Self-consistent Gorkov Green's function calculations of one-nucleon spectral properties

V. Somà

CEA-Saclay, IRFU/Service de Physique Nucléaire, F-91191 Gif-sur-Yvette, France

T. Duguet

CEA-Saclay, IRFU/Service de Physique Nucléaire, F-91191 Gif-sur-Yvette, France
National Superconducting Cyclotron Laboratory and Department of Physics and Astronomy, Michigan State University, East Lansing, MI 48824, USA

C. Barbieri

Department of Physics, University of Surrey, Guildford GU2 7XH, UK

Abstract. Results from the newly developed Gorkov self-consistent Green's function approach are presented. Ab-initio spectral strength distributions for one-nucleon addition or removal calculated in doubly-closed shell ^{40}Ca and in semi-magic ^{44}Ca are briefly discussed. The object of the present communication is to illustrate the potential spectroscopic reach of the method.

1. Introduction

In the last decade the reach of ab-initio nuclear structure calculations has extended up to the region of medium-mass systems. Despite the significant progress both from the theoretical and computational point of view, methods as coupled-cluster (CC) [1] or Dyson self-consistent Green's function [2] (Dyson-SCGF) are however currently limited to a few doubly-magic nuclei. A few tens of neighbor isotopes with ± 1 or ± 2 nucleons can also be reached with particle attachment or removal formalisms [3, 4].

One way of tackling truly open-shell nuclei may involve the development of a multi-reference scheme, such as e.g. multi-reference CC [5]. Alternatively, one can build the correlated many-body state starting from a reference state that already incorporates zeroth-order pairing correlations, as in the case of e.g. Bogoliubov theory. We are currently following this second route and developing [6] a many-body method based on the self-consistent Green's function theory in the Gorkov formalism. Such method explicitly accounts for pairing correlations through the introduction of anomalous propagators, treated on the same footings as (and coupled to) the normal propagators of Dyson theory. This generalization of the standard Green's function approach is then applicable to several hundreds of (semi-magic +/-1) nuclei, including systems up to, e.g., the tin isotopic chain.

In the current implementation the method starts from realistic 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

Let us introduce a basis $\{a_a^\dagger\}$ of the one-body Hilbert space $\mathcal{H}_1$ that can be divided into two blocks according to the value (or more precisely to the sign) of an appropriate quantum number. In the present calculations such a basis will be identified with the harmonic oscillator basis; notice however that the formalism is more generally valid for any basis that possesses this property.

To any state a belonging to the first block, a single-particle state $\bar{a}$ belonging to the second block and having the same quantum numbers as a, except for the one differentiating the two blocks, can be associated through a transformation, i.e. time-reversal in the present case. With that in mind one can define a basis $\{\bar{a}_a^\dagger\}$ dual to the basis $\{a_a^\dagger\}$ through

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

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 $\eta_a\,\eta_{\bar{a}} = -1$.

Using the second quantized operators $\{a_a^\dagger, a_a\}$ and their dual counterparts $\{\bar{a}_a^\dagger, \bar{a}_a\}$ one defines an "annihilation" column vector

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

and a "creation" row vector

$$\mathbf{A}_a^\dagger(t) \equiv \begin{pmatrix} a_a^\dagger(t) & \bar{a}_a(t) \end{pmatrix}\,. \tag{2b}$$

The four Gorkov propagators [7] are then constructed by means of these generalized operators through

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

Here $|\Psi_0\rangle$ represents the ground state 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. Notice that the state $|\Psi_0\rangle$ is a priori not an eigenstate of N, i.e. it is likely to break particle number symmetry.

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

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

Here $\mathbf{G}_{ab}^{(0)}(\omega)$ indicates 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

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

Any actual solution of Gorkov equations involves a truncation of the diagrammatic expansion of the irreducible self-energies. Such an expansion is performed in terms of dressed propagators, which implies that at every order an infinite subset of self-energy insertions is implicitly resummed. It is easy to see that such a prescription goes beyond perturbation theory. In more practical terms, the solution of Gorkov equations is typically achieved via an iterative procedure that ends when a suitably chosen quantity (e.g. the chemical potential) has reached the desired degree of convergence.

Figure 1 (2) shows the corresponding diagrammatic contribution 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. The first- and second-order contributions to the self-energy are computed and inserted into Eq. 4, which is then solved iteratively to convergence. Extensive details regarding both the formalism and the computational scheme will be reported in a forthcoming publication [6].

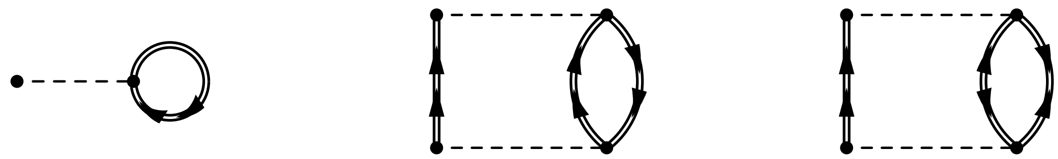

Figure 1. First- and second-order contributions to the normal self-energy Σ^{11}.

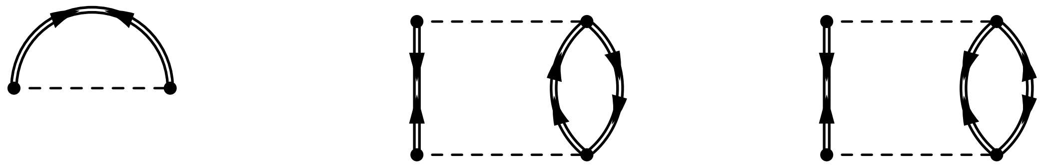

Figure 2. First- and second-order contributions to the anomalous self-energy Σ^{21}.

3. Results

The knowledge of the single-particle propagator gives access not only to the total energy and to all one-body observable of the targeted A-body ground state but also to one-nucleon separation energies and spectroscopic amplitudes to eigenstates of $A \pm 1$ systems. In order to retrieve the spectroscopic content of the one-body Gorkov Green's function it is convenient to express it in its so-called spectral or Lehmann representation [8, 6]

$$\mathbf{G}_{ab}(\omega) = \sum_k \left\{ \frac{\mathbf{X}_a^k \, \mathbf{X}_b^{k\dagger}}{\omega - E_k^+ - \mu + i\eta} + \frac{\mathbf{Y}_a^{k\dagger} \, \mathbf{Y}_b^k}{\omega - E_k^- - \mu - i\eta} \right\} , \tag{6}$$

with $\mathbf{X}_a^{k\dagger} \equiv \langle \Psi_k | \mathbf{A}_a^\dagger | \Psi_0 \rangle$, $\mathbf{Y}_a^k \equiv \langle \Psi_k | \mathbf{A}_a | \Psi_0 \rangle$ and where $E_k^\pm$ represent one-nucleon addition and removal separation energies. A pole's position and residue of the Gorkov propagator therefore carry information respectively on the separation energies to $A \pm 1$ systems excited states and the spectroscopic amplitudes associated with such states.

In the present calculations we restrict ourselves to the case of a $J^\Pi = 0^+$ many-body target state, with J being its total angular momentum and Π its parity. A natural choice for labeling single-particle basis states in this context is $a \equiv (n_a, \pi_a, j_a, m_a, q_a)$, where n_a represents the principal quantum number, π_a is the parity, j_a is the total angular momentum, m_a is the projection of the total angular momentum along the z axis and q_a is the isospin projection. In this case all relevant objects in the theory turn out to be independent of m and block-diagonal in j, π and q. In particular one can define block-diagonal spectroscopic amplitudes according to $\mathbf{X}_a^k \equiv \delta_{\alpha\kappa} \delta_{m_a m_k} \mathbf{X}_{n_a[\kappa]}^{n_k}$ and $\mathbf{Y}_a^k \equiv \delta_{\alpha\kappa} \delta_{m_a m_k} \mathbf{Y}_{n_a[\kappa]}^{n_k}$, where we have introduced $\alpha \equiv \{j_a, \pi_a, q_a\}$.

Suitable quantities to analyze the spectroscopic information contained in the single-particle Green's function are the spectroscopic factors

$$\mathbf{F}^{-}_{n_k[\kappa]} \equiv \sum_{n_a} \left| \mathbf{Y}^{n_k}_{n_a[\kappa]} \right|^2 , \qquad \mathbf{F}^{+}_{n_k[\kappa]} \equiv \sum_{n_a} \left| \mathbf{X}^{n_k}_{n_a[\kappa]} \right|^2 , \tag{7}$$

and the spectral strength distribution (SSD)

$$\mathbf{S}_{[\kappa]}(\omega) \equiv \sum_{n_k} \mathbf{F}^{-}_{n_k[\kappa]} \, \delta(\omega - E^{-}_{k}) + \sum_{n_k} \mathbf{F}^{+}_{n_k[\kappa]} \, \delta(\omega - E^{+}_{k}) , \tag{8}$$

that can be interpreted as a generalized probability distribution for adding/removing a nucleon to/from the ground state while leaving the $A\pm1$ system in the many-body state κ with (relative) energy ω.

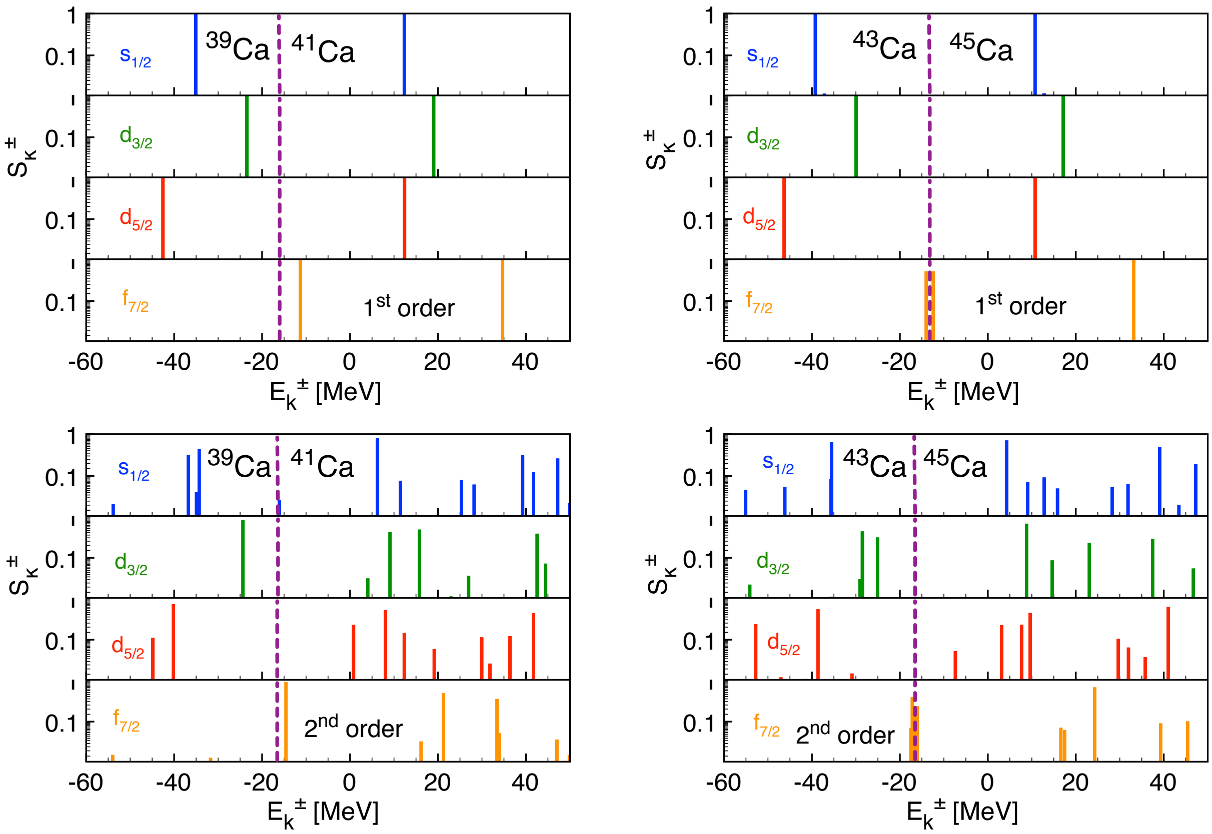

Figure 3. Neutron spectral strength distributions for different values of angular momentum and parity in ^{40}Ca (left) and ^{44}Ca (right). Results are displayed for self-consistent first-order (top) and second-order (bottom) approximations to the self-energy. The dashed vertical line denotes the Fermi energy. Calculations are performed using the $\Lambda = 500$ MeV chiral two-nucleon interaction [9] evolved down to $\Lambda = 2.1$ fm^{-1} through renormalization group technique [10]. Three-nucleon forces are omitted.

In Fig. 3 results for the normal neutron SSDs $\mathrm{S}^{11}_{[\kappa]}(\omega)$ in ^{40}Ca and ^{44}Ca are plotted for different values of angular momentum and parity as a function of ω. SSDs are shown for two different truncations of the self-energy expansion, i.e. at first and second order, respectively.

Calculations are performed using the $\Lambda = 500$ MeV chiral two-nucleon interaction [9] evolved down to $\Lambda = 2.1$ fm^{-1} through renormalization group technique [10]; three-nucleon forces are omitted. The model space consists of 7 major oscillator shells.

Both spectroscopic factors and SSDs represent an analysis tool to investigate correlations arising in the many-body system. Spectral peaks close to unity denote states that possess a single-particle character, i.e. that can be described to a good approximation as one nucleon added to or removed from an $A-$particle core. This is the case of ^{40}Ca when only first-order self-energies are included (top left in Fig. 3). When going from a doubly-closed shell systems as ^{40}Ca to one with a genuinely open-shell structure as ^{44}Ca, however, the arising of (static) pairing correlations can be detected. This is evident when focusing on the $f_{7/2}$ orbital in the top plots of Fig. 3: the lowest quasiparticle peak in ^{40}Ca breaks into two peaks of approximately equal strength right across the Fermi surface in ^{44}Ca, reflecting the partial filling of the neutron shell that can not be described in a single quasi-particle picture. The inclusion of the energy-dependent normal and anomalous second-order self-energies further fragment the single-particle strength into many states distributed over a wide range of energies. In most cases a single quasi-particle peak that carries 80 to 90 % of the strength is still visible. For the $f_{7/2}$ orbital the splitting of such main peak across the Fermi surface do not seem to be much affected by dynamical pairing correlations and remains similar to the first-order case.

4. Conclusions

Spectral strength distributions for one-nucleon addition and removal in ^{40}Ca and ^{44}Ca from Gorkov self-consistent Green's functions calculations have been presented. Although quantitatively not yet realistic due to the limited model space and the absence of three-nucleon forces, such calculations already show many of the features one requires from an ab-initio method that has access to spectroscopic quantities. The onset of static pairing correlations when filling up the neutron $f_{7/2}$ orbital going from ^{40}Ca to ^{48}Ca is reflected in the splitting of the quasi-particle peak across the Fermi surface in ^{44}Ca. The inclusion of energy-dependent self-energies accounts for dynamical correlations that result into a diffused fragmentation of the single-particle strength over a considerable range of energies.

More systematic application of Gorkov self-consistent Green's functions method are in progress [6] and will aim to describe for the first time in an ab-initio fashion the properties of long isotopic chains in the medium-mass region.

Acknowledgments

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.

References

[1] G. Hagen, T. Papenbrock, D. J. Dean, M. Hjorth-Jensen, Phys. Rev. C82, 034330 (2010).
[2] C. Barbieri, M. Hjorth-Jensen, Phys. Rev. C79, 064313 (2009).
[3] C. Barbieri, C. Giusti, F. D. Pacati, and W. H. Dickhoff, Phys. Rev. C70, 014606 (2004).
[4] G. R. Jansen, M. Hjorth-Jensen, G. Hagen, and T. Papenbrock, Phys. Rev. C 83, 054306 (2011).
[5] B. Jeziorski, H. J. Monkhorst, Phys. Rev. A24, 1668 (1981).
[6] V. Somà, T. Duguet, C. Barbieri, *unpublished* (2011).
[7] L. P. Gorkov, Sov. Phys. JETP 7, 505 (1958).
[8] H. Lehmann, Nuovo Cim. 11, 342 (1954).
[9] D. R. Entem, R. Machleidt, Phys. Rev. C68, 041001 (2003).
[10] S. K. Bogner, T. T. S. Kuo, A. Schwenk, Phys. Rept. 386, 1 (2003).
[11] T. Duguet, J. Sadoudi, V. Somà, G. Hagen, C. Barbieri, *unpublished* (2011).