Extension of self-consistent Gorkov-Green's function theory

Towards the Spectroscopy of even-even semi-magic Nuclei

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AB INITIO NUCLEAR MANY-BODY PROBLEM

- Adopting realistic interactions, nuclei are described in terms of Z ***protons*** and N ***neutrons***, with the aim of

  understanding how nucleons organise themselves into nuclei (pairing, clustering ...)

  providing reliable predictions for nuclear observables (excited states, transitions ...)

Tool: the A-body Schrödinger equation $H\Psi_k^A = E_k^A \Psi_k^A$

where Ψ_k^A is the A-body wavefunction, associated with the energy eigenvalue E_k^A

- In H, realistic interactions are drawn from ***Chiral Effective Field Theory***, which provides

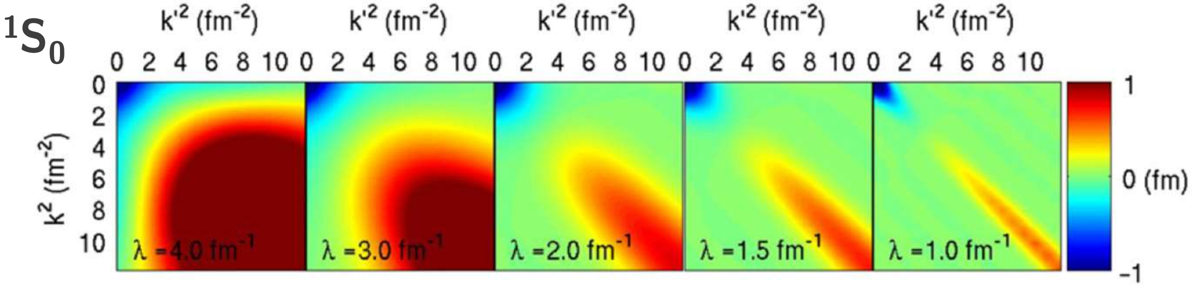
  a direct link with low-energy QCD and its symmetries

  a systematic framework to construct many-body interactions

  a theoretical error, stemming from the truncation of the expansion in powers of Q/Λ_χ

  where Λ_χ *is the chiral-symmetry-breaking scale* Q *is the 'small momentum' or pion mass*

In practice, ChEFT forces are preprocessed via the ***similarity renormalization group***, in order to quench the coupling between low and high momenta in the Hamiltonian



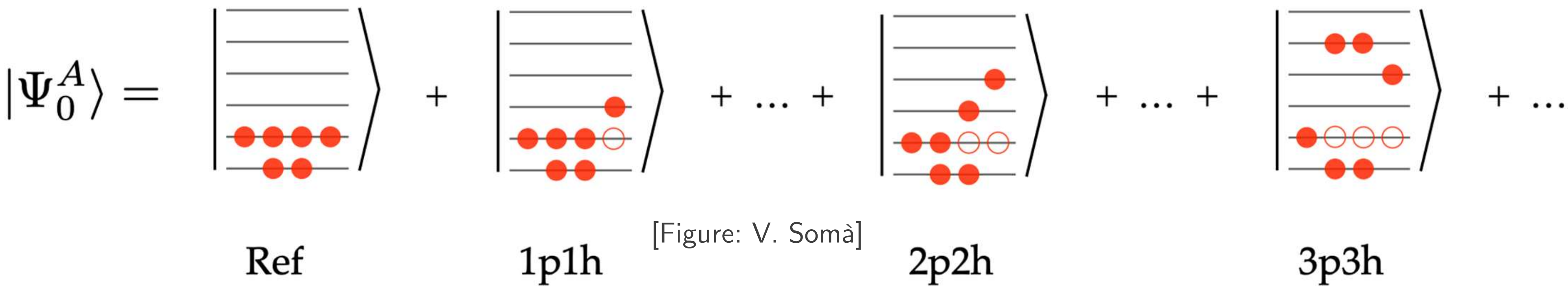
[S. Bogner et al. 2010]

Ab Initio Nuclear Wavefunction

Efficient approximation schemes for the nuclear wavefunction entail ***a polynomial scaling*** in the size M of the space of single-particle excitations $\rightsquigarrow M^\alpha$ with $\alpha \geq 4$

Correlation-expansion methods: expansion of the exact nuclear wavefunction into the space of particle-hole excitations built through the correlator Ω on a given *reference state*:

$$|\Psi_0^A\rangle = \Omega|\Phi_0^A\rangle = |\Phi_0^A\rangle + |\Phi_0^{A\,1p1h}\rangle + \ldots + |\Phi_0^{A\,2p2h}\rangle + \ldots + |\Phi_0^{A\,3p3h}\rangle + \ldots$$



[Figure: V. Somà]

where Ψ_0^A is the exact ground eigenstate of the A-body Hamiltonian, H_0

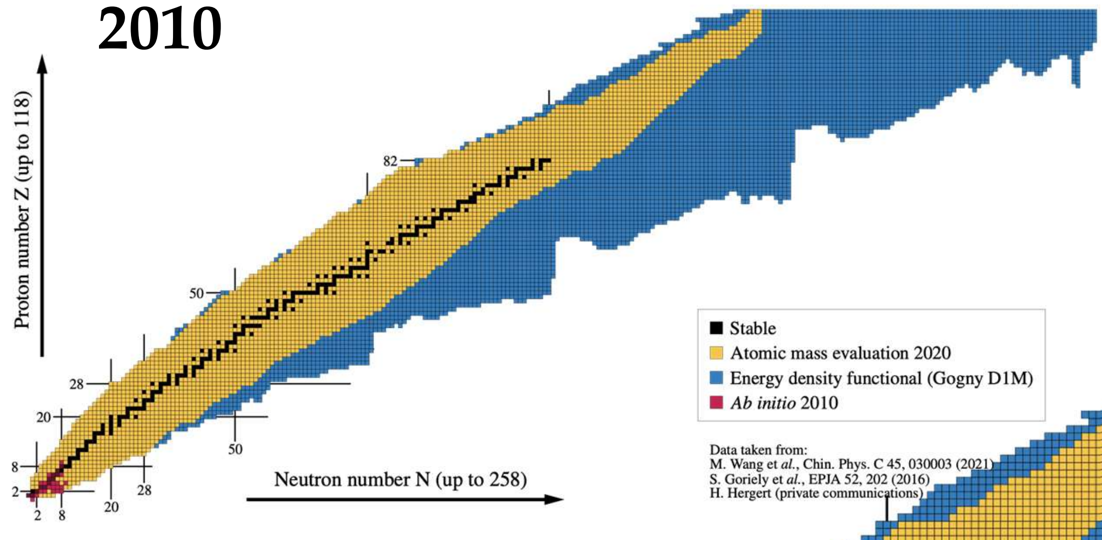
and the reference state Φ_0^A is the ground state of H, a solvable Hamiltonian, splitting the original one into $H = H_0 + H_I$ where H_I contains the 2-, 3-, ... -body interactions

Problem: *In open-shell nuclei, the ground state is almost degenerate with respect to the excitation of pairs of nucleons in the same single-particle energy level*

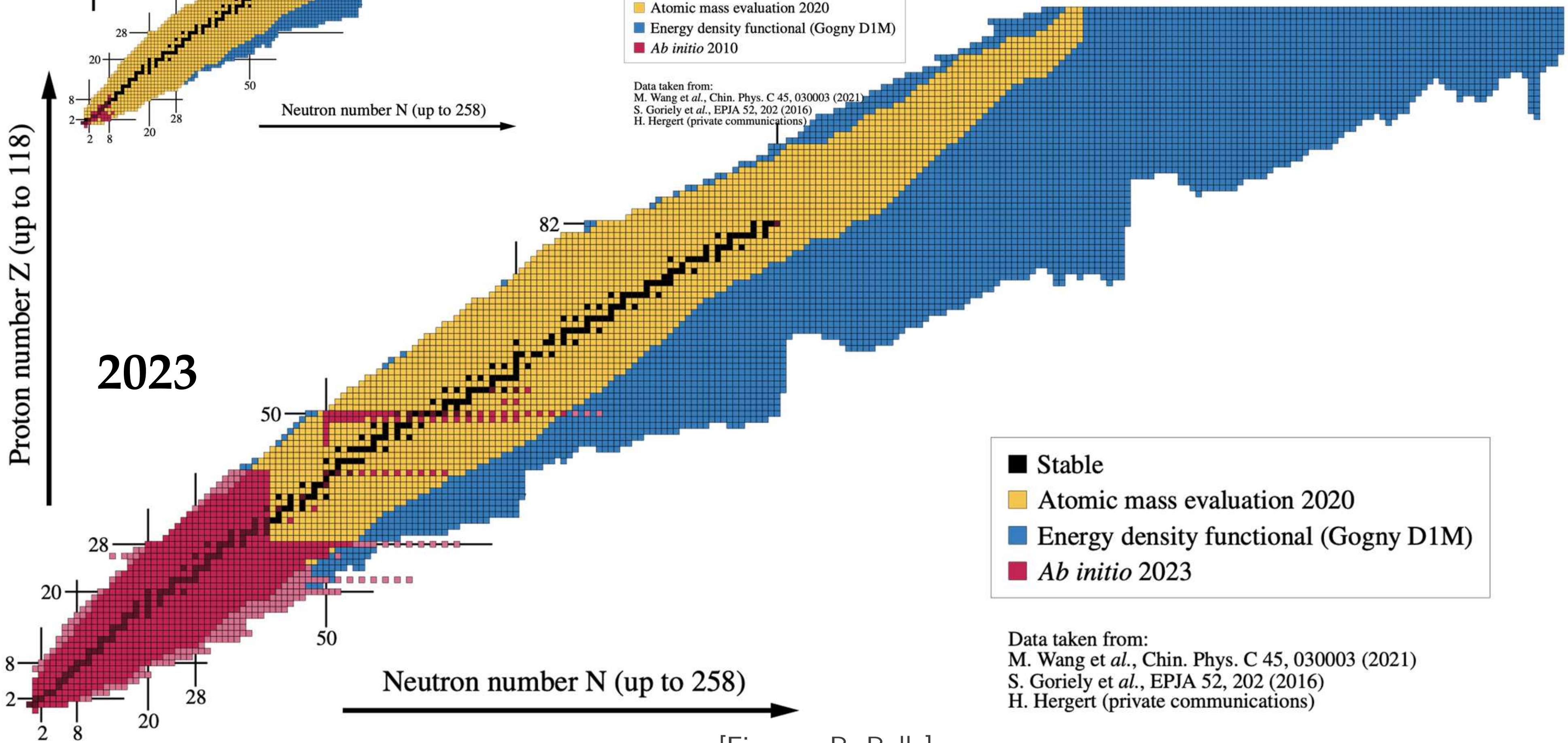
$\Downarrow$ $\Downarrow$ $\Downarrow$

Solution: in the reference state, breaking the symmetry associated to **particle number**, (semi-magic nuclei) together with **rotational symmetry** (doubly-open-shell nuclei)

AB INITIO NUCLEAR CHART



- A very significant **increase** in the reach of *ab-initio approaches* took place in the last decade...



[Figures: B. Bally]

Ab initio models of Nuclear Structure

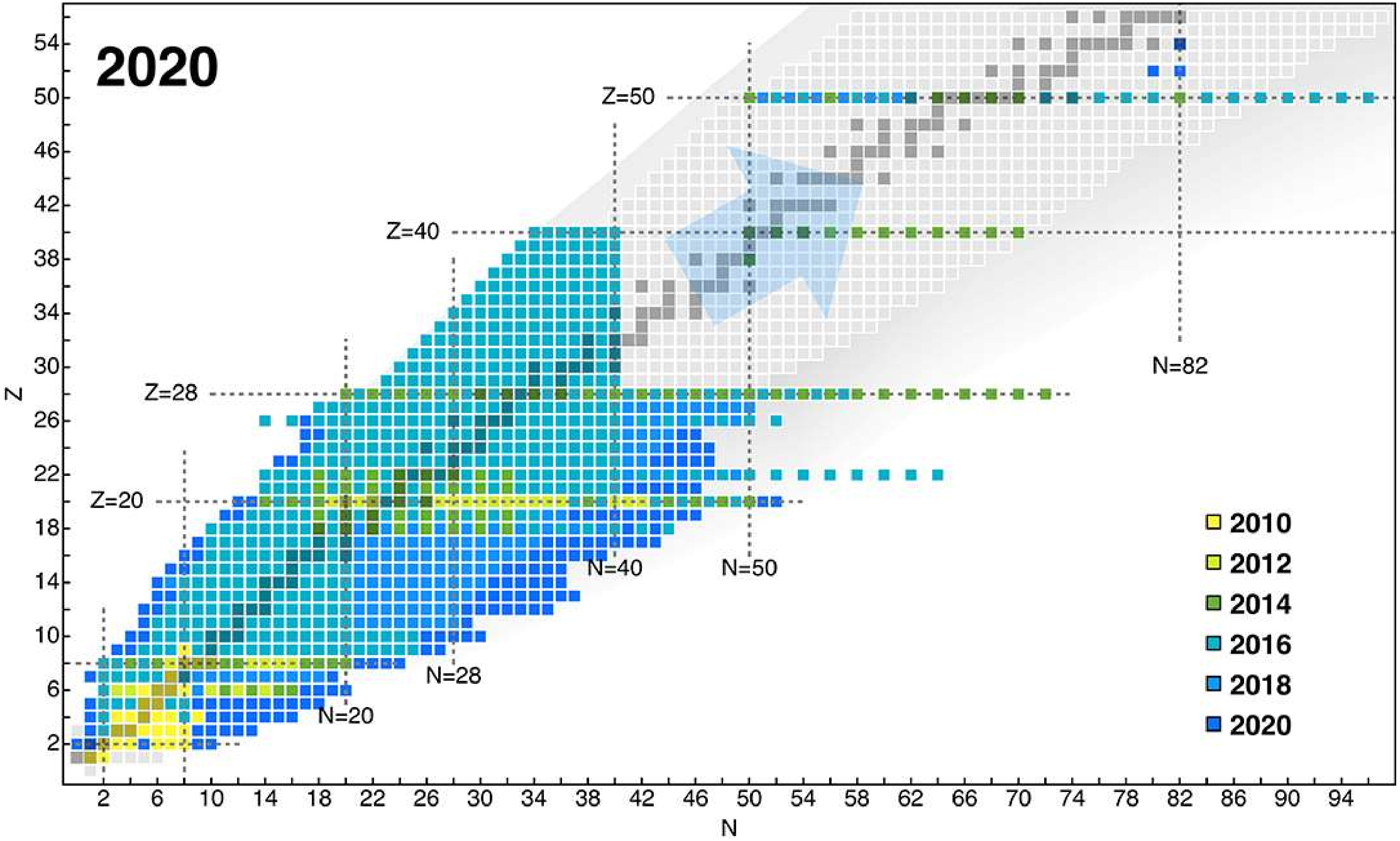
Main approaches:

Magic nuclei: MBPT, SCGF, IMSRG, CI, CC ...

Semi-magic nuclei: MR-IMSRG, BMBPT, SCGGF, BCC, ...

Doubly open-shell nuclei: MR-IMSRG, BMBPT, SCGGF$^+$, CC, ...

Passepartout: FCI, NCSM, NLEFT, LQCD ($A < 4$), PGCM-PT ...



[Figure: H. Hergert]

STATE OF THE ART

The salient novelty of the self-consistent Gorkov-Green's function approach consists in the

- Breaking of the symmetry associated with *particle-number:* $U_Z(1) \times U_N(1)$
  ⇝ V. Somà et al. *Phys. Rev. C* **84**, 064317 (2011)

  ^{44}Ca and ^{74}Ni: binding energy
  ^{43}Ca and ^{45}Ca: neutron addition and removal spectral distribution
  ^{45}Cl, ^{47}Cl and ^{49}Cl: ground and excited state energies, spectroscopic factors
  $18 \leq Z \leq 24$ isotopic chains: binding energy, two neutron shell gaps, one and two-proton/neutron separation energy, charge radius
  ^{50}Cr, ^{52}Cr and ^{54}Cr: charge density distribution
  Lepton scattering in ^{40}Ar and ^{48}Ti: neutron spectral function, charge density distr.
  O, Ca and Ni isotopes: binding energy, two-neutron separation energy, charge radius
  ^{47}Ca, ^{49}Ca, ^{51}Ca, ^{55}Ca, ^{53}K and ^{55}Sc: low-lying excited states

  ADC(2) with 2N forces
  Phys. Rev. C **87**, 011303 (2013)
  Phys. Rev. C **89**, 024323 (2014)

  ADC(2) with 2N+3N forces
  Phys. Rev. C **89**, 061301 (2014)
  Phys. Rev. C ***100***, 062501 (2019)
  Eur. Phys. J A **57**, 135 (2021)
  Phys. Rev. Lett. **128**, 022502 (2022)

  Extension of the algebraic diagrammatic construction to third order in progress ⇝ ADC(3)

- Additional breaking *of the symmetry associated with angular momentum:*

  $U_Z(1) \times U_N(1) \times SU(2)$ ⇝ A. Scalesi et al. (in progress)

THEORETICAL FRAMEWORK

The model conveniently is formulated in second-quantization formalism.

- The **single-particle space** $\mathscr{H}_1$ is split into two blocks, characterized by the sign of the total angular mom. projection along the z axis, j_z. $\Longrightarrow$ two pairs of creation/annihilation operators:

$$a_b,\ a_{\bar{b}} \qquad a_b^\dagger,\ a_{\bar{b}}^\dagger$$

where the *involution* In s.p. space (⇝ *time reversal*) is defined:

$$a_{\bar{b}} = \eta_b a_{\tilde{b}} \qquad a_{\bar{b}}^\dagger = \eta_b a_{\tilde{b}}^\dagger$$

with

$$\tilde{b} \equiv (n, \ell, j, -m, q) \qquad b \equiv (n, \ell, j, m, q)$$

where

$$\eta_b = (-1)^{\ell - j - m} \qquad \eta_b \eta_b^* = \eta_b^2 = 1 \qquad \eta_b \eta_{\tilde{b}} = -1$$

and q $\Longrightarrow$ z-component of the isospin

- The two partitions of the single-particle space constitute the **Nambu space** (2-dimens.) Introducing the superscripts $g = 1, 2$ one groups the creation/annihilation oper. into

$$\mathbf{A}_a \equiv \begin{pmatrix} a_a \\ \bar{a}_a^\dagger \end{pmatrix} \qquad \mathbf{A}_a^\dagger = \begin{pmatrix} a_a^\dagger & \bar{a}_a \end{pmatrix}$$

and $\mathbf{A}_a^* \equiv (\mathbf{A}_a^\dagger)^T$, obeying the canonical anticommutation rules

$$\left\{A_a^g, A_b^{g'}\right\} = \delta_{a\bar{b}}\delta_{g\bar{g}'} \qquad \left\{A_a^g, A_b^{\dagger\, g'}\right\} = \delta_{ab}\delta_{gg'} \qquad \left\{A_a^{\dagger\, g}, A_b^{\dagger\, g'}\right\} = \delta_{g\bar{g}'}\delta_{a\bar{b}}$$

with $\bar{g} = \begin{cases} 1 \text{ if } g = 2 \\ 2 \text{ if } g = 1 \end{cases}$

involution in Nambu space

These define the elements of a *metric tensor*

$\Longrightarrow$ Nambu-Covariant Pertubation Theory (appendix)

Theoretical Framework

- The system is described by the grand-canonical potential Ω, replacing the Hamiltonian:

$$\Omega = \underbrace{T + U - \mu_p Z - \mu_n N}_{\equiv \Omega_U} + \underbrace{V^{\rm NN} - U}_{\equiv \Omega_I}$$

where

$$T = \sum_{ab} T_{ab}\, a^\dagger_a a_b \qquad \text{with} \qquad T_{ab} \equiv (\bar{a}|T|b)$$ is the *kinetic energy* operator

$$V = \sum_{\substack{ab\\cd}} \frac{1}{(2!)^2} \bar{V}_{abcd}\, a^\dagger_a a^\dagger_b a_d a_c \qquad \text{with} \qquad \bar{V}_{abcd} \equiv \left[(ab|V^{\rm NN}|cd) - (ab|V^{\rm NN}|dc)\right]$$

is the partially antisymmetrized two-body *potential energy* operator

and
$$U = \sum_{ab} [U_{ab}\, a^\dagger_b a_b - U_{ab}\, a_{\bar{a}} a^\dagger_{\bar{b}} + \tilde{U}_{ab}\, a^\dagger_a a^\dagger_{\bar{b}} + \tilde{U}^\dagger_{ab}\, a_{\bar{a}} a_b]$$

is a one-body *auxiliary potential*, explicitly **breaking** particle number symmetry U(1).

- **Paradigm**: expansion scheme around a single reference state that builds the correlated state on top of a Bogoliubov vacuum that incorporates static pairing correlations

Physical symmetry	Group	Correlations
Particle number	$U_Z(1) \times U_N(1)$	*Pairing / superfluidity*
Rotations in 3 dim. space	$SU(N)$	*Quadrupole deformation*

Theoretical Framework

- **Method**: the degeneracy wrt *ph*-excitations is lifted via the *Bogoliubov reference state* and transferred into a degeneracy wrt the operations of the symmetry group $U_Z(1) \times U_N(1)$

$$\Omega_0^{A+2}(\mathrm{Z}+2,\mathrm{N}) \approx \Omega_0^A(\mathrm{Z},\mathrm{N}) \quad \Longrightarrow \quad E_0^{Z+2}(\mathrm{Z}+2,\mathrm{N}) - E_0^A(\mathrm{Z},\mathrm{N}) \approx E_0^A(\mathrm{Z},\mathrm{N}) - E_0^{A-2}(\mathrm{Z}-2,\mathrm{N}) \approx \ldots \approx 2\mu_p$$

$$\Omega_0^{A+2}(\mathrm{Z},\mathrm{N}+2) \approx \Omega_0^A(\mathrm{Z},\mathrm{N}) \quad \Longrightarrow \quad E_0^{A+2}(\mathrm{Z},\mathrm{N}+2) - E_0^A(\mathrm{Z},\mathrm{N}) \approx E_0^A(\mathrm{Z},\mathrm{N}) - E_0^{A-2}(\mathrm{Z},\mathrm{N}-2) \approx \ldots \approx 2\mu_n$$

  the constituents can be added or removed *at the same energy cost*, irrespective of A.

- **Observation**: The choice of *U* corresponds to selecting a superfluid unperturbed *g.s.*, acting as reference for the application of *Wick's theorem*. The exact eigenstates of Ω, preserve A:

$$H|\Psi_0^A\rangle = E_0^A|\Psi_0^A\rangle \qquad \Omega|\Psi_0^A\rangle = (E_0^A - \mu_p\mathrm{Z} - \mu_n\mathrm{N})|\Psi_0^A\rangle \equiv \Omega_0^A|\Psi_0^A\rangle$$

Considering the superposition of the g.s. of the nuclear systems with even number of constituents

$$|\Psi_0^{\mathrm{SB}}\rangle = \sum_{\mathrm{n}}^{\mathrm{even}} c_{\mathrm{n}}|\Psi_0^{\mathrm{n}}\rangle$$

one **replaces** $|\Psi_0\rangle \equiv |\Psi_0^A\rangle$ with $|\Psi_0^{\mathrm{SB}}\rangle$

where the coefficients of the expansion in the Fock space minimize:

$$\Omega_0^{\mathrm{SB}} \equiv \langle\Psi_0^{\mathrm{SB}}|\Omega|\Psi_0^{\mathrm{SB}}\rangle \gtrsim \Omega_0^A$$

subject to three constraints:

$$\mathrm{Z} = \langle\Psi_0^{\mathrm{SB}}|Z|\Psi_0^{\mathrm{SB}}\rangle \qquad \mathrm{N} = \langle\Psi_0^{\mathrm{SB}}|N|\Psi_0^{\mathrm{SB}}\rangle \qquad \langle\Psi_0^{\mathrm{SB}}|\Psi_0^{\mathrm{SB}}\rangle = \sum_{\mathrm{n}}^{\mathrm{even}} |c_{\mathrm{n}}|^2 = 1$$

THE ONE-BODY PROPAGATOR

- The Gorkov-Green's function in Nambu space and time repr. is defined as

$$i\mathbf{G}_{ab}(t,t') \equiv \langle \Psi_0 | T\{\mathbf{A}_a(t) \odot \mathbf{A}_b^*(t')\} | \Psi_0 \rangle$$

Since the Hamiltonian is time-independent, the FT of the one-body propagator becomes

$$\mathbf{G}_{ab}(\omega) = \int_{-\infty}^{+\infty} \mathrm{d}(t-t')\, e^{i\omega(t-t')} \mathbf{G}_{ab}(t-t')$$

Carrying out the integration, the *Lehmann representation* can be recast as

$$G_{ab}^{gg'}(\omega) = \sum_k \frac{{}^k\chi_a^g \; {}^k\chi_b^{g'*}}{\omega - (\Omega_k - \Omega_0)/\hbar + i\eta} + \sum_k \frac{{}^k\Upsilon_a^g \; {}^k\Upsilon_b^{g'*}}{\omega + (\Omega_k - \Omega_0)/\hbar - i\eta}$$

where $E_k^{(u)\pm} \equiv \mu_u \pm (\Omega_k - \Omega_0)$ with $u = p,\, n$ are the ***separation energies*** between the g.s. of the A-body system and the excited state *k* of the $A \pm 1$-body system.

$$E_k^{(p)\pm} \approx \pm(\langle \Psi_k^{\mathrm{SB}} | H | \Psi_k^{\mathrm{SB}} \rangle - \langle \Psi_0^{\mathrm{SB}} | H | \Psi_0^{\mathrm{SB}} \rangle) \mp \mu_p [\langle \Psi_k^{\mathrm{SB}} | Z | \Psi_k^{\mathrm{SB}} \rangle - (Z \pm 1)]$$

$$E_k^{(n)\pm} \approx \pm(\langle \Psi_k^{\mathrm{SB}} | H | \Psi_k^{\mathrm{SB}} \rangle - \langle \Psi_0^{\mathrm{SB}} | H | \Psi_0^{\mathrm{SB}} \rangle) \mp \mu_n [\langle \Psi_k^{\mathrm{SB}} | N | \Psi_k^{\mathrm{SB}} \rangle - (N \pm 1)]$$

whereas the residues of the poles are proportional to the ***spectroscopic amplitudes***

$${}^k\Upsilon_b^1 \equiv \langle \Psi_k | A_b^1 | \Psi_0 \rangle = \langle \Psi_k | a_b | \Psi_0 \rangle \qquad {}^k\chi_b^1 \equiv \langle \Psi_0 | A_b^1 | \Psi_k \rangle = \langle \Psi_0 | a_b | \Psi_k \rangle$$

$${}^k\Upsilon_b^2 \equiv \langle \Psi_k | A_b^2 | \Psi_0 \rangle = \langle \Psi_k | a_{\bar{b}}^\dagger | \Psi_0 \rangle \qquad {}^k\chi_b^2 \equiv \langle \Psi_0 | A_b^2 | \Psi_k \rangle = \langle \Psi_0 | a_{\bar{b}}^\dagger | \Psi_k \rangle$$

- The spectroscopic amplitudes are not *independent*: $[{}^k\chi_a^g]^* = {}^k\Upsilon_{\bar{a}}^{\bar{g}}$

- Gorkov *spectral functions*:

$$\mathbf{S}^{+}_{ab}(\omega) = -\frac{1}{\pi}\Im\mathfrak{m}\ \mathbf{G}_{ab}(\omega) = \sum_k {}^k\boldsymbol{\chi}_a\ {}^k\boldsymbol{\chi}_b^{\dagger}\delta(\omega - \omega_k)$$

with $\omega > 0$

$$\mathbf{S}^{-}_{ab}(\omega) = +\frac{1}{\pi}\Im\mathfrak{m}\ \mathbf{G}_{ab}(\omega) = \sum_k {}^k\boldsymbol{\Upsilon}_a\ {}^k\boldsymbol{\Upsilon}_b^{\dagger}\delta(\omega + \omega_k)$$

with $\omega < 0$

From the normal components, one nucleon removal and addition amplitudes are extracted:

$$S^h_{ab}(\omega) \equiv S^{11}_{ab}(\omega)$$
$$S^p_{ab}(\omega) \equiv S^{+}_{ab}(\omega)$$

- One and two-neutron separation energies:

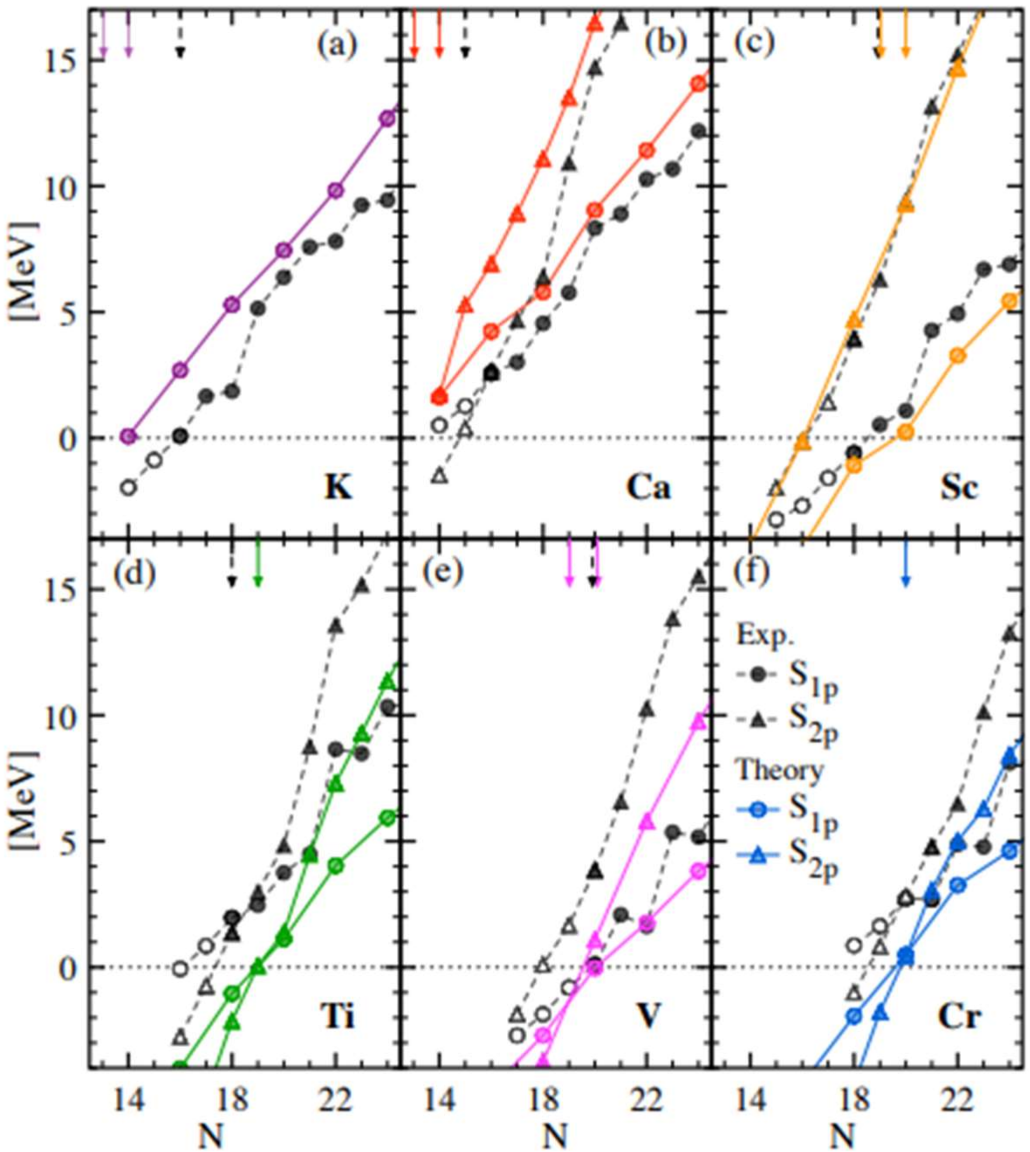
$$S_n(N,Z) \equiv |E(N,Z)| - |E(N-1,Z)|$$
$$S_{2n}(N,Z) \equiv |E(N,Z)| - |E(N-2,Z)|$$

- One and two-proton separation energies:

$$S_p(N,Z) \equiv |E(N,Z)| - |E(N,Z-1)|$$
$$S_{2p}(N,Z) \equiv |E(N,Z)| - |E(N,Z-2)|$$

where $E(N,Z) \rightsquigarrow$ g.s. energy

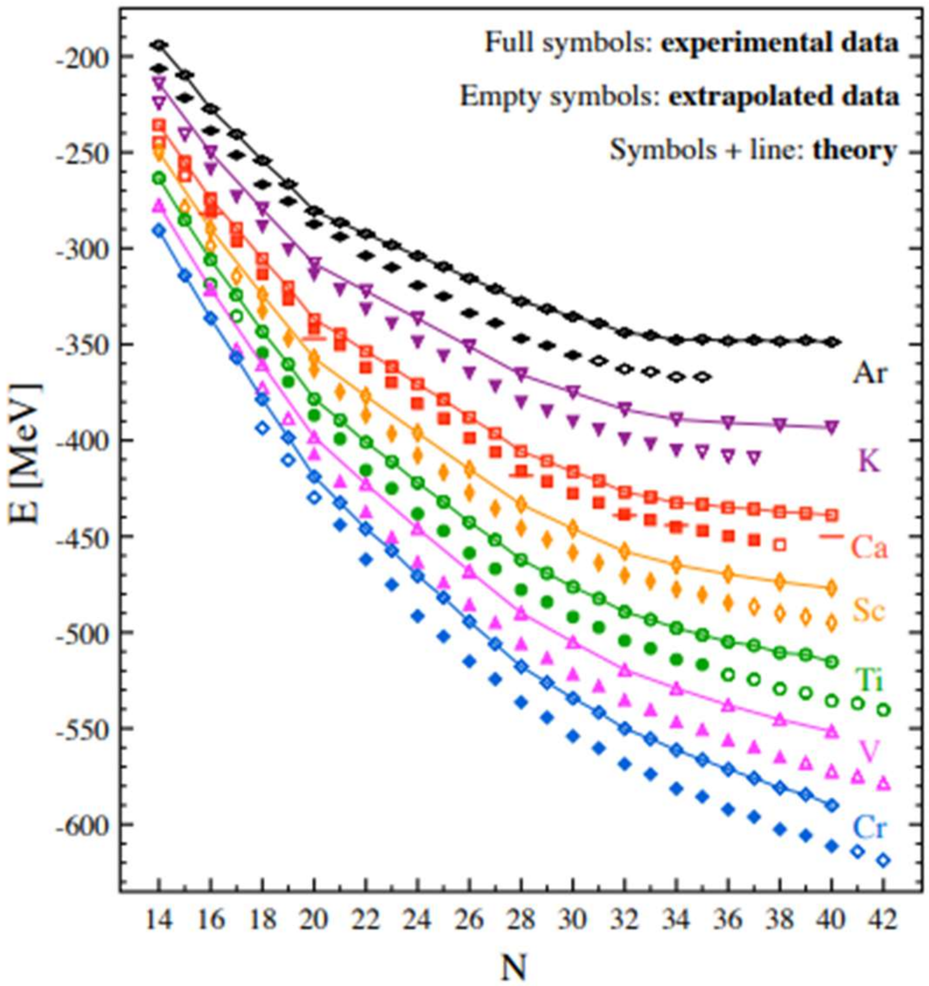
$S_p(N,Z)$ and $S_{2p}(N,Z)$



[*Eur. Phys. J A* **57**, 135 (2021)]

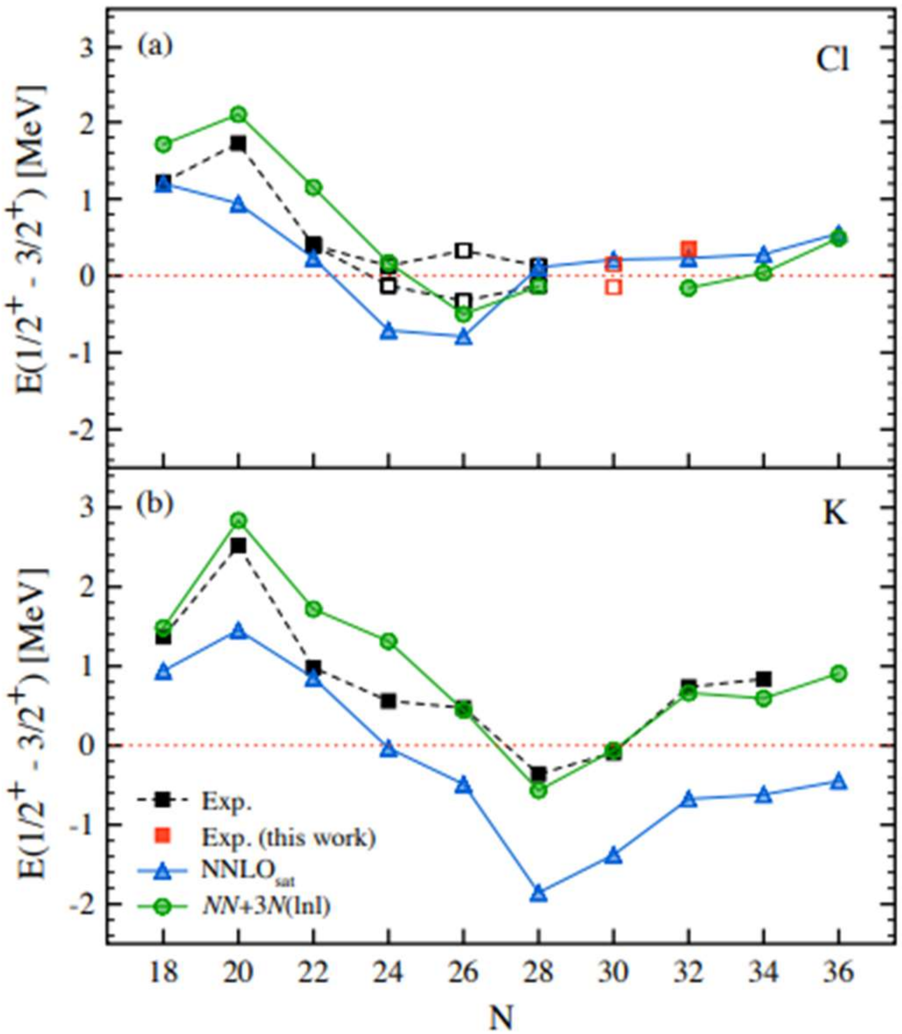
Physical Observables
from the one-body propagator

- Binding energy of even-even isotopic chains: the $18 \leq Z \leq 24$ nuclei



[*Eur. Phys. J A* **57**, 135 (2021)]

- Energies of the excited states of odd-even systems: the first $1/2^+$ and $3/2^+$ levels (Cl & K)



[*Phys. Rev. C* ***104***, 044331 (2021)]

The Polarization Propagator

The construction of the Gorkov response functions recalls the Dyson case:

$$R^{gg'g''g'''}_{abcd}(t,t',t'',t''') \equiv G^{gg'g''g'''}_{abcd}(t,t',t'',t''') - G^{gg''}_{ac}(t,t'')G^{g'g'''}_{bd}(t',t''')$$

where the two-body propagator is a rank-four tensor (16 elements) in Nambu space,

$$i^2\mathbf{G}_{abcd}(t,t',t'',t''') \equiv \langle\Psi_0|T\{\mathbf{A}_a(t)\odot\mathbf{A}_b(t')\odot\mathbf{A}^*_d(t''')\odot\mathbf{A}^*_c(t'')\}|\Psi_0\rangle$$

with the convention of J. Schirmer, *Phys. Rev. A* ***26***, 5, 2395-2416 (1982)

▶ Switching to the two-time limit the Gorkov *polarization propagator* is obtained:

$$\Pi^{gg''g'''g'}_{acdb}(t,t') \equiv \lim_{\substack{t''\to t^+ \\ t'''\to t'^+}} R^{gg'g''g'''}_{abcd}(t,t',t'',t''')$$

Explicitly:

$$\Pi^{gg''g'''g'}_{acdb}(t,t') = -i\langle\Psi^A_0|T\Big\{A^g_a(t)A^{g'}_b(t')A^{\dagger\, g'''}_d(t'^+)A^{\dagger\, g''}_c(t^+)\Big\}|\Psi^A_0\rangle$$
$$+i\langle\Psi^A_0|T\Big\{A^g_a(t)A^{\dagger\, g''}_c(t^+)\Big\}|\Psi^A_0\rangle\langle\Psi^A_0|T\Big\{A^{g'}_b(t')A^{\dagger\, g'''}_d(t'^+)\Big\}|\Psi^A_0\rangle$$

Analogously, the Fourier Transform of the polarization propagator yields

$$\Pi^{gg''g'''g'}_{acdb}(\omega) \equiv \int_{-\infty}^{+\infty} \mathrm{d}(t-t')e^{i\omega(t-t')}\Pi^{gg''g'''g'}_{acdb}(t-t')$$

and fulfills the symmetry properties under *time reversal* (left) and *complex conjugation* (right):

$$\Pi^{gg''g'''g'}_{acdb}(\omega) = \Pi^{g'g'''g''g}_{bdca}(-\omega) \qquad \Pi^{gg''g'''g'}_{acdb}(\omega) = [\Pi^{\bar{g}'''\bar{g}'\bar{g}\bar{g}''}_{d\bar{b}\bar{a}\bar{c}}(-\omega)]^*$$

The Polarization Propagator

- The Lehmann representation of the Gorkov polarization propagator gives

$$\Pi^{gg''g'''g}_{acdb}(\omega) \equiv \Pi^{+}{}^{gg''g'''g}_{acdb}(\omega) + \Pi^{-}{}^{gg''g'''g}_{acdb}(\omega)$$

The two contributions contain the same information and are again related by complex conjugation

$$[\Pi^{+}{}^{\bar{g}''\bar{g}\bar{g}'\bar{g}'''}_{\bar{c}\bar{a}\bar{b}\bar{d}}(-\omega)]^* = \Pi^{-}{}^{gg''g'''g'}_{acdb}(\omega)$$

where the l.h.s. (r.h.s.) is analytical in the upper (lower) part of the complex plane for ω,

$$\Pi^{+}{}^{gg''g'''g'}_{acdb}(\omega) = \sum_{k\neq 0} \frac{{}^k\chi^{gg''}_{ac} \; {}^k\chi^{*g'''g'}_{db}}{\omega - (\Omega_k - \Omega_0)/\hbar + i\eta} \qquad \Pi^{-}{}^{gg''g'''g'}_{acdb}(\omega) = -\sum_{k\neq 0} \frac{{}^k\Upsilon^{gg''}_{ac} \; {}^k\Upsilon^{*\,g'''g'}_{db}}{\omega + (\Omega_k - \Omega_0)/\hbar - i\eta}$$

the poles, for U(1)-cons. states, coincide with the energy of the excited states of the A-body system with respect to the g.s. energy $E_k \equiv \Omega_k - \Omega_0$ and the transition matrix elements, fulfilling

$${}^k\Upsilon^{gg'}_{ab} = [{}^k\chi^{\bar{g}'\bar{g}}_{\bar{b}\bar{a}}]^*$$

have been defined and orthogonality between the A-body states has been exploited. Explicitly

$${}^k\chi^{22}_{bc} \equiv \langle\Psi_0|A^2_b A^{\dagger\,2}_c|\Psi_k\rangle = \langle\Psi_0|a^\dagger_{\bar{b}} a_{\bar{c}}|\Psi_k\rangle \qquad {}^k\Upsilon^{22}_{bc} \equiv \langle\Psi_k|A^2_b A^{\dagger\,2}_c|\Psi_0\rangle = \langle\Psi_k|a^\dagger_{\bar{b}} a_{\bar{c}}|\Psi_0\rangle$$

$${}^k\chi^{12}_{bc} \equiv \langle\Psi_0|A^1_b A^{\dagger\,2}_c|\Psi_k\rangle = \langle\Psi_0|a_b a_{\bar{c}}|\Psi_k\rangle \qquad {}^k\Upsilon^{12}_{bc} \equiv \langle\Psi_k|A^1_b A^{\dagger\,2}_c|\Psi_0\rangle = \langle\Psi_k|a_b a_{\bar{c}}|\Psi_0\rangle$$

$${}^k\chi^{11}_{bc} \equiv \langle\Psi_0|A^1_b A^{\dagger\,1}_c|\Psi_k\rangle = \langle\Psi_0|a_b a^\dagger_c|\Psi_k\rangle \qquad {}^k\Upsilon^{21}_{bc} \equiv \langle\Psi_k|A^2_b A^{\dagger\,1}_c|\Psi_0\rangle = \langle\Psi_k|a^\dagger_{\bar{b}} a^\dagger_c|\Psi_0\rangle$$

$${}^k\chi^{21}_{bc} \equiv \langle\Psi_0|A^2_b A^{\dagger\,1}_c|\Psi_k\rangle = \langle\Psi_0|a^\dagger_{\bar{b}} a^\dagger_c|\Psi_k\rangle \qquad {}^k\Upsilon^{11}_{bc} \equiv \langle\Psi_k|A^1_b A^{\dagger\,1}_c|\Psi_0\rangle = \langle\Psi_k|a_b a^\dagger_c|\Psi_0\rangle$$

as in the one-body GF case, the anomalous elements *vanish* between U(1)-conserving states.

GORKOV'S BETHE-SALPETER EQUATIONS

- Gorkov's polarization propagator has proven to fulfill the following *self-consistent* equations

$$\Pi^{g_4 g_3 g_2 g_1}_{feba}(t,t^+,s^+,s) = \underbrace{\Pi^{\mathrm{D}\, g_4 g_3 g_2 g_1}_{feba}(t,t^+,s^+,s)} + \underbrace{\Pi^{\mathrm{B}\, g_4 g_3 g_2 g_1}_{feba}(t,t^+,s^+,s)} + \frac{1}{\hbar}\sum_{\substack{gg' \\ g''g'''}}\sum_{\substack{cd \\ hl}}\int_{-\infty}^{+\infty} \mathrm{d}t_1$$

$$\times \int_{-\infty}^{+\infty}\mathrm{d}t_2\int_{-\infty}^{+\infty}\mathrm{d}t_3\int_{-\infty}^{+\infty}\mathrm{d}t_4\, \underbrace{\Pi^{\mathrm{D}\, g_1 g_2 g g'}_{abcd}(t,t^+,t_1,t_2)}\, \underbrace{\Gamma^{ph\, gg'g''g'''}_{cdhl}(t_1,t_2,t_3,t_4)}\, \overbrace{\Pi^{g_4 g_3 g''' g''}_{felh}(s,s^+,t_4,t_3)}$$

disj. direct pol. propagator

disj. Bogoliubov pol. propagator

three-time pol. propagator

disjoint direct three-time pol. propagator

where

$$\Sigma^{\phi\, gg''}_{ad}(t,t'') = -i\sum_{bcef}\sum_{g'}(\bar{V}_{acef}\delta_{1g}+\bar{V}_{c\bar{e}\bar{a}f}\delta_{g2})\int_{-\infty}^{+\infty}\mathrm{d}t' G^{\phi\, g1g'1}_{efbc}(t,t,t',t^+)G^{\phi-1\, g'g''}_{bd}(t',t'') \quad \Leftarrow \quad \Gamma^{ph\, gg'g''g'''}_{cdhl}(t_1,t_2,t_3,t_4) = \left.\frac{\delta\Sigma^{\phi\, gg'}_{cd}(t_1,t_2)}{\delta G^{g''g'''}_{hl}(t_3,t_4)}\right|_{\phi(t)=0}$$

self-energy, in terms of the two-body propagator

particle-hole vertex

In energy representation, Gorkov's Bethe-Salpeter equations (GBSE) become

$$\Pi^{g_4 g_3 g_2 g_1}_{feba}(\omega) = \Pi^{\mathrm{D}\, g_4 g_3 g_2 g_1}_{feba}(\omega) + \Pi^{\mathrm{B}\, g_4 g_3 g_2 g_1}_{feba}(\omega) + \frac{1}{\hbar}\sum_{cdhl}\sum_{\substack{gg' \\ g''g'''}}\int_{-\infty}^{+\infty}\frac{\mathrm{d}\Omega_1}{(2\pi)}\int_{-\infty}^{+\infty}\frac{\mathrm{d}\Omega_2}{(2\pi)}\Pi^{\mathrm{D}\, g_1 g_2 g g'}_{abcd}\left(\tfrac{\omega-\Omega_1}{2},\tfrac{\omega+\Omega_1}{2}\right)$$

$$\times\Gamma^{ph\, gg'g''g'''}_{cdhl}\left(\tfrac{\omega-\Omega_1}{2},\omega,\omega-2\Omega_2\right)\Pi^{g_4 g_3 g''' g''}_{felh}(2\Omega_2,\omega-2\Omega_2) \; .$$

In contrast with Gorkovs equation, in energy repr. it remains an integral equation!

- By defining a particle-hole Kernel, the GBSE can be recast into a algebraic equations...

$$\Pi^{g_4 g_3 g_2 g_1}_{dcba}(\omega) = \Pi^{\mathrm{D}\, g_4 g_3 g_2 g_1}_{dcba}(\omega) + \Pi^{\mathrm{B}\, g_4 g_3 g_2 g_1}_{dcba}(\omega) + \sum_{\substack{g_5 g_6 \\ g_7 g_8}}\sum_{efgh}\Pi^{\mathrm{D}\, g_1 g_2 g_5 g_6}{}_{abfe}(\omega)K^{ph\, g_5 g_6 g_7 g_8}{}_{efgh}(\omega)\Pi^{g_7 g_8 g_3 g_4}_{ghcd}(\omega)$$

W. Czyz, *Acta. Phys. Pol.* ***20***, 737 (1961).

Caveat: there's no diagram-based approach to determine $K^{ph}_{efgh}(\omega)$! (except approx. such as RPA)

Perturbation Expansion

of the polarization propagator

- As an alternative to the solution of the GBSE, one considers the *perturbation expansion* of Gorkov's polarization propagator in terms of Ω_I, in the interaction picture

⇝ J. Schirmer, *Phys. Rev. A* **26**, 5, 2395-2416 (1982)

$$\Pi^{g_1 g_2 g_3 g_4}_{acdb}(t,t^+,t'^+,t') = -i\sum_{l=0}^{+\infty}\left(\frac{-i}{\hbar}\right)^l \frac{1}{l!}\int_{-\infty}^{+\infty} dt_1 \ldots \int_{-\infty}^{+\infty} dt_l \overbrace{\langle\Phi_0|T\Big\{\Omega_I(t_1)\ldots\Omega_I(t_l)A_{I\,a}^{g_1}(t)A_{I\,b}^{g_2}(t')A_{I\,d}^{\dagger\,g_4}(t'^+)A_{I\,c}^{\dagger\,g_3}(t^+)\Big\}|\Phi_0\rangle_{\text{conn}}}^{(P)}$$
$$+\; i\left[\sum_{m=0}\left(\frac{-i}{\hbar}\right)^m \frac{1}{m!}\int_{-\infty}^{+\infty} dt_1 \ldots \int_{-\infty}^{+\infty} dt_m \langle\Phi_0|T\Big\{\Omega_I(t_1)\ldots\Omega_I(t_m)A_{I\,a}^{g_1}(t)A_{I\,c}^{\dagger\,g_3}(t^+)\Big\}|\Phi_0\rangle_{\text{conn}}\right]$$
$$\times\left[\sum_{n=0}\left(\frac{-i}{\hbar}\right)^n \frac{1}{n!}\int_{-\infty}^{+\infty} dt_1 \ldots \int_{-\infty}^{+\infty} dt_n \underbrace{\langle\Phi_0|}\, T\Big\{\Omega_I(t_1)\ldots\Omega_I(t_n)A_{I\,b}^{g_2}(t')A_{I\,d}^{\dagger\,g_4}(t'^+)\Big\}|\Phi_0\rangle_{\text{conn}}\right]$$

where

unperturbed reference state

connected contributions only!

- Time ordered products are evaluated by means of the Wick theorem, converting them into fully-contracted normal-ordered products of second-quantization operators.

Caveat: the contractions between two creation and annihilation operators do not vanish!

Diagrammatics: see the term (P)

Contraction	$\underbrace{a^{\dagger}_{I\,a}(t)\, a^{\dagger}_{I\,b}(t')}$	$\underbrace{a_{I\,a}(t)\, a_{I\,b}(t')}$
$\exists!\, a \vee b \in$ *interaction vertex*	$G^{(0)\,21}_{ab}(t,t')$	$G^{(0)\,12}_{ab}(t,t')$
$a \wedge b \in$ *external legs*	$G^{(0)\,21}_{\bar{a}b}(t,t')$	$G^{(0)\,12}_{a\bar{b}}(t,t')$
$\bar{a} \wedge \bar{b} \in$ *external legs*	$G^{(0)\,21}_{a\bar{b}}(t,t')$	$G^{(0)\,12}_{\bar{a}b}(t,t')$

DIAGRAMMATIC EXPANSION

of the polarization propagator

- Alternative to the Wick theorem, the diagrams appearing at any order *n* in perturbation theory can be generated via *Feynman rules* for the polarization prop. in *time representation*:

I. diagrams have *n* interaction lines and *2n+2* propagation lines

II. discard disconnected diag. and disjoint linked diag. and direct type

III. label the vertices and the endpoints of the external legs with a single particle (s.p.) index and a time index

IV. write $\bar{V}_{abcd}$ for each two-b. vertex

V. write a factor $i^{2n+2} \cdot i(-i/\hbar)^n$

VI. write a factor 1/2 for each pair of prop. starting and ending at the same two-body vertex

VII. write a factor 1/2 for each anomalous prop. starting and ending at the same int. vertex.

VIII. in the Abrikosov-Hügenholtz notation, check the global sign

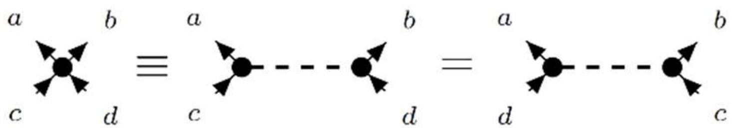
IX. interpret the equal time prop.

X. write a fact. $(-1)^{N_c+N_a}$ where:
N_c ⇝ number of closed loops
N_a ⇝ number of anomalous contractions.

XI. sum over free s.p. indices

XII. integrate over free time variables

- Two-body vertex:



$\bar{V}_{abcd} = \bar{V}_{badc}$ $\quad -\bar{V}_{abdc} = -\bar{V}_{bacd}$

Abrikosov – Hügenholtz notation

Extended or Bloch-Brandow notation

- Unperturbed one-body propagator:

$G^{(0)\,11}_{ab}(t,t') \equiv$

$G^{(0)\,12}_{ab}(t,t') \equiv$

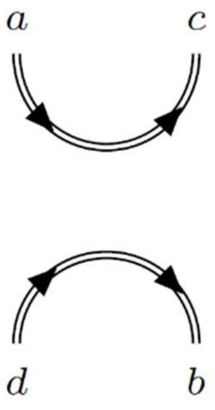
$G^{(0)\,21}_{ab}(t,t') \equiv$

$G^{(0)\,22}_{ab}(t,t') \equiv$

DIAGRAMMATIC EXPANSION

of the polarization propagator

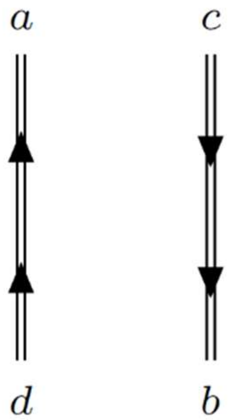
Converting each sequence of normal-ordered second quantization operators in (P) into diagrammatic form, at any order the graphs can be grouped into 5 categories:



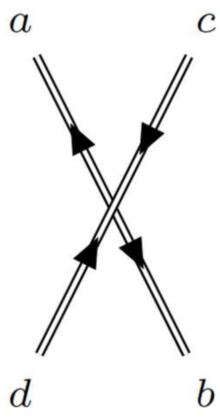
(i) $\notin \Pi^{1111}_{acdb}$

- *Disjoint linked diagrams of **exchange** type*

- *Disjoint linked diagrams of **direct** type*

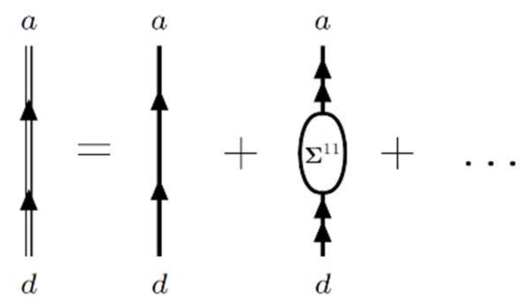


(ii)



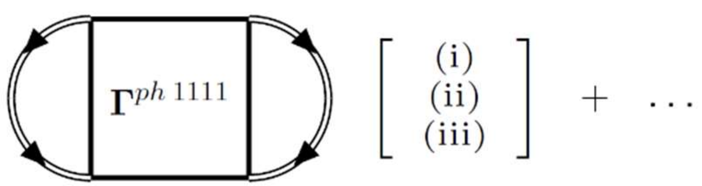
(iii) $\in \Pi^{1111}_{acdb}$ $\in \Pi^{1122}_{ac\bar{b}\bar{d}}$

- *Disjoint linked diagrams of **Bogoliubov** type*



G^{11}_{ad}

dressed one-body propagator

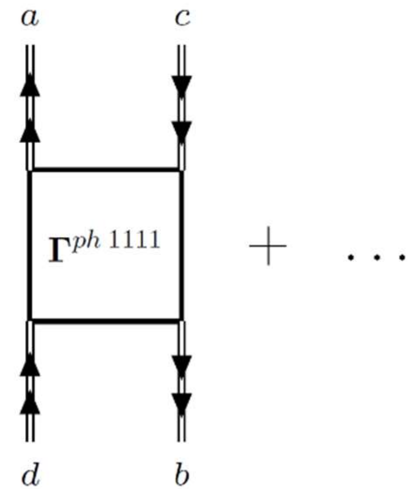


multiple disconnected parts

(iv) $\notin \Pi^{1111}_{acdb}$

- ***Disconnected** (=disjoint unlinked) diagrams*

- ***Conjoint** diagrams*



(v)

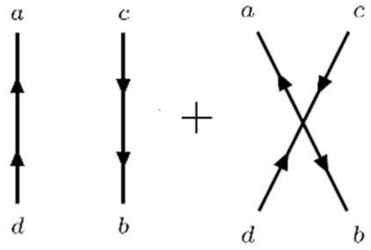
Leading and First Order Diagrams

of the polarization propagator

Example: perturbation expansion of $\Pi^{1111}_{acdb}(t,t')$

- *Leading order:*

$$-i\, G^{(0)\,11}_{ad}(t,t'^{+})\, G^{(0)\,11}_{cb}(t^{+},t') \longleftarrow$$

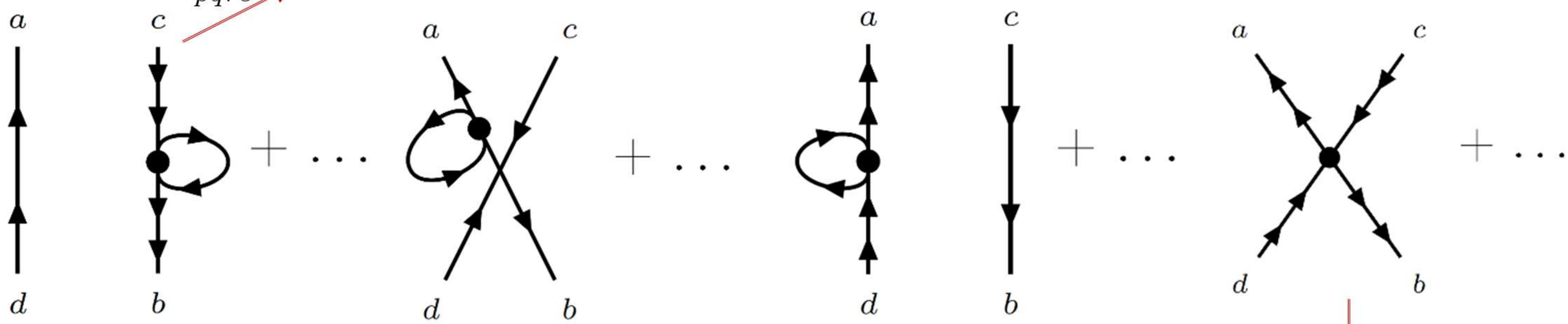


$$\longrightarrow i\, G^{(0)\,1\bar{1}}_{a\bar{b}}(t,t')\, G^{(0)\,\bar{1}1}_{\bar{d}c}(t'^{+},t^{+})$$

i.e. the LO disjoint exchange and Bogoliubov diagrams!

- *Subleading order:*

$$-\frac{1}{\hbar}\sum_{pqrs}\bar{V}_{pqrs}\, iG^{(0)\,11}_{ad}(t,t'^{+})\int_{-\infty}^{+\infty}\mathrm{d}t_1\, iG^{(0)\,11}_{rp}(t_1,t^{+})\, iG^{(0)\,11}_{bq}(t',t_1)\, iG^{(0)\,11}_{sc}(t_1,t^{+})$$



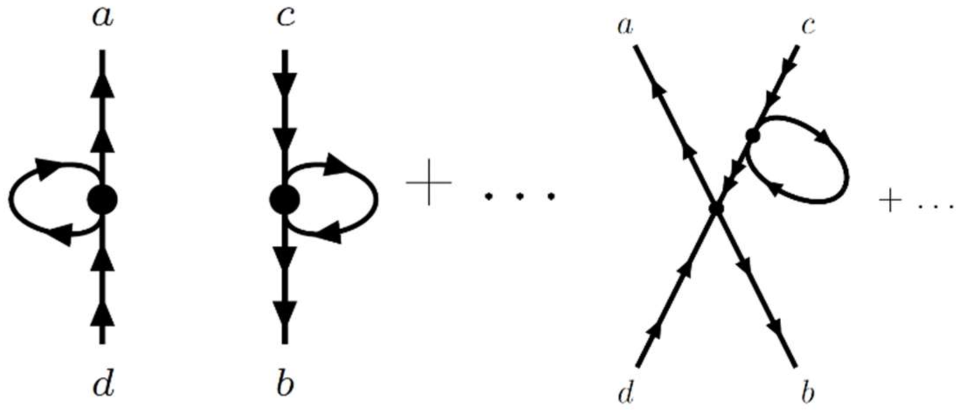
Ellipsis: Bogoliubov diagrams with a bubble on the $G^{(0)\,\bar{1}1}_{\bar{d}c}$ propagator plus graphs with at least a pair of anomalous propagators

$$-\frac{1}{\hbar}\frac{1}{2}\sum_{pqrs}\bar{V}_{pqrs}\int_{-\infty}^{+\infty}\mathrm{d}t_1\, iG^{(0)\,11}_{bp}(t',t_1)\, iG^{(0)\,11}_{aq}(t,t_1)\, iG^{(0)\,11}_{sc}(t_1,t^{+})\, iG^{(0)\,11}_{rd}(t_1,t'^{+})$$

Example (continued): perturbation expansion of $\Pi^{1111}_{acdb}(t,t')$

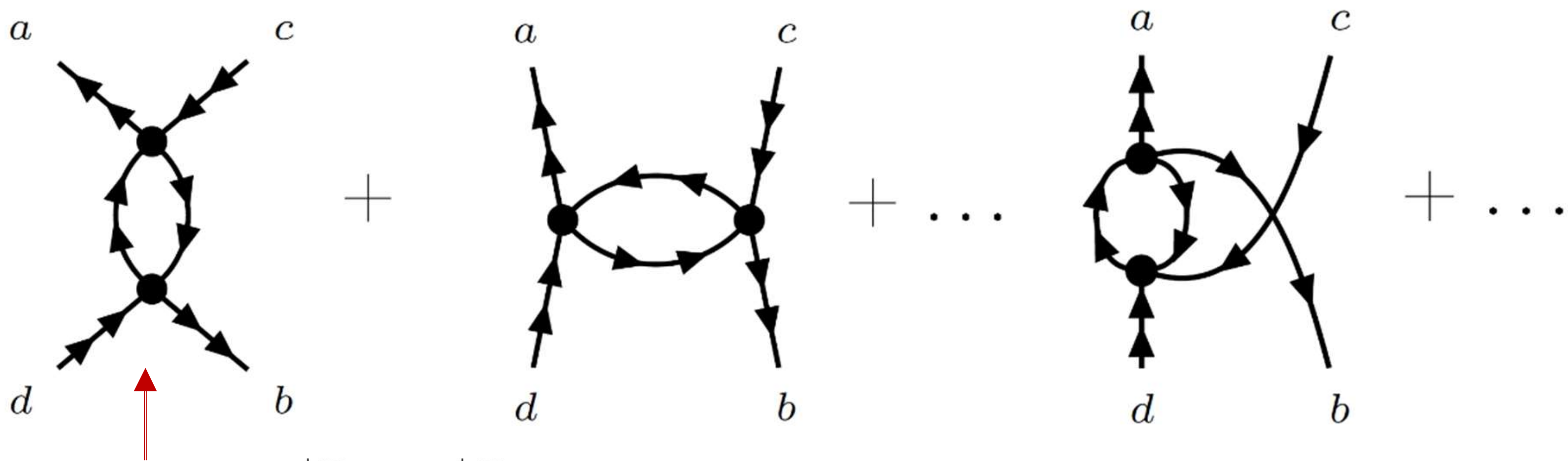
- *Next to next to leading order:*

Composite diagrams:



Ellipsis: Bogoliubov plus other composite diagrams and graphs with the same structure and (even) anomalous propagators

Skeleton diagrams:



Ellipsis: graphs with the same structure and (even) anomalous propagators

$$\frac{i}{\hbar^2}\sum_{\substack{pqrs\\tuvw}}\bar{V}_{pqrs}\bar{V}_{tuvw}\int_{-\infty}^{+\infty}\mathrm{d}t_1\int_{-\infty}^{+\infty}\mathrm{d}t_2\, iG^{(0)\,11}_{aq}(t,t_1)\,iG^{(0)\,11}_{sc}(t_1,t)\,iG^{(0)\,11}_{vp}(t_2,t_1)\,iG^{(0)\,11}_{rt}(t_1,t_2)\,iG^{(0)\,11}_{wd}(t_2,t')\,iG^{(0)\,11}_{bu}(t',t_2)$$

Algebraic Diagrammatic Construction

for the one-body propagator

It is an approximation scheme deveoped for the *polarization propagator* (J. Schirmer, *Phys. Rev. A* **26**, 5, 2395-2416 (1982)) and the *one-body propagator* (J. Schirmer, *Phys. Rev. A* **28**, 3, 1237-1259 (1983)) in SCGF theory. At present, only the extension to Gorkov's one-body propagators is operational.

Motivation: the ADC scheme permits to rewrite Gorkov's equations (in energy repr.) as an energy-independent eigenvalue problem, preserving the analytic structure of the self-energy.

⇝ V. Somà et al. *Phys. Rev. C 84, 064317 (2011)*

- Splitting of the *proper* self-energy into a static and a dynamic part:

$$\tilde{\mathbf{\Sigma}}_{ab}(\omega) = -\mathbf{U}_{ab} + \mathbf{\Sigma}^{(\mathrm{stat})}_{ab} + \mathbf{\Sigma}^{(\mathrm{dyn})}_{ab}$$

whose structure is

$$\mathbf{\Sigma}^{(\mathrm{dyn})}_{ab}(\omega) = \mathbf{\Sigma}^{(\mathrm{dyn})\,+}_{ab} + \mathbf{\Sigma}^{(\mathrm{dyn})\,-}_{ab} = \sum_k \left[\frac{{}^k\mathbf{M}_a\, {}^k\mathbf{M}^\dagger_b}{\omega - \Omega_k/\hbar + i\eta} + \frac{{}^k\mathbf{N}_a\, {}^k\mathbf{N}^\dagger_b}{\omega + \Omega_k/\hbar - i\eta} \right]$$

It is sufficient to consider only $\mathbf{\Sigma}^{(\mathrm{dyn})\,+}_{ab} \equiv \mathbf{M}_a(\mathbb{1}\omega - \mathbf{E})\mathbf{M}^\dagger_b$

- The ADC scheme postulates $\mathbf{\Sigma}^{(\mathrm{dyn})\,+}_{ab} \overset{\mathrm{ADC}}{=} \mathbf{C}_a(\omega\mathbb{1} - \mathbf{W} - \mathbf{P})^{-1}\mathbf{C}^\dagger_b$

where the matrices $\mathbf{C}_a$ and $\mathbf{P}$ in Nambu and k-space are expanded oder by order

$\mathbf{C}_a \equiv \mathbf{C}^{(1)}_a + \mathbf{C}^{(2)}_a + \dots \qquad \mathbf{P} \equiv \mathbf{P}^{(1)} + \mathbf{P}^{(2)} + \dots \qquad \mathbf{W} \Rightarrow$ Matrix of the unperturbed eigenvalues (Ω_U)

By exploiting the geometric series, the ADC ansatz can be rewritten as

$$\mathbf{\Sigma}^{(\mathrm{dyn})\,+}_{ab} \overset{\mathrm{ADC}}{=} \mathbf{C}_a(\omega\mathbb{1} - \mathbf{W})^{-1} \sum_{n=0}^{+\infty} \left\{ \mathbf{P}(\omega\mathbb{1} - \mathbf{W})^{-1} \right\}^n \mathbf{C}^\dagger_b$$

Matching procedure with the standard pert. expansion yields the expressions for $\mathbf{C}_a$, $\mathbf{P}$ and $\mathbf{W}$

$$\mathbf{\Sigma}^{(\mathrm{dyn})\,+}_{ab}(\omega) \equiv \mathbf{\Sigma}^{(\mathrm{dyn},1)\,+}_{ab} + \mathbf{\Sigma}^{(\mathrm{dyn},2)\,+}_{ab} + \dots$$

Algebraic Diagrammatic Construction

for the polarization propagator

- It has been applied directly to the *polarization propagator* (instead of $\Gamma^{ph}_{cdhl}(\frac{\omega-\Omega_1}{2},\omega,\omega-2\Omega_2)$).

Starting from the one-body transition operator

$$\mathcal{D} = \sum_{rs} D_{rs} a^\dagger_r a_s$$

for particle-number conserving operators, such as EM trans. oper. $D_{rs} \equiv D^{11}_{rs}$ or D^{22}_{rs}

Thanks to the complex-conj. property, one may consider only $\Pi^{+\,g_1g_3g_4g_2}_{acdb}(\omega)$

Defining the transition function as $$T(\omega) \equiv \sum_{abcd} D^*_{ac} \Pi^{+\,1111}_{acdb}(\omega) D_{db}$$

Lehmann's repr. permits to write $$T(\omega) \equiv \mathbf{T}^\dagger(\omega\mathbb{1} - \mathbf{\Delta})\mathbf{T}$$

where $\Delta_{jk} \equiv \langle\Psi_j|\Omega - \Omega_0|\Psi_k\rangle/\hbar \implies$ *secular matrix* and $T_k = \langle\Psi_k|\mathcal{D}|\Psi_0\rangle \implies$ *vector of transition ampl.*

- Construction of the ADC ansatz, similar to the one for $\mathbf{\Sigma}^{(\mathrm{dyn})\,+}_{ab}$

$$T(\omega) \equiv \mathbf{F}^\dagger(\omega\mathbb{1} - \mathbf{K} - \mathbf{C})\mathbf{F}$$

where $\mathbf{K} \Rightarrow$ *matrix of diff. betw. the eigenvalues associated with* Ω_U: $K_{ij,kl} = \delta_{ik}\delta_{jl}(\omega_i - \omega_j)/\hbar$

As for the self-energy, the matrices admit an order by order expansion

$$\mathbf{C} \equiv \mathbf{C}^{(1)} + \mathbf{C}^{(2)} + \dots \qquad \mathbf{F} \equiv \mathbf{F}^{(0)} + \mathbf{F}^{(1)} + \mathbf{F}^{(2)} + \dots$$

Again the geometric series gives...

$$T(\omega) \overset{\text{ADC}}{=} \mathbf{F}^\dagger(\omega\mathbb{1} - \mathbf{K})^{-1} \sum_{n=0}^{+\infty} \left\{\mathbf{C}(\omega\mathbb{1} - \mathbf{K})^{-1}\right\}^n \mathbf{F}$$

Matching procedure with the standard pert. expansion yields the expressions for $\mathbf{F}$, $\mathbf{C}$ and $\mathbf{K}$

$$T(\omega) \equiv T(\omega)^{(0)} + T(\omega)^{(1)} + T(\omega)^{(2)} + \dots$$

Goldstone Diagrams

for the polarization propagator

The ADC splits the problem of determing **T** into two tasks: the *construction* of the modified transition ampl. **F** and the *diagonalization* proc. for the modified. interaction matrix, **C** + **K**

- In the ADC formulation for the polariz. propagator, it is useful to disentangle the time integrations, by considering the *n+2!* possible orderings of the time vertices at order *n*

Time-ordered or *Goldstone* diagrams are obtained by multiplying each Feynman graph by

$$1 = \theta(t-t') + \theta(t'-t)$$

$$\begin{aligned} 1 &= \theta(t-t')\theta(t_1-t) + \theta(t-t')\theta(t'-t_1) + \theta(t-t_1)\theta(t_1-t') \\ &+ \theta(t'-t)\theta(t_1-t') + \theta(t'-t)\theta(t-t_1) + \theta(t'-t_1)\theta(t_1-t) \\ 1 &= \theta(t'-t_1)\theta(t-t')\theta(t_2-t) + \theta(t_2-t_1)\theta(t'-t_2)\theta(t-t') \\ &+ \theta(t'-t_1)\theta(t_2-t')\theta(t-t_2) + \theta(t_1-t_2)\theta(t'-t_1)\theta(t-t') \\ &+ \theta(t_1-t)\theta(t-t')\theta(t'-t_2) + \dots \end{aligned}$$

- In practice: each Feynman diagram in $\Pi^{+\,g_1g_3g_4g_1}_{acdb}(t,t')$ corresponds to:

1 Goldstone graph at leading order

3 Goldstone graphs first order

12 Goldstone graphs at second order

...

Diagrammatic rules for the Goldstone graphs of the SCGF polarization prop. in energy repr. exist...

⇝ J. Schirmer, *Phys. Rev. A* ***26***, 5, 2395-2416 (1982)

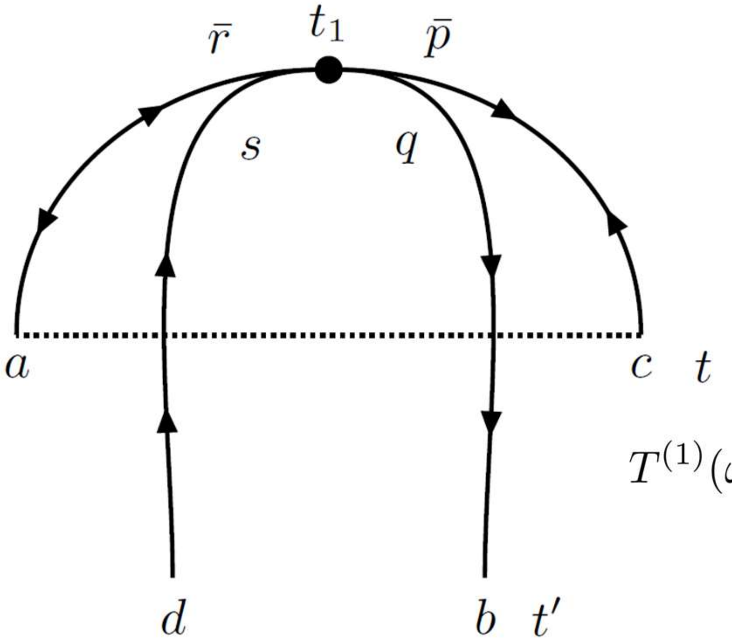
FIRST-ORDER GOLDSTONE DIAGRAMS

for the polarization propagator

- Example of a first-order diagram contributing to $\Pi^{+\,1111}_{acdb}(\omega)$ (conventionally $t > t'$):

in time representation:

$$\Pi^{+\,1111}_{acdb}(t,t') = \ldots + \frac{1}{\hbar}\sum_{pqrs}\bar{V}_{\bar{p}q\bar{r}s}\int_{-\infty}^{+\infty} \mathrm{d}t_1\, iG^{(0)\,21}_{pc}(t_1,t^+)iG^{11}_{(0)\,bq}(t',t_1) \times iG^{(0)\,11}_{sd}(t_1,t'^+)iG^{(0)\,12}_{ar}(t,t_1)\theta(t-t')\theta(t_1-t) + \ldots$$



- Performing the FT, this Goldstone graph translates into the following contribution to the first order transition function:

$$T^{(1)}(\omega) = \ldots + \sum_{abcd}\sum_{pqrs}\sum_{\substack{k_1\,k_2\\k_3\,k_4}} D^*_{ac}\bar{V}_{\bar{p}q\bar{r}s}\frac{{}^{k_1}\chi^{(0)\,2}_{p}\;{}^{k_1}\Upsilon^{(0)\,1}_{c}\;{}^{k_4}\chi^{(0)\,2}_{r}\;{}^{k_4}\Upsilon^{(0)\,1}_{a}}{\omega_{k_1,0}+\omega_{k_2,0}+\omega_{k_3,0}+\omega_{k_4,0}} \times \frac{{}^{k_2}\chi^{(0)\,1}_{a}\;{}^{k_2}\Upsilon^{(0)\,1}_{b}\;{}^{k_3}\chi^{(0)\,1}_{s}\;{}^{k_3}\Upsilon^{(0)\,1}_{d}}{\omega-\omega_{k_3,0}-\omega_{k_2,0}+i\eta}D_{db} + \ldots$$

Time ordering:

$$t_1 > t > t'$$

- Due to the SB in Ψ_0, the connection of the ‘energies’ in the denominators

$$\omega_{k_m0} \equiv \omega_{k_m} - \omega_0$$

with the single-particle excitation energies is *less transparent*:

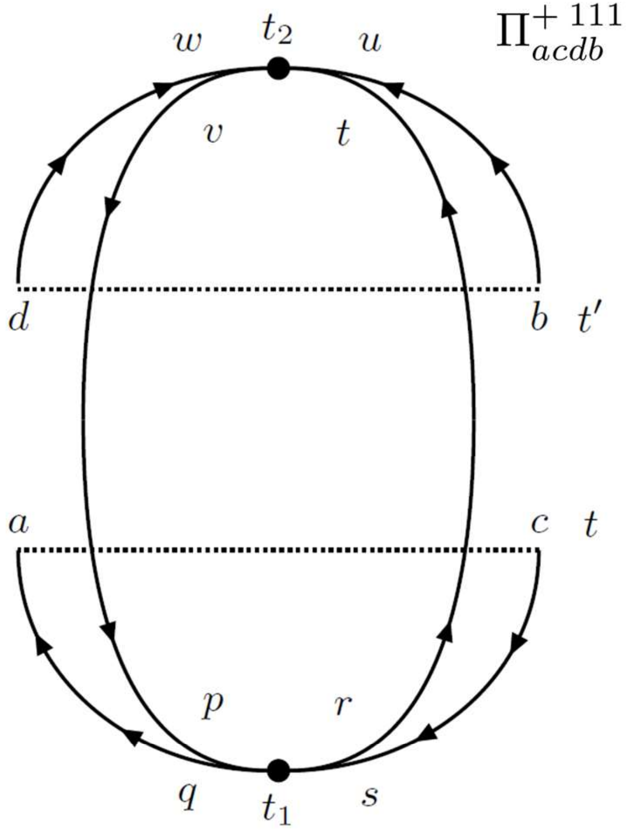
$\omega_{k_1}, \omega_{k_2}, \omega_{k_3}, \omega_{k_4} \Longrightarrow$ Eigenvalues of Ω for states with an odd number of nucleons on average

$\rightsquigarrow$ largest exp. contrib. $= A \pm 1$ states

SECOND-ORDER GOLDSTONE DIAGRAMS

for the polarization propagator

- Example of a second-order Goldstone graph contributing to $\Pi^{+\,1111}_{acdb}(\omega)$ $(t > t')$, corresponding to the time ordering $t_2 > t > t' > t_1$ In time representation, it gives:



$$\Pi^{+\,1111}_{acdb}(t,t') = \ldots + \frac{i}{\hbar^2}\sum_{pqrs}\sum_{tuwv}\bar{V}_{pqrs}\bar{V}_{tuvw} iG^{(0)\,11}_{aq}(t,t_1)$$
$$\times\ iG^{(0)\,11}_{sc}(t_1,t)\, iG^{(0)\,11}_{vp}(t_2,t_1)\, iG^{(0)\,11}_{rt}(t_1,t_2)\, iG^{(0)\,11}_{wd}(t_2,t')$$
$$\times\ iG^{(0)\,11}_{bu}(t',t_2)\theta(t'-t_1)\theta(t-t')\theta(t_2-t) + \ldots$$

The presence of the sole *normal* propagators guarantees that

$\omega_{k_2}, \omega_{k_4}, \omega_{k_6} \Longrightarrow$ states with odd number of nucleons (largest exp. contrib. $= A-1$ state)

$\omega_{k_1}, \omega_{k_3}, \omega_{k_5} \Longrightarrow$ states with odd number of nucleons (largest exp. contrib. $= A+1$ state)

- In energy repr. this Goldstone graph translates into the following contribution to the second order transition function:

$$T^{(2)}(\omega) = \ldots - i\sum_{abcd}\sum_{pqrs}\sum_{tuwv}\sum_{\substack{k_1\\k_3}}\sum_{\substack{k_2\ k_4\\k_6}}\sum_{k_5} D^{*}_{ac}\bar{V}_{pqrs}\bar{V}_{tuvw}\frac{{}^{k_1}\chi^{(0)\,1}_{a}\ {}^{k_1}\Upsilon^{(0)\,1}_{q}\ {}^{k_2}\chi^{(0)\,1}_{c}\ {}^{k_2}\Upsilon^{(0)\,1}_{s}}{\omega_{k_1,0}+\omega_{k_2,0}+\omega_{k_3,0}+\omega_{k_4,0}}$$
$$\times\ \frac{{}^{k_5}\chi^{(0)\,1}_{v}\ {}^{k_3}\Upsilon^{(0)\,1}_{p}\ {}^{k_4}\chi^{(0)\,1}_{t}\ {}^{k_4}\Upsilon^{(0)\,1}_{r}}{\omega-(\omega_{k_1,0}+\omega_{k_2,0}+\omega_{k_3,0}+\omega_{k_4,0}+\omega_{k_5,0}+\omega_{k_6,0})/\hbar}\frac{{}^{k_5}\chi^{(0)\,1}_{w}\ {}^{k_5}\Upsilon^{(0)\,1}_{d}\ {}^{k_6}\chi^{(0)\,1}_{u}\ {}^{k_6}\Upsilon^{(0)\,1}_{b}}{\omega_{k_3,0}+\omega_{k_4,0}+\omega_{k_5,0}+\omega_{k_6,0}}D_{db} + \ldots$$

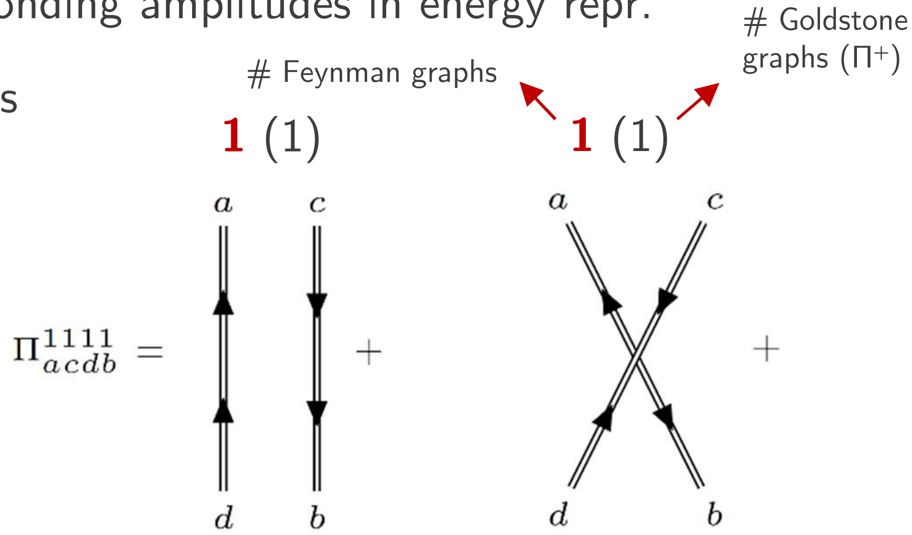
A code generating the diagrammatic contrib. for Gorkov's polarization propagator as Wick theorem contractions at first and second order in perturbation theory has been developed.

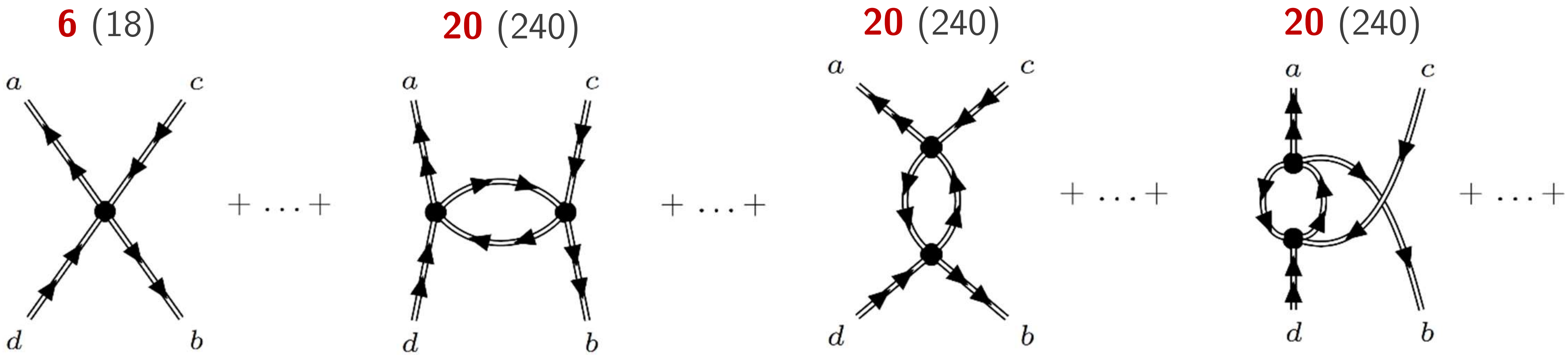
- **Tool**: for any time ordering, the *diagrammatic rules* for *Goldstone diagrams* in energy representation permit to bridge the sequences of contracted second-quantization op. in time repr. and the amplitudes and the corresponding amplitudes in energy repr.

Alternatively, the time integrals can be evaluated as in the *Automated Diagram Generation* code:

⇝ P. Arthuis et al. *Comp. Math. Comm.* **240**, 202-227 (2019)

- **Improvement**: self-consistent dressing of the one-body propagators in the *skeleton* graphs (up to 2^{nd} order), output of the existing *Boccadorata* codes





- For a general one-body operator that mediates the transition between two the A-body states

$$\langle \Psi_p | \mathcal{O} | \Psi_0 \rangle = \sum_{ab} (a|\mathcal{O}|b) \langle \Psi_p | a_b^\dagger a_a | \Psi_0 \rangle$$

  - **Example**: reduced *electric* ($R{=}E$) and *magnetic* ($R{=}M$) multipole transition probabilities between states with angular momentum J_0 and J_p

$$B(J_0 \to J_p, R\ell) \equiv \frac{1}{2J_0+1} \sum_{M_0} \sum_{M_p} \sum_{m} |\langle \Psi_p | \Omega_{\ell m}(R) | \Psi_0 \rangle|^2$$

where $\Omega_{\ell m}(R)$ are the transition operators with angular momentum ℓ and projection m

$$\langle \Psi_p | \Omega_{\ell m}(R) | \Psi_0 \rangle = \sum_{ab} (a|\Omega_{\ell m}(R)|b) \langle \Psi_p | [A_a^{1\,\dagger} \otimes A_b^1]^\ell_m | \Psi_0 \rangle$$

which are expressed in terms of the angular-momentum-coupled transition matrix elements

$$[A_a^{\dagger\,1} \otimes A_b^1]^\ell_m = [a_a^\dagger \otimes a_b]^\ell_m = \sum_{m_a m_b} (j_a j_b \ell | m_a - m_b m)(-1)^{-m_b} a_a^\dagger a_b$$

and the matrix elements between the s.p. states and the EM mult. transition oper. are given by

$$(a|\Omega_{\ell m}(E)|b) = \int \mathrm{d}^3 r \; (a| r^\ell Y_\ell^m(\theta,\phi) \rho(\mathbf{r}) |b)$$

$$(a|\Omega_{\ell m}(M)|b) = \int \mathrm{d}^3 r \; (a| \mathbf{j}(\mathbf{r}) \cdot \mathbf{L} r^\ell Y_\ell^m(\theta,\phi) |b)$$

where $\rho(\mathbf{r}) = e\delta(\mathbf{r}-\mathbf{r}')$ and $\mathbf{j}(\mathbf{r}) = \frac{\hbar}{2mi}[\delta(\mathbf{r}-\mathbf{r}')\overrightarrow{\nabla}' - \overleftarrow{\nabla}'\delta(\mathbf{r}-\mathbf{r}')]$ (pointlike charge distrib.)

CONCLUSION

- Motivated by the successes of SCGGF theory in the prediction of physical observables from the one-body propagator, we are extending the approach to quantities accessible from the polarization propagator, such as the excitation spectrum of even-even semi-magic nuclei and reduced EM multipole transition probabilities. In particular, we have
  - ✓ briefly recapitulated the progress brought by the introduction of the particle-number SB mechanism (binding energy, two-nucleon separation energy, charge radius, shell gaps, energy levels of odd nuclei ...) in SCGF theory;
  - ✓ defined the polarization propagator in Gorkov's formalism, in time and energy representation, together with its symmetry properties;
  - ✓ derived the self-consistent equation obeyed by Gorkov's polarization propagator, thus generalizing the Bethe-Salpeter equation;
  - ✓ outlined the diagrammatic contributions up to the second order in perturbation theory, exploiting the expansion formula for the polarization propagator;
  - ✓ shortly illustrated the ADC approach, its application to the irreducible self-energy and to the polariz. propagator, so far exploited in quantum chemistry;
  - ✓ examples of Goldstone diagrams up to second order, instrumental for the implementation of the ADC, have been shown in time representation.

Thank you for the attention!

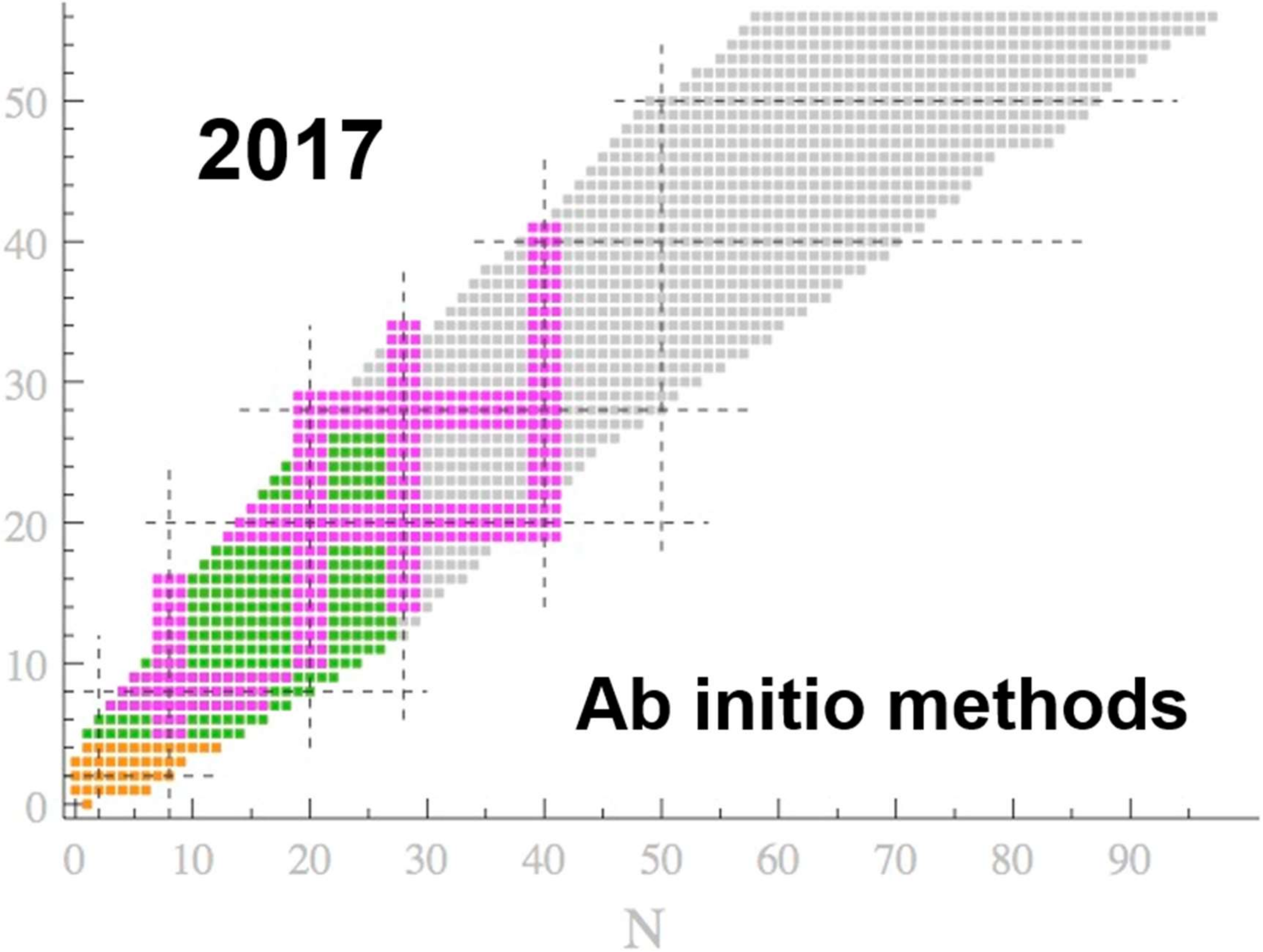
Ab initio models of Nuclear Structure

Exact solution of the Schr. equation: *exponential* or factorial scaling with the system size (A)
Approximate solution: polynomial scaling with A in the correlation expansion methods

Approximate solution for magic and semi-magic nuclei with A > 11.
Tools: MBPT/BMBPT, SCGF/SCGGF, IMSRG, CC/BCC ...

Approximate solution for open-shell nuclei with A > 11
Tools: BMBPT, CI, BCC, MR-IMSRG...

Exact solution for nuclei with A < 12
Tools: MBPT, NLEFT, NCSM, LQCD (A < 4)...



NAMBU COVARIANT PERTURBATION THEORY

We adopt the formalism of Nambu-covariant perturbation theory (NCPT) M. Drissi et al, arXiv:2107.09763

Purpose: extension of the SCGF approach to tackle the near-degeneracy of the ground states of singly open-shell nuclei with respect to creation/annihilation of pairs of nucleons with opposite j_z

Duplication of the Hilbert space associated to a single-nucleon $\mathscr{H}_1^e \equiv \mathscr{H}_1 \otimes \mathscr{H}_1^\dagger$
where $\mathcal{B} \subset \mathscr{H}_1$ is a basis and $\bar{\mathcal{B}} \subset \mathscr{H}_1^\dagger$ its dual and $|b\rangle,\ |\bar{b}\rangle \in \mathcal{B},\ \langle b|,\ \langle \bar{b}| \in \mathcal{B}^\dagger$

- Second quantization operators: $a_b,\ a_{\bar{b}}$ and $a_b^\dagger,\ a_{\bar{b}}^\dagger$

  where the *involution* (s.p. space) is defined: $a_{\bar{b}} = \eta_b a_{\tilde{b}} \quad a_{\bar{b}}^\dagger = \eta_b a_{\tilde{b}}^\dagger$ with $\tilde{b} \equiv (n, \ell, j, -m, q)$, $b \equiv (n, \ell, j, m, q)$ where $\eta_b = (-1)^{\ell - j - m}$, $\eta_b \eta_b^* = \eta_b^2 = 1$, $\eta_b \eta_{\tilde{b}} = -1$

  ...which are grouped into *Nambu* vectors:

$$\bar{B}_{(b,1)} \equiv a_b^\dagger \qquad \bar{B}_{(b,2)} \equiv \eta_b a_{\tilde{b}} = a_{\bar{b}}$$

$$B^{(b,1)} \equiv a_b \qquad B^{(b,2)} \equiv \eta_b a_{\tilde{b}}^\dagger = a_{\bar{b}}^\dagger$$

...and $l = 1, 2$ are Nambu indices.

- The canonical anticommutation rules

$$\left\{\bar{B}_\mu, \bar{B}_\nu\right\} = g_{\mu\nu} \qquad \left\{\bar{B}_\mu, B^\nu\right\} = g_\mu{}^\nu \qquad \left\{B^\mu, \bar{B}_\nu\right\} = g^\mu{}_\nu \qquad \left\{B^\mu, B^\nu\right\} = g^{\mu\nu}$$

define the elements of the *metric tensor*:

$$g^{\alpha\beta} \equiv \delta_{a\tilde{b}} \delta_{l_a \bar{l}_b} [\delta_{1 l_a} \eta_{\tilde{a}} + \delta_{2 l_a} \eta_a] \qquad g_{\alpha\beta} \equiv \delta_{a\tilde{b}} \delta_{l_a \bar{l}_b} [\delta_{1 l_a} \eta_{\tilde{a}} + \delta_{2 l_a} \eta_a] \qquad g^\alpha{}_\beta = g^{\alpha\gamma} g_{\gamma\beta} = \delta_{ab} \delta_{l_a l_b}$$

$g^{\alpha\beta} \wedge g_{\alpha\beta}$ are antidiagonal in both the Nambu and the s.p. space! $\quad g_\alpha{}^\beta = g_{\alpha\gamma} g^{\gamma\beta} = \delta_{ab} \delta_{l_a l_b}$

Time Evolution of Operators and States

- **Heisenberg's picture**: time evolution of Nambu second-quantization operators follows

$$\mathbf{A}_b(t) = \mathbf{A}_{\Omega\, b}(t) \equiv e^{i\Omega t/\hbar}\mathbf{A}_b e^{-i\Omega t/\hbar}$$
$$\mathbf{A}_b^\dagger(t) = [\mathbf{A}_{\Omega\, b}(t)]^\dagger \equiv e^{i\Omega t/\hbar}\mathbf{A}_b^\dagger e^{-i\Omega t/\hbar}$$

As in standard Heisenberg's picture, the states are time-independent:

$$|\Psi_0\rangle \equiv |\Psi_0(t)\rangle = |\Psi_0(t_0)\rangle \quad \forall\ t, t_0$$

- **Interaction picture**: time evolution of Nambu second-quantization operators follows

$$\mathbf{A}_{I\, b}(t) \equiv e^{i\Omega_U t/\hbar}\mathbf{A}_b e^{-i\Omega_U t/\hbar}$$
$$[\mathbf{A}_{I\, b}(t)]^\dagger \equiv e^{i\Omega_U t/\hbar}\mathbf{A}_b^\dagger e^{-i\Omega_U t/\hbar}$$

States evolve as in the standard interaction picture:

$$|\Psi_{I\,0}\rangle \equiv e^{i\Omega_U/\hbar}e^{-i\Omega/\hbar}|\Psi_0\rangle$$

- **Field picture**: time evolution of Nambu second-quantization operators follows

$$\mathbf{A}_{F\, b}(t) \equiv e^{i\Omega t/\hbar}\mathbf{A}_b e^{-i\Omega t/\hbar}$$
$$[\mathbf{A}_{F\, b}(t)]^\dagger \equiv e^{i\Omega t/\hbar}\mathbf{A}_b^\dagger e^{-i\Omega t/\hbar}$$

where $\Omega_I^\phi = \Omega_I + \phi$ contains the ext. field $\phi(t)$ and the states evolve as

$$|\Psi_{F\,0}\rangle \equiv e^{i\Omega/\hbar}U_S^\phi(t,0)|\Psi_0\rangle$$

and $U_S^\phi(t,0)$ is Schrödinger's time evolution operator wrt the grand canonical potential $\Omega_U + \Omega_I^\phi$

GORKOV'S EQUATIONS

- The one-body Gorkov-Green's functions obey the following generalization of Dyson's equation:

$$G^{\alpha}{}_{\beta}(\omega) = G^{(0)\alpha}{}_{\beta}(\omega) + \sum_{\gamma\delta} G^{(0)\alpha}{}_{\gamma}(\omega)\tilde{\Sigma}^{\gamma}{}_{\delta}(\omega)G^{\delta}{}_{\beta}(\omega)$$

where the self-energy can be subdivided into a proper part and a contribution from the aux. potential

$$\tilde{\Sigma}^{\alpha}{}_{\beta}(\omega) \equiv \Sigma^{\alpha}{}_{\beta}(\omega) - U^{\alpha}{}_{\beta} - \tilde{U}^{\alpha}{}_{\beta}$$

and $G^{(0)\alpha}{}_{\beta}(\omega)$ are the unperturbed propagators.

Since U acts as a mean field, the Hartree-Fock-Bogoliubov (HFB) one-body propagators, solution of the problem $\Omega_U = \Omega_{\text{HFB}}$ can be exploited for $G^{(0)\alpha}{}_{\beta}(\omega)$ as well as an input for $G^{\alpha}{}_{\beta}(\omega)$ at the r.h.s. of the self-consistent equation. The numerical $G^{\alpha}{}_{\beta}(\omega)$ are obtained though ***BcDor* codes**

- *in practice*: energy-independent self-consistent equations for $G^{\alpha}{}_{\beta}(\omega)$ are solved.

EXAMPLES (proper self-energy to first order):

$$\Sigma^{(a,1)}{}_{(b,1)}(\omega)\Big|_1 \equiv -i \sum_{c,l_c}\sum_{d,l_d}\int_{C\uparrow}\frac{d\omega'}{2\pi}\frac{1}{3!} \times V^{(a,1)(c,l_c)}{}_{(d,l_d)(b,1)}G^{(d,l_d)}{}_{(c,l_c)}(\omega)$$

$$\Sigma^{(a,2)}{}_{(b,2)}(\omega)\Big|_1 \equiv -i \sum_{c,l_c}\sum_{d,l_d}\int_{C\downarrow}\frac{d\omega'}{2\pi}\frac{1}{3!} \times V_{(b,2)(d,l_d)}{}^{(c,l_c)(a,2)}G^{(d,l_d)}{}_{(c,l_c)}(\omega)$$

$$\Sigma^{(a,1)}{}_{(b,2)}(\omega)\Big|_1 \equiv -i \sum_{c,l_c}\sum_{d,l_d}\int_{C\uparrow}\frac{d\omega'}{2\pi}\frac{1}{3!} \times V^{(a,1)}{}_{(b,2)}{}^{(d,l_d)}{}_{(c,l_c)}G^{(c,l_c)}{}_{(d,l_d)}(\omega)$$

$$\Sigma^{(a,2)}{}_{(b,1)}(\omega)\Big|_1 \equiv -i \sum_{c,l_c}\sum_{d,l_d}\int_{C\uparrow}\frac{d\omega'}{2\pi}\frac{1}{3!} \times V_{(c,l_c)}{}^{(d,l_d)}{}_{(b,1)}{}^{(a,2)}G^{(c,l_c)}{}_{(d,l_d)}(\omega)$$

Dyson's Polarization Propagator

- In SCGF theory, the *polarization propagator* is obtained from the two-body response function.

  Adopting the covention of J. Schirmer, *Phys. Rev. A* ***26***, 5, 2395-2416 (1982), the latter reads:

$$\mathcal{R}^{(A,A)}_{abcd}(t,t';t'',t''') \equiv \mathcal{G}^{(A,A)}_{abcd}(t,t',t'',t''') - \mathcal{G}^{(A,A)}_{ac}(t,t'')\mathcal{G}^{(A,A)}_{bd}(t',t''')$$

where $\mathcal{G}^{(A,A)}_{abcd}(t,t',t'',t''') \equiv (-i)^2\langle\Psi^A_0|T\Big\{a_a(t)a_b(t')a^\dagger_d(t''')a^\dagger_c(t'')\Big\}|\Psi^A_0\rangle$

... is the two-body Green's function.

and $\mathcal{G}^{(A,A)}_{ab}(t,t') \equiv (-i)\langle\Psi^A_0|T\Big\{a_a(t)a^\dagger_b(t')\Big\}|\Psi^A_0\rangle$

... is the one-body Green's function.

- Taking the two-time limit the *polarization propagator* is obtained:

$$\Pi_{acdb}(t,t') = \lim_{\substack{t''\to t^+\\ t'''\to t'^+}} i\mathcal{R}^{(A,A)}_{abcd}(t,t';t'',t''')$$

alternatively, the limits $t''\to t'^+ \ \wedge \ t'''\to t''^+$ can be considered. In the first case, one writes

$$\Pi_{acdb}(t,t') = -i\langle\Psi^A_0|T\Big\{a^\dagger_c(t)a_a(t)a^\dagger_d(t')a_b(t')\Big\}|\Psi^A_0\rangle$$
$$+i\langle\Psi^A_0|T\Big\{a^\dagger_c(t)a_a(t)\Big\}|\Psi^A_0\rangle\langle\Psi^A_0|T\Big\{a^\dagger_d(t')a_b(t')\Big\}|\Psi^A_0\rangle$$

Dyson's Polarization Propagator

If the Schrödinger problem is time-independent, the Fourier transform is function of one frequency

$$\Pi_{acdb}(\omega) = \int_{-\infty}^{+\infty} \mathrm{d}(t-t') e^{i\omega(t-t')} \Pi_{acdb}(t,t')$$

The ensuing Lehmann representation can be decomposed into two interrelated parts,

$$\Pi_{acdb}(\omega) = \Pi^{+}_{acdb}(\omega) + \Pi^{-}_{acdb}(\omega)$$

analytical in the upper part of the complex plane ...

... and in the lower one.

$$\Pi^{+}_{acdb}(\omega) \equiv \sum_{k\neq 0} \frac{\langle \Psi^A_0 | a^\dagger_c a_a | \Psi^A_k \rangle \langle \Psi^A_k | a^\dagger_d a_b | \Psi^A_0 \rangle}{\omega - (E^A_k - E^A_0) + i\eta}$$

$$\Pi^{-}_{acdb}(\omega) = -\sum_{k\neq 0} \frac{\langle \Psi^A_0 | a^\dagger_d a_b | \Psi^A_k \rangle \langle \Psi^A_k | a^\dagger_c a_a | \Psi^A_0 \rangle}{\omega + (E^A_k - E^A_0) - i\eta}$$

The relation between the two reads:

$$\Pi^{+\,*}_{cabd}(-\omega) = \Pi^{-}_{acdb}(\omega)$$

- Symmetry relations:

time reversal of H

$$\Pi_{acdb}(\omega) = \Pi_{bdca}(-\omega)$$

complex-conjugation

$$\Pi_{acdb}(\omega) = -\Pi^{*}_{dbac}(-\omega)$$

- The poles coincide with the energy of the *excited states* of the even-even system wrt the g.s.
- The residues of the poles are proportional to the *transition matrix elements*:

$$^{k}X_{db} \equiv \langle \Psi^A_0 | a^\dagger_d a_b | \Psi^A_k \rangle \qquad ^{k}Y_{ca} \equiv \langle \Psi^A_k | a^\dagger_c a_a | \Psi^A_0 \rangle$$

- Transition mediated by a one-body operator:

$$\langle \Psi^A_p | \mathcal{O} | \Psi^A_0 \rangle = \sum_{ab} (a|\mathcal{O}|b) \langle \Psi^A_p | a^\dagger_a a_b | \Psi^A_0 \rangle$$

DYSON'S POLARIZATION PROPAGATOR

Approximation methods

In SCGF theory, the determination of the polarization propagator in Lehmann representation may follow three different paths:

- the **direct** approach: the ADC scheme applied directly to the polarization propagator

J. Schirmer, *Phys. Rev. A* ***26***, 5, 2395-2416 (1982),

approx. scheme for the time-ordered diagrams contributing to the trans. function, linked to Π via a unitary transf.

...so far adopted in *molecular systems* (quantum chemistry): *Comput. Mol. Sci.* **5**, 82-95 (2015)

ADC(2)

Adv. Chem. Phys ***69***, *22*, 201-240 (1987)

J. of Chem. Phys **112**, *22*, 4173-4185 (2000)

ADC(3)

J. of Chem. Phys **111**, 9982-9999 (1999)

J. of Chem. Phys **117**, 6402-6409 (2002)

- the **self-consistent** (SC) approach: possible application of the ADC scheme on the interaction kernel K_{fegh}. In time repr. the SC equation for the *three-time* polarization prop. reads

$$\Pi_{acdb}(t,t',t'',t''^{+}) = \Pi^{(0)}_{acdb}(t,t',t'',t''^{+}) + \frac{i}{\hbar}\sum_{efgh}\int \mathrm{d}t_1 \int \mathrm{d}t_2 \int \mathrm{d}t_2 \int \mathrm{d}t_3 \Pi^{(0)}_{acef}(t,t',t_1,t_2)$$
$$\times K_{fegh}(t_2,t_1,t_3,t_4)\Pi_{ghdb}(t_3,t_4,t'',t''^{+})$$

Tool: the SC equation for the *two-time* polarization propagator in energy representation

W. Czyz, *Acta. Phys. Polonica* ***20***, 737 (1961).

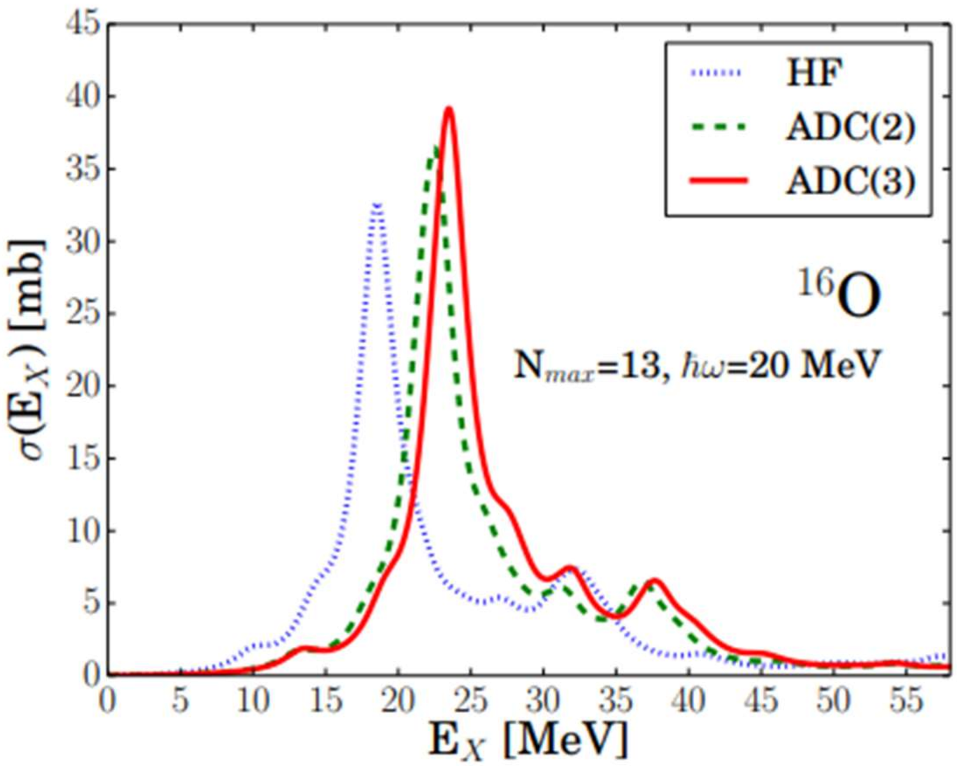
- the **random phase approximation**: although self-consistent, it neglects interactions betw.

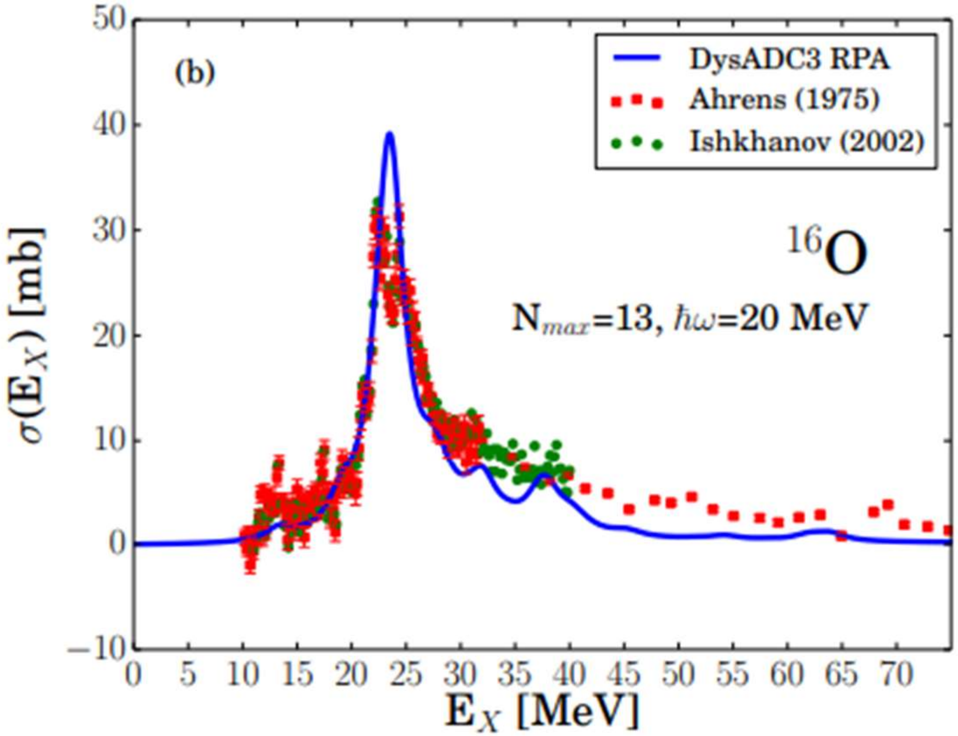
$$\Pi_{acdb}(\omega) = \Pi^{(0)}_{acdb}(\omega) + \Pi^{(0)}_{acef}(\omega)\bar{V}_{ehfg}\Pi_{ghdb}(\omega)$$

particles/holes propagating in different 'bubbles'. It is widely applied also in *nuclear systems*.

In SCGF theory, dressed RPA including some 2p-2h excitations is adopted for EM properties of semimagic nuclei with Z = 8, 20, 28 in Dyson GF theory.

Giant dipole resonances are studied, with different parameters of the HO s.p. basis and different implementations of the ADC scheme





[*Phys. Rev. C* ***99***, 054327 (2019)]

THE POLARIZATION PROPAGATOR IN THE SC APPROACH

- Derivation of a *self-consistent equation* for the Gorkov polarization propagator in momentum space.

W. Czyz, *Acta. Phys. Pol.* **20**, 737 (1961).

- Application of the *algebraic diagrammatic construction* scheme to the interaction Kernel

- Possible *approximation* of the SC equation.

F. Raimondi et al., *Phys. Rev. C* **99**, 054327 (2019).

- Possible *automatisation* of the construction of the necessary Feynman/Goldstone diagrams (ADG).

- Implementation of the *angular momentum coupling* (AMC) scheme

A. Tichai et al., *Eur. Phys. J. A* **56**, 272 (2020).

- Redrafting of the *BcDor codes* to include Π

t

- Application to **semi-magic nuclei**

Publication of exp. results concerning nuclear spectroscopy campaigns in the period 2014-2017:

Around Z = 20

- ^{47}Cl and ^{49}Cl: *Phys. Rev. C* ***104***, *044331* (2021).
- ^{50}Ar *Phys. Rev. C* ***102***, 064320 (2020), ^{51}Ar *Phys. Lett. B* ***814***, *136108* (2021) and ^{52}Ar *Phys. Rev. Lett.* ***122***, 074502 (2019).
- ^{51}K, ^{53}K *Phys. Lett. B* ***802***, 135215 (2020) and ^{55}K *Phys. Lett. B* ***827,*** 136953 (2022).
- ^{54}Ca *Phys. Rev. Lett.* ***126***, 252501 (2019), ^{55}Ca and ^{57}Ca *Phys. Lett. B* ***827,*** 136953 (2022).
- ^{62}Ti *Phys. Lett. B* ***800,*** 135071 (2020).
- ^{63}V *Phys. Rev. C* ***827,*** 064308 (2021).

Around Z = 28

- ^{72}Fe *Phys. Rev. Lett.* ***115,*** 192501 (2015).
- ^{66}Cr *Phys. Rev. Lett.* ***115,*** 192501 (2015).
- ^{76}Ni *Phys. Rev. C* ***99,*** 014312 (2019) and ^{78}Ni *Nature (London)* ***569,*** 53 (2019).
- ^{79}Cu *Phys. Rev. Lett.* ***119,*** 192501 (2017).
- ^{67}Mn *Phys. Lett. B* ***784,*** 392 (2018).
- ^{84}Zn *Phys. Lett. B* ***773,*** 492 (2017).
- ^{69}Co, ^{71}Co and ^{73}Co *Phys. Rev. C* ***101,*** 034314 (2020).

LEGEND: one-body propagator; one-body+polarization propagator; not yet investigated;