LXXIX ESNT WORKSHOP «NUCLEAR AB INITIO SPECTROSCOPY»

Spectroscopy of even-even singly open-shell nuclei

via self-consistent Gorkov-Green's function calculations:

the polarization propagator in perturbation theory and beyond

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Très Grand Centre de calcul du CEA

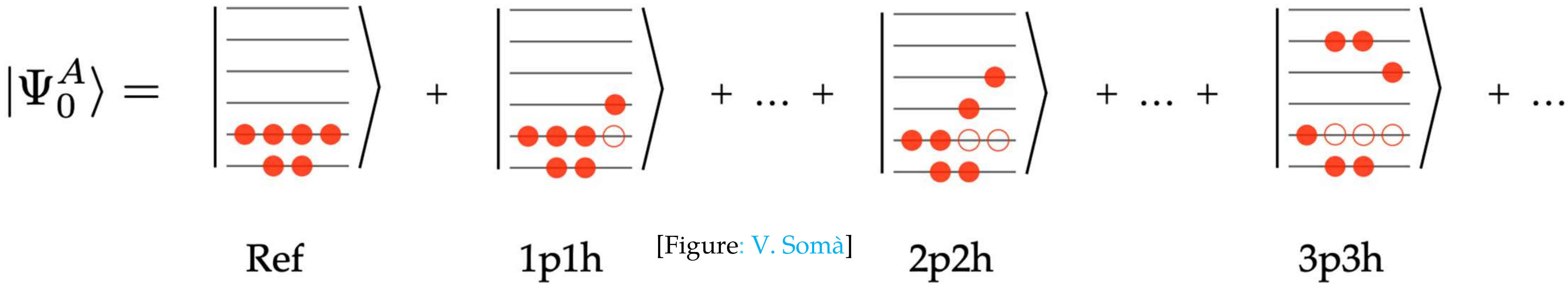
Self-consistent Gorkov-Green's function theory

- Ab-initio approach, extending the Self-consistent Green's function theory to semimagic nuclei. The Z *protons* and N *neutrons* interact through *Chiral Effective Field Theory* (χEFT) potentials

Practically, χEFT forces are preprocessed via the similarity renormalization group, in order to quench the coupling between low and high momenta in the Hamiltonian

SCGGF avails of an efficient approximation scheme for the nuclear wavefunction, entailing a *polynomial scaling* in the size M of the space of single-particle excitations M^{α} with $\alpha \geq 4$

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



[Figure: V. Somà]

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

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

Remark: *In open-shell nuclei, the ground state is almost degenerate with respect to the excitation of pairs of nucleons in the lowest-lying single-particle energy levels*

State of the art

- The salient feature of the self-consistent Gorkov-Green's function approach consists in the Breaking of the symmetry associated with *particle-number:* $U_Z(1) \times U_N(1)$

$\rightsquigarrow$ V. Somà et al. *Phys. Rev. C* **84**, 064317 (2011)

Applications:

^{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
^{15}C ^{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)
Phys. Rev. C **105**, 044330 (2022)

- ADC(2) with 2N+3N forces

Phys. Rev. C **89**, 061301 (2014)
Phys. Rev. C **100**, 062501 (2019)
Phys. Rev. Lett. **128**, 022502 (2022)
Eur. Phys. J A **57**, 135 (2021)
ArXiv:2302.08382
ArXiv:2310.19547

Excited-state energies, reduced EM multipole transition probabilities, γ-emission/absorption cross-sections… of even-even open-shell nuclei: $\rightsquigarrow$ *Gorkov's polarization propagator*

- Breaking of angular momentum symmetry: $SU(2)$ $\rightsquigarrow$ Scalesi's talk on Wednesday

Nambu formalism

Operators are conveniently expressed in terms of second-quantization operators, carrying

- a single-particle index $\rightsquigarrow$ $b \equiv (n, \ell, j, m, q)$

principal quantum number; total angular momentum; total angular momentum z-projection; isospin z-projection

- a Nambu index $\rightsquigarrow$ $g = 1, 2$

The single-particle space $\mathscr{H}_1$ is *split* into two blocks, characterized by the sign of the total angular momentum projection along the z axis, j_z. The partitions are mapped one another by means of *time-reversal*, corresponding to the *involution* in s.p. space: $b \mapsto \bar{b}$

- Hence, involuted creation $a^\dagger_{\bar{b}} = \eta_b a^\dagger_{\tilde{b}}$ and $a_{\bar{b}} = \eta_b a_{\tilde{b}}$ annihilation operators are introduced,

where $\tilde{b} \equiv (n, \ell, j, -m, q)$ and $\eta_b = (-1)^{\ell - j - m}$ such that $\eta_b \eta_{\tilde{b}} = -1$ and $\eta_b \eta^*_b = \eta^2_b = 1$

The two partitions of the s.p. space constitute the Nambu space (2-dimens.)

- The second-quantization operators are rearranged into two rank-one tensors,

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

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

$$\left\{ A^g_a, A^{g'}_b \right\} = \delta_{a\bar{b}} \delta_{g\bar{g}'} \qquad \left\{ A^g_a, A^{\dagger\, g'}_b \right\} = \delta_{ab} \delta_{gg'} \qquad \left\{ A^{\dagger\, g}_a, A^{\dagger\, g'}_b \right\} = \delta_{g\bar{g}'} \delta_{a\bar{b}}$$

involution in Nambu space:

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

Grand-canonical potential

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

$$H = T + V^{2N} \quad \rightsquigarrow \quad \Omega = \underbrace{T + U - \mu_p Z - \mu_n N}_{\equiv \Omega_U} + \underbrace{V^{2N} - U}_{\equiv \Omega_I}$$

where $T = \sum_{ab} t_{ab}\, a_a^\dagger a_b$ with $t_{ab} \equiv (a|T|b)$ is the *kinetic energy* operator

$$V^{2N} = \sum_{\substack{ab\\cd}} \frac{1}{(2!)^2} \bar{v}_{abcd}\, a_a^\dagger a_b^\dagger a_d a_c \quad \text{with} \quad \bar{v}_{abcd} \equiv \left[(ab|V^{2N}|cd) - (ab|V^{2N}|dc)\right]$$

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

and $$U = \frac{1}{2}\sum_{ab}\left[u^{11}_{ab}\, a_a^\dagger a_b + u^{22}_{ab}\, a_{\bar{a}} a_{\bar{b}}^\dagger + u^{12}_{ab}\, a_a^\dagger a_{\bar{b}}^\dagger + u^{21}_{ab}\, a_{\bar{a}} a_b\right]$$

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 3D space	$SU(2)$	*Quadrupole deformation*

One-body propagator

- The Gorkov-Green's function in Nambu space and time representation 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 grand-canonical pot. is time-independent, the FT of the one-body prop. 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

$$G^{gg'}_{ab}(\omega) = \sum_k \frac{{}^k\chi^g_a \; {}^k\chi^{g'*}_b}{\omega - (\Omega_k - \Omega_0)/\hbar + i\eta} + \sum_k \frac{{}^k\Upsilon^g_a \; {}^k\Upsilon^{g'*}_b}{\omega + (\Omega_k - \Omega_0)/\hbar - i\eta}$$

where $E^{(u)\pm}_k \equiv \mu_u \pm (\Omega_k - \Omega_0)$ 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.

$$E^{(p)\pm}_k \approx \pm(\langle \Psi^{\mathrm{SB}}_k | H | \Psi^{\mathrm{SB}}_k \rangle - \langle \Psi^{\mathrm{SB}}_0 | H | \Psi^{\mathrm{SB}}_0 \rangle) \mp \mu_p [\langle \Psi^{\mathrm{SB}}_k | Z | \Psi^{\mathrm{SB}}_k \rangle - (Z \pm 1)]$$

$$E^{(n)\pm}_k \approx \pm(\langle \Psi^{\mathrm{SB}}_k | H | \Psi^{\mathrm{SB}}_k \rangle - \langle \Psi^{\mathrm{SB}}_0 | H | \Psi^{\mathrm{SB}}_0 \rangle) \mp \mu_n [\langle \Psi^{\mathrm{SB}}_k | N | \Psi^{\mathrm{SB}}_k \rangle - (N \pm 1)]$$

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

$${}^k\Upsilon^1_b \equiv \langle \Psi_k | A^1_b | \Psi_0 \rangle = \langle \Psi_k | a_b | \Psi_0 \rangle \qquad {}^k\chi^1_b \equiv \langle \Psi_0 | A^1_b | \Psi_k \rangle = \langle \Psi_0 | a_b | \Psi_k \rangle$$

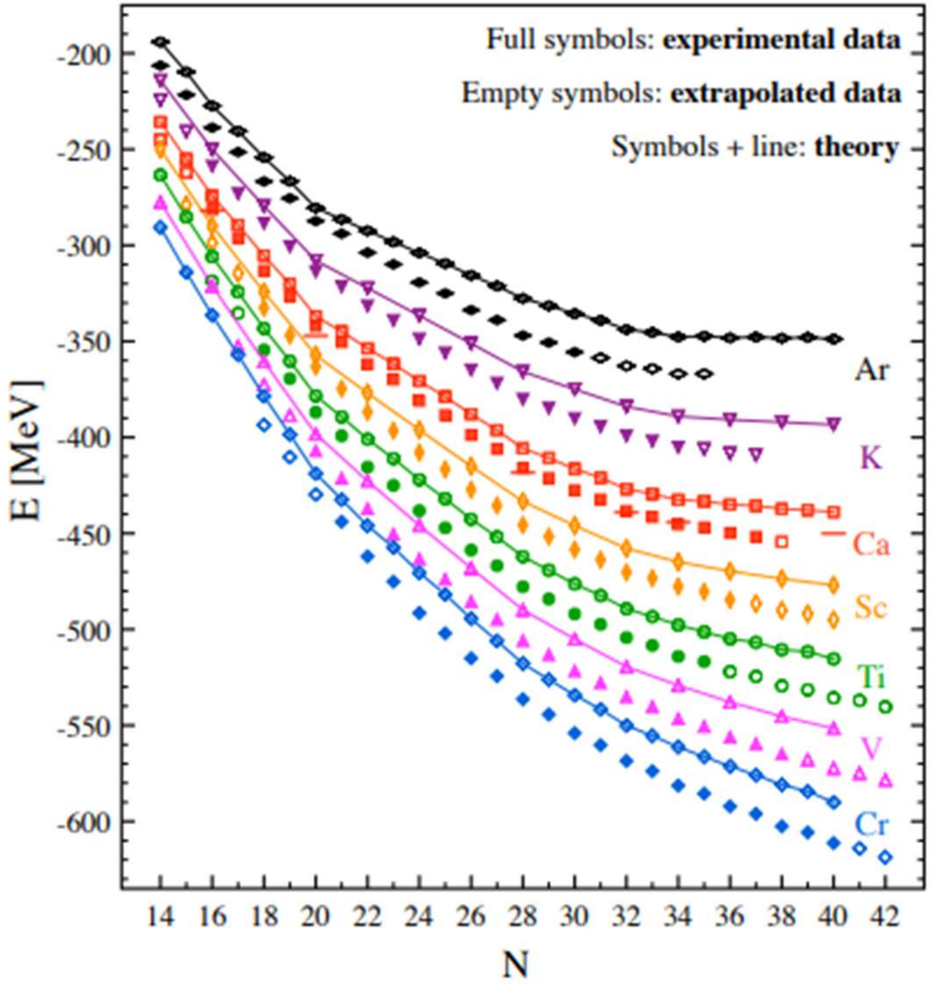
$${}^k\Upsilon^2_b \equiv \langle \Psi_k | A^2_b | \Psi_0 \rangle = \langle \Psi_k | a^\dagger_{\bar{b}} | \Psi_0 \rangle \qquad {}^k\chi^2_b \equiv \langle \Psi_0 | A^2_b | \Psi_k \rangle = \langle \Psi_0 | a^\dagger_{\bar{b}} | \Psi_k \rangle$$

The spectroscopic amplitudes are not *independent*: $(-1)^g \; [{}^k\chi^g_a]^* = {}^k\,\Upsilon^{\bar{g}}_{\bar{a}}$

Physical observables that can be evaluated from $i\mathbf{G}_{ab}(t,t')$ see the Appendix !

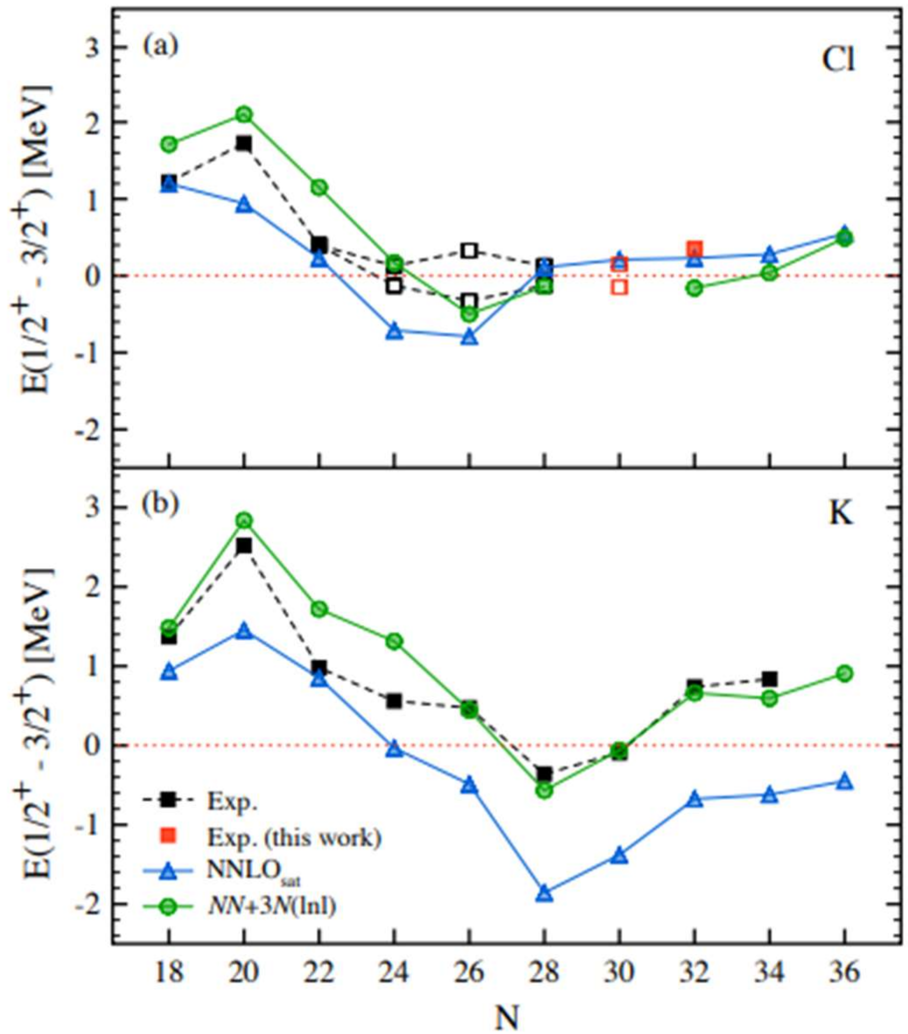
Physical observables

- 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



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

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

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

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

It has 10 anomalous and 6 normal components: '1111', '1212', '2121', '1221', '2112' and '2222'.

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 following symmetry property under complex conjugation:

$$\Pi^{gg''g'''g'}_{acdb}(\omega) = (-1)^{\bar g+\bar g'+\bar g''+\bar g'''}\ [\Pi^{\bar g\bar g''\bar g'''\bar g'}_{\bar a\bar c\bar d\bar b}(-\omega)]^*$$

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 related by complex conjugation

$$\Pi^{+\,gg''g'''g'}_{acdb}(\omega) = (-1)^{\bar{g}+\bar{g}'+\bar{g}''+\bar{g}'''}[\Pi^{+\,\bar{g}\bar{g}''\bar{g}'''\bar{g}'}_{\bar{a}\bar{c}\bar{d}\bar{b}}(-\omega)]^*$$

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

$$-(-1)^{g+g'}\;{}^k\Upsilon^{gg'}_{ab} = [{}^k\chi^{\bar{g}\bar{g}'}_{\bar{a}\bar{b}}]^*$$

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

$$
\begin{aligned}
{}^k\chi^{22}_{bc} &\equiv \langle\Psi_0|A^2_b A^{\dagger\,2}_c|\Psi_k\rangle = \langle\Psi_0|a^\dagger_{\bar{b}} a_{\bar{c}}|\Psi_k\rangle &\qquad {}^k\Upsilon^{22}_{bc} &\equiv \langle\Psi_k|A^2_b A^{\dagger\,2}_c|\Psi_0\rangle = \langle\Psi_k|a^\dagger_{\bar{b}} a_{\bar{c}}|\Psi_0\rangle \\
{}^k\chi^{12}_{bc} &\equiv \langle\Psi_0|A^1_b A^{\dagger\,2}_c|\Psi_k\rangle = \langle\Psi_0|a_b a_{\bar{c}}|\Psi_k\rangle &\qquad {}^k\Upsilon^{12}_{bc} &\equiv \langle\Psi_k|A^1_b A^{\dagger\,2}_c|\Psi_0\rangle = \langle\Psi_k|a_b a_{\bar{c}}|\Psi_0\rangle \\
{}^k\chi^{11}_{bc} &\equiv \langle\Psi_0|A^1_b A^{\dagger\,1}_c|\Psi_k\rangle = \langle\Psi_0|a_b a^\dagger_c|\Psi_k\rangle &\qquad {}^k\Upsilon^{21}_{bc} &\equiv \langle\Psi_k|A^2_b A^{\dagger\,1}_c|\Psi_0\rangle = \langle\Psi_k|a^\dagger_{\bar{b}} a^\dagger_c|\Psi_0\rangle \\
{}^k\chi^{21}_{bc} &\equiv \langle\Psi_0|A^2_b A^{\dagger\,1}_c|\Psi_k\rangle = \langle\Psi_0|a^\dagger_{\bar{b}} a^\dagger_c|\Psi_k\rangle &\qquad {}^k\Upsilon^{11}_{bc} &\equiv \langle\Psi_k|A^1_b A^{\dagger\,1}_c|\Psi_0\rangle = \langle\Psi_k|a_b a^\dagger_c|\Psi_0\rangle
\end{aligned}
$$

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

Phisical observables

- 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

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

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

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

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

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

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

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.)

Perturbative expansion

- Let us consider the *perturbative expansion* of Gorkov's polarization propagator in terms of $\Omega_I = V^{2\mathrm{N}} - U$, with the implied second-quantization operators the interaction picture:

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

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

where

unperturbed reference state

connected contributions only!

- Time ordered products in (P) are evaluated by means of Wick's theorem, converting them into fully-contracted normal-ordered products of second-quantization operators.

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

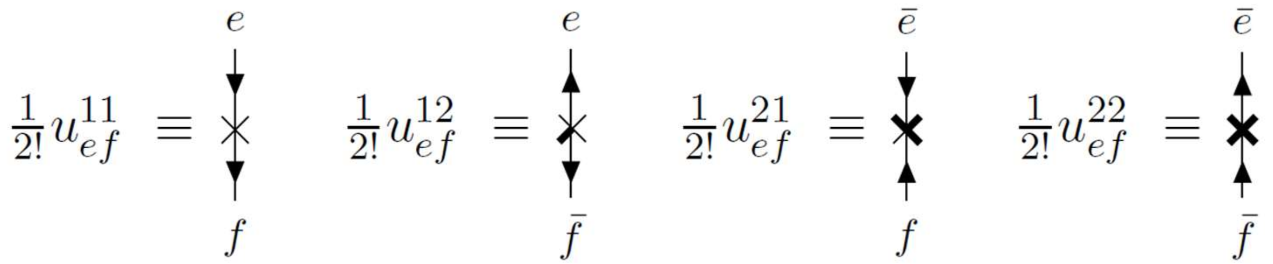
- ***Example***: conventions for non-canonical contractions, valid for all but *Bogoliubov* contributions

Contr. / Indic.	$\underbrace{a_e a_f}$	$\underbrace{a_{\bar e} a_{\bar f}}$	$\underbrace{a_e^\dagger a_f^\dagger}$	$\underbrace{a_{\bar e}^\dagger a_{\bar f}^\dagger}$	$\underbrace{a_e a_{\bar f}^\dagger}$	$\underbrace{a_e^\dagger a_{\bar f}}$
e, f internal	$iG^{(0)\ 12}_{ef}$ $f \mapsto \bar f$	$iG^{(0)\ 12}_{ef}$ $\bar e \mapsto e$	$iG^{(0)\ 21}_{ef}$ $e \mapsto \bar e$	$iG^{(0)\ 21}_{ef}$ $\bar f \mapsto f$	$-iG^{(0)\ 22}_{fe}$ $e \mapsto \bar e$	$iG^{(0)\ 22}_{ef}$ $e \mapsto \bar e$
e external f internal	$iG^{(0)\ 12}_{ef}$ $f \mapsto \bar f$	$-iG^{(0)\ 12}_{fe}$ $\bar f \mapsto f$	$-iG^{(0)\ 21}_{fe}$ $f \mapsto \bar f$	$iG^{(0)\ 21}_{ef}$ $\bar f \mapsto f$	$iG^{(0)\ 11}_{ef}$ $\bar f \mapsto f$	$-iG^{(0)\ 11}_{fe}$ $\bar f \mapsto f$
e internal f external	$-iG^{(0)\ 12}_{fe}$ $e \mapsto \bar e$	$iG^{(0)\ 12}_{ef}$ $\bar e \mapsto e$	$iG^{(0)\ 21}_{ef}$ $e \mapsto \bar e$	$-iG^{(0)\ 21}_{fe}$ $\bar e \mapsto e$	$-iG^{(0)\ 22}_{fe}$ $e \mapsto \bar e$	$iG^{(0)\ 22}_{ef}$ $e \mapsto \bar e$
e, f external	–	–	–	–	–	–

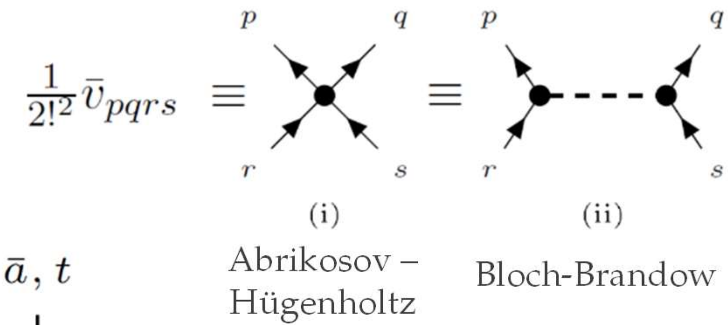
Diagrammatic representation

- Graphical interpretation of fully-contracted Wick's-theorem contributions in terms of Feynman diagrams for the polarization propagator in time representation. The conventions below hold:

One-body vertices: four inequivalent types

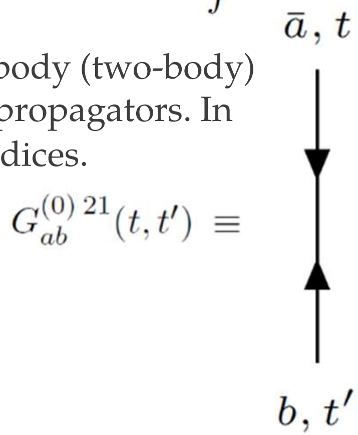


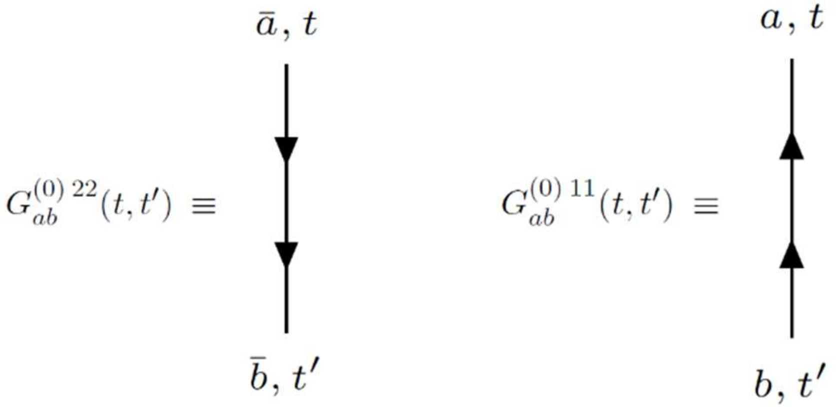
Two-body vertex: two notations

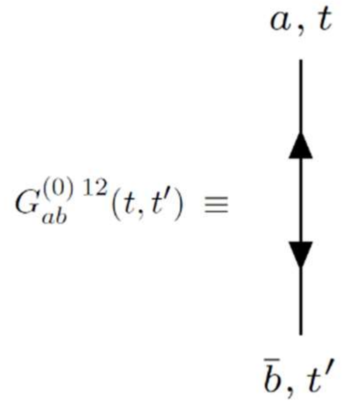


Feynman diagrams of order $l=n+m$ are graphs with m (n) one-body (two-body) vertices linked one another by $2n+m+2$ unperturbed one-body propagators. In the latter, the orientation of the arrows depend on the Nambu indices.

Unperturbed one-body propagators:
2 anomalous: '21' & '12'
and *2* normal: '11' & '22'





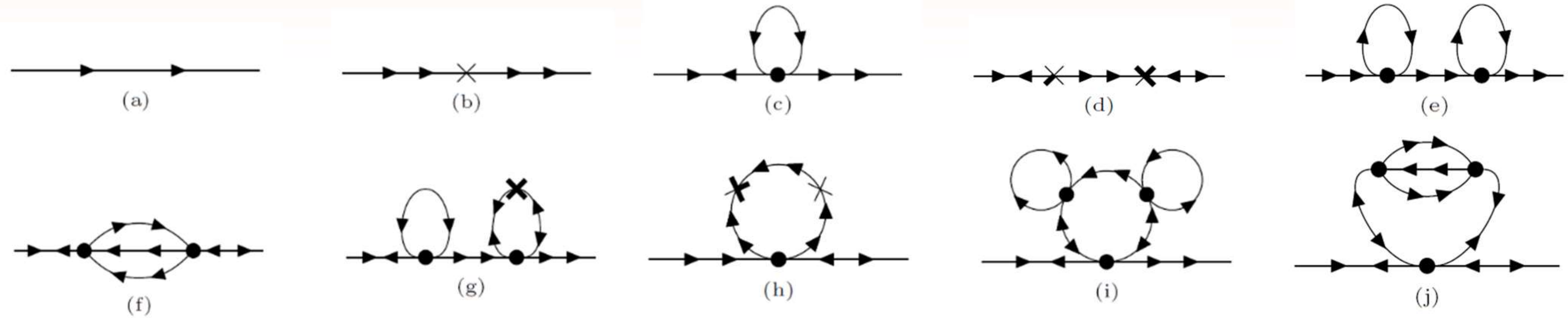


External single-particle indices

$g_1 \downarrow$	$g_2 \downarrow$ \ $g_3 \rightarrow$ / $g_4 \rightarrow$	1 / 1	1 / 2	2 / 1	2 / 2
1	1	$a\ c$ $d\ b$	$a\ c$ $\bar{d}\ b$	$a\ \bar{c}$ $d\ b$	$a\ \bar{c}$ $\bar{d}\ b$
1	2	$a\ c$ $d\ \bar{b}$	$a\ c$ $\bar{d}\ \bar{b}$	$a\ \bar{c}$ $d\ \bar{b}$	$a\ \bar{c}$ $\bar{d}\ \bar{b}$
2	1	$\bar{a}\ c$ $d\ b$	$\bar{a}\ c$ $\bar{d}\ b$	$\bar{a}\ \bar{c}$ $d\ b$	$\bar{a}\ \bar{c}$ $\bar{d}\ b$
2	2	$\bar{a}\ c$ $d\ \bar{b}$	$\bar{a}\ c$ $\bar{d}\ \bar{b}$	$\bar{a}\ \bar{c}$ $d\ \bar{b}$	$\bar{a}\ \bar{c}$ $\bar{d}\ \bar{b}$

Diagrammatic categories

- A dressing of order p in a Feynman diagram of order $l \geq p$ is a sub-graph with conn. vertices which can be isolated by cutting two propagation lines. Examples for the one-body prop. :



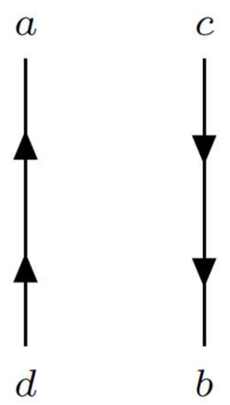
To specify the topology of a graph, the *orientation* of all propagation lines must be specified. A Feynman diagram devoid of arrows in the propagation lines is called unoriented.

- The application of Wick's theorem to the term (P) of the perturbation expansion gives rise to contributions which can be classified according to their topology into 5 categories:

Example:

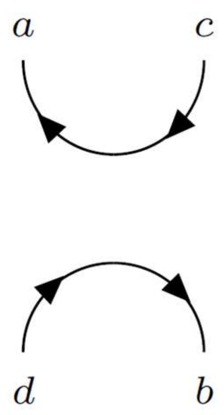
$\Pi^{1111}_{acdb}(t, t')$

- *Disjoint diagrams of direct type* →



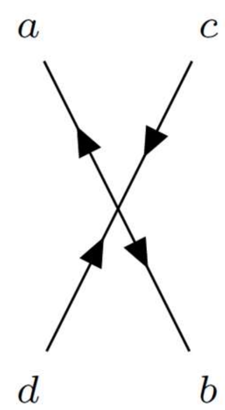
(i)

- *Disjoint diagrams of exchange type* →



(ii)

- *Disjoint diagrams of Bogoliubov type* →



(iii)

Diagrammatic categories

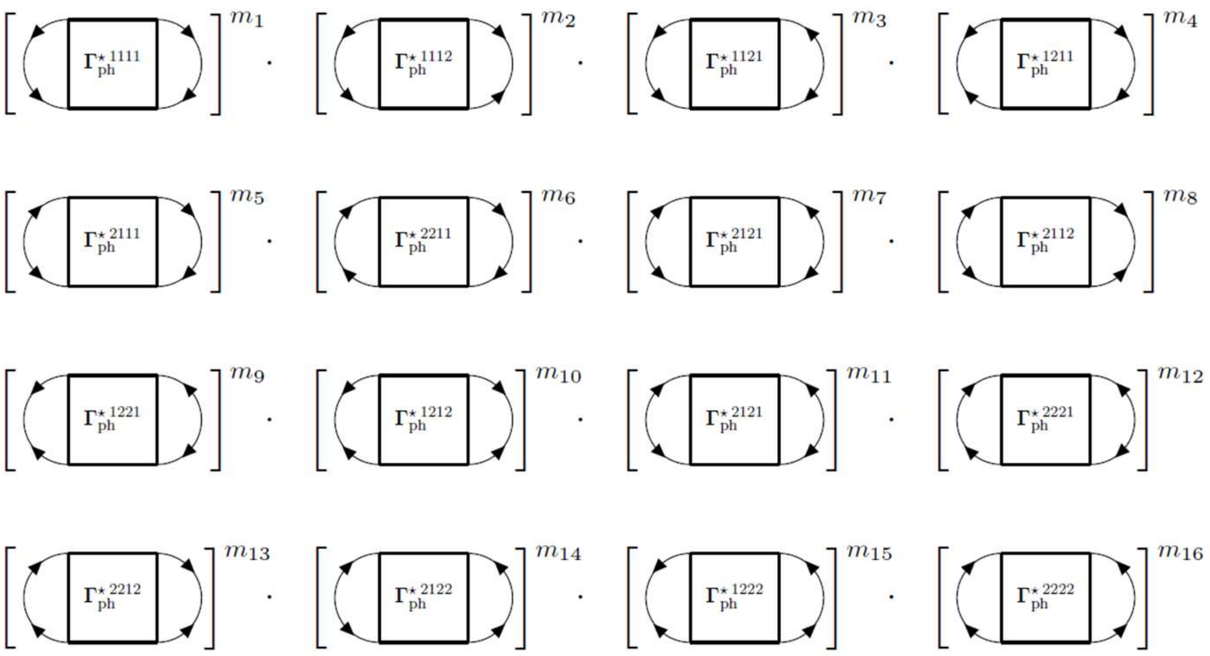
Composite diagrams contain at least one vertex that can be reabsorbed as a dressing in one unperturbed one-body propagators. Otherwise, the diagram is of *skeleton* type.

▶ **Example:** $\Pi^{1111}_{acdb}(t,t')$

Conjoint diagrams →

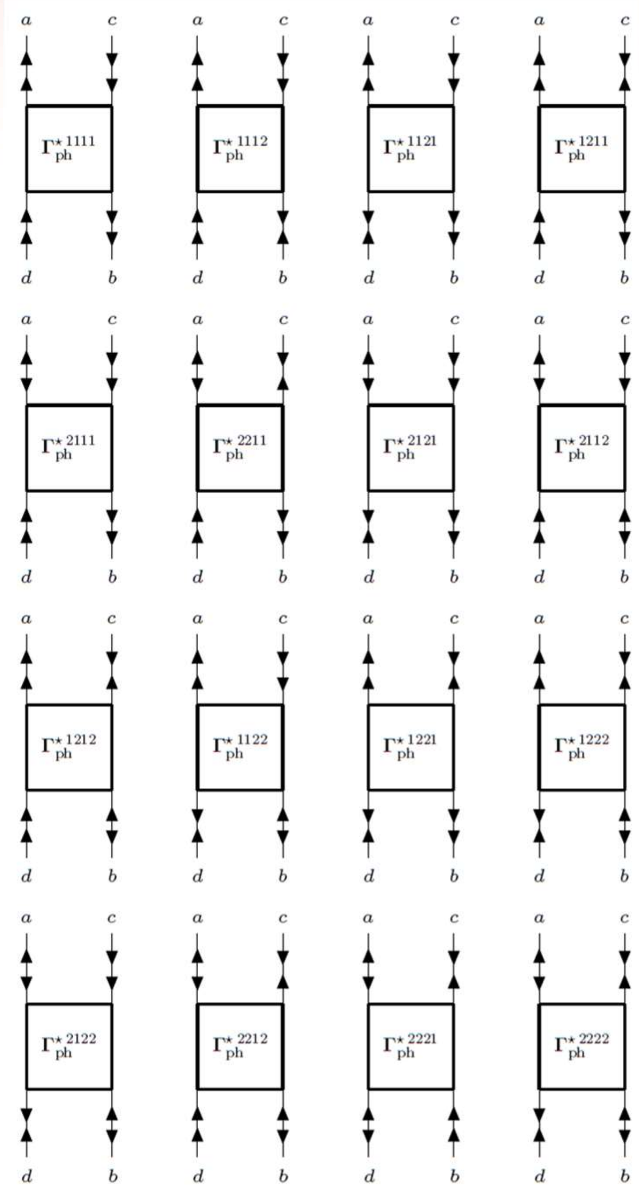
proper particle-hole vertex

[(i) (ii) (iii) (iv)] ·



(v)

Disconnected diagrams



(iv)

Gorkov's Bethe-Salpeter equations

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

$$\Pi^{gg''g'''g'}_{acdb}(t,t^+,t'^+,t') = \underbrace{\Pi^{\mathrm{D}\,gg''g'''g'}_{acdb}(t,t^+,t'^+,t')}_{\text{disj. direct pol. propagator}} + \underbrace{\Pi^{\mathrm{B}\,gg''g'''g'}_{acdb}(t,t^+,t'^+,t')}_{\text{disj. Bogoliubov pol. propagator}} + \frac{1}{\hbar}\sum_{\substack{g_1g_2\\g_3g_4}}\sum_{\substack{ef\\gh}}\int_{-\infty}^{+\infty}\mathrm{d}s_1$$

$$\cdot \int_{-\infty}^{+\infty}\mathrm{d}s_2\int_{-\infty}^{+\infty}\mathrm{d}s_3\int_{-\infty}^{+\infty}\mathrm{d}s_4\,\underbrace{\Pi^{\mathrm{D}\,g_2g_1g'''g'}_{fedb}(s_2,s_1,t^+,t)}_{\text{disjoint direct three-time pol. propagator}}\,\underbrace{\Gamma^{\star\,g_1g_2g_3g_4}_{\mathrm{ph}\,efgh}(s_1,s_2,s_3,s_4)}\,\overbrace{\Pi^{gg''g_4g_3}_{achg}(t',t'^+,s_4,s_3)}^{\text{three-time pol. propagator}}$$

where

$$\Sigma^{\star gg''}_{ad}(t,t'') = -i\sum_{bcef}\sum_{g'}(\bar{v}_{acef}\delta_{1g}+\bar{v}_{c\bar{e}\bar{a}f}\delta_{g2})\int_{-\infty}^{+\infty}\mathrm{d}t'\,G^{g1g'1}_{efbc}(t,t,t',t^+)G^{-1\,g'g''}_{bd}(t',t'') \quad \Leftarrow \quad \Gamma^{\star\,g_1g_2g_3g_4}_{\mathrm{ph}\,efgh}(s_1,s_2,s_3,s_4) = i\frac{\delta\Sigma^{\star g_1g_2}_{ef}(s_1,s_2)}{\delta G^{g_3g_4}_{gh}(s_3,s_4)}$$

proper *self-energy*, in terms of the two-body propagator — proper *particle-hole vertex*

- Where the two and three-time polarization propagator of direct and Bogoliubov types are special limits of the four-time polarization propagator ($\propto R^{g_1g_2g_3g_4}_{abcd}(t_1,t_2,t_3,t_4)$):

$$\Pi^{\mathrm{D}\,gg''g'''g'}_{acdb}(t_1,t_2,t_3,t_4) = -iG^{gg'''}_{ad}(t_1,t_4)G^{g'g''}_{bc}(t_2,t_3) \qquad \Pi^{\mathrm{B}\,gg''g'''g'}_{acdb}(t_1,t_2,t_3,t_4) = i(-1)^{g'+g'''}G^{\bar{g}'''g'}_{\bar{d}c}(t_4,t_3)G^{g\bar{g}'}_{a\bar{b}}(t_1,t_2)$$

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

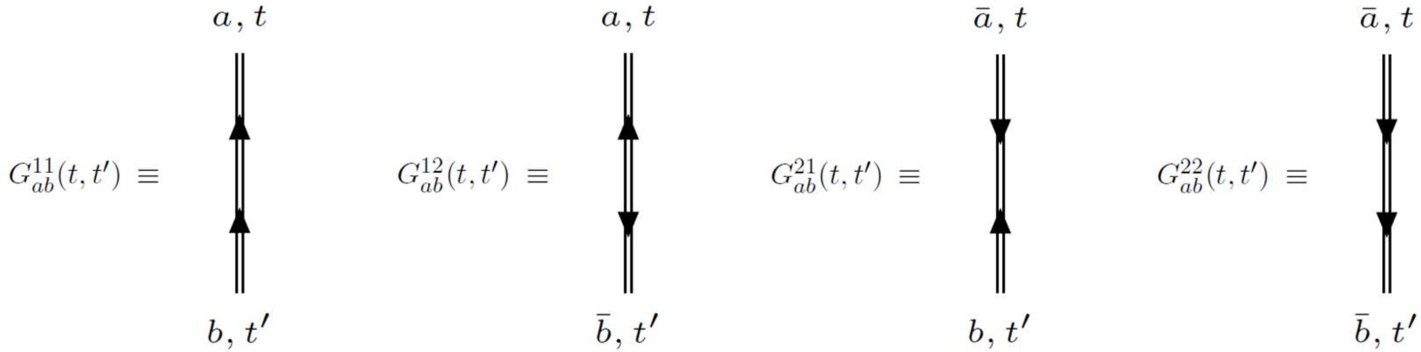
$$\Pi^{gg''g'''g'}_{acdb}(\omega) = \Pi^{\mathrm{D}\,gg''g'''g'}_{acdb}(\omega) + \Pi^{\mathrm{B}\,gg''g'''g'}_{acdb}(\omega) + \frac{1}{\hbar}\sum_{efgh}\sum_{\substack{g_1g_2\\g_3g_4}}\int_{-\infty}^{+\infty}\frac{\mathrm{d}\Omega_1}{(2\pi)}\int_{-\infty}^{+\infty}\frac{\mathrm{d}\Omega_2}{(2\pi)}\Pi^{\mathrm{D}\,g_2g_1g'''g'}_{fedb}\left(\tfrac{\omega+\Omega_1}{2},\tfrac{\omega-\Omega_1}{2}\right)$$

$$\cdot\Gamma^{\star\,g_1g_2g_3g_4}_{\mathrm{ph}\,efgh}\left(\tfrac{\omega-\Omega_1}{2},\omega,\omega-2\Omega_2\right)\Pi^{gg''g_4g_3}_{achg}(2\Omega_2,\omega-2\Omega_2)\ .$$

In contrast with Gorkov's equations, in energy repr. it remains an *integral* equation!

Particle-hole vertex

- For the analysis of the proper particle-hole vertex, the perturbative expansion of the proper self-energy is instrumental. In order to perform the functional derivation, the self-energy must be expressed in terms of *fully-dressed* one-body propagators (GGFs).
  - Convention for one-body propagators dressed to all orders in perturbation theory:



Resummation: the perturbative contributions to the self-energy (SE) of different orders are grouped according to their skeleton structure, then summed again, thus giving rise to a self-consistent expansion:

$\rightsquigarrow$ V. Somà et al. *Phys. Rev. C* **84**, 064317 (2011)
C. Barbieri et al. *Phys. Rev. C* *105*, 044330 (2022)

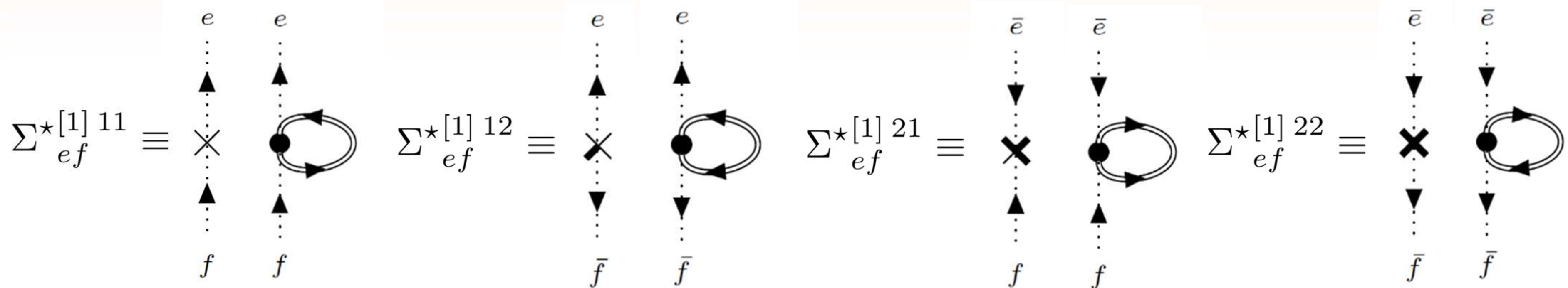
$$\mathbf{\Sigma}^{\star}_{ef}(s_1, s_2) = \mathbf{\Sigma}^{\star\,[1]}_{ef}(s_1, s_2) + \mathbf{\Sigma}^{\star\,[2]}_{ef}(s_1, s_2) + \mathbf{\Sigma}^{\star\,[3]}_{ef}(s_1, s_2) + \dots$$

Skeleton contributions do not contain any proper self-energy insertion of lower order. At order l, the latter are the lowest-order members of each grouping, $\mathbf{\Sigma}^{\star\,[l]}_{ef}(s_1, s_2)$. The composite ones are obtained by dressing the GGFs with a self-energy insertion.

Remark: The contributions of each self-consistent grouping can be diagrammatically represented by a sum of skeleton graphs, with the unperturbed GGFs replaced by the fully-dressed ones.

Particle-hole vertex

Leading order (self-consistent proper SE): 4 one-body vertces + 4 two-body vertices with a tadpole



Remark: first-order self-consistent one-body contributions independent on the dressed GGFs!

Performing the functional derivative $\Gamma^{\star\, g_1 g_2 g_3 g_4}_{\mathrm{ph}\; efgh}(s_1,s_2,s_3,s_4) = i\dfrac{\delta\Sigma^{\star g_1 g_2}_{ef}(s_1,s_2)}{\delta G^{g_3 g_4}_{gh}(s_3,s_4)}$ one obtains the self-consistent expansion of the proper particle-hole vertex:

$$\boldsymbol{\Gamma}^{\star}_{\mathrm{ph}\,efgh}(s_1,s_2,s_3,s_4) = \boldsymbol{\Gamma}^{\star\,[1]}_{\mathrm{ph}\,efgh}(s_1,s_2,s_3,s_4)+\boldsymbol{\Gamma}^{\star\,[2]}_{\mathrm{ph}\,efgh}(s_1,s_2,s_3,s_4)+\boldsymbol{\Gamma}^{\star\,[3]}_{\mathrm{ph}\,efgh}(s_1,s_2,s_3,s_4)+\dots$$

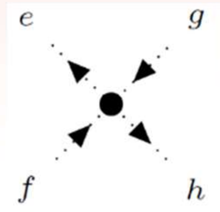
- Diagrammatically, the self-consistent expansion of $\Gamma^{\star\, g_1 g_2 g_3 g_4}_{\mathrm{ph}\; efgh}$ contains conjoint skeleton polarization propagator diagrams with dressed GGFs and amputated external legs.
- *Disjoint* polarization propagator diagrams with stripped legs are relevant only for the *improper* particle-hole vertex, in which the functional derivative is performed on the full SE.

Order zero terms do not contribute, as they do not belong to the self-energy: $\Gamma^{\star\,[0]\; g_1 g_2 g_3 g_4}_{\mathrm{ph}\quad efgh}(s_1,s_2,s_3,s_4) = 0$

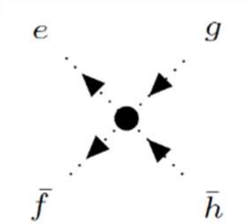
Outlook: in self-consistent approx. for $\Gamma^{\star\, g_1 g_2 g_3 g_4}_{\mathrm{ph}\; efgh}$, the dressed GGFs can be conveniently implemented in the optimized reference state (OpRS) scheme $\rightsquigarrow$ Barbieri's talk on Thursday

Particle-hole vertex

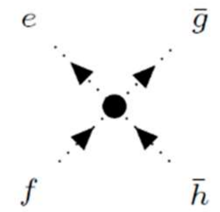
- The explicit calculation of the first-order contributions to $\Gamma^{\star}_{\mathrm{ph}}{}^{g_1 g_2 g_3 g_4}_{efgh}$ yields:



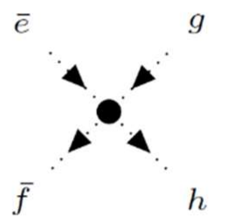
$$\Gamma^{\star}_{\mathrm{ph}}{}^{[1]}{}^{1111}_{efgh}(s_1,s_2,s_3,s_4) = \frac{1}{2}\delta(s_1-s_2)\delta(s_2-s_3)\delta(s_3-s_4)\bar{v}_{ehfg}$$



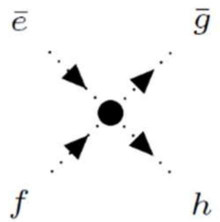
$$\Gamma^{\star}_{\mathrm{ph}}{}^{[1]}{}^{1212}_{efgh}(s_1,s_2,s_3,s_4) = \frac{1}{2}\delta(s_1-s_2)\delta(s_2-s_3)\delta(s_3-s_4)\bar{v}_{\bar{f}e\bar{h}g}$$



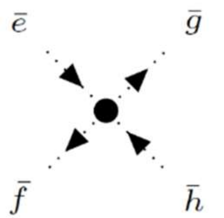
$$\Gamma^{\star}_{\mathrm{ph}}{}^{[1]}{}^{1122}_{efgh}(s_1,s_2,s_3,s_4) = \frac{1}{2}\delta(s_1-s_2)\delta(s_2-s_3)\delta(s_3-s_4)\bar{v}_{\bar{g}ef\bar{h}}$$



$$\Gamma^{\star}_{\mathrm{ph}}{}^{[1]}{}^{2211}_{efgh}(s_1,s_2,s_3,s_4) = \frac{1}{2}\delta(s_1-s_2)\delta(s_2-s_3)\delta(s_3-s_4)\bar{v}_{h\bar{f}\bar{e}g}$$



$$\Gamma^{\star}_{\mathrm{ph}}{}^{[1]}{}^{2121}_{efgh}(s_1,s_2,s_3,s_4) = \frac{1}{2}\delta(s_1-s_2)\delta(s_2-s_3)\delta(s_3-s_4)\bar{v}_{h\bar{g}f\bar{e}}$$



$$\Gamma^{\star}_{\mathrm{ph}}{}^{[1]}{}^{2222}_{efgh}(s_1,s_2,s_3,s_4) = \frac{1}{2}\delta(s_1-s_2)\delta(s_2-s_3)\delta(s_3-s_4)\bar{v}_{\bar{f}\bar{g}\bar{e}\bar{h}}$$

for the *normal* components of $\boldsymbol{\Gamma}^{\star}_{\mathrm{ph}\ efgh}$ The *anomalous* components vanish at first-order:

$$\Gamma^{\star}_{\mathrm{ph}}{}^{[1]}{}^{1112}_{efgh}(s_1,s_2,s_3,s_4) = \Gamma^{\star}_{ph}{}^{[1]}{}^{1121}_{efgh}(s_1,s_2,s_3,s_4) = \Gamma^{\star}_{\mathrm{ph}}{}^{[1]}{}^{1211}_{efgh}(s_1,s_2,s_3,s_4) = \Gamma^{\star}_{\mathrm{ph}}{}^{[1]}{}^{2111}_{efgh}(s_1,s_2,s_3,s_4) = 0$$

$$\Gamma^{\star}_{\mathrm{ph}}{}^{[1]}{}^{1222}_{efgh}(t_1,t_2,t_3,t_4) = \Gamma^{\star}_{\mathrm{ph}}{}^{[1]}{}^{2122}_{efgh}(t_1,t_2,t_3,t_4) = \Gamma^{\star}_{\mathrm{ph}}{}^{[1]}{}^{2212}_{efgh}(t_1,t_2,t_3,t_4) = \Gamma^{\star}_{\mathrm{ph}}{}^{[1]}{}^{2221}_{efgh}(t_1,t_2,t_3,t_4) = 0$$

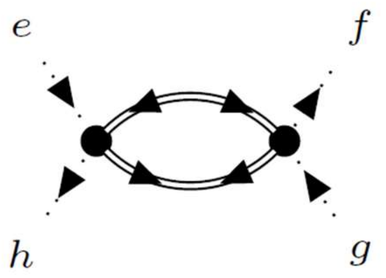
$$\Gamma^{\star}_{\mathrm{ph}}{}^{[1]}{}^{1221}_{efgh}(s_1,s_2,s_3,s_4) = \Gamma^{\star}_{\mathrm{ph}}{}^{[1]}{}^{2112}_{efgh}(s_1,s_2,s_3,s_4) = 0$$

the first-order self-consistent contributions correspond to the *random phase approximation*!

Particle-hole vertex

The explicit calculation of the second-order contributions to $\Gamma^{\star}_{\text{ph}}{}^{g_1g_2g_3g_4}_{efgh}$ yields:

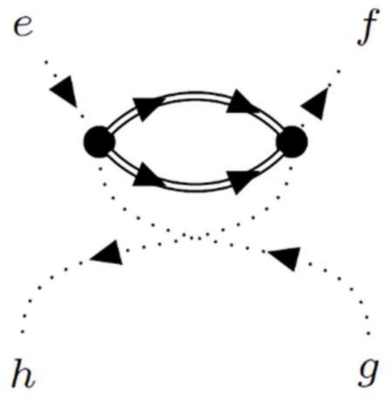
$$\boxed{\begin{aligned}
\Gamma^{\star\,[2]}_{\text{ph}}{}^{1111}_{efgh}(s_1,s_2,s_3,s_4) = &-\frac{i}{2\hbar}\sum_{pquv}\bar{v}_{\bar{p}fug}\bar{v}_{qhe\bar{v}}G^{21}_{pq}(s_2,s_1)G^{12}_{uv}(s_2,s_1)\delta(s_2-s_3)\delta(s_1-s_4)\\
&+\frac{i}{4\hbar}\sum_{pquv}\bar{v}_{hfup}\bar{v}_{qveg}G^{11}_{pq}(s_2,s_1)G^{11}_{uv}(s_2,s_1)\delta(s_1-s_3)\delta(s_2-s_4)\\
&+\frac{i}{2\hbar}\sum_{pquv}\bar{v}_{qfug}\bar{v}_{hvep}G^{11}_{pq}(s_1,s_2)G^{11}_{uv}(s_2,s_1)\delta(s_2-s_3)\delta(s_1-s_4)
\end{aligned}}$$



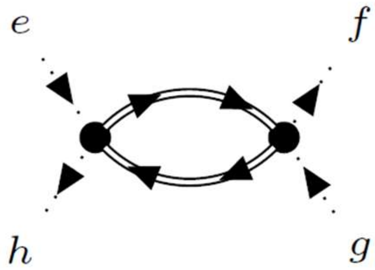
$$\Gamma^{\star\,[2]}_{\text{ph}}{}^{1112}_{efgh}(s_1,s_2,s_3,s_4) = -\frac{i}{\hbar}\sum_{pquv}\bar{v}_{\bar{p}fgu}\bar{v}_{qve\bar{h}}G^{21}_{pq}(s_2,s_1)G^{11}_{uv}(s_2,s_1)\delta(s_2-s_3)\delta(s_1-s_4)$$

$$\Gamma^{\star\,[2]}_{\text{ph}}{}^{1121}_{efgh}(s_1,s_2,s_3,s_4) = -\frac{i}{\hbar}\sum_{pquv}\bar{v}_{\bar{g}fup}\bar{v}_{hqe\bar{v}}G^{11}_{pq}(s_2,s_1)G^{12}_{uv}(s_2,s_1)\delta(s_2-s_3)\delta(s_1-s_4)$$

$$\begin{aligned}
\Gamma^{\star\,[2]}_{\text{ph}}{}^{1122}_{efgh}(s_1,s_2,s_3,s_4) = &\frac{i}{2\hbar}\sum_{pquv}\bar{v}_{\bar{p}fu\bar{h}}\bar{v}_{q\bar{g}e\bar{v}}G^{21}_{pq}(s_2,s_1)G^{12}_{uv}(s_2,s_1)\delta(s_1-s_3)\delta(s_2-s_4)\\
&-\frac{i}{4\hbar}\sum_{pquv}\bar{v}_{\bar{g}f\bar{u}\bar{p}}\bar{v}_{\bar{q}\bar{v}e\bar{h}}G^{22}_{qp}(s_1,s_2)G^{22}_{vu}(s_1,s_2)\delta(s_2-s_3)\delta(s_1-s_4)\\
&-\frac{i}{2\hbar}\sum_{pquv}\bar{v}_{\bar{q}f\bar{u}\bar{h}}\bar{v}_{\bar{g}\bar{v}e\bar{p}}G^{22}_{qp}(s_2,s_1)G^{22}_{vu}(s_1,s_2)\delta(s_1-s_3)\delta(s_2-s_4)
\end{aligned}$$



$$\begin{aligned}
\Gamma^{\star\,[2]}_{\text{ph}}{}^{1211}_{efgh}(s_1,s_2,s_3,s_4) = &-\frac{i}{2\hbar}\sum_{pquv}\bar{v}_{\bar{p}v\bar{f}g}\bar{v}_{qheu}G^{21}_{pq}(s_2,s_1)G^{11}_{uv}(s_1,s_2)\delta(s_2-s_3)\delta(s_1-s_4)\\
&-\frac{i}{2\hbar}\sum_{pquv}\bar{v}_{\bar{p}h\bar{f}u}\bar{v}_{qveg}G^{21}_{pq}(s_2,s_1)G^{11}_{uv}(s_2,s_1)\delta(s_1-s_3)\delta(s_2-s_4)
\end{aligned}$$

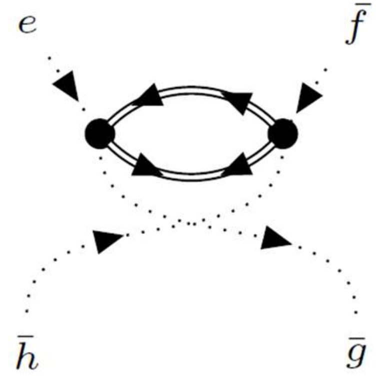


$$\Gamma^{\star\,[2]}_{\text{ph}}{}^{1212}_{efgh}(s_1,s_2,s_3,s_4) = -\frac{i}{2\hbar}\sum_{pquv}\bar{v}_{\bar{p}\bar{u}\bar{f}g}\bar{v}_{qve\bar{h}}G^{21}_{pq}(s_2,s_1)G^{21}_{uv}(s_2,s_1)\delta(s_2-s_3)\delta(s_1-s_4)$$

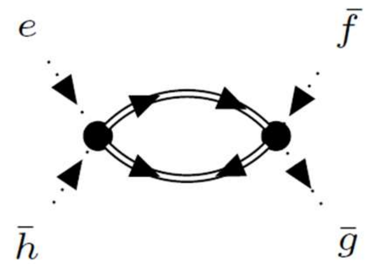
Particle-hole vertex

$$\Gamma^{\star\,[2]\;\;1221}_{\mathrm{ph}\;\;\;\;efgh}(s_1,s_2,s_3,s_4) = -\frac{i}{\hbar}\sum_{pquv}\bar{v}_{\bar{g}v\bar{f}p}\bar{v}_{hqeu}G^{11}_{pq}(s_2,s_1)G^{11}_{uv}(s_1,s_2)\delta(s_2-s_3)\delta(s_1-s_4)$$
$$-\frac{i}{\hbar}\sum_{pquv}\bar{v}_{\bar{g}\bar{u}\bar{f}p}\bar{v}_{hve\bar{q}}G^{12}_{pq}(s_2,s_1)G^{21}_{uv}(s_2,s_1)\delta(s_2-s_3)\delta(s_1-s_4)$$

$$\boxed{\begin{aligned}\Gamma^{\star\,[2]\;\;1222}_{\mathrm{ph}\;\;\;\;efgh}(s_1,s_2,s_3,s_4) &= -\frac{i}{2\hbar}\sum_{pquv}\bar{v}_{\bar{p}\bar{v}\bar{f}\bar{h}}\bar{v}_{q\bar{g}e\bar{u}}G^{21}_{pq}(s_2,s_1)G^{22}_{vu}(s_2,s_1)\delta(s_1-s_3)\delta(s_2-s_4)\\ &\quad -\frac{i}{2\hbar}\sum_{pquv}\bar{v}_{\bar{p}\bar{g}\bar{f}\bar{u}}\bar{v}_{q\bar{v}e\bar{h}}G^{21}_{pq}(s_2,s_1)G^{22}_{vu}(s_1,s_2)\delta(s_2-s_3)\delta(s_1-s_4)\end{aligned}}$$

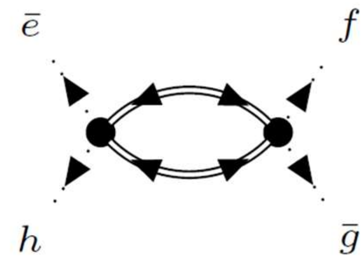


$$\Gamma^{\star\,[2]\;\;2111}_{\mathrm{ph}\;\;\;\;efgh}(s_1,s_2,s_3,s_4) = -\frac{i}{2\hbar}\sum_{pquv}\bar{v}_{hfup}\bar{v}_{q\bar{e}\bar{v}g}G^{11}_{pq}(s_2,s_1)G^{12}_{uv}(s_2,s_1)\delta(s_2-s_3)\delta(s_1-s_4)$$
$$-\frac{i}{2\hbar}\sum_{pquv}\bar{v}_{qfug}\bar{v}_{h\bar{e}\bar{v}p}G^{11}_{pq}(s_2,s_1)G^{12}_{uv}(s_2,s_1)\delta(s_2-s_3)\delta(s_1-s_4)$$



$$\Gamma^{\star\,[2]\;\;2112}_{\mathrm{ph}\;\;\;\;efgh}(s_1,s_2,s_3,s_4) = -\frac{i}{\hbar}\sum_{pquv}\bar{v}_{\bar{p}fug}\bar{v}_{q\bar{e}\bar{v}\bar{h}}G^{21}_{pq}(s_2,s_1)G^{12}_{uv}(s_1,s_2)\delta(s_2-s_3)\delta(s_1-s_4)$$
$$-\frac{i}{\hbar}\sum_{pquv}\bar{v}_{qfgu}\bar{v}_{v\bar{e}\bar{h}p}G^{11}_{pq}(s_1,s_2)G^{12}_{uv}(s_2,s_1)\delta(s_1-s_3)\delta(s_2-s_4)$$

$$\boxed{\Gamma^{\star\,[2]\;\;2121}_{\mathrm{ph}\;\;\;\;efgh}(s_1,s_2,s_3,s_4) = -\frac{i}{2\hbar}\sum_{pquv}\bar{v}_{\bar{g}fup}\bar{v}_{h\bar{e}\bar{v}\bar{q}}G^{12}_{pq}(s_2,s_1)G^{12}_{uv}(s_2,s_1)\delta(s_2-s_3)\delta(s_1-s_4)}$$



$$\Gamma^{\star\,[2]\;\;2122}_{\mathrm{ph}\;\;\;\;efgh}(s_1,s_2,s_3,s_4) = -\frac{i}{2\hbar}\sum_{pquv}\bar{v}_{\bar{g}fu\bar{p}}\bar{v}_{\bar{q}\bar{e}\bar{v}\bar{h}}G^{22}_{qp}(s_1,s_2)G^{12}_{uv}(s_2,s_1)\delta(s_1-s_3)\delta(s_2-s_4)$$
$$-\frac{i}{2\hbar}\sum_{pquv}\bar{v}_{\bar{q}fu\bar{h}}\bar{v}_{\bar{g}\bar{e}\bar{v}\bar{p}}G^{22}_{qp}(s_1,s_2)G^{12}_{uv}(s_2,s_1)\delta(s_1-s_3)\delta(s_2-s_4)$$

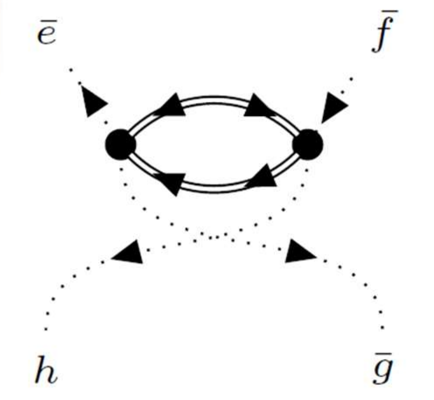
Particle-hole vertex

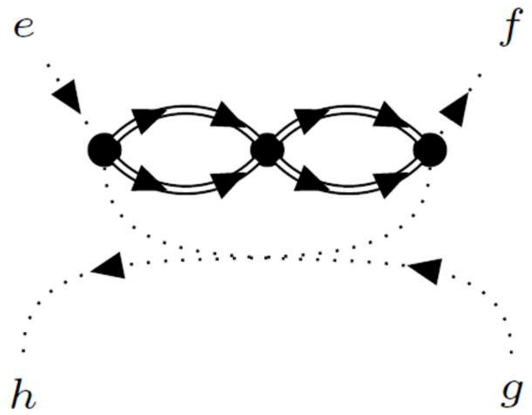
$$\Gamma^{\star\,[2]\,2211}_{\text{ph}\;efgh}(s_1,s_2,s_3,s_4) = -\frac{i}{2\hbar}\sum_{pquv} \bar{v}_{\bar{p}\bar{e}ug}\bar{v}_{qh\bar{v}\bar{f}}\, G^{21}_{pq}(s_1,s_2)G^{12}_{uv}(s_1,s_2)\delta(s_1-s_3)\delta(s_2-s_4)$$
$$-\frac{i}{4\hbar}\sum_{pquv} \bar{v}_{h\bar{e}\bar{u}\bar{p}}\bar{v}_{\bar{q}\bar{v}\bar{f}g}\, G^{22}_{qp}(s_2,s_1)G^{22}_{vu}(s_2,s_1)\delta(s_2-s_3)\delta(s_1-s_4)$$
$$-\frac{i}{2\hbar}\sum_{pquv} \bar{v}_{\bar{q}\bar{e}g\bar{u}}\bar{v}_{\bar{v}h\bar{f}\bar{p}}\, G^{22}_{qp}(s_1,s_2)G^{22}_{vu}(s_2,s_1)\delta(s_1-s_3)\delta(s_2-s_4)$$

$$\Gamma^{\star\,[2]\,2212}_{\text{ph}\;efgh}(s_1,s_2,s_3,s_4) = -\frac{i}{\hbar}\sum_{pquv} \bar{v}_{\bar{p}\bar{e}gu}\bar{v}_{qv\bar{h}\bar{f}}\, G^{21}_{pq}(s_1,s_2)G^{11}_{uv}(s_1,s_2)\delta(s_1-s_3)\delta(s_2-s_4)$$

$$\boxed{\Gamma^{\star\,[2]\,2221}_{\text{ph}\;efgh}(s_1,s_2,s_3,s_4) = -\frac{i}{\hbar}\sum_{pquv} \bar{v}_{\bar{g}\bar{e}up}\bar{v}_{hq\bar{v}\bar{f}}\, G^{11}_{pq}(s_1,s_2)G^{12}_{uv}(s_1,s_2)\delta(s_1-s_3)\delta(s_2-s_4)}$$

$$\Gamma^{\star\,[2]\,2222}_{\text{ph}\;efgh}(s_1,s_2,s_3,s_4) = \frac{i}{2\hbar}\sum_{pquv} \bar{v}_{\bar{p}\bar{e}u\bar{h}}\bar{v}_{q\bar{g}\bar{v}\bar{f}}\, G^{21}_{pq}(s_1,s_2)G^{12}_{uv}(s_1,s_2)\delta(s_1-s_3)\delta(s_2-s_4)$$
$$+\frac{i}{4\hbar}\sum_{pquv} \bar{v}_{\bar{g}\bar{e}\bar{u}\bar{p}}\bar{v}_{\bar{q}\bar{v}\bar{f}\bar{h}}\, G^{22}_{qp}(s_1,s_2)G^{22}_{vu}(s_2,s_1)\delta(s_1-s_3)\delta(s_2-s_4)$$
$$+\frac{i}{2\hbar}\sum_{pquv} \bar{v}_{\bar{q}\bar{e}\bar{u}\bar{h}}\bar{v}_{\bar{g}\bar{v}\bar{f}\bar{p}}\, G^{22}_{qp}(s_1,s_2)G^{22}_{vu}(s_2,s_1)\delta(s_2-s_3)\delta(s_1-s_4)$$





The explicit calculation of the third-order contributions to $\Gamma^{\star\;g_1g_2g_3g_4}_{\text{ph}\;efgh}$ yields:

$$\boxed{\begin{aligned}\Gamma^{\star\,[3]\,1111}_{\text{ph}\;efgh}(s_1,s_2,s_3,s_4) = -\frac{1}{\hbar^2}\sum_{pquv}\sum_{knsw}\int_{-\infty}^{+\infty} \mathrm{d}t_1\; \bar{v}_{pqus}\bar{v}_{vhfw}\bar{v}_{kegn}\, G^{21}_{wp}(s_2,t_1)G^{11}_{sv}(t_1,s_2)G^{11}_{uk}(t_1,s_1)\\ G^{11}_{nq}(s_1,t_1)\delta(s_1-s_3)\delta(s_2-s_4)+\ldots\end{aligned}}$$

Automated calculation techniques recommended: *work in progress!*

Automated implementation of Wick's theorem

A code implementing Wick's theorem in the term (P) of the expansion formula for Gorkov's polarization propagator has been developed in **Mathematica** and Jupyter up to third order.

- At order $l = m+n$ with m (n) one-body (two-body) vertices there are $4n{+}2m\text{-}3!!$ contributions

Generation Process

Key: encode fully-contracted contributions into 2-dim. arrays of integers (≡ rectang. matrices)

- **Example**: *third order*

$V^{2N}(t_1)$	$U(t_2)$	$U(t_3)$
$\overbrace{p\ q\ s\ r}$	$\overbrace{e\ f}$	$\overbrace{g\ h}$
1 2 3 4	5 6	7 8

$V^{2N}(t_1)$	$V^{2N}(t_2)$	$U(t_3)$
$\overbrace{p\ q\ s\ r}$	$\overbrace{t\ u\ w\ v}$	$\overbrace{e\ f}$
1 2 3 4	5 6 7 8	9 10

$U(t_1)$	$U(t_2)$	$U(t_3)$
$\overbrace{e\ f}$	$\overbrace{g\ h}$	$\overbrace{i\ j}$
1 2	3 4	5 6

$V^{2N}(t_1)$	$V^{2N}(t_2)$	$V^{2N}(t_3)$
$\overbrace{p\ q\ s\ r}$	$\overbrace{t\ u\ w\ v}$	$\overbrace{k\ l\ n\ m}$
1 2 3 4	5 6 7 8	9 10 11 12

▲ one and two-body vertices

$A_a^{g_1}(t)$	$A_b^{g_2}(t')$	$A_d^{\dagger\, g_4}(t')$	$A_c^{\dagger\, g_3}(t)$	
a	b	c	d	ORD.
1	2	3	4	0^{th}
5	6	7	8	1^{st}
9	10	11	12	2^{nd}
13	14	15	16	3^{rd}

▲ external legs

the s.-p. indices of 2nd-quantization operators contracted together are stored in the same *row*.

All contrib. are generated by means of transp. from the *canonical* sequence (1st elem. of `Acomb`)

- **Example**: *third order* `Acomb[[1]] = {{1,2},{3,4},{5,6},{7,8},{9,10},{11,12},{13,14},{15,16}}`

$$a_p^\dagger(t_1)a_q^\dagger(t_1)a_s(t_1)a_r(t_1)a_t^\dagger(t_2)a_u^\dagger(t_2)a_w(t_2)a_v(t_2) \cdot a_k^\dagger(t_3)a_l^\dagger(t_3)a_n(t_3)a_m(t_3)a_a^\dagger(t)a_b(t')a_d^\dagger(t')a_c^\dagger(t) \mapsto$$

```
Acomb[[d_1]] = {{1,4},{5,16},{6,8},
{11,12},{9,13},{2,14},{3,7},{10,15}}
```

Automated implementation of Wick's theorem

- Next, elementary *topological rules* are exploited in order to separate the Wick's-theorem contributions according to the diagram *category* and *type* they are associated with.

	Order $l = m + n$ →	0	1		2			3			
Category	Type \ (m,n) →	$(0,0)$	$(1,0)$	$(0,1)$	$(2,0)$	$(1,1)$	$(0,2)$	$(3,0)$	$(2,1)$	$(1,2)$	$(0,3)$
Conjoint	Skeleton	0	0	24	0	0	1,728	0	0	0	311,040
	Composite	0	0	0	0	768	2,304	0	19,200	193,536	718,848
Disjoint Direct	Non-Dressed	1	0	0	0	0	0	0	0	0	0
	Left or Right-Dr.	0	16	24	160	576	1,536	1,920	11,520	61,440	228,096
	Left and Right-Dr.	0	0	0	80	192	288	1920	7,680	26,112	55,296
Disjoint Bogoliubov	Non-Dressed	1	0	0	0	0	0	0	0	0	0
	Diag. or Antidiag.-Dr.	0	16	24	160	576	1,536	1,920	11,520	61,440	228,096
	Diag. and Antidiag.-Dr.	0	0	0	80	192	288	1920	7,680	26,112	55,296
Relevant		2	32	72	480	2,304	7,680	7,680	57,600	368,640	1,596,672
Disjoint Exchange	Non-Dressed	1	0	0	0	0	0	0	0	0	0
	Above or Below-Dr.	0	16	24	160	576	1,536	1,920	11,520	61,440	228,096
	Above and Below-Dr.	0	0	0	80	192	288	1920	7,680	26,112	55,296
Disconnected		0	12	9	330	708	891	7,380	27,150	84,348	146,961
Total		3	60	105	1,050	3,780	10,395	18,900	103,950	540,540	2,027,025

At third order, there are 2,690,415 fully-contracted terms in total!

Automated implementation of Wick's theorem

Filtration Process

- The *equivalent* Wick's-theorem contrib. are identified and their multiplicity is stored, thanks to:
  - the exchange symmetry of identical one and two-body vertices (*external* s.-p. index permutations)
    - the partial antisymmetry of the two-body vertex, (*internal* s.-p. index permutations)

Category	Order $l = m + n$ →	0	1		2			3			
	Type \ (m, n) →	$(0,0)$	$(1,0)$	$(0,1)$	$(2,0)$	$(1,1)$	$(0,2)$	$(3,0)$	$(2,1)$	$(1,2)$	$(0,3)$
Conjoint	Skeleton	0	0	6	0	0	60	0	0	0	924
	Composite	0	0	0	0	192	96	0	3,840	7,200	2,880
Disjoint Direct	Non-Dressed	1	0	0	0	0	0	0	0	0	0
	Left or Right-Dr.	0	16	8	128	176	76	1,024	2,704	2,720	1,032
	Left and Right-Dr.	0	0	0	64	64	16	1,024	1,920	1,312	304
Disjoint Bogoliubov	Non-Dressed	1	0	0	0	0	0	0	0	0	0
	Diag. or Antidiag.-Dr.	0	16	8	128	176	76	1,024	2,704	2,720	1,032
	Diag. and Antidiag.-Dr.	0	0	0	64	64	16	1,024	1,920	1,312	304
Relevant		2	32	22	384	672	340	4,096	13,088	15,264	6,476
Disjoint Exchange	Non-Dressed	1	0	0	0	0	0	0	0	0	0
	Above or Below-Dr.	0	16	8	128	176	76	1,024	2,704	2,720	1,032
	Above and Below-Dr.	0	0	0	64	64	16	1,024	1,920	1,312	304
Disconnected		0	12	6	282	288	99	4,308	7,788	5,604	1,524
Total		3	60	36	858	1200	531	10,452	25,500	24,900	9,336

Automated implementation of Wick's theorem

- The *equivalent* Wick's-theorem contrib. are identified and their multiplicity is stored, thanks to:
  - ⇝ the exchange symmetry of identical one and two-body vertices (*external* s.-p. index permutations)
    - ⇝ the partial antisymmetry of the two-body vertex, (*internal* s.-p. index permutations)

	Order $l = m + n$ →	0	1		2			3			
Category	Type \ (m,n) →	$(0,0)$	$(1,0)$	$(0,1)$	$(2,0)$	$(1,1)$	$(0,2)$	$(3,0)$	$(2,1)$	$(1,2)$	$(0,3)$
Conjoint	Skeleton	0	0	6	0	0	60	0	0	0	924
	Composite	0	0	0	0	192	96	0	3,840	7,200	2,880
Disjoint Direct	Non-Dressed	1	0	0	0	0	0	0	0	0	0
	Left or Right-Dr.	0	16	8	128	176	76	1,024	2,704	2,720	1,032
	Left and Right-Dr.	0	0	0	64	64	16	1,024	1,920	1,312	304
Disjoint Bogoliubov	Non-Dressed	1	0	0	0	0	0	0	0	0	0
	Diag. or Antidiag.-Dr.	0	16	8	128	176	76	1,024	2,704	2,720	1,032
	Diag. and Antidiag.-Dr.	0	0	0	64	64	16	1,024	1,920	1,312	304
Relevant		2	32	22	384	672	340	4,096	13,088	15,264	6,476
Disjoint Exchange	Non-Dressed	1	0	0	0	0	0	0	0	0	0
	Above or Below-Dr.	0	16	8	128	176	76	1,024	2,704	2,720	1,032
	Above and Below-Dr.	0	0	0	64	64	16	1,024	1,920	1,312	304
Disconnected		0	12	6	282	288	99	4,308	7,788	5,604	1,524
Total		3	60	36	858	1200	531	10,452	25,500	24,900	9,336

At third order, there are 70,188 inequivalent fully-contracted terms in total!

Automated implementation of Wick's theorem

Evaluation Process

▶ The inequivalent Wick's-theorem contributions are converted into *analytical* expressions. The latter are in one-to-one correspondence with the amplitudes of the *Feynman graphs* in time representation.

The procedure entails:

- ✓ the conversion of contractions into *one-body Gorkov-Green's functions*;
- ✓ the writing of the *summation* and *integration signs*;
- ✓ the writing of *multiplication factors* (interaction matrix elements, multiplicity, ...)
- ✓ the determination of the *sign*;

t'	t_3	t_2	t_1	t	
$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	$\downarrow$	ORD.
1	–	–	–	2	0^{th}
1	–	–	2	3	1^{st}
1	–	2	3	4	2^{nd}
1	2	3	4	5	3^{rd}

convention for the encoding of the time indices of one.body Gorkov-Green's functions.

convention for the conversion of *canonical contractions* for Wick's-theorem contributions of Bogoliubov type

CONTR. / INDIC.	$\underbrace{a_e a_{\bar f}}$	$\underbrace{a^\dagger_{\bar e} a^\dagger_f}$	$\underbrace{a_e a^\dagger_f}$	$\underbrace{a^\dagger_{\bar e} a_{\bar f}}$
$e,\ f$ INTERNAL	$iG^{(0)\ 12}_{ef}$	$iG^{(0)\ 21}_{ef}$	$iG^{(0)\ 11}_{ef}$	$iG^{(0)\ 22}_{ef}$
$e = a, c$ EXT. f INTERNAL	$iG^{(0)\ 12}_{ef}$	$iG^{(0)\ 21}_{ef}$	$iG^{(0)\ 11}_{ef}$	$iG^{(0)\ 22}_{ef}$
$e = b, d$ EXT. f INTERNAL	$iG^{(0)\ 12}_{f\bar e}$ $\bar f \mapsto f$	$-iG^{(0)\ 21}_{f\bar e}$ $f \mapsto \bar f$	$iG^{(0)\ 22}_{f\bar e}$ $f \mapsto \bar f$	$-iG^{(0)\ 11}_{f\bar e}$ $\bar f \mapsto f$
e INTERNAL $f = a, c$ EXT.	$iG^{(0)\ 12}_{ef}$	$iG^{(0)\ 21}_{ef}$	$iG^{(0)\ 11}_{ef}$	$iG^{(0)\ 22}_{ef}$
e INTERNAL $f = b, d$ EXT.	$-iG^{(0)\ 12}_{\bar f e}$ $e \mapsto \bar e$	$iG^{(0)\ 21}_{\bar f e}$ $\bar e \mapsto e$	$iG^{(0)\ 22}_{\bar f e}$ $e \mapsto \bar e$	$-iG^{(0)\ 11}_{\bar f e}$ $\bar e \mapsto e$
$e,\ f$ EXTERNAL	–	–	–	–

Output: amplitudes of *conjoint-composite* Feynman diagrams of Gorkov's polarization propagator at third order with $(m,n) = (1,2)$ and Nambu component '*1111*'

```
In[∘]:= For[u = 1, u ≤ 1800, u++,
  If [GGFNambu⟦u, 1, 1⟧ == 1 && GGFNambu⟦u, 1, 2⟧ == 1 && GGFNambu⟦u, 2, 1⟧ == 1 && GGFNambu⟦u, 2, 2⟧ == 1 && GGFNambu⟦u, 3, 1⟧ == 1 && GGFNambu⟦u, 3, 2⟧ == 1 &&
    GGFNambu⟦u, 4, 1⟧ == 1 && GGFNambu⟦u, 4, 2⟧ == 1 && GGFNambu⟦u, 5, 1⟧ == 1 && GGFNambu⟦u, 5, 2⟧ == 1 && GGFNambu⟦u, 6, 1⟧ == 1 && GGFNambu⟦u, 6, 2⟧ == 1 &&
    GGFNambu⟦u, 7, 1⟧ == 1 && GGFNambu⟦u, 7, 2⟧ == 1 , Print[u, "     ", GGFFeynmanAmplitude⟦u⟧, "\n"]]]
```

374 $\frac{1}{2\hbar^3}\sum_{pqrs}\sum_{tuvw}\sum_{ef} \bar{v}_{pqrs}\, \bar{v}_{tuvw}\, u^{11}_{ef}\int_{-\infty}^{+\infty} dt_2 \int_{-\infty}^{+\infty} dt_3 \int_{-\infty}^{+\infty} dt_4\, G^{(0)}{}_{sp}{}^{11}(t_4,t_4)\, G^{(0)}{}_{wq}{}^{11}(t_3,t_4)\, G^{(0)}{}_{ft}{}^{11}(t_2,t_3)\, G^{(0)}{}_{rd}{}^{11}(t_4,t_1)\, G^{(0)}{}_{ae}{}^{11}(t_5,t_2)\, G^{(0)}{}_{bu}{}^{11}(t_1,t_3)\, G^{(0)}{}_{vc}{}^{11}(t_3,t_5)$

376 $-\frac{1}{2\hbar^3}\sum_{pqrs}\sum_{tuvw}\sum_{ef} \bar{v}_{pqrs}\, \bar{v}_{tuvw}\, u^{11}_{ef}\int_{-\infty}^{+\infty} dt_2 \int_{-\infty}^{+\infty} dt_3 \int_{-\infty}^{+\infty} dt_4\, G^{(0)}{}_{sp}{}^{11}(t_4,t_4)\, G^{(0)}{}_{wq}{}^{11}(t_3,t_4)\, G^{(0)}{}_{ft}{}^{11}(t_2,t_3)\, G^{(0)}{}_{rd}{}^{11}(t_4,t_1)\, G^{(0)}{}_{be}{}^{11}(t_1,t_2)\, G^{(0)}{}_{au}{}^{11}(t_5,t_3)\, G^{(0)}{}_{vc}{}^{11}(t_3,t_5)$

Automated implementation of Wick's theorem

The inequivalent Wick's-theorem contributions are converted into *analytical* expressions. The latter are in one-to-one correspondence with the amplitudes of the *Feynman graphs* in time representation.

Amplitude of third-order conjoint composite diagrams contributing to Π_{acdb}

with a one-body and two two-body interaction vertices

Conventions

The fully-contracted terms processed henceforth correspond to fully-contracted conjoint composite contributions generated by the application of Wick's theorem to the following matrix element (cf. expansion formula of Gorkov's polarization propagator),

$$\Pi^{g_1g_3g_4g_2}_{acdb}|_{\text{third order}} \equiv +3i\left(\frac{-i}{\hbar}\right)^3\frac{1}{3!}\int dt_1\int dt_2\int dt_3\,\langle\Phi_0|T\{\bar{V}(t_1)\bar{V}(t_2)U(t_3)A_{I\,a}^{g_1}(t)A_{I\,b}^{g_2}(t')A_{I\,d}^{\dagger g_4}(t')A_{I\,c}^{\dagger g_3}(t)\}|\Phi_0\rangle_{\text{conn}}$$

... ...

```
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Framed[20,RoundingRadius->10]" "GGFFeynmanAmplitude[[20]]
Framed[21,RoundingRadius->10]" "GGFFeynmanAmplitude[[21]]
Framed[22,RoundingRadius->10]" "GGFFeynmanAmplitude[[22]]
Framed[23,RoundingRadius->10]" "GGFFeynmanAmplitude[[23]]
Framed[24,RoundingRadius->10]" "GGFFeynmanAmplitude[[24]]
```

Out[83]:

(1) $\frac{1}{2\hbar^3}\sum_{ef}\sum_{pqrs}\sum_{tuvw}\bar{v}_{tuvw}\,\bar{v}_{pqrs}\,u_{e\bar{f}}^{11}\int_{-\infty}^{+\infty}dt_2\int_{-\infty}^{+\infty}dt_3\int_{-\infty}^{+\infty}dt_4$

$G^{(0)}{}_{pc}^{21}(t_4,t_5)\;G^{(0)}{}_{sq}^{11}(t_4,t_4)\;G^{(0)}{}_{rt}^{11}(t_4,t_3)\;G^{(0)}{}_{wd}^{11}(t_3,t_1)\;G^{(0)}{}_{ue}^{21}(t_3,t_2)\;G^{(0)}{}_{af}^{12}(t_5,t_2)\;G^{(0)}{}_{bv}^{12}(t_1,t_3)$

(2) $\frac{1}{4\hbar^3}\sum_{ef}\sum_{pqrs}\sum_{tuvw}\bar{v}_{tuvw}\,\bar{v}_{pqrs}\,u_{ef}^{11}\int_{-\infty}^{+\infty}dt_2\int_{-\infty}^{+\infty}dt_3\int_{-\infty}^{+\infty}dt_4$

$G^{(0)}{}_{pq}^{21}(t_4,t_4)\;G^{(0)}{}_{st}^{11}(t_4,t_3)\;G^{(0)}{}_{re}^{11}(t_4,t_2)\;G^{(0)}{}_{aw}^{12}(t_5,t_3)\;G^{(0)}{}_{bu}^{11}(t_1,t_3)\;G^{(0)}{}_{vd}^{11}(t_3,t_1)\;G^{(0)}{}_{fc}^{11}(t_2,t_5)$

(3) $-\frac{1}{4\hbar^3}\sum_{ef}\sum_{pqrs}\sum_{tuvw}\bar{v}_{tuvw}\,\bar{v}_{pqrs}\,u_{ef}^{11}\int_{-\infty}^{+\infty}dt_2\int_{-\infty}^{+\infty}dt_3\int_{-\infty}^{+\infty}dt_4$

$G^{(0)}{}_{pq}^{21}(t_4,t_4)\;G^{(0)}{}_{st}^{11}(t_4,t_3)\;G^{(0)}{}_{re}^{11}(t_4,t_2)\;G^{(0)}{}_{aw}^{12}(t_5,t_3)\;G^{(0)}{}_{bu}^{11}(t_1,t_3)\;G^{(0)}{}_{vc}^{11}(t_3,t_5)\;G^{(0)}{}_{fd}^{11}(t_2,t_1)$

(4) $-\frac{1}{4\hbar^3}\sum_{ef}\sum_{pqrs}\sum_{tuvw}\bar{v}_{tuvw}\,\bar{v}_{pqrs}\,u_{ef}^{11}\int_{-\infty}^{+\infty}dt_2\int_{-\infty}^{+\infty}dt_3\int_{-\infty}^{+\infty}dt_4$

$G^{(0)}{}_{pq}^{21}(t_4,t_4)\;G^{(0)}{}_{st}^{11}(t_4,t_3)\;G^{(0)}{}_{re}^{11}(t_4,t_2)\;G^{(0)}{}_{aw}^{12}(t_5,t_3)\;G^{(0)}{}_{ud}^{21}(t_3,t_1)\;G^{(0)}{}_{bv}^{12}(t_1,t_3)\;G^{(0)}{}_{fc}^{11}(t_2,t_5)$

(5) $\frac{1}{\ldots}\sum_{ef}\sum_{pqrs}\sum_{tuvw}\bar{v}_{tuvw}\,\bar{v}_{pqrs}\,u_{e\bar{f}}^{11}\int_{-\infty}^{+\infty}dt_2\int_{-\infty}^{+\infty}dt_3\int_{-\infty}^{+\infty}dt_4$

Entrée [107]:

```
For[u = 1, u <= 1800, u++, If [GGFNambu[[u, 1, 1]] == 1 && GGFNambu[[u, 1, 2]] == 1 && GGFNambu[[u, 2, 1]] == 1
GGFNambu[[u, 3, 1]] == 1 && GGFNambu[[u, 3, 2]] == 1 && GGFNambu[[u, 4, 1]] == 1 && GGFNambu[[u, 4, 2]] == 1 &&
GGFNambu[[u, 7, 1]] == 1 && GGFNambu[[u, 7, 2]] == 1, Print["Framed[",u, ",RoundingRadius->10]\" \"GGFFeynmanAm
```

Output: amplitudes of *conjoint-composite* Feynman diagrams of Gorkov's polarization propagator at third order with $(m,n) = (1,2)$ and Nambu component '*1111*'

Automated implementation of Wick's theorem

Example: fully-contracted second-order Bogoliubov contribution to $\Pi^{1211}_{acdb}(t,t')$ with $(m,n)=(0,2)$

```
CombBog[[1]] = {{1,2},{3,9},{5,6},{7,11},{4,10},{8,12}};
GGFMult[[1]] = 8;
```

- Recasting of the contractions into unperturbed one-body Gorkov-Green's functions (GGFs) and determination of the phase factor:

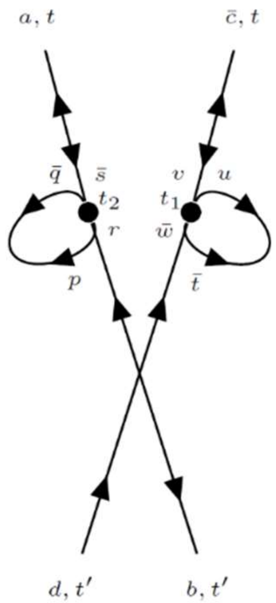
Converting the integers in `CombBog[[1]]` into letters in a string and following the conventions on the second-quantization operators in the matrix elements in the term (P) of the expansion formula, one finds:

$$[pqsatuwdrbvc] \mapsto [pqsrtuwvabdc]$$

$$\underbrace{a_p^\dagger(t_1)a_q^\dagger(t_1)}\,\underbrace{a_s(t_1)a_a(t)}\,\underbrace{a_t^\dagger(t_2)a_u^\dagger(t_2)}\,\underbrace{a_w(t_2)a_d^\dagger(t')}\cdot\underbrace{a_r(t_1)a_b(t')}\,\underbrace{a_v(t_2)a_{\bar c}(t)} \longmapsto a_p^\dagger(t_1)a_q^\dagger(t_1)a_s(t_1)a_r(t_1)a_t^\dagger(t_2)a_u^\dagger(t_2)a_w(t_2)a_v(t_2)\cdot a_a(t)a_b(t')a_d^\dagger(t')a_{\bar c}(t)\ ,$$

the number of transpositions necessary to restore the canonical sequence of 2nd-quantiza -tion operators is 12. Two additional *sign-changing* operations are performed, in order to obey the conventions for the conversion of contractions into one-body GGFs: factor $(-1)^2$

$$(-1)^T(-i)^{2m+n+1}i^{m+2n+2} \longmapsto i^3(-1)^{14}=-i$$



- Introducing the rest of the necessary symbols and the multiplicity factor in `GGFMult[[1]]`, the Feynman amplitude is finally found:

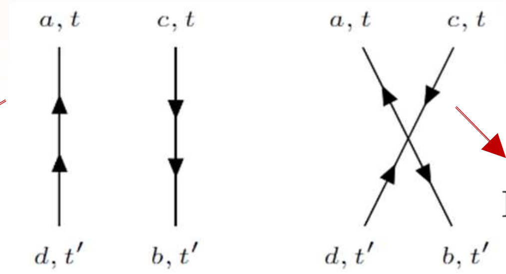
$$-\frac{i}{4\hbar^2}\sum_{pqrs}\sum_{tuvw}\bar v_{\bar p q r \bar s}\bar v_{t \bar u v \bar w}\int_{-\infty}^{+\infty}\mathrm{d}t_1\int_{-\infty}^{+\infty}\mathrm{d}t_2\ G^{(0)\ 21}_{pq}(t_1,t_1^+)G^{(0)\ 12}_{as}(t,t_1)\cdot G^{(0)\ 21}_{tu}(t_2,t_2^+)G^{(0)\ 22}_{\bar d w}(t',t_2)G^{(0)\ 12}_{r\bar b}(t_1,t')G^{(0)\ 12}_{vc}(t_1,t)$$

Zeroth and first-order Feynman diagrams

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

- Zeroth order:

$$\Pi^{1111\,(0a)}_{acdb}(t,t') = -i\, G^{(0)\,11}_{ad}(t,t'^{+})\, G^{(0)\,11}_{cb}(t^{+},t')$$



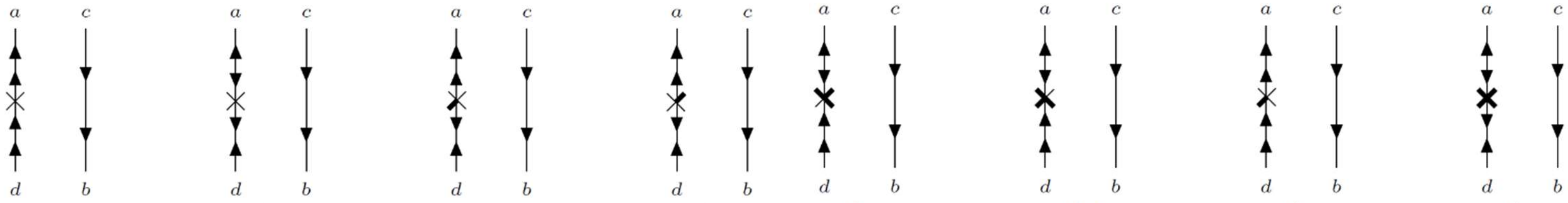
(0a) (0b)

$$\Pi^{1111\,(0b)}_{acdb}(t,t') = i\, G^{(0)\,12}_{a\bar{b}}(t,t')\, G^{(0)\,21}_{\bar{d}c}(t'^{+},t^{+})$$

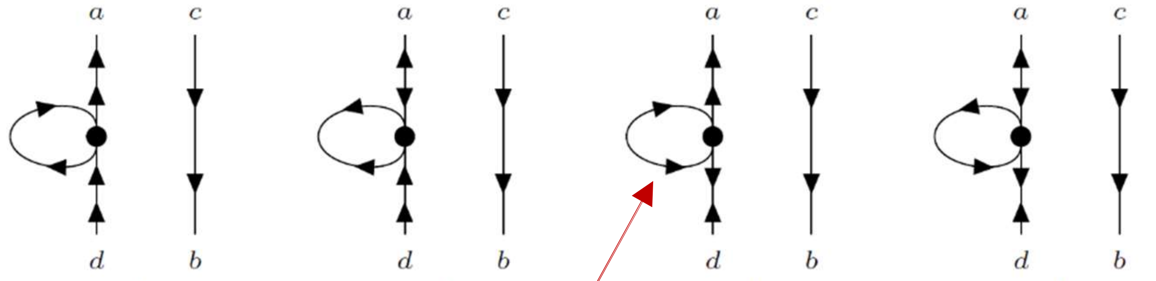
i.e. the LO disjoint direct and Bogoliubov diagrams!

- First order:

left-dressed direct diagrams



(1′aa) (1′ab) (1′ac) (1′ad) (1′ae) (1′af) (1′ag) (1′ah)



(1′ai) (1′aj) (1′ak) (1′al)

Anomalous loop!

$$\Pi^{1111\,(1'ak)}_{acdb}(t,t') = +\boxed{\frac{1}{2\hbar}} \sum_{pqrs} \bar{v}_{p\bar{q}\bar{r}s} \int_{-\infty}^{+\infty} \mathrm{d}t_1 G^{(0)\,11}_{ap}(t,t_1) \boxed{G^{(0)\,12}_{sr}(t_1,t_1^{+})} G^{(0)\,11}_{qd}(t_1,t'^{+}) G^{(0)\,22}_{bc}(t',t^{+})$$

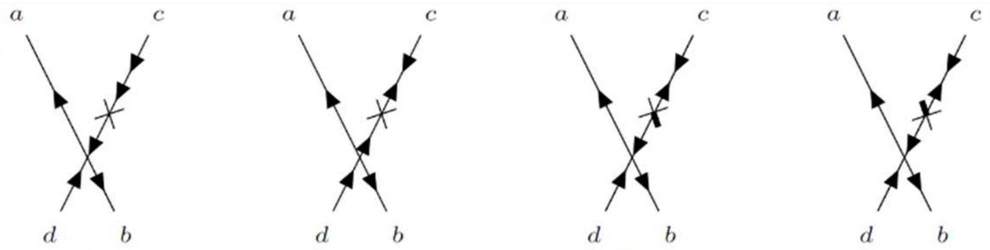
Ellipsis: *right-dressed* direct diagrams

First-order Feynman diagrams

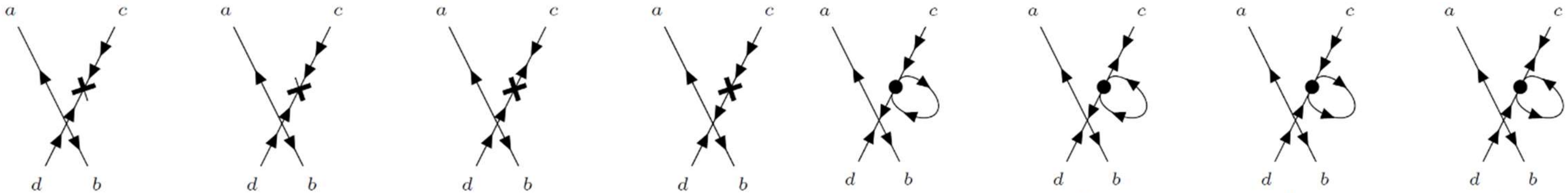
Example: perturbative expansion of $\Pi^{1111}_{acdb}(t,t')$

- First order:

  - *antidiagonally-dressed* Bogoliubov diagrams



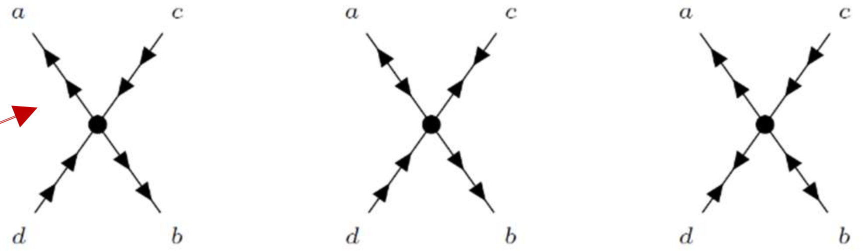
(1″aa) (1″ab) (1″ac) (1″ad)



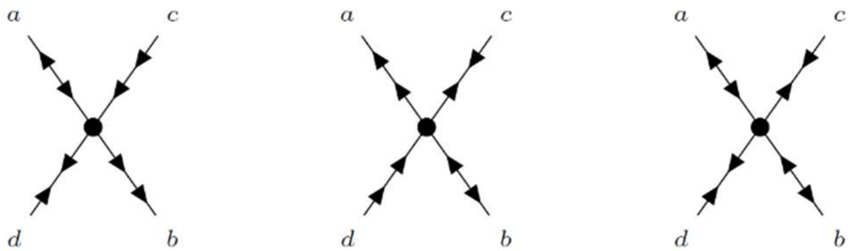
(1″ae) (1″af) (1″ag) (1″ah) (1″ai) (1″aj) (1″ak) (1″al)

  - conjoint skeleton diagrams

$$\Pi^{1111\,(1a)}_{acdb}(t,t') = -\frac{1}{\hbar}\sum_{pqrs} \bar{v}_{pqrs}\int_{-\infty}^{+\infty} \mathrm{d}t_1\, G^{(0)\,11}_{bq}(t',t_1)\, G^{(0)\,11}_{ap}(t,t_1) G^{(0)\,11}_{rc}(t_1,t^+)\, G^{(0)\,11}_{sd}(t_1,t'^+)$$



(1a) (1b) (1c)



(1d) (1e) (1f)

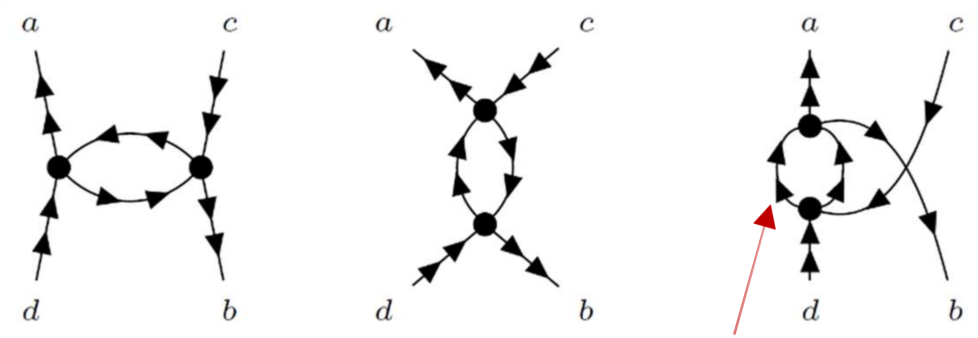
Ellipsis: *diagonally-dressed* Bogoliubov diagrams

Second-order Feynman diagrams

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

- Second order:
  - conjoint skeleton diagrams

Equivalent propagators!

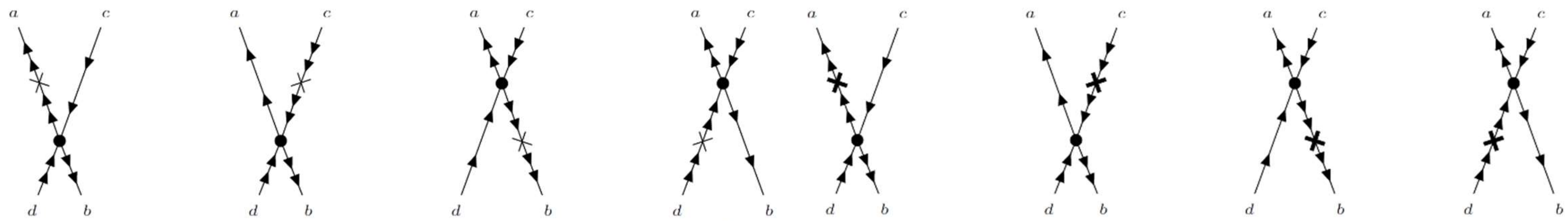


(2a) (2b) (2c)

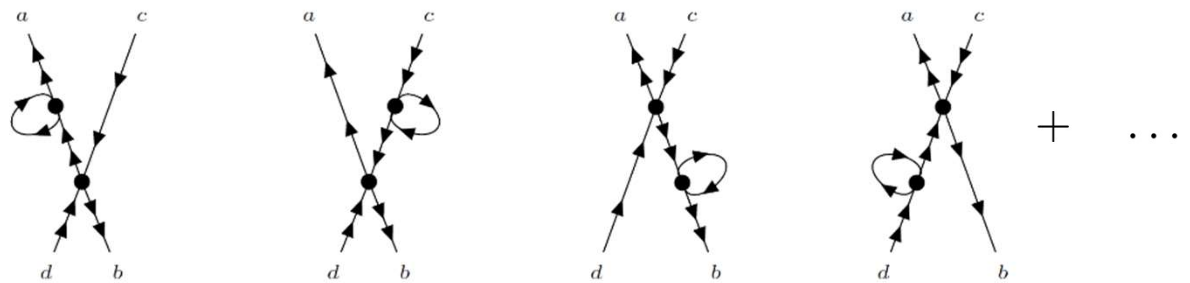
Ellipsis: conjoint skeleton diagrams containing anoma-lous propagators

$$\Pi^{1111\,(2c)}_{acdb}(t,t') = -\boxed{\frac{i}{2\hbar^2}} \sum_{\substack{pqrs\\tuvw}} \bar{v}_{pqrs}\bar{v}_{tuvw} \int_{-\infty}^{+\infty} \mathrm{d}t_1 \int_{-\infty}^{+\infty} \mathrm{d}t_2 \boxed{G^{(0)\,11}_{wp}(t_2,t_1)} G^{(0)\,11}_{sd}(t_1,t'^{+}) G^{(0)\,11}_{at}(t,t_2) \boxed{G^{(0)\,11}_{vq}(t_2,t_1)} G^{(0)\,11}_{bu}(t',t_1) G^{(0)\,11}_{rc}(t_1,t^{+})$$

- conjoint *composite* diagrams



(2′a) (2′b) (2′c) (2′d) (2′e) (2′f) (2′g) (2′h)



(2′i) (2′j) (2′k) (2′l)

$+ \quad \ldots$

Ellipsis: conjoint composite diagrams containing anomalous propagators

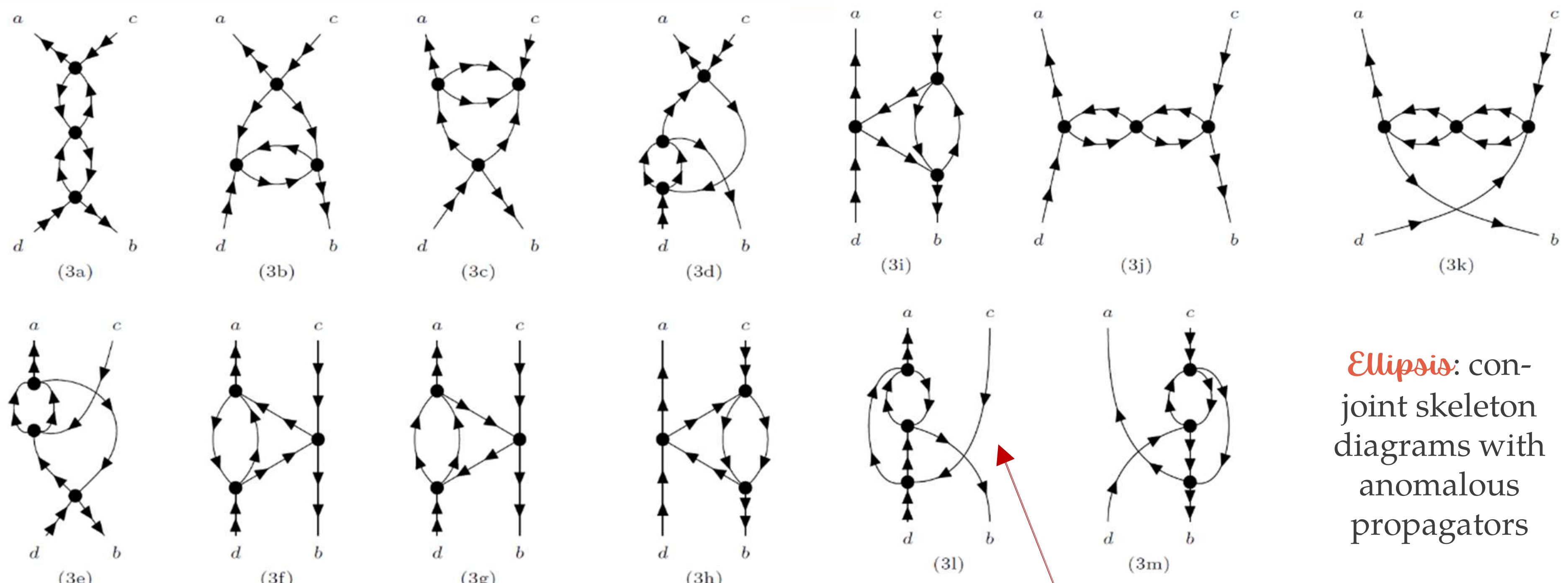
Other contributions: disjoint direct and Bogoliubov diagrams

Third-order Feynman diagrams

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

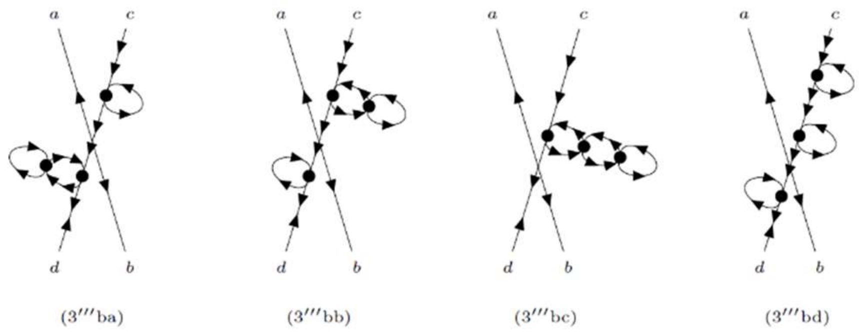
- Third order:

conjoint *skeleton* diagrams



Ellipsis: conjoint skeleton diagrams with anomalous propagators

antidiagonally-dressed disjoint Bogoliubov diagrams



$+ \quad \ldots$

$$\Pi^{1111\,(3l)}_{acdb}(t,t') = -\frac{1}{\hbar^3}\sum_{pqrs}\sum_{tuvw}\sum_{klmn}\bar{v}_{pqrs}\bar{v}_{tuvw}\bar{v}_{klmn}\int_{-\infty}^{+\infty}\mathrm{d}t_1\int_{-\infty}^{+\infty}\mathrm{d}t_2\int_{-\infty}^{+\infty}\mathrm{d}t_3$$
$$\cdot G^{(0)\,11}_{wp}(t_2,t_1)\,G^{(0)\,11}_{st}(t_1,t_2):\; G^{(0)\,11}_{rk}(t_1,t_3)\,G^{(0)\,11}_{aq}(t,t_1)G^{(0)\,11}_{bu}(t',t_2)$$
$$\cdot G^{(0)\,11}_{nd}(t_3,t'^{+})\,G^{(0)\,11}_{vl}(t_2,t_3)\,G^{(0)\,11}_{mc}(t_3,t^{+})$$

Ellipsis: *antidiagonally-dr.* disjoint Bogoliubov diagrams containing *one-body vertices* and more than one anomalous propagator

Third-order Feynman diagrams

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

- Third order:

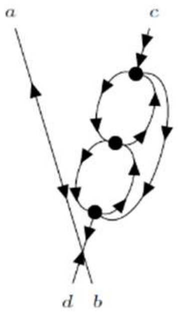
antidiagonally-dressed disjoint Bogoliubov diagrams

$(3'''\text{be})$

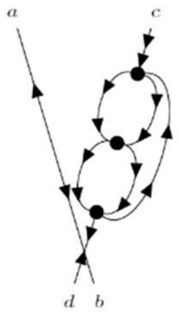
$(3'''\text{bf})$

$(3'''\text{bg})$

$(3'''\text{bh})$

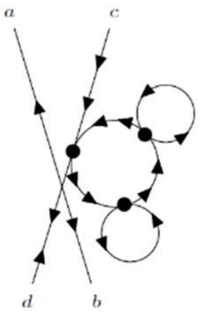


$(3'''\text{bi})$



$(3'''\text{bj})$

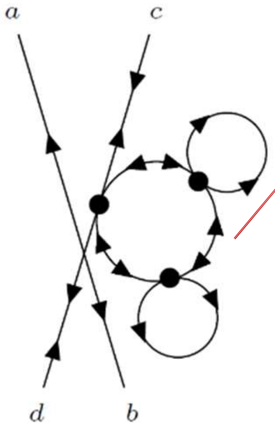
$(3'''\text{bk})$



$(3'''\text{bl})$

$+ \quad \dots$

$$\Pi^{1111\ (3'''bm)}_{acdb}(t,t') = -\boxed{\frac{1}{8\hbar^3}} \sum_{pqrs}\sum_{tuvw}\sum_{klmn} \boxed{\bar v_{\bar p q\bar r s}\bar v_{\bar t u\bar v w}}\, \bar v_{\bar k l\bar m n} \int_{-\infty}^{+\infty} dt_1 \int_{-\infty}^{+\infty} dt_2 \int_{-\infty}^{+\infty} dt_3 \boxed{G^{21\ (0)}_{tu}(t_2,t_2^+)G^{21\ (0)}_{pq}(t_1,t_1^+)}\, G^{12\ (0)}_{wm}(t_2,t_3) G^{12\ (0)}_{sv}(t_1,t_2) G^{12\ (0)}_{nr}(t_3,t_1) G^{21\ (0)}_{kc}(t_3,t) G^{21\ (0)}_{\bar d l}(t_3,t') G^{12\ (0)}_{a\bar b}(t,t')$$

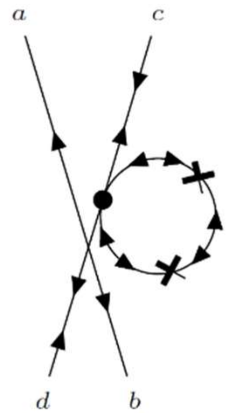


$(3'''\text{bm})$

Equivalent vertices

& two anomalous loops!

Remark: *Equivalent vertices* can be also of one-body type



$(3'''\text{bn})$

Ellipsis: antidiagonally-dr. disjoint Bogoliubov diagrams containing *one-body vertices* and more than one anomalous propagator

Other contributions: conjoint composite, disjoint direct and further disjoint Bogoliubov diagrams

Algebraic diagrammatic construction

Starting-point: the one-body transition operator $\mathcal{D} = \sum_{rs} D_{rs} a_r^\dagger a_s$

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

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

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

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

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 the self energy ($\mathbf{\Sigma}_{ab}^{(\mathrm{dyn})\,+}$)

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

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

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

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 $\mathbf{K}$

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

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

Goldstone diagrams

- In the ADC scheme for the polarization propagator in energy representation, time integrations are carried out by considering the $m+n+2!$ possible orderings of the time indices of the m one-body vertices and n two-body vertices at order $l=m+n$.

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

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

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

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

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 at first order

12 Goldstone graphs at second order

60 Goldstone graphs at third order

360 Goldstone graphs at fourth order

...

Goldstone diagrams

- In the *evaluation* part of the AIWT code, the time-ordered Feynman (≡ *Goldstone*) amplitudes are Fourier-transformed. The $m+n$ time integrations are performed, exploiting the Fourier representation of the *Dirac deltas* and the *theta functions*. The ensuing expressions are given in terms of *spectroscopic amplitudes*.

Example: code for the amplitudes of *disjoint-direct* Goldstone diagrams contributing to $\Pi^{+\,2221}_{acdb}(t,t')$ at third order with $(m,n) = (2,1)$

Entrée [191]:

```
For[r = 1, r <= NcMax, r++,
 For[j = 1, j <= 6, j++,
  For[i = 1, i <= 2, i++,
    If[GGFSParticle[[r, j, i]] == 1 && GGFNambu[[r, j, i]] == 1, SPLIndex[[1]] = "p"];
    If[GGFSParticle[[r, j, i]] == 1 && GGFNambu[[r, j, i]] == 2, SPLIndex[[1]] = OverBar["p"]];
    If[GGFSParticle[[r, j, i]] == 2 && GGFNambu[[r, j, i]] == 1, SPLIndex[[2]] = "q"];
    If[GGFSParticle[[r, j, i]] == 2 && GGFNambu[[r, j, i]] == 2, SPLIndex[[2]] = OverBar["q"]];
    If[GGFSParticle[[r, j, i]] == 3 && GGFNambu[[r, j, i]] == 1, SPLIndex[[3]] = "s"];
    If[GGFSParticle[[r, j, i]] == 3 && GGFNambu[[r, j, i]] == 2, SPLIndex[[3]] = OverBar["s"]];
    If[GGFSParticle[[r, j, i]] == 4 && GGFNambu[[r, j, i]] == 1, SPLIndex[[4]] = "r"];
    If[GGFSParticle[[r, j, i]] == 4 && GGFNambu[[r, j, i]] == 2, SPLIndex[[4]] = OverBar["r"]];
    If[GGFSParticle[[r, j, i]] == 5 && GGFNambu[[r, j, i]] == 1, SPLIndex[[5]] = "e"];
    If[GGFSParticle[[r, j, i]] == 5 && GGFNambu[[r, j, i]] == 2, SPLIndex[[5]] = OverBar["e"]];
    If[GGFSParticle[[r, j, i]] == 6 && GGFNambu[[r, j, i]] == 1, SPLIndex[[6]] = "f"];
    If[GGFSParticle[[r, j, i]] == 6 && GGFNambu[[r, j, i]] == 2, SPLIndex[[6]] = OverBar["f"]];
    If[GGFSParticle[[r, j, i]] == 7 && GGFNambu[[r, j, i]] == 1, SPLIndex[[7]] = "g"];
    If[GGFSParticle[[r, j, i]] == 7 && GGFNambu[[r, j, i]] == 2, SPLIndex[[7]] = OverBar["g"]];
    If[GGFSParticle[[r, j, i]] == 8 && GGFNambu[[r, j, i]] == 1, SPLIndex[[8]] = "h"];
    If[GGFSParticle[[r, j, i]] == 8 && GGFNambu[[r, j, i]] == 2, SPLIndex[[8]] = OverBar["h"]];
    ];
  ];
 Pref = StringForm["``", (-1)^AmplSign[[r]] 3 (-I)^4/ℏ^3 (1/-I)^4 GGFMult[[r]]/96 UMult[[NuIdx]]];
 Vind1 = StringForm["`1``2``3``4`",SPLIndex[[1]], SPLIndex[[2]], SPLIndex[[4]], SPLIndex[[3]]];
 Uins1 = Superscript[Superscript[Subscript["u",Subscript[•,SPLIndex[[5]] SPLIndex[[6]]]],UNambu[[NuIdx,1]]],UNa
 Uins2 = Superscript[Superscript[Subscript["u",Subscript[•,SPLIndex[[7]] SPLIndex[[8]]]],UNambu[[NuIdx,1]]],UNa
 Symb1 = Subscript["∑",Subscript[•,Subscript[k,1]Subscript[k,2]Subscript[k,3]]]
    Subscript["∑",Subscript[•,Subscript[k,4]Subscript[k,5]Subscript[k,6]]]
    Subscript["∑",Subscript[•,pqrs]] Subscript["∑",Subscript[•,efgh]];
 Symb2 = Subscript[OverBar["v"],Subscript[•,Vind1]] Uins1 Uins2;
  TimeIntegralSolutions1 = Solve[Coefficient[GGFTotalPolynomial[[r]], Subscript[t,TimeClassOrdPlus[[T, 2]]]] ==
     Coefficient[GGFTotalPolynomial[[r]], Subscript[t,TimeClassOrdPlus[[T, 3]]]] == 0 &&
     Coefficient[GGFTotalPolynomial[[r]], Subscript[t,TimeClassOrdPlus[[T, 4]]]] == 0, {ϵ, γ, ι}];
  {ϵ, γ, ι} = TimeIntegralSolutions1 // Values // Flatten;
  TimeIntegralSolutions2 = Solve[Coefficient[GGFTotalPolynomial[[r]], Subscript[t,TimeClassOrdPlus[[T, 1]]]] ==
  {ƒ} = TimeIntegralSolutions2 // Values // Flatten;
  GGFGoldstoneAmplitude[[r]] = StringForm["`1``2``3`·`4`·`5`·`6`·`7`", Pref, Symb1,Symb2,
      GGFAmplitude[[r, 1]] GGFAmplitude[[r, 2]]/(ϵ + I Superscript[η,"(0)"]), GGFAmplitude[[r, 3]] GGFAmplitude[
      GGFAmplitude[[r, 5]]/(γ + I Superscript[η,"(2)"]), GGFAmplitude[[r, 6]]/(ι + I Superscript[η,"(3)"])];
  Clear[ƒ];
  Clear[ϵ];
  Clear[γ];
  Clear[ι];
  Clear[TimeIntegralSolutions1];
  Clear[TimeIntegralSolutions2];
  ];
```

Goldstone diagrams

Output: amplitudes of *disjoint-direct* Goldstone diagrams of

$$\Pi^{+\,2221}_{acdb}(t,t')$$

at third order with $(m,n) = (2,1)$ and time ordering

$$t > t_1 > t_2 > t_3 > t'$$

Non-identical one-body vertices of type u^{21}_{ef} and u^{22}_{ef} : multiplicity = *1*

Amplitude of third-order left-and-right-dressed disjoint direct diagrams contributing to Π_{acdb}

with one two-body and two one-body interaction vertices

Conventions

The fully-contracted terms processed henceforth correspond to fully-contracted left-and-right-dressed disjoint direct contributions generated by the application of Wick's theorem to the following matrix element (cf. expansion formula of Gorkov's polarization propagator),

$$\Pi_{acdb}{}^{g_1 g_3 g_4 g_2}\big|_{\text{second order}} = -i\left(\frac{-i}{\hbar}\right)^3 \frac{1}{3!}\, 3 \int dt_1 \int dt_2 \int dt_3 \langle \Phi_0 | \, T\{ \bar{V}(t_1)\, U(t_2)\, U(t_3)\, A_{la}{}^{g_1}(t) A_{lb}{}^{g_2}(t') A_{ld}{}^{\dagger g_4}(t') A_{lc}{}^{\dagger g_3}(t) | \Phi_0\rangle$$

where the one-body and the two-body potential insertions, $\bar{V}(t_1)$ $U(t_2)$ and $U(t_3)$, take the form

$$\bar{V}(t_1) = \frac{1}{4}\sum_{pqrs} \bar{V}_{pqrs}\, a_p^\dagger(t_1)\, a_q^\dagger(t_1)\, a_s(t_1)\, a_r(t_1),$$

$$U(t_2) = \frac{1}{2}\sum_{ef}\left[u_{ef}{}^{11} a_e^\dagger(t_2)\, a_f(t_2) + u_{ef}{}^{22} a_{\bar e}(t_2)\, a_{\bar f}^\dagger(t_2) + u_{ef}{}^{12} a_e^\dagger(t_2)\, a_{\bar f}^\dagger(t_2) + u_{ef}{}^{21} a_{\bar e}(t_2)\, a_f(t_2)\right],$$

$$U(t_3) = \frac{1}{2}\sum_{gh}\left[u_{gh}{}^{11} a_g^\dagger(t_3)\, a_h(t_3) + u_{gh}{}^{22} a_{\bar g}(t_3)\, a_{\bar h}^\dagger(t_3) + u_{gh}{}^{12} a_g^\dagger(t_3)\, a_{\bar h}^\dagger(t_3) + u_{gh}{}^{21} a_{\bar g}(t_3)\, a_h(t_3)\right].$$

. . . .

Results with T = 4, corresponding to {1,2,3,4,5}

```
In[152]:= For[u = 1, u ≤ 24, u++, Print[u, "     ", GGFGoldstoneAmplitude[[u]]]]
```

1 $$-\frac{1}{8\hbar^3}\sum_{k_1k_2k_3}\sum_{k_4k_5k_6}\sum_{pqrs}\sum_{efgh} \bar V_{\bar p q \bar r s}\, u^{21}_{ef}\, u^{22}_{gh} \frac{\chi_p{}^{2k_1}\chi_s{}^{1k_2}\bar\chi_e{}^{2k_2}\bar\chi_q{}^{1k_1}}{-\frac{\Omega_{k_2}-\Omega_{k_3}}{\hbar}+i\eta}\cdot\frac{\chi_a{}^{2k_3}\chi_g{}^{1k_4}\bar\chi_b{}^{2k_4}\bar\chi_r{}^{2k_3}}{\frac{\omega\hbar+2\Omega_0-\Omega_{k_4}-\Omega_{k_5}}{\hbar}+i\eta'}\cdot\frac{\chi_f{}^{1k_5}\bar\chi_d{}^{2k_5}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_5}+\Omega_{k_6}}{\hbar}+i\eta''}\cdot\frac{-\Upsilon_h{}^{2k_6}\bar\Upsilon_c{}^{2k_6}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_3}+\Omega_{k_6}}{\hbar}+i\eta'''}$$

2 $$-\frac{1}{8\hbar^3}\sum_{k_1k_2k_3}\sum_{k_4k_5k_6}\sum_{pqrs}\sum_{efgh} \bar V_{\bar p q \bar r s}\, u^{21}_{ef}\, u^{22}_{gh} \frac{\chi_p{}^{2k_1}\chi_s{}^{1k_2}\bar\chi_e{}^{2k_2}\bar\chi_q{}^{1k_1}}{-\frac{\Omega_{k_2}-\Omega_{k_3}}{\hbar}+i\eta}\cdot\frac{-\Upsilon_g{}^{1k_4}\chi_a{}^{2k_3}\bar\Upsilon_c{}^{2k_4}\bar\chi_r{}^{2k_3}}{\frac{\omega\hbar+2\Omega_0-\Omega_{k_5}-\Omega_{k_6}}{\hbar}+i\eta'}\cdot\frac{\chi_f{}^{1k_5}\bar\chi_d{}^{2k_5}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_4}+\Omega_{k_5}}{\hbar}+i\eta''}\cdot\frac{-\Upsilon_b{}^{1k_6}\bar\Upsilon_h{}^{1k_6}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_3}+\Omega_{k_4}}{\hbar}+i\eta'''}$$

3 $$\frac{1}{8\hbar^3}\sum_{k_1k_2k_3}\sum_{k_4k_5k_6}\sum_{pqrs}\sum_{efgh} \bar V_{\bar p q \bar r s}\, u^{21}_{ef}\, u^{22}_{gh} \frac{\chi_p{}^{2k_1}\chi_s{}^{1k_2}\bar\chi_e{}^{2k_2}\bar\chi_q{}^{1k_1}}{-\frac{-2\Omega_0+\Omega_{k_2}+\Omega_{k_3}}{\hbar}+i\eta}\cdot\frac{-\Upsilon_b{}^{1k_3}\chi_a{}^{2k_4}\bar\Upsilon_r{}^{2k_3}\bar\chi_g{}^{2k_4}}{\frac{\omega\hbar+2\Omega_0-\Omega_{k_3}-\Omega_{k_5}}{\hbar}+i\eta'}\cdot\frac{\chi_h{}^{2k_5}\bar\chi_d{}^{2k_5}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_3}+\Omega_{k_4}}{\hbar}+i\eta''}\cdot\frac{-\Upsilon_f{}^{1k_6}\bar\Upsilon_c{}^{2k_6}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_4}+\Omega_{k_6}}{\hbar}+i\eta'''}$$

4 $$-\frac{1}{8\hbar^3}\sum_{k_1k_2k_3}\sum_{k_4k_5k_6}\sum_{pqrs}\sum_{efgh} \bar V_{\bar p q \bar r s}\, u^{21}_{ef}\, u^{22}_{gh} \frac{\chi_p{}^{2k_1}\chi_s{}^{1k_2}\bar\chi_e{}^{2k_2}\bar\chi_q{}^{1k_1}}{-\frac{-2\Omega_0+\Omega_{k_2}+\Omega_{k_3}}{\hbar}+i\eta}\cdot\frac{-\Upsilon_b{}^{1k_3}\chi_g{}^{1k_4}\bar\Upsilon_r{}^{2k_3}\bar\chi_d{}^{2k_4}}{\frac{\omega\hbar+2\Omega_0-\Omega_{k_3}-\Omega_{k_4}}{\hbar}+i\eta'}\cdot\frac{\chi_a{}^{2k_5}\bar\chi_h{}^{1k_5}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_3}+\Omega_{k_5}}{\hbar}+i\eta''}\cdot\frac{-\Upsilon_f{}^{1k_6}\bar\Upsilon_c{}^{2k_6}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_5}+\Omega_{k_6}}{\hbar}+i\eta'''}$$

5 $$\frac{1}{8\hbar^3}\sum_{k_1k_2k_3}\sum_{k_4k_5k_6}\sum_{pqrs}\sum_{efgh} \bar V_{\bar p qrs}\, u^{21}_{ef}\, u^{22}_{gh} \frac{\chi_p{}^{2k_1}\chi_s{}^{1k_2}\bar\chi_e{}^{2k_2}\bar\chi_q{}^{1k_1}}{-\frac{-2\Omega_0+\Omega_{k_2}+\Omega_{k_3}}{\hbar}+i\eta}\cdot\frac{\chi_g{}^{1k_4}\chi_r{}^{1k_3}\bar\chi_b{}^{2k_4}\bar\chi_d{}^{2k_3}}{\frac{\omega\hbar+2\Omega_0-\Omega_{k_3}-\Omega_{k_4}}{\hbar}+i\eta'}\cdot\frac{\chi_a{}^{2k_5}\bar\chi_f{}^{2k_5}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_3}+\Omega_{k_6}}{\hbar}+i\eta''}\cdot\frac{-\Upsilon_h{}^{2k_6}\bar\Upsilon_c{}^{2k_6}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_5}+\Omega_{k_6}}{\hbar}+i\eta'''}$$

6 $$\frac{1}{8\hbar^3}\sum_{k_1k_2k_3}\sum_{k_4k_5k_6}\sum_{pqrs}\sum_{efgh} \bar V_{\bar p qrs}\, u^{21}_{ef}\, u^{22}_{gh} \frac{\chi_p{}^{2k_1}\chi_s{}^{1k_2}\bar\chi_e{}^{2k_2}\bar\chi_q{}^{1k_1}}{-\frac{-2\Omega_0+\Omega_{k_2}+\Omega_{k_3}}{\hbar}+i\eta}\cdot\frac{-\Upsilon_g{}^{1k_4}\chi_r{}^{1k_3}\bar\Upsilon_c{}^{2k_4}\bar\chi_d{}^{2k_3}}{\frac{\omega\hbar+2\Omega_0-\Omega_{k_3}-\Omega_{k_6}}{\hbar}+i\eta'}\cdot\frac{\chi_a{}^{2k_5}\bar\chi_f{}^{2k_5}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_3}+\Omega_{k_4}}{\hbar}+i\eta''}\cdot\frac{-\Upsilon_b{}^{1k_6}\bar\Upsilon_h{}^{1k_6}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_4}+\Omega_{k_5}}{\hbar}+i\eta'''}$$

7 $$-\frac{1}{8\hbar^3}\sum_{k_1k_2k_3}\sum_{k_4k_5k_6}\sum_{pqrs}\sum_{efgh} \bar V_{\bar p qrs}\, u^{21}_{ef}\, u^{22}_{gh} \frac{\chi_p{}^{2k_1}\chi_s{}^{1k_2}\bar\chi_e{}^{2k_2}\bar\chi_q{}^{1k_1}}{-\frac{\Omega_{k_2}-\Omega_{k_3}}{\hbar}+i\eta}\cdot\frac{-\Upsilon_r{}^{1k_3}\chi_a{}^{2k_4}\bar\Upsilon_c{}^{2k_3}\bar\chi_g{}^{2k_4}}{\frac{\omega\hbar+2\Omega_0-\Omega_{k_5}-\Omega_{k_6}}{\hbar}+i\eta'}\cdot\frac{\chi_h{}^{2k_5}\bar\chi_d{}^{2k_5}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_4}+\Omega_{k_6}}{\hbar}+i\eta''}\cdot\frac{-\Upsilon_b{}^{1k_6}\bar\Upsilon_f{}^{2k_6}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_3}+\Omega_{k_4}}{\hbar}+i\eta'''}$$

Goldstone diagrams

Output: amplitudes of *disjoint-direct* Goldstone diagrams of

$$\Pi^{+\,2221}_{acdb}(t,t')$$

at third order with $(m,n) = (2,1)$ and time ordering

$$t > t_1 > t_2 > t_3 > t'$$

Identical one-body vertices of type u^{11}_{ef}: multipl. = *2!*

Amplitude of third-order left-and-right-dressed disjoint direct diagrams contributing to Π_{acdb}

with a two-body and two one-body interaction vertices

Conventions

The fully-contracted terms processed henceforth correspond to fully-contracted left-and-right-dressed disjoint direct contributions generated by the application of Wick's theorem to the following matrix element (cf. expansion formula of Gorkov's polarization propagator),

... ...

Results with T = 4, corresponding to {1,2,3,4,5}

Entrée [ ]:

```
For[u = 1, u <= NcMax, u++, Print["Framed[",u,",RoundingRadius->10]\" \"GGFGoldstoneAmplitude[[",u,"]]"]]
```

Entrée [226]:

```
Framed[1,RoundingRadius->10]" "GGFGoldstoneAmplitude[[1]]
Framed[2,RoundingRadius->10]" "GGFGoldstoneAmplitude[[2]]
Framed[3,RoundingRadius->10]" "GGFGoldstoneAmplitude[[3]]
Framed[4,RoundingRadius->10]" "GGFGoldstoneAmplitude[[4]]
Framed[5,RoundingRadius->10]" "GGFGoldstoneAmplitude[[5]]
Framed[6,RoundingRadius->10]" "GGFGoldstoneAmplitude[[6]]
Framed[7,RoundingRadius->10]" "GGFGoldstoneAmplitude[[7]]
Framed[8,RoundingRadius->10]" "GGFGoldstoneAmplitude[[8]]
Framed[9,RoundingRadius->10]" "GGFGoldstoneAmplitude[[9]]
Framed[10,RoundingRadius->10]" "GGFGoldstoneAmplitude[[10]]
Framed[11,RoundingRadius->10]" "GGFGoldstoneAmplitude[[11]]
Framed[12,RoundingRadius->10]" "GGFGoldstoneAmplitude[[12]]
Framed[13,RoundingRadius->10]" "GGFGoldstoneAmplitude[[13]]
Framed[14,RoundingRadius->10]" "GGFGoldstoneAmplitude[[14]]
Framed[15,RoundingRadius->10]" "GGFGoldstoneAmplitude[[15]]
Framed[16,RoundingRadius->10]" "GGFGoldstoneAmplitude[[16]]
Framed[17,RoundingRadius->10]" "GGFGoldstoneAmplitude[[17]]
Framed[18,RoundingRadius->10]" "GGFGoldstoneAmplitude[[18]]
```

Out[226]:

$$(1)\ \frac{1}{8\hbar^3}\sum_{efgh}\sum_{pqrs}\sum_{k_1k_2k_3}\sum_{k_4k_5k_6}V_{pqrs}\,u_{ef}^{11}\,u_{gh}^{11}\cdot-\frac{\chi_p^{2k_1}\Upsilon_s^{1k_2}\bar\chi_q^{1k_1}\bar\Upsilon_e^{1k_2}}{-\frac{2\Omega_0-\Omega_{k_2}-\Omega_{k_3}}{\hbar}+i\eta^{(0)}}\cdot-\frac{\chi_a^{2k_3}\Upsilon_b^{1k_4}\bar\chi_r^{2k_3}\bar\Upsilon_g^{1k_4}}{\frac{\omega\hbar+2\Omega_0-\Omega_{k_4}-\Omega_{k_5}}{\hbar}+i\eta^{(1)}}\cdot\frac{\chi_f^{1k_5}\bar\chi_d^{2k_5}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_5}+\Omega_{k_6}}{\hbar}+i\eta^{(2)}}\cdot-\frac{\Upsilon_h^{1k_6}\bar\Upsilon_c^{2k_6}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_3}+\Omega_{k_6}}{\hbar}+i\eta^{(3)}}$$

$$(2)\ -\frac{1}{8\hbar^3}\sum_{efgh}\sum_{pqrs}\sum_{k_1k_2k_3}\sum_{k_4k_5k_6}V_{pqrs}\,u_{ef}^{11}\,u_{\bar g\bar h}^{11}\cdot-\frac{\chi_p^{2k_1}\Upsilon_s^{1k_2}\bar\chi_q^{1k_1}\bar\Upsilon_e^{1k_2}}{-\frac{2\Omega_0-\Omega_{k_2}-\Omega_{k_3}}{\hbar}+i\eta^{(0)}}\cdot-\frac{\chi_a^{2k_3}\Upsilon_g^{2k_4}\bar\chi_r^{2k_3}\bar\Upsilon_c^{2k_4}}{\frac{\omega\hbar+2\Omega_0-\Omega_{k_5}-\Omega_{k_6}}{\hbar}+i\eta^{(1)}}\cdot\frac{\chi_f^{1k_5}\bar\chi_d^{2k_5}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_4}+\Omega_{k_5}}{\hbar}+i\eta^{(2)}}\cdot-\frac{\Upsilon_b^{1k_6}\bar\Upsilon_h^{2k_6}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_3}+\Omega_{k_4}}{\hbar}+i\eta^{(3)}}$$

$$(3)\ \frac{1}{8\hbar^3}\sum_{efgh}\sum_{pqrs}\sum_{k_1k_2k_3}\sum_{k_4k_5k_6}V_{pqrs}\,u_{ef}^{11}\,u_{gh}^{11}\cdot-\frac{\chi_p^{2k_1}\Upsilon_s^{1k_2}\bar\chi_q^{1k_1}\bar\Upsilon_e^{1k_2}}{-\frac{-\Omega_{k_2}+\Omega_{k_3}}{\hbar}+i\eta^{(0)}}\cdot-\frac{\chi_a^{2k_4}\Upsilon_b^{1k_3}\bar\chi_g^{1k_4}\bar\Upsilon_r^{2k_3}}{\frac{\omega\hbar+2\Omega_0-\Omega_{k_3}-\Omega_{k_5}}{\hbar}+i\eta^{(1)}}\cdot\frac{\chi_h^{1k_5}\bar\chi_d^{2k_5}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_3}+\Omega_{k_4}}{\hbar}+i\eta^{(2)}}\cdot-\frac{\Upsilon_f^{1k_6}\bar\Upsilon_c^{2k_6}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_4}+\Omega_{k_6}}{\hbar}+i\eta^{(3)}}$$

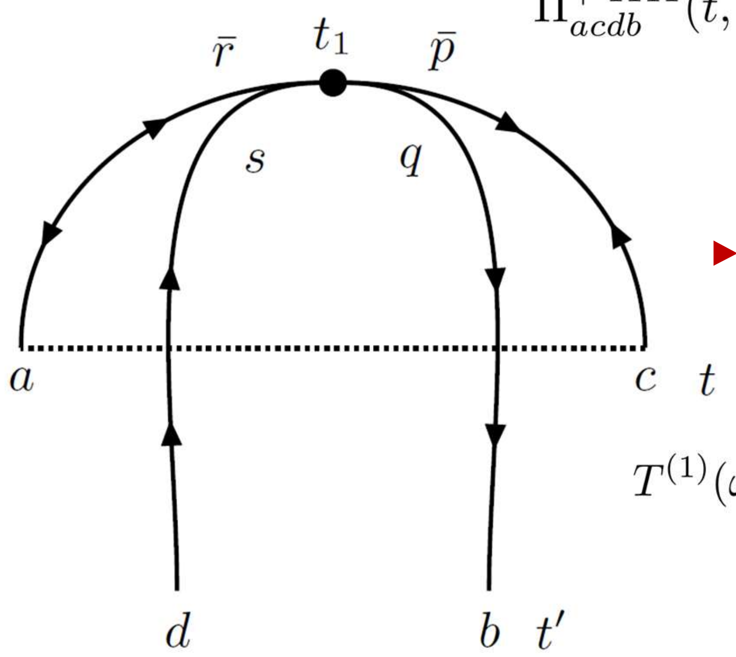
$$(4)\ -\frac{1}{8\hbar^3}\sum_{efgh}\sum_{pqrs}\sum_{k_1k_2k_3}\sum_{k_4k_5k_6}V_{pqrs}\,u_{ef}^{11}\,u_{\bar g\bar h}^{11}\cdot-\frac{\chi_p^{2k_1}\Upsilon_s^{1k_2}\bar\chi_q^{1k_1}\bar\Upsilon_e^{1k_2}}{-\frac{-\Omega_{k_2}+\Omega_{k_3}}{\hbar}+i\eta^{(0)}}\cdot-\frac{\chi_g^{2k_4}\Upsilon_b^{1k_3}\bar\chi_d^{2k_4}\bar\Upsilon_r^{2k_3}}{\frac{\omega\hbar+2\Omega_0-\Omega_{k_3}-\Omega_{k_4}}{\hbar}+i\eta^{(1)}}\cdot\frac{\chi_a^{2k_5}\bar\chi_h^{2k_5}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_3}+\Omega_{k_5}}{\hbar}+i\eta^{(2)}}\cdot-\frac{\Upsilon_f^{1k_6}\bar\Upsilon_c^{2k_6}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_5}+\Omega_{k_6}}{\hbar}+i\eta^{(3)}}$$

$$(5)\ -\frac{1}{8\hbar^3}\sum_{efgh}\sum_{pqrs}\sum_{k_1k_2k_3}\sum_{k_4k_5k_6}V_{pqrs}\,u_{gh}^{11}\,u_{ef}^{11}\cdot-\frac{\chi_p^{2k_1}\Upsilon_s^{1k_2}\bar\chi_q^{1k_1}\bar\Upsilon_e^{1k_2}}{-\frac{-\Omega_{k_2}+\Omega_{k_3}}{\hbar}+i\eta^{(0)}}\cdot-\frac{\chi_r^{1k_3}\Upsilon_b^{1k_4}\bar\chi_d^{2k_3}\bar\Upsilon_g^{1k_4}}{\frac{\omega\hbar+2\Omega_0-\Omega_{k_3}-\Omega_{k_4}}{\hbar}+i\eta^{(1)}}\cdot\frac{\chi_a^{2k_5}\bar\chi_f^{2k_5}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_3}+\Omega_{k_6}}{\hbar}+i\eta^{(2)}}\cdot-\frac{\Upsilon_h^{1k_6}\bar\Upsilon_c^{2k_6}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_5}+\Omega_{k_6}}{\hbar}+i\eta^{(3)}}$$

$$(6)\ \frac{1}{8\hbar^3}\sum_{efgh}\sum_{pqrs}\sum_{k_1k_2k_3}\sum_{k_4k_5k_6}V_{pqrs}\,u_{ef}^{11}\,u_{gh}^{11}\cdot-\frac{\chi_p^{2k_1}\Upsilon_s^{1k_2}\bar\chi_q^{1k_1}\bar\Upsilon_e^{1k_2}}{-\frac{-\Omega_{k_2}+\Omega_{k_3}}{\hbar}+i\eta^{(0)}}\cdot-\frac{\chi_r^{1k_3}\Upsilon_g^{2k_4}\bar\chi_d^{2k_3}\bar\Upsilon_c^{2k_4}}{\frac{\omega\hbar+2\Omega_0-\Omega_{k_3}-\Omega_{k_6}}{\hbar}+i\eta^{(1)}}\cdot\frac{\chi_a^{2k_5}\bar\chi_f^{2k_5}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_3}+\Omega_{k_4}}{\hbar}+i\eta^{(2)}}\cdot-\frac{\Upsilon_b^{1k_6}\bar\Upsilon_h^{2k_6}}{-\frac{-\omega\hbar-2\Omega_0+\Omega_{k_4}+\Omega_{k_5}}{\hbar}+i\eta^{(3)}}$$

First-order Goldstone diagrams

- Example of a *first-order* diagram contributing to $\Pi^{+\,1111}_{acdb}(\omega)$ $(t > t')$, corresponding to corresponding to the time ordering $t_1 > t > t'$ in time representation.



$$\Pi^{+\,1111}_{acdb}(t,t') = \ldots + \frac{1}{\hbar}\sum_{pqrs} \bar{v}_{\bar{p}q\bar{r}s} \int_{-\infty}^{+\infty} dt_1\, G^{(0)\,21}_{pc}(t_1,t^+) G^{11}_{(0)\,bq}(t',t_1) \cdot G^{(0)\,11}_{sd}(t_1,t'^+) G^{(0)\,12}_{ar}(t,t_1)\theta(t-t')\theta(t_1-t) + \ldots$$

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

$$T^{(1)}(\omega) = \ldots + \sum_{abcd}\sum_{pqrs}\sum_{\substack{k_1\,k_2\\k_3\,k_4}} D^*_{ac}\bar{v}_{\bar{p}q\bar{r}s} \frac{{}^{k_1}\chi^{(0)\,2}_{p}\,{}^{k_1}\Upsilon^{(0)\,1}_{c}\,{}^{k_4}\chi^{(0)\,2}_{r}\,{}^{k_4}\Upsilon^{(0)\,1}_{a}}{\omega_{k_{1,0}}+\omega_{k_{2,0}}+\omega_{k_{3,0}}+\omega_{k_{4,0}}} \cdot \frac{{}^{k_2}\chi^{(0)\,1}_{a}\,{}^{k_2}\Upsilon^{(0)\,1}_{b}\,{}^{k_3}\chi^{(0)\,1}_{s}\,{}^{k_3}\Upsilon^{(0)\,1}_{d}}{\omega-\omega_{k_{3,0}}-\omega_{k_{2,0}}+i\eta} D_{db} + \ldots$$

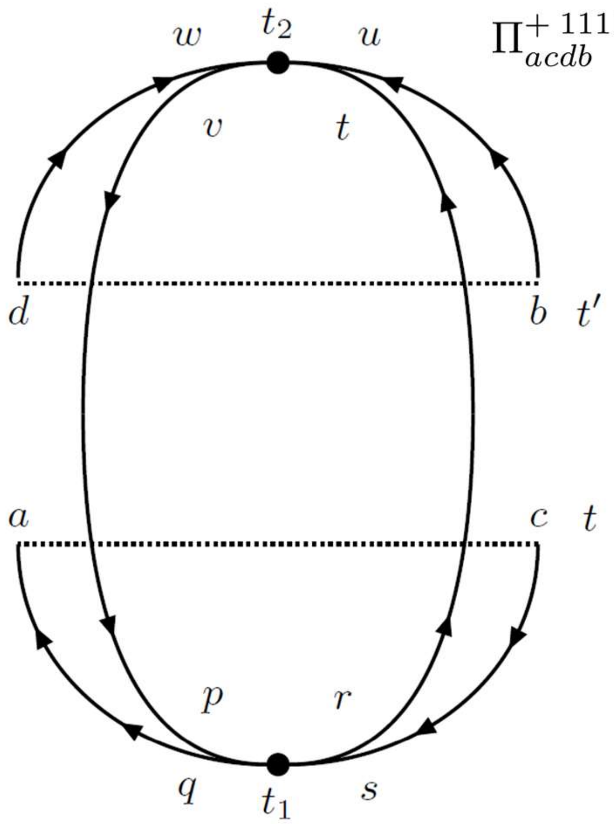
- Due to the SB in Ψ_0, the connection of the 'energies' in the denominators
$$\omega_{k_{m0}} \equiv \omega_{k_m} - \omega_0$$
with the single-particle excitation energies is *less transparent*:

$\omega_{k_1}, \omega_{k_2}, \omega_{k_3}, \omega_{k_4} \Longrightarrow$ 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

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



$$\Pi^{+\,1111}_{acdb}(t,t') = \ldots - \frac{i}{\hbar^2} \sum_{pqrs} \sum_{tuwv} \bar{v}_{pqrs} \bar{v}_{tuvw} \int_{-\infty}^{+\infty} \mathrm{d}t_1 \int_{-\infty}^{+\infty} \mathrm{d}t_2 \, G^{(0)\,11}_{aq}(t,t_1)$$
$$\cdot \; G^{(0)\,11}_{sc}(t_1,t)\, G^{(0)\,11}_{vp}(t_2,t_1)\, G^{(0)\,11}_{rt}(t_1,t_2)\, G^{(0)\,11}_{wd}(t_2,t')$$
$$\cdot \; G^{(0)\,11}_{bu}(t',t_2)\theta(t'-t_1)\theta(t-t')\theta(t_2-t) + \ldots$$

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:

$$T^{(2)}(\omega) = \ldots - i \sum_{abcd} \sum_{pqrs} \sum_{tuwv} \sum_{\substack{k_1 k_2\\ k_3}} \sum_{\substack{k_4 k_5\\ k_6}} D^*_{ac} \bar{v}_{pqrs} \bar{v}_{tuvw} \frac{{}^{k_1}\chi^{(0)\,1}_a \; {}^{k_1}\Upsilon^{(0)\,1}_q \; {}^{k_2}\chi^{(0)\,1}_c \; {}^{k_2}\Upsilon^{(0)\,1}_s}{\omega_{k_1,0} + \omega_{k_2,0} + \omega_{k_3,0} + \omega_{k_4,0}}$$
$$\cdot \; \frac{{}^{k_5}\chi^{(0)\,1}_v \; {}^{k_3}\Upsilon^{(0)\,1}_p \; {}^{k_4}\chi^{(0)\,1}_t \; {}^{k_4}\Upsilon^{(0)\,1}_r}{\omega - (\omega_{k_1,0} + \omega_{k_2,0} + \omega_{k_3,0} + \omega_{k_4,0} + \omega_{k_5,0} + \omega_{k_6,0})/\hbar} \frac{{}^{k_5}\chi^{(0)\,1}_w \; {}^{k_5}\Upsilon^{(0)\,1}_d \; {}^{k_6}\chi^{(0)\,1}_u \; {}^{k_6}\Upsilon^{(0)\,1}_b}{\omega_{k_3,0} + \omega_{k_4,0} + \omega_{k_5,0} + \omega_{k_6,0}} D_{db} + \ldots$$

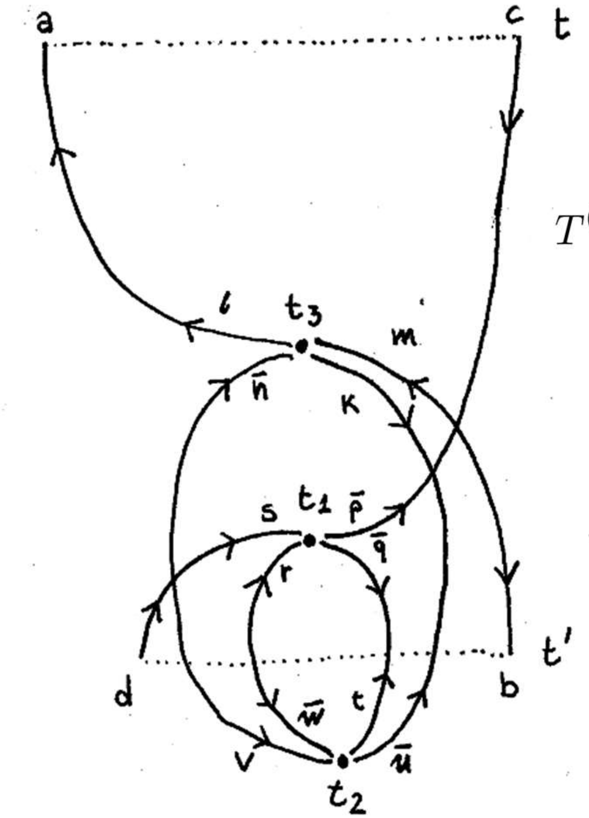
Third-order Goldstone diagrams

Example of a *third-order* Goldstone graph contributing to $\Pi^{+\,1111}_{acdb}(\omega) \quad (t > t')$, corresponding to the time ordering $t > t_3 > t_1 > t' > t_2$ In time representation, it gives:

$$\Pi^{+\,1111}_{acdb}(t,t') = \ldots + \frac{1}{\hbar^3} \sum_{pqrs} \sum_{tuvw} \sum_{klmn} \bar{v}_{\bar{p}\bar{q}rs} \bar{v}_{t\bar{u}v\bar{w}} \bar{v}_{kl\bar{m}\bar{n}} \int_{-\infty}^{+\infty} \mathrm{d}t_1 \int_{-\infty}^{+\infty} \mathrm{d}t_2 \int_{-\infty}^{+\infty} \mathrm{d}t_3$$

$$\cdot \quad G^{(0)\,21}_{pc}(t_1,t) G^{(0)\,11}_{sd}(t_1,t')\, G^{(0)\,21}_{qt}(t_1,t_2)\, G^{(0)\,12}_{rw}(t_1,t_2)\, G^{(0)\,21}_{uk}(t_2,t_3) G^{(0)\,12}_{vn}(t_2,t_3)$$

$$\cdot \quad G^{(0)\,12}_{al}(t,t_3) G^{(0)\,12}_{bm}(t',t_3) \theta(t'-t_2)\theta(t_1-t')\theta(t_3-t_1)\theta(t-t_3) + \ldots$$



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

$$T^{(3)}(\omega) = \ldots - \frac{1}{\hbar^3} \sum_{abcd} \sum_{pqrs} \sum_{tuwv} \sum_{klmn} \sum_{\substack{k_1\\k_3}} \sum_{\substack{k_2\\k_4}} \sum_{\substack{k_5\\k_7}} \sum_{\substack{k_6\\k_8}} D^*_{ac} \bar{v}_{\bar{p}\bar{q}rs}$$

$$\cdot \quad \bar{v}_{t\bar{u}v\bar{w}} \bar{v}_{kl\bar{m}\bar{n}} \frac{{}^{k_5}\chi^{(0)\,2}_{u}\; {}^{k_6}\chi^{(0)\,1}_{v}\; {}^{k_5}\bar{\chi}^{(0)\,1}_{k}\; {}^{k_6}\bar{\chi}^{(0)\,2}_{n}}{\omega + (\omega_{k_{2,0}} - \omega_{k_{5,0}} - \omega_{k_{6,0}} - \omega_{k_{7,0}})/\hbar - i\eta'}$$

$$\cdot \quad \frac{{}^{k_3}\Upsilon^{(0)\,2}_{q}\; {}^{k_4}\Upsilon^{(0)\,1}_{r}\; {}^{k_3}\bar{\Upsilon}^{(0)\,1}_{t}\; {}^{k_4}\bar{\Upsilon}^{(0)\,2}_{w}}{\omega + (\omega_{k_{2,0}} + \omega_{k_{8,0}})/\hbar + i\eta} \frac{{}^{k_7}\chi^{(0)\,1}_{a}\; {}^{k_8}\chi^{(0)\,1}_{b}\; {}^{k_7}\bar{\chi}^{(0)\,1}_{l}\; {}^{k_8}\bar{\chi}^{(0)\,2}_{m}}{\omega - (\omega_{k_{1,0}} + \omega_{k_{7,0}})/\hbar - i\eta''}$$

$$\cdot \quad \frac{{}^{k_1}\Upsilon^{(0)\,2}_{p}\; {}^{k_2}\Upsilon^{(0)\,1}_{s}\; {}^{k_1}\bar{\Upsilon}^{(0)\,1}_{c}\; {}^{k_2}\bar{\Upsilon}^{(0)\,1}_{d}}{\omega_{k_{1,0}} + \omega_{k_{2,0}} + \omega_{k_{3,0}} + \omega_{k_{4,0}}} D_{db} + \ldots$$

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 state-of-the-art of Gorkov's SCGF theory;
  - ✓ defined the polarization propagator in Gorkov's formalism, in time and energy representation, together with its symmetry properties;
  - ✓ derived the self-consistent GBSE obeyed by Gorkov's polarization propagator, and displayed the components of the proper particle-hole vertex up to second SC order;
  - ✓ introduced the *automated implementation of Wick's theorem* (AIWT) code for the perturbative expansion of the polarization propagator up to third order;
  - ✓ displayed examples in diagrammatic form of contributions up to third order in perturbation theory, generated automatically by the AIWT code;
  - ✓ shortly illustrated the ADC approach, its application to the irreducible self-energy and to the polarization propagator, so far exploited in quantum chemistry;
  - ✓ shown examples of Goldstone diagrams, corresponding to expressions in energy repr. generated by the AIWT code, instrumental for the application of the ADC.

Thank you for the attention!

coming soon

LXXXII ESNT Workshop:

«Light Nuclei between single-particle and clustering features»

26^{th}-29^{th} November 2024

Light
Nuclei
Workshop
CEA Paris-Saclay
2024

Commissariat à l'Énergie Atomique et aux Énergies Alternatives - www.cea.fr

Ab initio nuclear many-body problem

- By 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

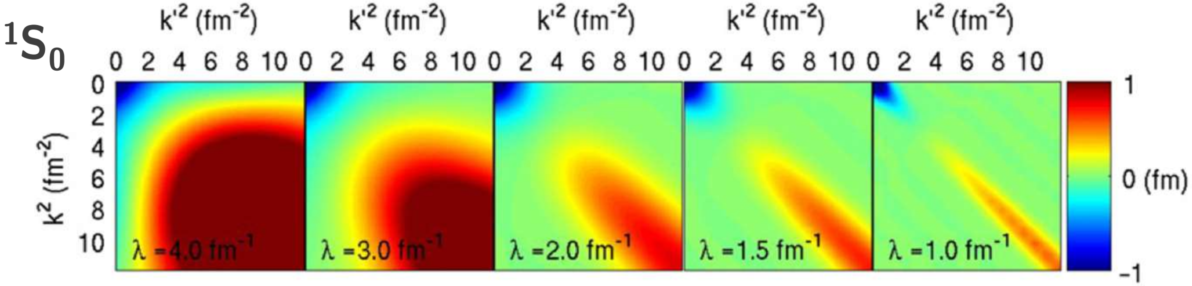
a direct link with low-energy QCD and its symmetries

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 models of nuclear structure

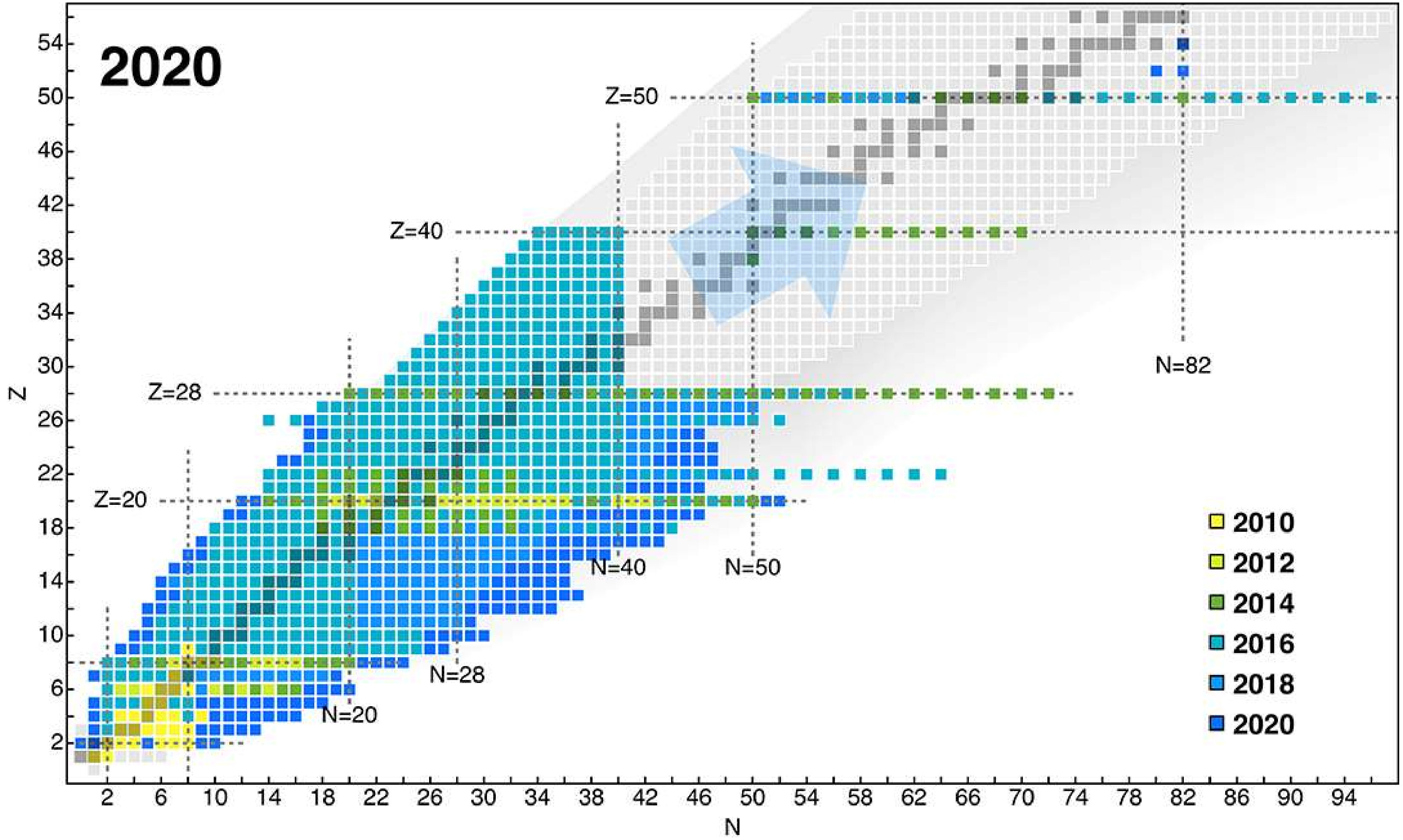
Main approaches:

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]

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 $|b\rangle, \ |\bar{b}\rangle, \in \mathcal{B} \quad \langle b|, \ \langle \bar{b}| \in \mathcal{B}^\dagger$

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:

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

...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*:

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

$$g^\alpha{}_\beta = g^{\alpha\gamma} g_{\gamma\beta} = \delta_{ab} \delta_{l_a l_b} \qquad g_\alpha{}^\beta = g_{\alpha\gamma} g^{\gamma\beta} = \delta_{ab} \delta_{l_a l_b}$$

$g^{\alpha\beta} \wedge g_{\alpha\beta}$ are antidiagonal in both the Nambu and the s.p. space!

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 $U_Z(1) \times U_N(1)$

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

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

the constituents can be added or removed almost *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:

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

Time evolution of operators and states

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

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

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

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

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

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

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 $\Omega_U + \Omega_I^\phi$

Physical observables

- Gorkov's *spectral functions*:

$$\mathbf{S}^{+}_{ab}(\omega) = -\frac{1}{\pi}\mathfrak{Im}\ \mathbf{G}_{ab}(\omega) = \sum_k {}^k\chi_a\ {}^k\chi_b^\dagger \delta(\omega - \omega_k)$$

with $\omega > 0$

$$\mathbf{S}^{-}_{ab}(\omega) = +\frac{1}{\pi}\mathfrak{Im}\ \mathbf{G}_{ab}(\omega) = \sum_k {}^k\Upsilon_a\ {}^k\Upsilon_b^\dagger \delta(\omega + \omega_k)$$

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:

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

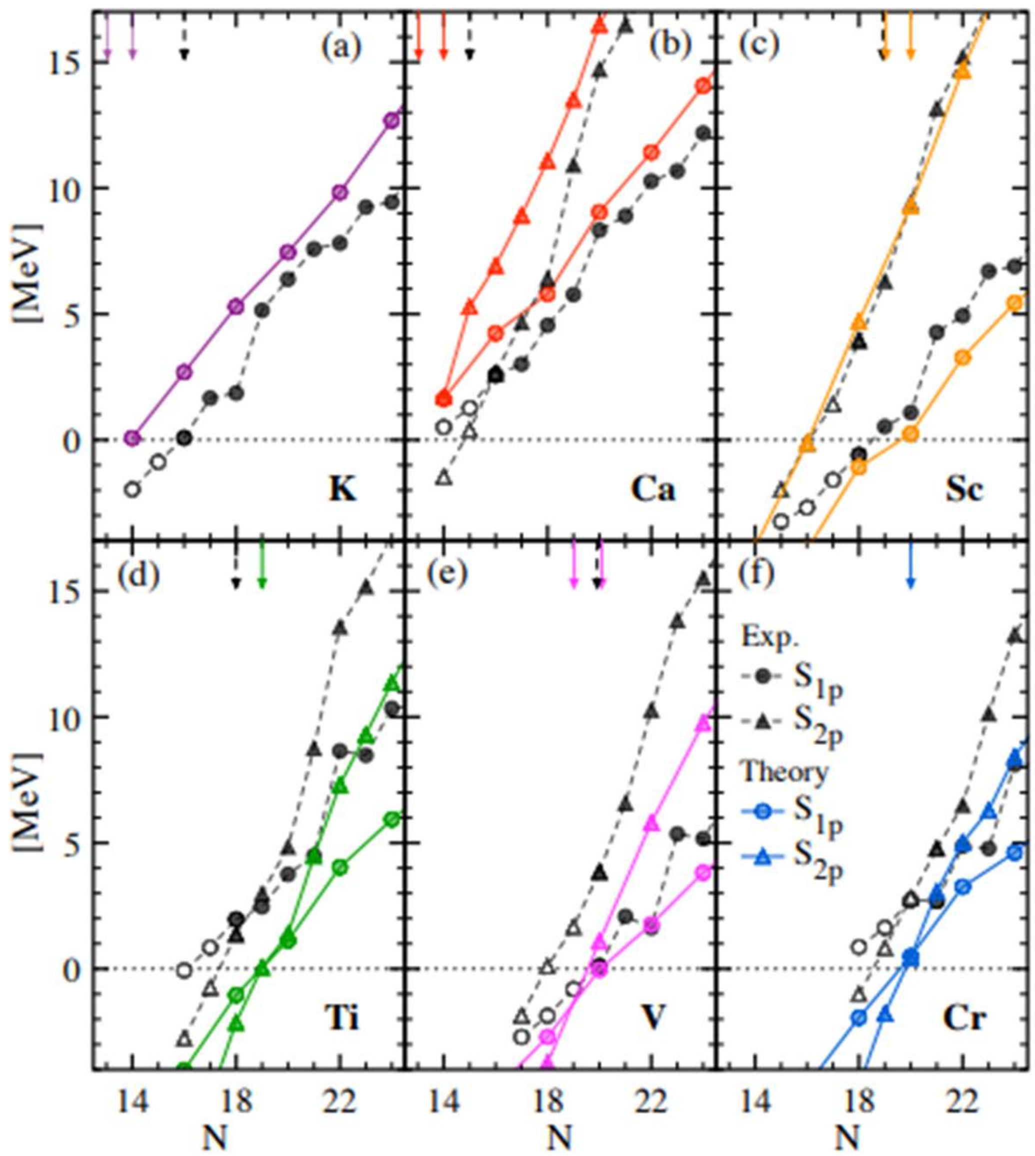
- One and two-proton separation energies:

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

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

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

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



Gorkov's equations

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

$$G_{ab}^{gg'}(t,t') = G_{ab}^{(0)\ gg'}(t,t') + \frac{1}{\hbar}\sum_{g_1 g_2}\sum_{ef}\int_{-\infty}^{+\infty} dt_1 \int_{-\infty}^{+\infty} dt_2\, G_{ae}^{(0)\ gg_1}(t,t_1)\Sigma_{ef}^{\star g_1 g_2}(t_1,t_2) G_{fb}^{g_2 g'}(t_2,t')$$

where the proper self-energy can be split into a two-body part and a contrib. from the aux. potential

$$\Sigma_{ef}^{\star g_1 g_2}(t,t') \equiv \tilde{\Sigma}_{ef}^{\star g_1 g_2}(t,t') - u_{ef}^{g_1 g_2}\delta(t_1 - t_2)$$

and the $G_{ab}^{(0)\ gg'}(t,t')$ are the unperturbed propagators.

Since U acts as a mean field, the Hartree-Fock-Bogoliubov (HFB) one-body propagators, solution of the problem $\Omega_U = \Omega_{\mathrm{HFB}}$ can be exploited for $G_{ab}^{(0)\ gg'}(t,t')$ as well as an input for $G_{ab}^{gg'}(t,t')$ at the r.h.s. of the self-consistent equation. The numerical $G_{ab}^{gg'}(t,t')$ 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 *self-consistent* order

$$\tilde{\Sigma}_{ef}^{\star[1]\ 11}(t_1,t_2) = -\frac{i}{2}\delta(t_1-t_2)\sum_{pq}\bar{v}_{eqfp}G_{pq}^{11}(t_1,t_1^+) + \frac{i}{2}\delta(t_1-t_2)\sum_{pq}\bar{v}_{e\bar{q}f\bar{p}}G_{qp}^{22}(t_1^+,t_1)$$

$$\tilde{\Sigma}_{ef}^{\star[1]\ 12}(t_1,t_2) = -\frac{i}{2}\delta(t_1-t_2)\sum_{pq}\bar{v}_{e\bar{f}p\bar{q}}G_{pq}^{12}(t_1,t_1^+)$$

$$\tilde{\Sigma}_{ef}^{\star[1]\ 21}(t,t') = -\frac{i}{2}\delta(t_1-t_2)\sum_{pq}\bar{v}_{\bar{p}q\bar{e}f}G_{pq}^{21}(t_1,t_1^+)$$

$$\tilde{\Sigma}_{ef}^{\star[1]\ 22}(t,t') = -\delta(t_1-t_2)\frac{i}{2}\sum_{pq}\bar{v}_{\bar{f}\bar{q}\bar{e}\bar{p}}G_{qp}^{22}(t_1^+,t_1) + \delta(t_1-t_2)\frac{i}{2}\sum_{pq}\bar{v}_{\bar{f}q\bar{e}p}G_{pq}^{11}(t_1,t_1^+)$$

Algebraic diagrammatic construction

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:

$$\boldsymbol{\Sigma}^{\star}_{ab}(\omega) = -\mathbf{U}_{ab} + \boldsymbol{\Sigma}^{\star(\text{stat})}_{ab} + \boldsymbol{\Sigma}^{\star(\text{dyn})}_{ab}$$

whose structure is

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

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

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

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

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

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

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

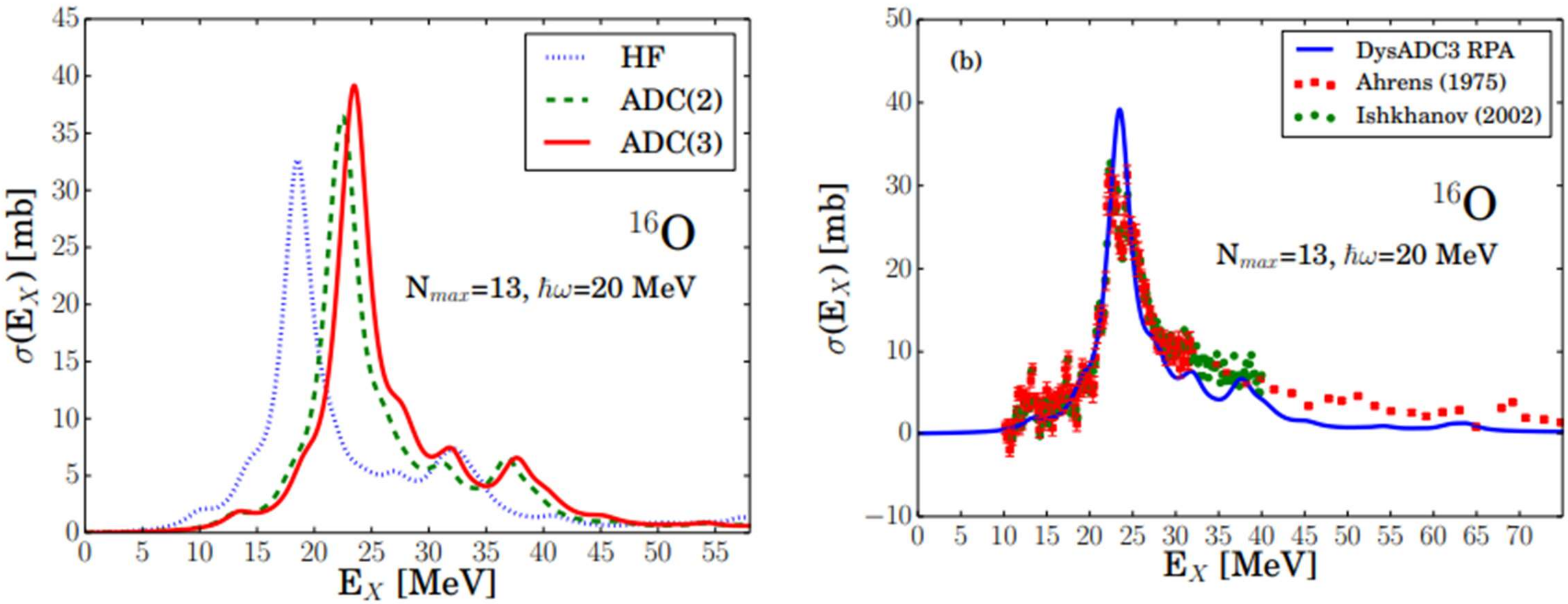
Matching procedure with the std pert. expansion yields the expressions for $\mathbf{C}_a, \mathbf{P}$ and $\mathbf{W}$

$$\boldsymbol{\Sigma}^{\star(\text{dyn})\,+}_{ab}(\omega) \equiv \boldsymbol{\Sigma}^{\star(\text{dyn},1)\,+}_{ab} + \boldsymbol{\Sigma}^{\star(\text{dyn},2)\,+}_{ab} + \dots$$

Phisical observables

- 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)]