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2011 J. Phys.: Conf. Ser. 321 012039

(http://iopscience.iop.org/1742-6596/321/1/012039)

Journal of Physics: Conference Series **321** (2011) 012039 doi:10.1088/1742-6596/321/1/012039

Gorkov self-consistent Green's function calculations of semi-magic nuclei

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Abstract. The first nuclear structure application of the newly developed Gorkov self-consistent Green's function method is presented. The approach aims to describe many-nucleon systems from an ab-initio standpoint featuring an explicit treatment of pairing correlations. In the present work calculations of binding energies of calcium isotopes are reported and compared with experimental data and other theoretical references.

1. Introduction

Although considerable progress has been made in recent years, e.g. using coupled-cluster (CC) [1] or Dyson self-consistent Green's function [2] (Dyson-SCGF) methods, ab-initio calculations of medium-mass nuclei are still limited to a few tens of (doubly-magic ± 1) nuclei. Besides the challenging numerical scaling of such ab-initio methods with nucleon number, there exists an intrinsic difficulty in going to truly open-shell nuclei. Indeed, doing so requires either to use a multi-reference based method, e.g. multi-reference CC [3], or to build the correlated state onto a zeroth-order reference state that already accounts for pairing correlations.

Following the second option, we are currently developing [4] a many-body method based on the self-consistent Green's function theory in the Gorkov formalism that allows for an explicit treatment of pairing correlations and that is therefore applicable to several hundreds of (semi-magic ± 1) nuclei, including systems up to, e.g., the tin isotopic chain. The present implementation of the method starts from realistic low-momentum interactions and consists in the self-consistent solution of Gorkov's equations on the basis of first- and second-order self-energies.

2. Gorkov Green's function theory

2.1. Elements of formalism

Let $\{c_a^\dagger\}$ be a basis of the one-body Hilbert space $\mathcal{H}_1$ that can be divided into two blocks mapped into each other by the time-reversal transformation. In our case, such a basis will correspond to the harmonic oscillator basis. To any state a belonging to the first block is associated a single-particle state $\bar{a}$ belonging to the second block and having the same quantum numbers as a, except for the sign of the third component of the j-coupled angular momentum. With that in mind one can define a basis $\{\bar{c}_a^\dagger\}$ dual to the basis $\{c_a^\dagger\}$ through

$$\bar{c}_a^\dagger(t) \equiv \eta_a c_{\bar{a}}^\dagger(t)\,, \qquad \bar{c}_a(t) \equiv \eta_a c_{\bar{a}}(t)\,, \tag{1}$$

which correspond to exchanging the state a by its partner $\bar{a}$ up to the phase η_a. By convention $\bar{\bar{a}} = a$ with $\eta_a\,\eta_{\bar{a}} = -1$.

In Gorkov formalism, one targets the ground state $|\Psi_0\rangle$ of the grand-canonical-like potential $\Omega = H - \mu N$, where μ is the chemical potential and N the particle-number operator, having the number $N = \langle\Psi_0|N|\Psi_0\rangle$ of particles in average. The state $|\Psi_0\rangle$ is a priori not an eigenstate of N, i.e. it is likely to break particle number symmetry. In order to access complete one-body information contained in $|\Psi_0\rangle$, one must introduce a set of four Green's functions, known as Gorkov propagators [5]. Gorkov's propagators can be conveniently grouped into a matrix representation, first introduced by Nambu [6]. After defining an "annihilation" column vector made of annihilation and creation operators

$$\mathbf{C}_a(t) \equiv \begin{pmatrix} c_a(t) \\ \bar{c}_a^\dagger(t) \end{pmatrix}\,, \tag{2a}$$

and a "creation" row vector

$$\mathbf{C}_a^\dagger(t) \equiv \begin{pmatrix} c_a^\dagger(t) & \bar{c}_a(t) \end{pmatrix}\,, \tag{2b}$$

one can write the four propagators through

$$i\,\mathbf{G}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{\mathbf{C}_a(t)\mathbf{C}_b^\dagger(t')\right\}|\Psi_0\rangle = i\begin{pmatrix} G_{ab}^{11}(t,t') & G_{ab}^{12}(t,t') \\ G_{ab}^{21}(t,t') & G_{ab}^{22}(t,t') \end{pmatrix}\,. \tag{3}$$

Similarly to the Dyson case, self-consistent, i.e. *dressed*, Gorkov propagators are solution of an equation of motion taking, in Nambu's notation and in the energy representation, the typical form

$$\mathbf{G}_{ab}(\omega) = \mathbf{G}_{ab}^{(0)}(\omega) + \sum_{cd}\mathbf{G}_{ac}^{(0)}(\omega)\,\tilde{\mathbf{\Sigma}}_{cd}(\omega)\,\mathbf{G}_{db}(\omega)\,. \tag{4}$$

In Eq. (4) $\mathbf{G}_{ab}^{(0)}(\omega)$ denotes the unperturbed Gorkov Green's function associated with a reference state of the Bogoliubov type, whereas $\tilde{\mathbf{\Sigma}}_{cd}(\omega)$ defines normal and anomalous irreducible self-energies through

$$\tilde{\mathbf{\Sigma}}_{ab}(\omega) \equiv \begin{pmatrix} \tilde{\Sigma}_{ab}^{11}(\omega) & \tilde{\Sigma}_{ab}^{12}(\omega) \\ \tilde{\Sigma}_{ab}^{21}(\omega) & \tilde{\Sigma}_{ab}^{22}(\omega) \end{pmatrix}\,. \tag{5}$$

2.2. Calculation scheme

Proceeding to an actual calculation and solving Eq. (4) relates to truncating the diagrammatic expansion of the irreducible self-energies. The latter expansion, originally based on perturbation theory, is re-expressed in terms of skeleton diagrams, i.e. in terms of dressed propagators solution

of Eq. (4). This key feature of *self-consistent* Green's function methods allows the resummation of self-energy insertions to all orders and makes the method intrinsically iterative.

In a first step, our objective is to perform self-consistent second-order calculations, i.e. include first- and second-order diagrams in the computation of the self-energies and solve Eq. (4) iteratively to convergence. Figure 1 (2) displays the corresponding diagrammatic contributions to the normal (anomalous) self-energy. In such diagrams, double lines denote self-consistent normal (two arrows in the same direction) and anomalous (two arrows in opposite directions) propagators, solutions of Eq. (4). Notice that this choice of diagrams constitutes a Kadanoff-Baym Φ-derivable approximation, which automatically ensures the exact fulfillment of conservation laws [7]. Extensive details regarding both the formalism and the computational scheme will be reported in a forthcoming publication [4].

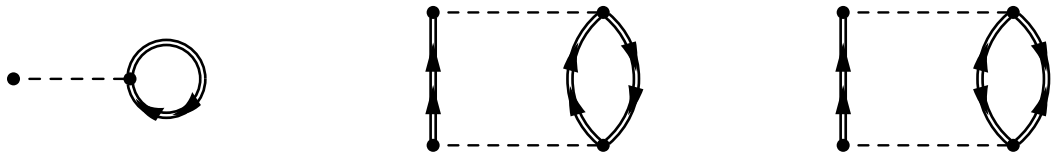

Figure 1. First- and second-order contributions to the normal self-energy Σ^{11}.

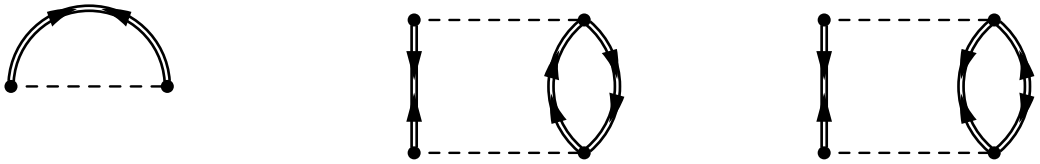

Figure 2. First- and second-order contributions to the anomalous self-energy Σ^{21}.

3. Results

A large set of observables are accessible as an outcome of Gorkov calculations, ranging from the binding energy and all one-body observables of the targeted A-body ground-state to one-nucleon separation energies to eigenstates of $A \pm 1$ systems. In the present paper, we simply wish to highlight the potential of this newly developed ab-initio method by reporting on one illustrative example, i.e. the binding energy evolution in the calcium isotopic chain. According to the Koltun-Galitskii sum rule [8], the total energy associated with a two-body operator can be accessed from the one-body (normal) dressed propagator, i.e.

$$E_0 \;=\; \sum_{ab} \frac{i}{4\pi} \int_{C\uparrow} d\omega \, G^{11}_{ba}(\omega) \left[t_{ab} + \omega \, \delta_{ab} \right] , \tag{6}$$

where the integration is performed over a closed contour in the upper half of the complex plane and where t_{ab} denotes the matrix elements of the kinetic energy operator.

Figure 3 displays the binding energy from ^{40}Ca to ^{48}Ca. Results obtained using various ab-initio methods and approximation schemes are compared, i.e. (i) first-order Gorkov self-consistent Green's function (GGF(1)), equivalent to self-consistent Hartree-Fock-Bogoliubov (HFB), (ii) second-order perturbation theory (MBPT(2)), (iii) second-order Gorkov self-consistent Green's function (GGF(2)) and (iv) coupled cluster in singles and doubles approximation (CCSD) [9] methods. All calculations are performed using the same $\Lambda = 500$ MeV chiral two-nucleon interaction [10], further evolved down to $\Lambda = 2.1$ fm^{-1} through

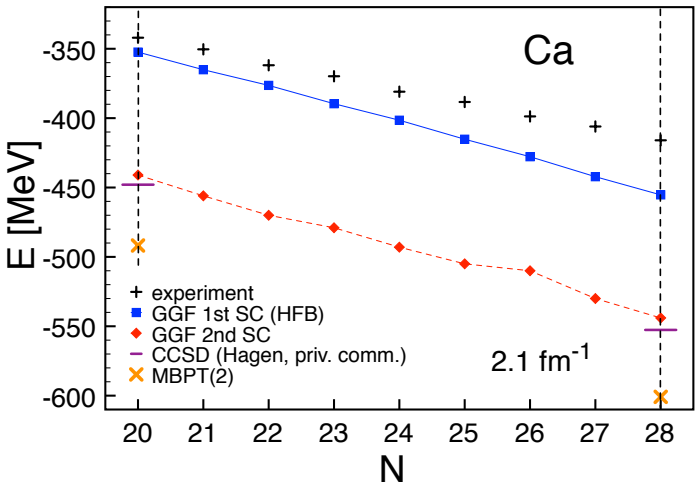

Figure 3. Binding energy in Ca isotopes from $N = 20$ to $N = 28$. Results of calculations from (i) HFB, (ii) MBPT(2), (iii) GGF(2) and (iv) CCSD [9] methods are reported and compared with experimental values. Calculations are performed using the $\Lambda = 500$ MeV chiral two-nucleon interaction [10] evolved down to $\Lambda = 2.1$ fm^{-1} through renormalization group technique [11]. Three-nucleon forces are omitted.

renormalization group technique [11]. Three-nucleon forces (TNF) are omitted in the present calculations.

As a consequence of the softness of the interaction and the omission of TNF the Hamiltonian employed is not expected to reproduce the experimental energies. All sets of results overbind the targeted nuclei. In this respect experimental values have to be considered a qualitative rather than quantitative reference. An additional signal for the need of TNF comes from the fact that, in all calculations, this overbinding increases with the mass number A.

Self-consistent second-order calculations correct MBPT(2) estimations reducing the overbinding of about 10%. This significant difference evidences the importance of a self-consistent treatment of the dynamical correlations introduced by second-order self-energy diagrams.

Binding energies from GGF(2) calculations are in the range of CCSD results in the doubly-closed shell ^{40}Ca and ^{48}Ca (note the large vertical scale). This rudimentary agreement, although in a small model space and with a relatively soft interaction, is a promising indication of the possible capabilities of the present method. It is in particular essential to note the qualitative improvement of GGF(2) over second order many-body perturbation theory that provides a clear overbinding compared to a CC calculation. This underlines the key role played by the self-consistent nature of GGF method and of the associated resummation of self-energy insertions to all orders. Starting from there, GGF approach allows us to address the trend of binding energy along the full isotopic chain. A thorough comparison between Dyson- and Gorkov-GF and CC approaches is in progress and will be object of a future publication [12].

4. Conclusions

Binding energies from ab-initio calculations of several calcium isotopes have been presented. In particular, first illustrative results from the newly developed Gorkov self-consistent Green's function method have been shown and compared with other many-body approaches. In this precursory application the GGF(2) approximation scheme shows to be in the range of CCSD results that employ the same interaction and model-space parameters. Thanks to the ability of tackling truly open-shell systems Gorkov self-consistent Green's function techniques represent a promising candidate for the first-time ab-initio description of long isotopic chains in the mid-mass region of the nuclear chart.

Acknowledgments
The authors wish to thank G. Hagen for providing them with unpublished results of CCSD calculations. Gorkov-SCGF calculations have been performed at the Centre de Calcul Recherche et Technologie (CCRT) of the Commissariat à l'Energie Atomique et aux Energies Alternatives (CEA), France. C.B. acknowledges support from the United Kingdom Science and Technology Facilities Council (STFC) through grant No. ST/I003363.

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