strength that is characteristic of correlated many-body systems. Overall the pattern is similar to the one found in doubly-magic nuclei [3]. Close to the Fermi energy, however, one notices a feature that is unique to open-shell nuclei, i.e. the $7/2^-$ strength is equally fragmented into addition and removal channels, which results in the fact that both ^{43}Ca and ^{45}Ca ground-states have angular momentum and parity $J^\pi = 7/2^-$. This reflects static pairing correlations that manifest themselves as a result of emerging degeneracies in the ground state of open-shell nuclei. It is the main strength of Gorkov-SCGF theory to explicitly handle such degeneracies and resulting pairing correlations.

The right column in the upper panel of Fig. 4 supplies a zoom of Fig. 3 around the Fermi energy for states with spectroscopic factors larger than 10%. The left column provides the same quantities for first-order (i.e. HFB) calculations. The center column displays effective single-neutron energies. The same information is provided for ^{74}Ni in the lower panel of Fig. 4. The main fragmentation of the strength is absent from first-order calculations, i.e. it is due to dynamical correlations that come in at second order and that are qualitatively

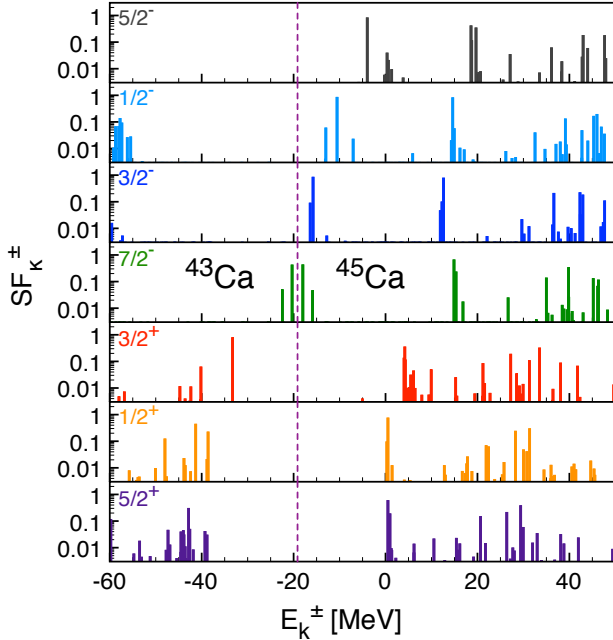


FIG. 3. (Color online) One-neutron addition and removal spectral strength distributions in ^{44}Ca obtained from second-order (sc0) Gorkov-SCGF calculations. For each final state in ^{43}Ca (left to the dashed line) and in ^{45}Ca (right to the dashed line), the spectroscopic factor is plotted as a function of its separation energy to the ground state of ^{44}Ca . Energies above 0 MeV correspond to $n+^{44}\text{Ca}$ scattering states [28]. Final states with different J^π values are separated for clarity. Results correspond to the minimum energy at $N_{\max}=13$ and $\hbar\omega=22$ MeV. Although center of mass motion is subtracted by using H_{int} , the variation of that correction going from A to $A\pm 1$ is neglected. The associated error is small in medium-mass nuclei [23].

the same as for closed-shell nuclei. Contrarily, the fragmentation of the strength in the vicinity of the Fermi energy into two peaks of (essentially) equal strength is qualitatively accounted for at first order and thus relates predominantly to static pairing correlations. One observes that the position of the dominant peak of a given J^π value is significantly modified by second-order effects such that the corresponding spectrum is more compressed than at first order. Further compression is expected from addition of 3N forces and coupling to collective fluctuations as in ADC(3).

Effective single-particle energies recollect the fragmented strength [13, 21, 22] from both one-nucleon addition and removal channels. Many-body correlations are largely screened out from ESPEs, which picture the averaged single-nucleon dynamics inside the correlated system. Two different features are identifiable in the ESPE spectrum e_a^{cent} when compared to observable one-nucleon addition and removal spectra E_k^\pm . The ESPE $e_{1f_{7/2}}^{\text{cent}}$ ($e_{1g_{9/2}}^{\text{cent}}$) located at the Fermi energy recollects the strength of the two equally important $7/2^-$ ($9/2^+$) states. Other ESPEs recollect the strength of a low-lying dominant peak and of a highly fragmented strength distributed at higher excitation energies such that they move away from the Fermi energy to closely match first-order, i.e. HFB, peaks. This is

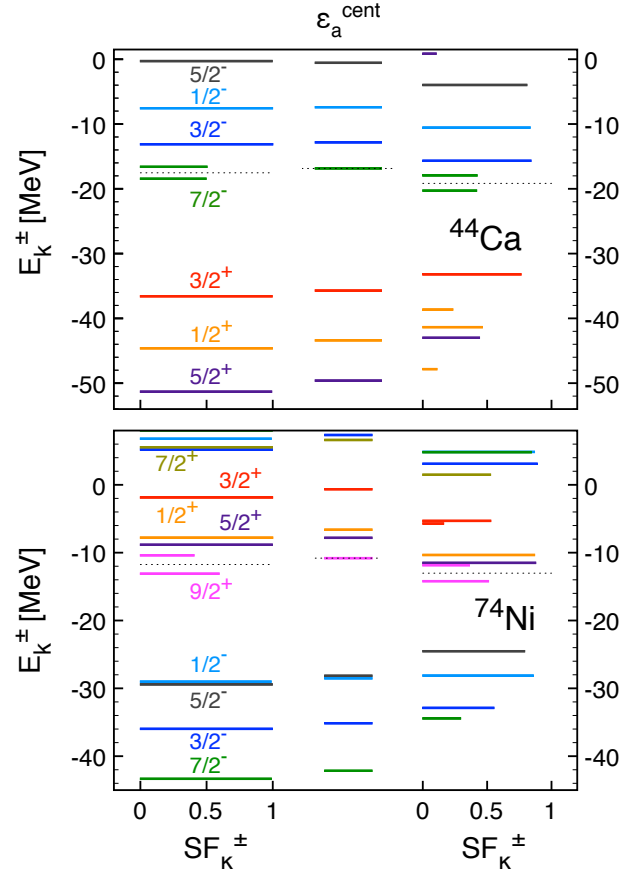


FIG. 4. (Color online) Left: One-neutron addition and removal spectral strength distribution obtained from first-order (HFB) Gorkov-SCGF calculations. Right: same as left panel for second-order (sc0) calculations. Center: Baranger ESPEs reconstructed from second-order (sc0) Gorkov-SCGF calculations. Upper panel: ^{44}Ca . Lower panel: ^{74}Ni .

consistent with the fact that ESPEs inform on the averaged, mean-field-like, one nucleon dynamics.

Conclusions. - We have presented the first ever calculations of medium-mass (truly) open-shell nuclei from *first principles*. Such calculations are based on the implementation of self-consistent Gorkov-Green's function theory on the basis of realistic nuclear interactions. Taking ^{44}Ca and ^{74}Ni as test cases, we have demonstrated the good convergence with respect to the basis size and discussed the possibility of extracting several quantities of experimental interests including ground-state energies, pairing gaps and particle addition/removal spectroscopy. Comparison with other ab-initio calculations for closed shells ^{40}Ca and ^{48}Ca shows that the method is capable of high accuracy upon extension to state-of-the-art Dyson-SCGF technique and incorporation of three-nucleon interactions. Work in this direction is in progress. The present results open a path to increase the reach of *ab-initio* theory in the mid-mass region tremendously. This will allow, in the near future, to perform systematic studies over long isotopic and isotonic chains, up to Nickel and to $N=28$

or 32 [23].

Acknowledgements. - We thank G. Hagen for providing the coupled cluster results of Fig. 1. This work was supported by the United Kingdom Science and Technology Facilities Council (STFC) under Grants ST/I003363 and ST/J00005, by the DFG through grant SFB 634 and by the Helmholtz Alliance Program, contract HA216/EMMI. V. S. acknowledges support from Espace de Structure Nucléaire Théorique (ESNT) at CEA/Saclay. Calculations were performed using HPC resources from GENCI-CCRT (Grant 2012- 050707).

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