Basics of many-body Green's function theory

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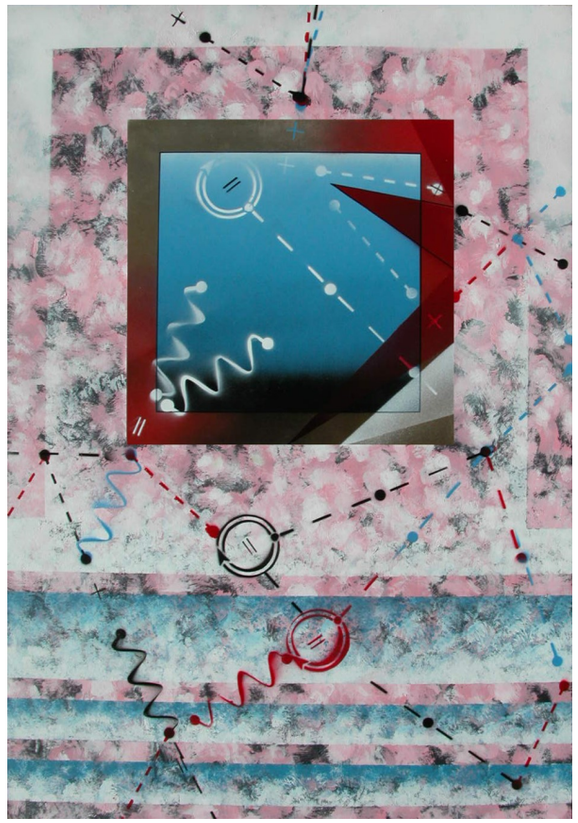
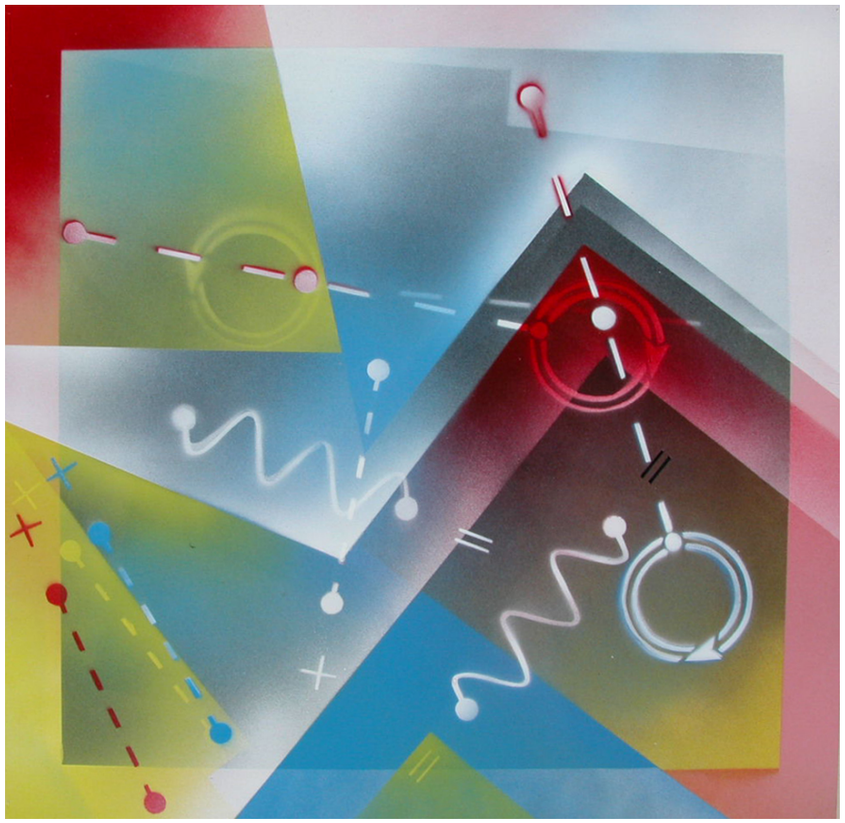


Forze nello spazio I



Forze nello spazio II

Meo Carbone (2014)

ESNT workshop

Near-degenerate systems in nuclear structure and quantum chemistry from ab initio many-body methods

30 March 2015

Outline

1. Introduction and definitions
2. Spectral representation and connection to experiments
3. Calculation methods
4. Approximations to the exact self-energy
5. Extra time: three-body forces and Gorkov formalism

Semantics & history

Many-body Green's function theory: set of techniques that originated in quantum field theory and have then been imported to the many-body problem.

Green's function: mathematical object (see next slide).

Many-body Green's functions are applicable to all sorts of complex/many-body systems: crystals, molecules, atoms, atomic nuclei, …

Self-consistent Green's functions: many-body Green's functions with dressed propagators (see later).

Many-body Green's functions are **not** *Green's function Monte Carlo.*

Late 1950s, 1960s: import of ideas from QFT and development of formalism.

1970s → today: applications and technical developments.

Green's function in maths

In *mathematics*: **solution** of a inhomogeneous **differential equation**

$$[z - L(\boldsymbol{r})]\, G\left(\boldsymbol{r}, \boldsymbol{r}'; z\right) = \delta\left(\boldsymbol{r} - \boldsymbol{r}'\right)$$

complex variable

hermitian operator

$L(\boldsymbol{r})\phi_n(\boldsymbol{r}) = \lambda_n \phi_n(\boldsymbol{r})$

Green's function

Contains information about **eigenstates** & **eigenvalues** of L

$$G(\boldsymbol{r}, \boldsymbol{r}'; z) = \langle \boldsymbol{r}| \frac{1}{z - L} \left[\sum_n |\phi_n\rangle\langle\phi_n|\right] |\boldsymbol{r}'\rangle = \sum_n \langle \boldsymbol{r}| \frac{1}{z - L} |\phi_n\rangle\langle\phi_n \,|\, \boldsymbol{r}'\rangle = \sum_n \frac{\langle \boldsymbol{r} \,|\, \phi_n\rangle\langle\phi_n \,|\, \boldsymbol{r}'\rangle}{z - \lambda_n}$$

more generally

$$G\left(\boldsymbol{r}, \boldsymbol{r}'; z\right) = \sum_n{}' \frac{\phi_n(\boldsymbol{r})\phi_n^*\left(\boldsymbol{r}'\right)}{z - \lambda_n} + \int \mathrm{d}c\, \frac{\phi_c(\boldsymbol{r})\phi_c^*\left(\boldsymbol{r}'\right)}{z - \lambda_c}$$

discrete spectrum

continuous spectrum

One-body system

Substituting $L(\boldsymbol{r}) \to \mathcal{H}(\boldsymbol{r})$, $\lambda \to E$ with $\mathcal{H}(\boldsymbol{r})$ a one-particle Hamiltonian

$$[E - \mathcal{H}(\boldsymbol{r})]G(\boldsymbol{r}, \boldsymbol{r}'; E) = \delta(\boldsymbol{r} - \boldsymbol{r}')$$

which corresponds to the one-particle Schrödinger equation

$$[E - \mathcal{H}(\boldsymbol{r})]\psi(\boldsymbol{r}) = 0$$

The Green's function in the case reads

$$G(\boldsymbol{r}, \boldsymbol{r}'; z) = \sum_n \frac{\phi_n(\boldsymbol{r})\phi_n^*(\boldsymbol{r}')}{z - E_n}$$

Many-body system

By introducing *second-quantised* **annihilation** & **creation** operators we can express

$$G(\boldsymbol{r},\boldsymbol{r}';z)=\sum_n \frac{\langle \boldsymbol{r}\,|\,\phi_n\rangle\langle\phi_n\,|\,\boldsymbol{r}'\rangle}{z-E_n}=\sum_n \frac{\langle 0|a_{\boldsymbol{r}}\,|\,\phi_n\rangle\langle\phi_n\,|\,a^\dagger_{\boldsymbol{r}'}|0\rangle}{z-E_n}$$

one-body

$$G(\boldsymbol{r},\boldsymbol{r}';z)=\sum_\mu \frac{\langle \Psi_0^N|a_{\boldsymbol{r}}\,|\,\Psi_\mu^{N+1}\rangle\langle\Psi_\mu^{N+1}\,|\,a^\dagger_{\boldsymbol{r}'}|\Psi_0^N\rangle}{z-E_\mu^+}+\sum_\nu \frac{\langle \Psi_0^N|a^\dagger_{\boldsymbol{r}'}\,|\,\Psi_\nu^{N-1}\rangle\langle\Psi_\nu^{N-1}\,|\,a_{\boldsymbol{r}}|\Psi_0^N\rangle}{z-E_\nu^-}$$

many-body

with

$|\Psi_0^N\rangle$ → (Exact) ground state of N-body system

$|\Psi_\kappa^{N\pm1}\rangle$ → κ-excited state of ($N\pm1$)-body system

$E_\mu^+\equiv E_\mu^{N+1}-E_0^N$ → one-particle (addition) separation energy

$E_\nu^-\equiv E_0^N-E_\nu^{N-1}$ → one-particle (removal) separation energy

Definition

General case

$$G_{ab}(t,t') \equiv -i\langle \Psi_0^N | \mathcal{T}\left[a_a(t)\, a_b^\dagger(t')\right] | \Psi_0^N \rangle$$

single-particle labels

time-ordering operator

(Exact) ground state of N-body system

➟ It describes the process of **adding** a particle at time t' and **removing** it at time t (or viceversa if $t'>t$)

➟ Hence the equivalent name of **single-particle propagator**

For time-independent Hamiltonians

$$G_{ab}(t,t') = G_{ab}(t-t') \xrightarrow[\text{Fourier transform}]{} G_{ab}(z)$$

Lehmann representation [Lehmann 1954]

$$G_{ab}(z) = \sum_\mu \frac{\langle \Psi_0^N | a_a \,|\, \Psi_\mu^{N+1}\rangle\langle \Psi_\mu^{N+1} \,|\, a_b^\dagger | \Psi_0^N\rangle}{z - E_\mu^+ + i\eta} + \sum_\nu \frac{\langle \Psi_0^N | a_b^\dagger \,|\, \Psi_\nu^{N-1}\rangle\langle \Psi_\nu^{N-1} \,|\, a_a | \Psi_0^N\rangle}{z - E_\nu^- - i\eta}$$

Many-particle Green's functions

One can define up to N-body Green's functions (GFs).

The two-body GF reads

$$G_{2\,abcd}(t_a, t_b, t_c, t_d) \equiv -i\langle \Psi_0^N | \mathcal{T}\left[a_b(t_b)\, a_a(t_a)\, a_c^\dagger(t_c)\, a_d^\dagger(t_d)\right] | \Psi_0^N \rangle$$

More precisely, this is called the **4-point GF**. Depending on the ordering of the 4 times one can then define the two-particle (or two-hole) GF

$$G_{abcd}^{pp/hh}(t, t') \equiv -i\langle \Psi_0^N | \mathcal{T}\left[a_b(t)\, a_a(t)\, a_c^\dagger(t')\, a_d^\dagger(t')\right] | \Psi_0^N \rangle$$

or the particle-hole (~polarisation) propagator

$$G_{abcd}^{ph}(t, t') \equiv -i\langle \Psi_0^N | \mathcal{T}\left[a_b^\dagger(t)\, a_a(t)\, a_c^\dagger(t')\, a_d(t')\right] | \Psi_0^N \rangle$$

Similarly, one can introduce up to $2N$-point GFs.

Observables

For one-body operators

$$\langle \Psi_0^N \,|\, \mathcal{O} \,|\, \Psi_0^N \rangle = \sum_{ab} \int \frac{dz}{2\pi i} G_{ba}(z)\, o_{ab} \qquad \text{with} \qquad o_{ab} = \langle a \,|\, \mathcal{O} | b \rangle$$

The only two-body expectation value that can be computed exactly solely from the one-particle GF is the **total ground-state energy**

$$E_0 = \langle \Psi_0^N \,|\, \mathcal{H} \,|\, \Psi_0^N \rangle = \frac{1}{2} \sum_{ab} \int \frac{dz}{2\pi i} G_{ba}(z)\ [t_{ab} + z\,\delta_{ab}]$$

Galitskii-Migdal-Koltun sum rule [Galitskii & Migdal 1958; Koltun 1972]

where t_{ab} are matrix elements of the kinetic energy operator.

All other two-body observables necessitate the two-body GF.

Single-particle Green's function ⇿ Schrödinger equation

Single-particle GF: matches (psychological & practical) needs of handling one-body objects.

For certain (typically one-body) properties, the **exact single-particle GF** contains the same information as the **exact many-body wave function**, e.g. expectation values of a one-body operator in the ground state.

For others it does not, and one need to resort to higher-body GFs.

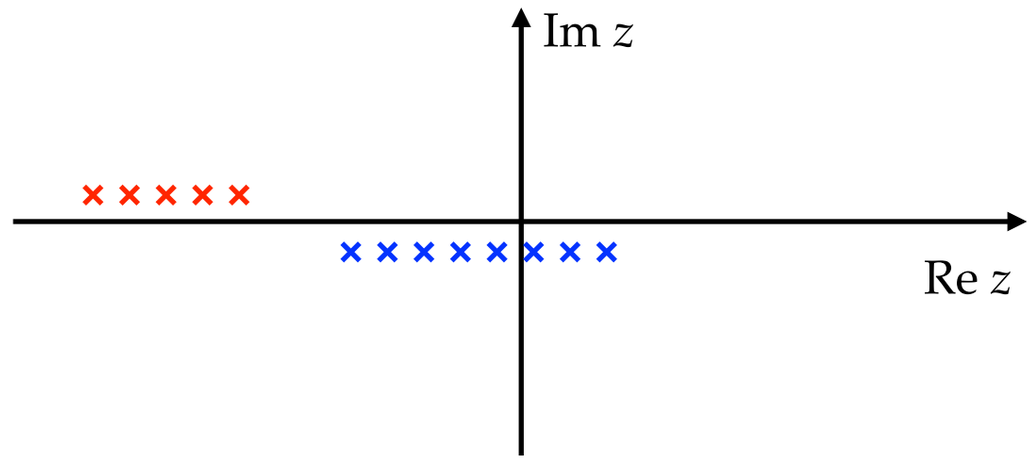
The knowledge of the (N-body) ground state gives us information about ($N\pm1$-body) excited states in a **single calculation** (the magic of Green's functions!).

Spectral representation: *finite* systems

Lehmann or **spectral** representation

$$G_{ab}(z) = \sum_{\mu} \frac{\langle \Psi_0^N | a_a \,|\, \Psi_\mu^{N+1} \rangle \langle \Psi_\mu^{N+1} \,|\, a_b^\dagger | \Psi_0^N \rangle}{z - E_\mu^+ + i\eta} + \sum_{\nu} \frac{\langle \Psi_0^N | a_b^\dagger \,|\, \Psi_\nu^{N-1} \rangle \langle \Psi_\nu^{N-1} \,|\, a_a | \Psi_0^N \rangle}{z - E_\nu^- - i\eta}$$

➟ Set of poles along the real energy axis



Poles represent one-particle excitation energies,
i.e. energies of the ***N*±1-body** system w.r.t. the ground state of the ***N*-body** system

$$E_\mu^+ \equiv E_\mu^{N+1} - E_0^N$$
$$E_\nu^- \equiv E_0^N - E_\nu^{N-1}$$

Spectral representation: *finite* systems

Lehmann or **spectral** representation

$$G_{ab}(z) = \sum_{\mu} \frac{\langle \Psi_0^N | a_a \,|\, \Psi_\mu^{N+1} \rangle \langle \Psi_\mu^{N+1} \,|\, a_b^\dagger | \Psi_0^N \rangle}{z - E_\mu^+ + i\eta} + \sum_{\nu} \frac{\langle \Psi_0^N | a_b^\dagger \,|\, \Psi_\nu^{N-1} \rangle \langle \Psi_\nu^{N-1} \,|\, a_a | \Psi_0^N \rangle}{z - E_\nu^- - i\eta}$$

spectroscopic amplitudes

$$U_\mu^b \equiv \langle \Psi_0^N | a_b \,|\, \Psi_\mu^{N+1} \rangle$$

$$V_\nu^b \equiv \langle \Psi_0^N | a_b^\dagger \,|\, \Psi_\nu^{N-1} \rangle$$

spectroscopic probabilities matrices

$$S_\mu^{+ab} \equiv \langle \Psi_0^{\mathrm{A}} | a_a | \Psi_\mu^{\mathrm{A}+1} \rangle \langle \Psi_\mu^{\mathrm{A}+1} | a_b^\dagger | \Psi_0^{\mathrm{A}} \rangle$$

$$S_\nu^{-ab} \equiv \langle \Psi_0^{\mathrm{A}} | a_a^\dagger | \Psi_\nu^{\mathrm{A\text{-}1}} \rangle \langle \Psi_\nu^{\mathrm{A\text{-}1}} | a_b | \Psi_0^{\mathrm{A}} \rangle$$

spectroscopic factors

$$SF_\mu^+ \equiv \mathrm{Tr}_{\mathcal{H}_1}\left[\mathbf{S}_\mu^+\right] = \sum_{a \in \mathcal{H}_1} \left|U_\mu^a\right|^2$$

$$SF_\nu^- \equiv \mathrm{Tr}_{\mathcal{H}_1}\left[\mathbf{S}_\nu^-\right] = \sum_{a \in \mathcal{H}_1} \left|V_\nu^a\right|^2$$

spectral function

$$\mathbf{S}(z) \equiv \sum_{\mu \in \mathcal{H}_{A+1}} \mathbf{S}_\mu^+ \, \delta(z - E_\mu^+) + \sum_{\nu \in \mathcal{H}_{A-1}} \mathbf{S}_\nu^- \, \delta(z - E_\nu^-)$$

spectral strength distribution

$$\mathcal{S}(z) \equiv \mathrm{Tr}_{\mathcal{H}_1}[\mathbf{S}(z)] = \sum_{\mu \in \mathcal{H}_{A+1}} SF_\mu^+ \, \delta(z - E_\mu^+) + \sum_{\nu \in \mathcal{H}_{A-1}} SF_\nu^- \, \delta(z - E_\nu^-)$$

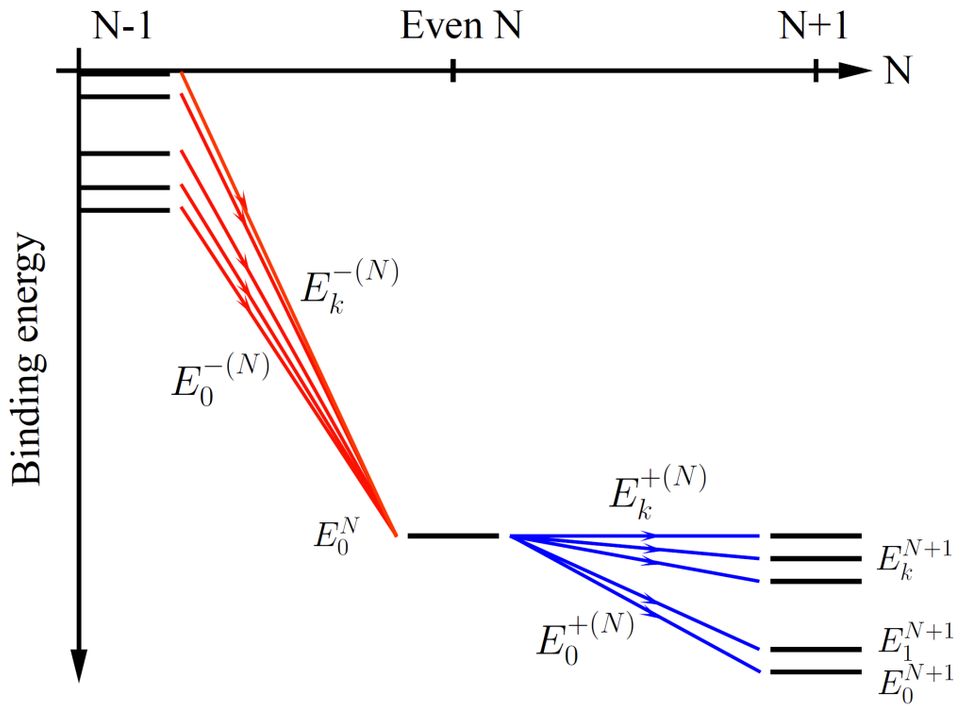
Spectral representation: *finite* systems

Lehmann or **spectral** representation

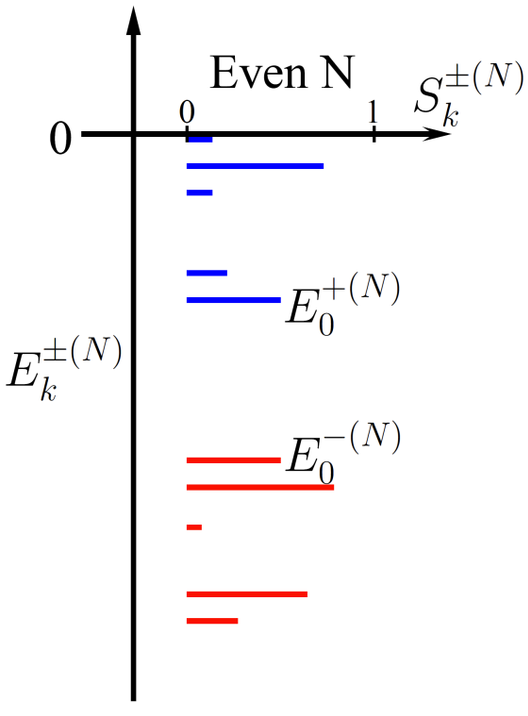
$$G_{ab}(z) = \sum_{\mu} \frac{\langle \Psi_0^N | a_a \mid \Psi_\mu^{N+1} \rangle \langle \Psi_\mu^{N+1} \mid a_b^\dagger | \Psi_0^N \rangle}{z - E_\mu^+ + i\eta} + \sum_{\nu} \frac{\langle \Psi_0^N | a_b^\dagger \mid \Psi_\nu^{N-1} \rangle \langle \Psi_\nu^{N-1} \mid a_a | \Psi_0^N \rangle}{z - E_\nu^- - i\eta}$$

Information contained in the GF

denominator



denominator + numerator

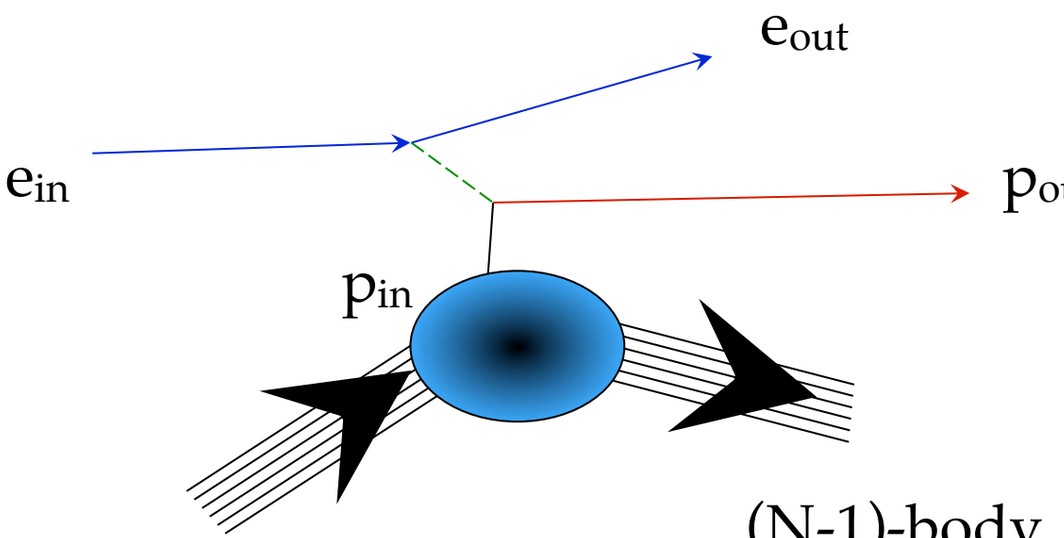


[figure from J. Sadoudi]

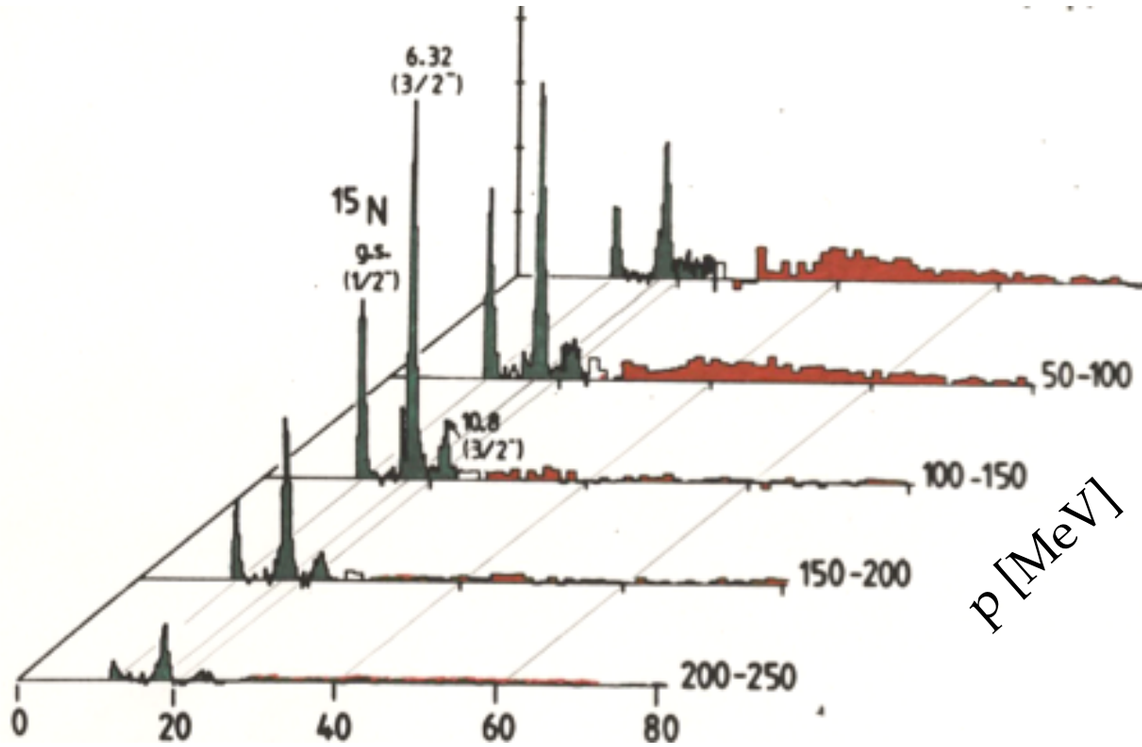
Connection with experiments

Basic idea: spectroscopy via **knock-out reactions**

Use a probe to eject a particle we are interested into



By measuring e_{in}, e_{out} and p_{out}
get information on p_{in}



[Mougey *et al.* 1980]

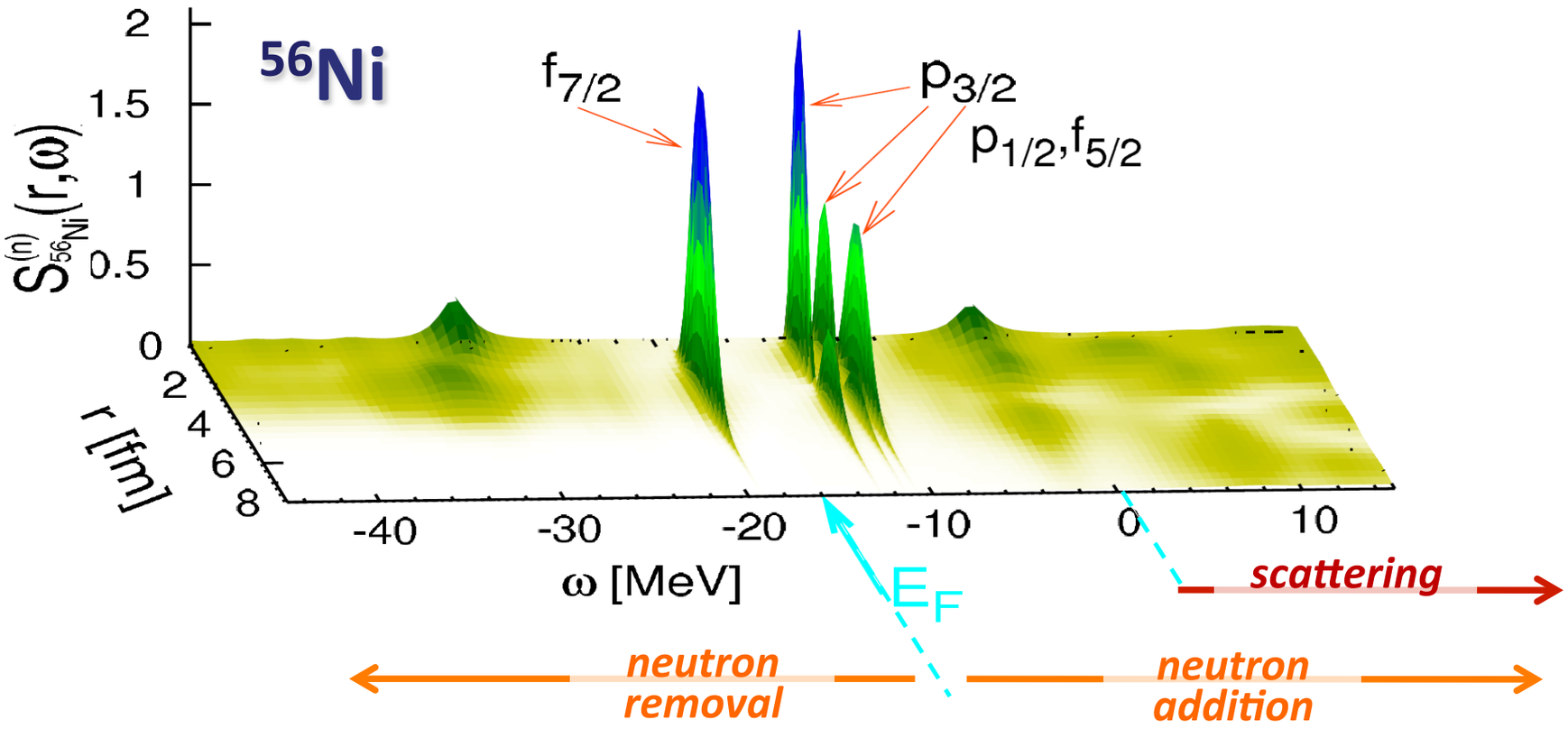
Results from (e,e'p) on ^{16}O
(here in **Saclay**)

➟ Spectral function **S**(ω)

Connection with experiments

Application to one-neutron removal/addition spectrum of ^{56}Ni.

Self-energy truncation: Faddeev RPA (see later).



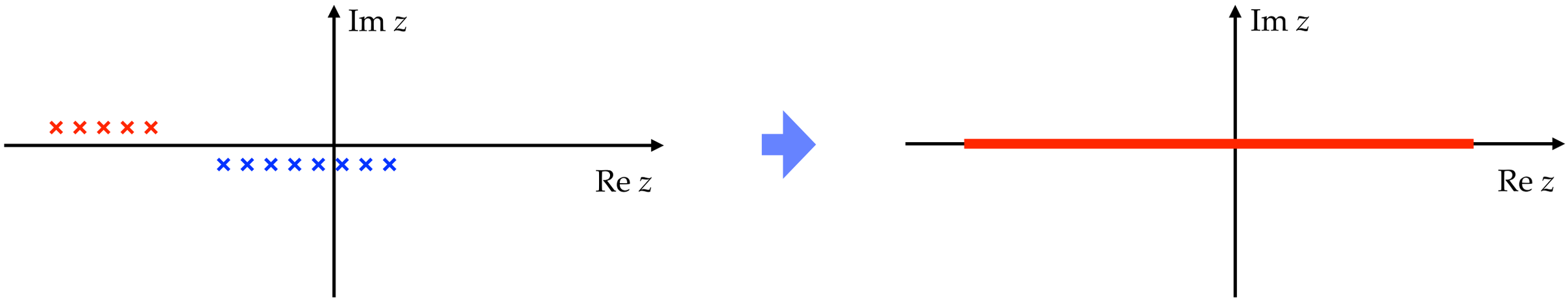
[Barbieri 2009]

Spectral representation: *infinite* systems

For extended systems (large N) excited states become highly degenerate.

Description in terms of isolated exact excitations no longer meaningful.

Smearing of **poles** into **branch cuts:**



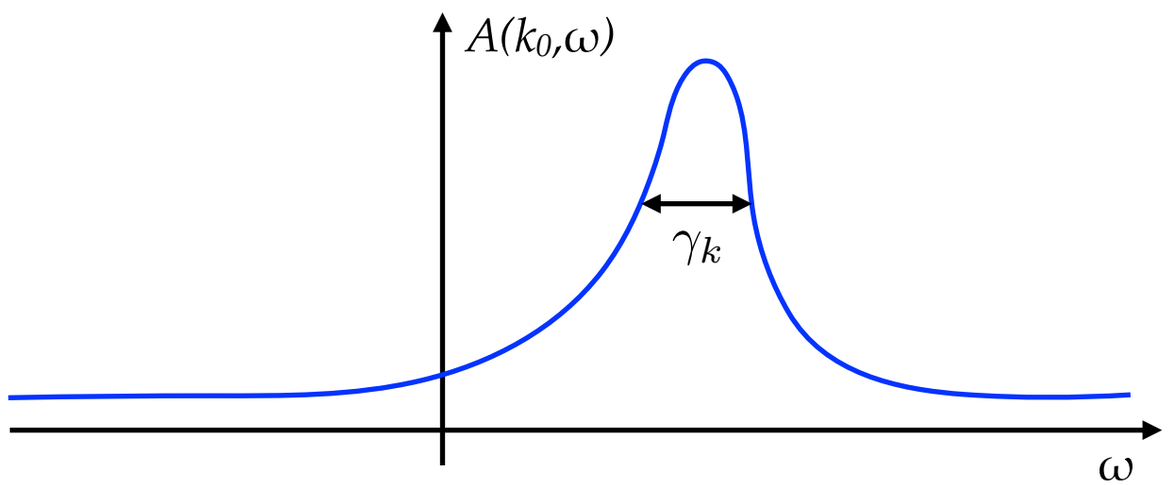
From finite to infinite systems, i.e. taking the thermodynamic limit ($N,V \to \infty$; N/V constant)

$$G_{ab}(z) \longrightarrow G(k,z) = \int \frac{d\omega}{2\pi} \frac{\mathcal{A}(k,\omega)}{z-\omega}$$

spectral function

Spectral representation and quasiparticles

The spectral function describes the dispersion in energy of modes with a given momentum. Excitation of the system would then show up as peaks in A.



Idea: associate a well-defined peak with a **quasiparticle.**

Quasiparticles will have, in general,

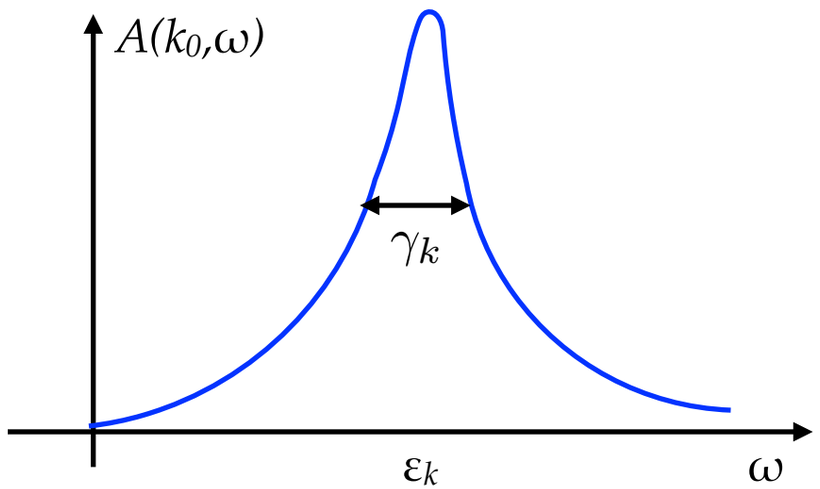
- ➟ Modified or *renormalised* "single-particle" properties (e.g. an effective mass)
- ➟ A **finite lifetime**, physically associated with the damping of the excitation

  The lifetime is given by the width of the quasiparticle peak

$$\tau \sim \gamma_k^{-1}$$

Spectral representation and quasiparticles

Example: Lorentzian spectral function



$$\mathcal{A}(k,\omega) = \frac{2\xi_k\gamma_k}{(\omega-\varepsilon_k)^2+\gamma_k}$$

In this case the Fourier transform can be computed analytically

$$\begin{aligned}\mathcal{A}(k,t) &= \int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}e^{-i\omega t}\frac{2\xi_k\gamma_k}{(\omega-\varepsilon_k)^2+\gamma_k^2} = \int_C\frac{\mathrm{d}z}{2\pi}e^{-izt}\frac{2\xi_k\gamma_k}{(z-z_k)(z-z_k^*)}\\ &= \xi_k e^{-i\varepsilon_k t}e^{-\gamma_k|t|}\end{aligned}$$

- ➟ Damped quasiparticles with a characteristic time $\tau \sim \gamma_k^{-1}$
- ➟ Damping arises from interactions with other quasiparticles
- ➟ Energy & width of the peak correspond to Re and Im of a pole of G

$$z_k = \varepsilon_k + i\gamma_k$$

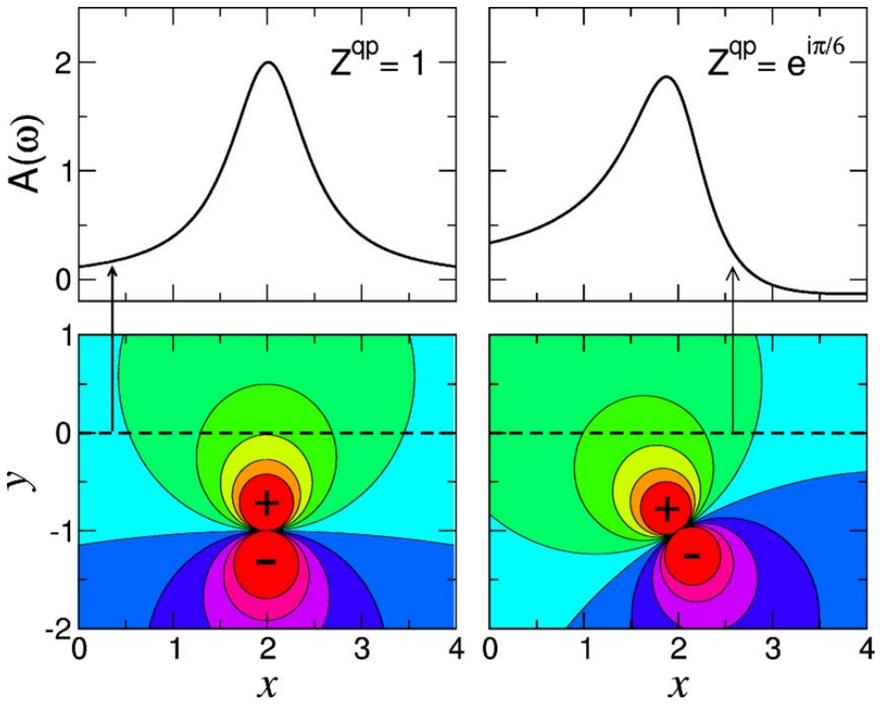
Ab initio quasiparticles

General case: look for a pole of G in the complex energy plane.

However, causality imposes analyticity of G in the upper half plane $\mathrm{Im}\, z > 0$.

Because of the reflection property $G(k,z)^* = G(k,z^*)$, i.e. there is **no pole**!

Solution: the pole appears in an *unphysical Riemann sheet* of G.



[Eiguren, Ambrosch-Draxl & Echenique 2008]

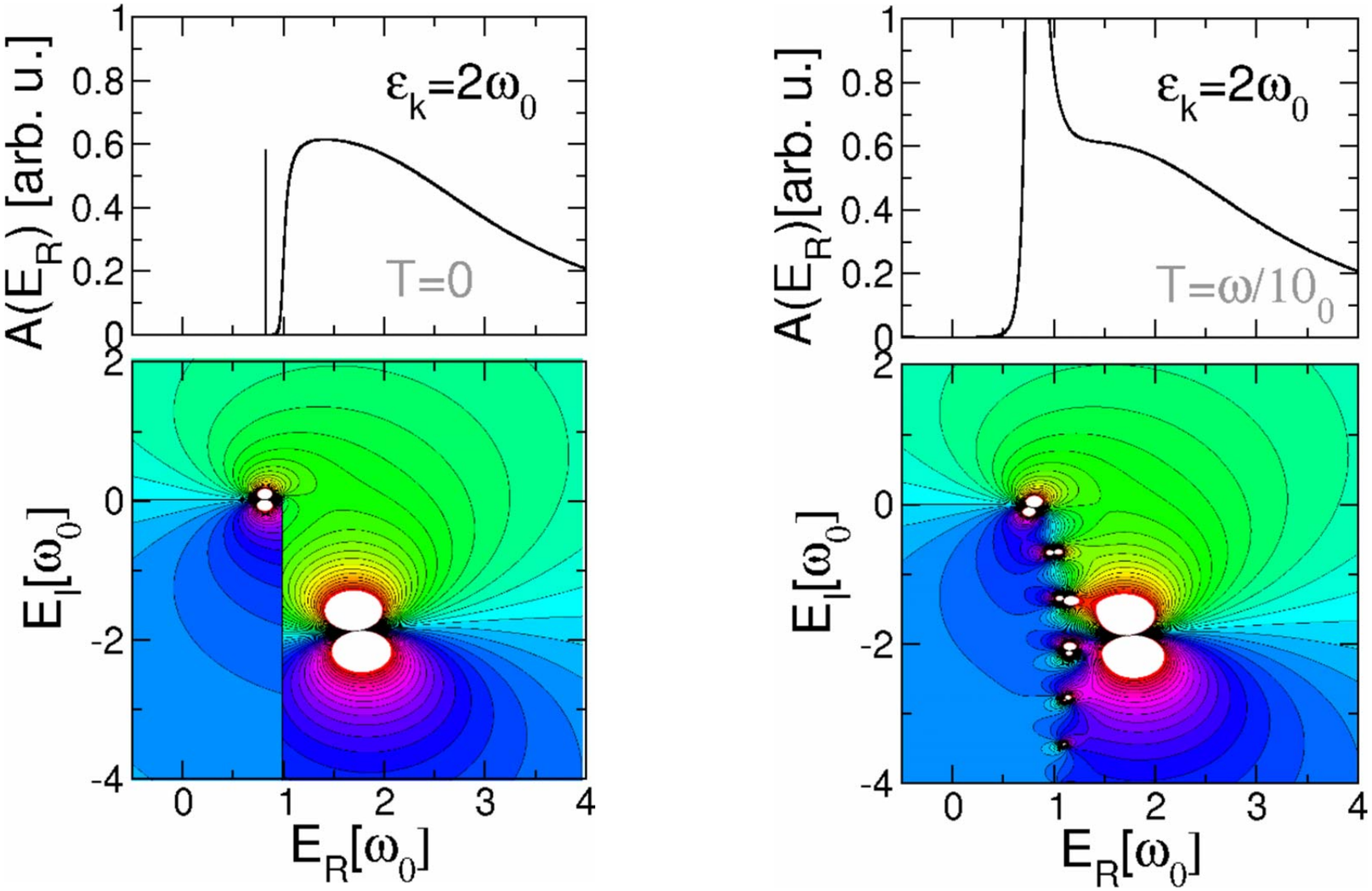
➟ Analytical continuation is performed from the physical Riemann sheet across the branch cut on the real axis

➟ Good control over the energy dependence of the propagator is needed

➟ Achieved only recently for electronic and nucleonic systems

Ab initio quasiparticles

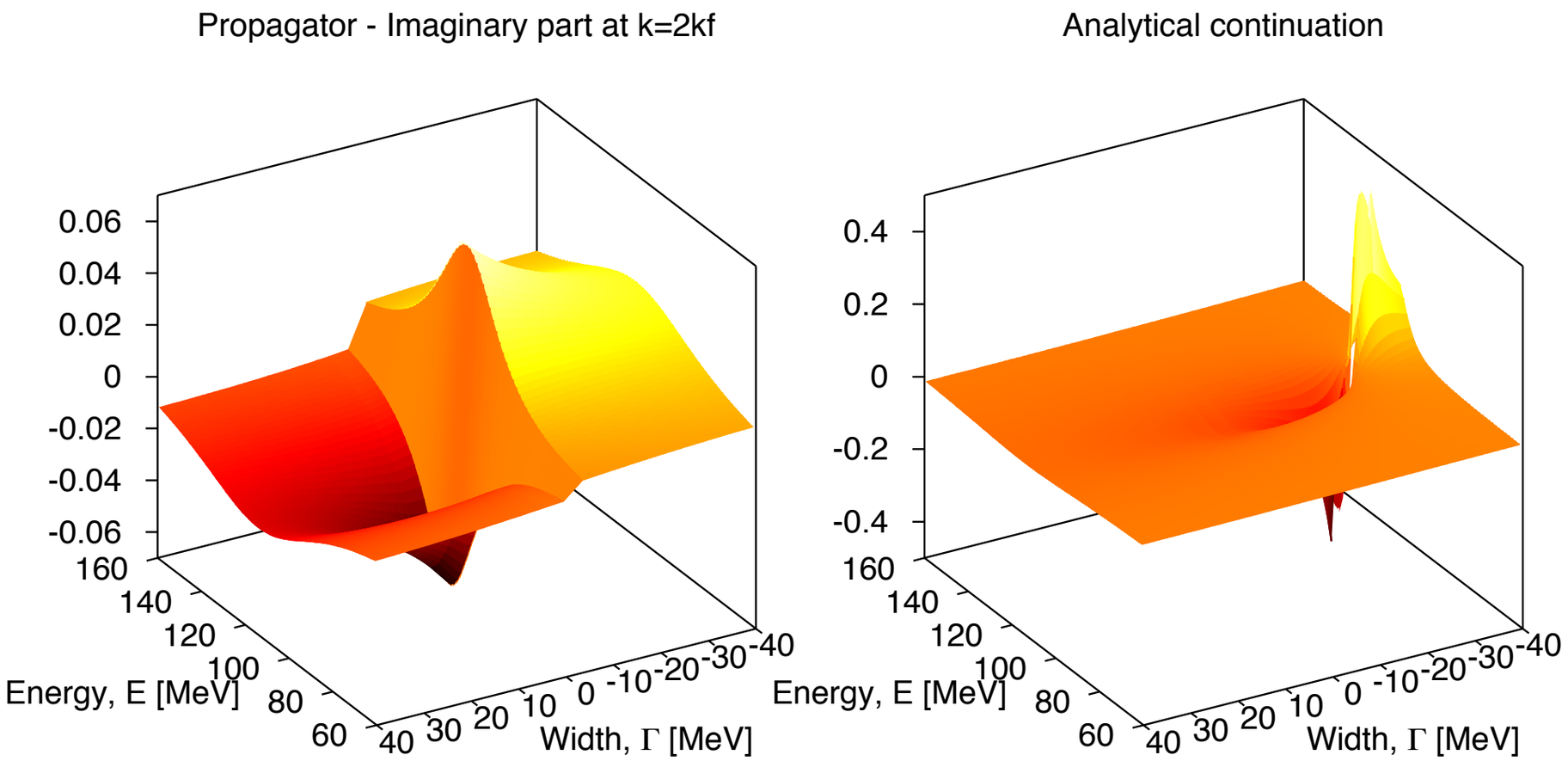
Electron-phonon Einstein model



[Eiguren, Ambrosch-Draxl & Echenique 2008]

Ab initio quasiparticles

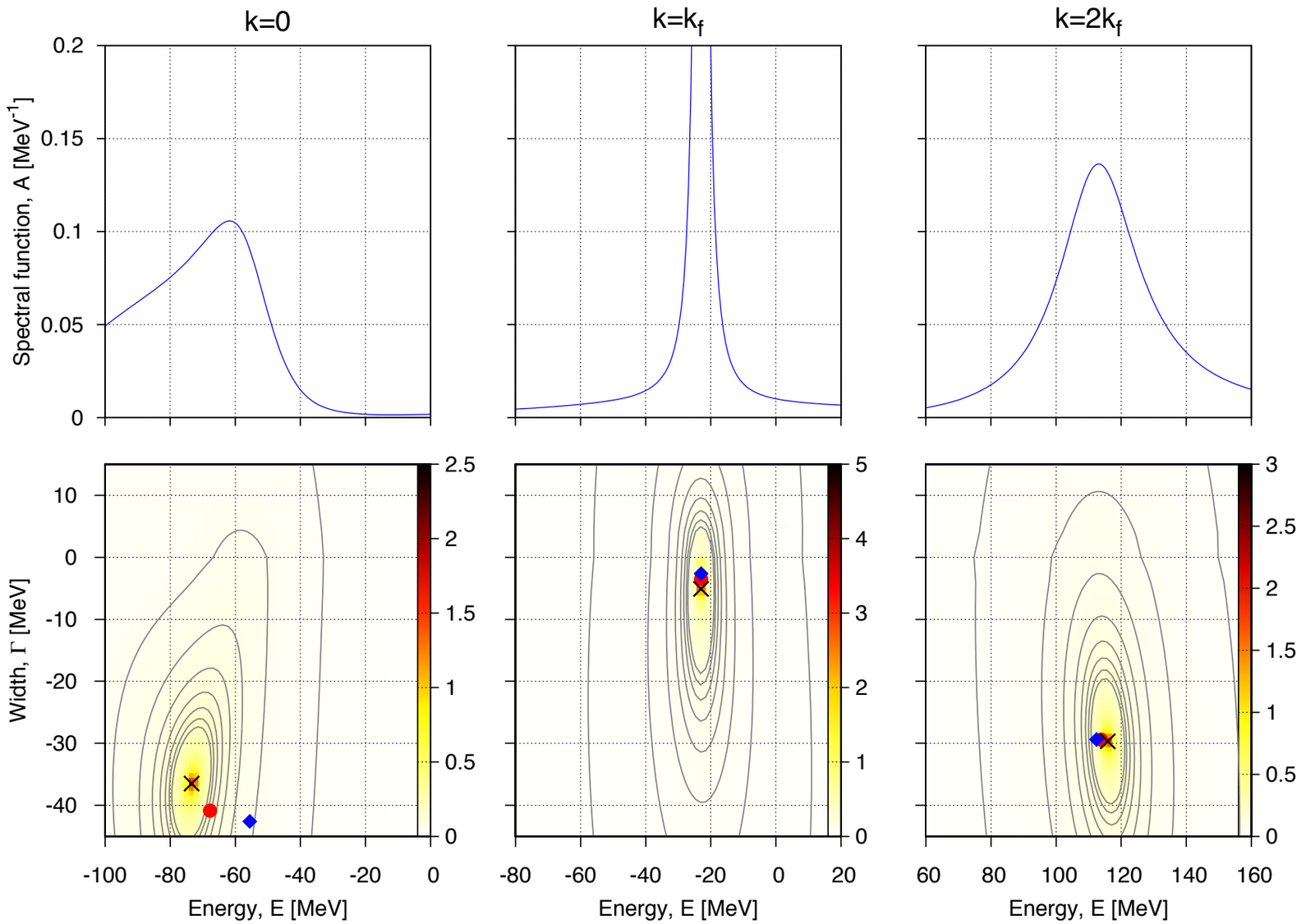
Infinite nuclear matter



[Rios & Somà 2012 + in preparation]

Ab initio quasiparticles

Infinite nuclear matter



[Rios & Somà 2012 + in preparation]

Recap

The *exact* **one-body** G contains some of the information contained in the *exact* ***N*-body** w.f.

- ➟ Specifically, all one-body properties + ground state energy
- ➟ *Finite systems:* spectroscopy of ***N*±*1*-body** neighbours
- ➟ *Infinite systems:* elementary **collective** or **coherent** excitations
- ➟ If we need more, compute G_2, G_3, …

In the following, let us look at how G is typically computed.

Calculation methods for G

I) Equation of motion method

The Green's functions for an interacting many-body system obey a hierarchy of equations (which can be derived starting from the eq. of motion of annihilation/creation operators).

The first one reads [$1 \equiv (\boldsymbol{r}_1, t_1)$]

$$\left(i\frac{\partial}{\partial t_1} + \frac{\nabla^2_{r_1}}{2m} \right) G(1,2) = \delta(1,2) - \int d\,3\, v(1^+,3)\, G_2(1,3;2,3^+)$$

The second one connects G_2 and G_3, and so on…

Simple example: Hartree approximation

$$G_2(1,2;1',2') \approx G(1,1')\, G(2,2')$$

$$\left[i\frac{\partial}{\partial t_1} + \frac{\nabla^2_{r_1}}{2m} + V_H(1) \right] G(1,2) = \delta(1,2) \qquad \text{with} \qquad V_H(1) \equiv \int d\,2\, v(1,2)\, G(2,2^+)$$

i.e. a particle that moves independently in the potential V_H.

Calculation methods for G

In general, one needs to decouple the system of N integro-differential equations.
Introduce an external fictitious time-dependent potential φ. Then

$$G_2(3,4;2,4^+;[\varphi]) = G(3,2;[\varphi])G(4,4^+;[\varphi]) - \frac{\delta G(3,2;[\varphi])}{\delta\varphi(4)}$$

$$G(1,2;[\varphi]) = G_0(1,2) + \int d3\, G_0(1,3)V_{\rm H}(3;[\varphi])G(3,2;[\varphi]) + \int d3\, G_0(1,3)\varphi(3)G(3,2;[\varphi]) + {\rm i}\int d4d3\, G_0(1,3)v(3^+,4)\frac{\delta G(3,2;[\varphi])}{\delta\varphi(4)}$$

Dyson equation

$$G(1,2) = G_0(1,2) + \int d3\, G_0(1,3)V_{\rm H}(3)G(3,2) + \int d4d3\, G_0(1,3)\Sigma(3,4)G(4,2)$$

where one has introduced the **self-energy**

$$\Sigma(1,3) = {\rm i}\int d4d2\, v(1^+,4)\frac{\delta G(1,2;[\varphi])}{\delta\varphi(4)}\Big|_{\varphi=0} G^{-1}(2,3)$$

➟ All many-body effects are transferred from N-body GFs to the self-energy

➟ In practise, approximations are performed at the self-energy level

Calculation methods for G

II) Diagrammatic method

Basic idea:

1) Separate full Hamiltonian into unperturbed part + perturbation

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$$

2) Compute unperturbed propagator

$$G_0(z) = (z - \mathcal{H}_0)^{-1}$$

3) Express full propagator in terms of G_0 and $\mathcal{H}_1$

Simple in the case of **one-particle** system:

$$\begin{aligned} G(z) = (z - \mathcal{H}_0 - \mathcal{H}_1)^{-1} &= \left\{ (z - \mathcal{H}_0) \left[1 - (z - \mathcal{H}_0)^{-1} \mathcal{H}_1 \right] \right\}^{-1} \\ &= \left[1 - (z - \mathcal{H}_0)^{-1} \mathcal{H}_1 \right]^{-1} (z - \mathcal{H}_0)^{-1} \\ &= \left[1 - G_0(z) \mathcal{H}_1 \right]^{-1} G_0(z) \, . \end{aligned}$$

expand $(1 - G_0 \mathcal{H}_1)^{-1}$ in power series

$$G = G_0 + G_0 \mathcal{H}_1 \left(G_0 + G_0 \mathcal{H}_1 G_0 + \cdots \right) = G_0 + G_0 \mathcal{H}_1 G$$

Calculation methods for G

Many-body case more complicated:

➟ Separation $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$ exploited by working in *interaction representation*

➟ One-body Green's function is expanded as (now $\mathcal{H}_1 = v$)

$$G(1,1') = \frac{\displaystyle\sum_n \cdots \int\int \cdots G^{(0)}_{2n+1}(\overbrace{1,1';2,2';3,3';\cdots}^{4n+2 \text{ variables}}) \overbrace{v\cdots v\cdots}^{n \text{ terms}}}{\displaystyle\sum_n \cdots \int\int \cdots G^{(0)}_{2n}(\underbrace{2,2';3,3';\cdots}_{4n \text{ variables}}) \underbrace{v\cdots v\cdots}_{n \text{ terms}}}$$

➟ *Unperturbed* many-body GFs can be written just as *products* of one-body GFs

$$G^{(0)}_{2n}(\underbrace{1,1';2,2';3,3';\cdots}_{4n \text{ variables}}) = \sum_{\text{permutations}} (-1)^P \underbrace{G^{(0)}(1,\tilde{1}')\cdots G^{(0)}(2n,\tilde{2n}')}_{2n \text{ one-body GFs}} \qquad \textbf{(Wick theorem)}$$

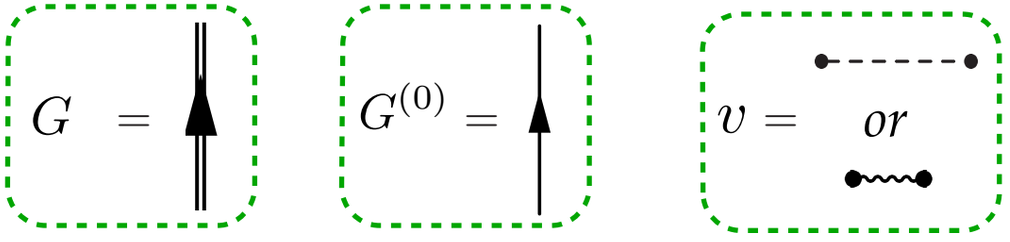
➟ Several terms cancel out (all disconnected combinations of variables), at the end:

$$G = \sum_n \sum_{\text{connected}} \underbrace{G^{(0)}\cdots G^{(0)}\cdots}_{2n+1 \text{ propagators}} \underbrace{v\cdots v\cdots}_{n \text{ interactions}}$$

Better to introduce **Feynman diagrams** and work out the expansion diagrammatically

Diagrammatic expansion

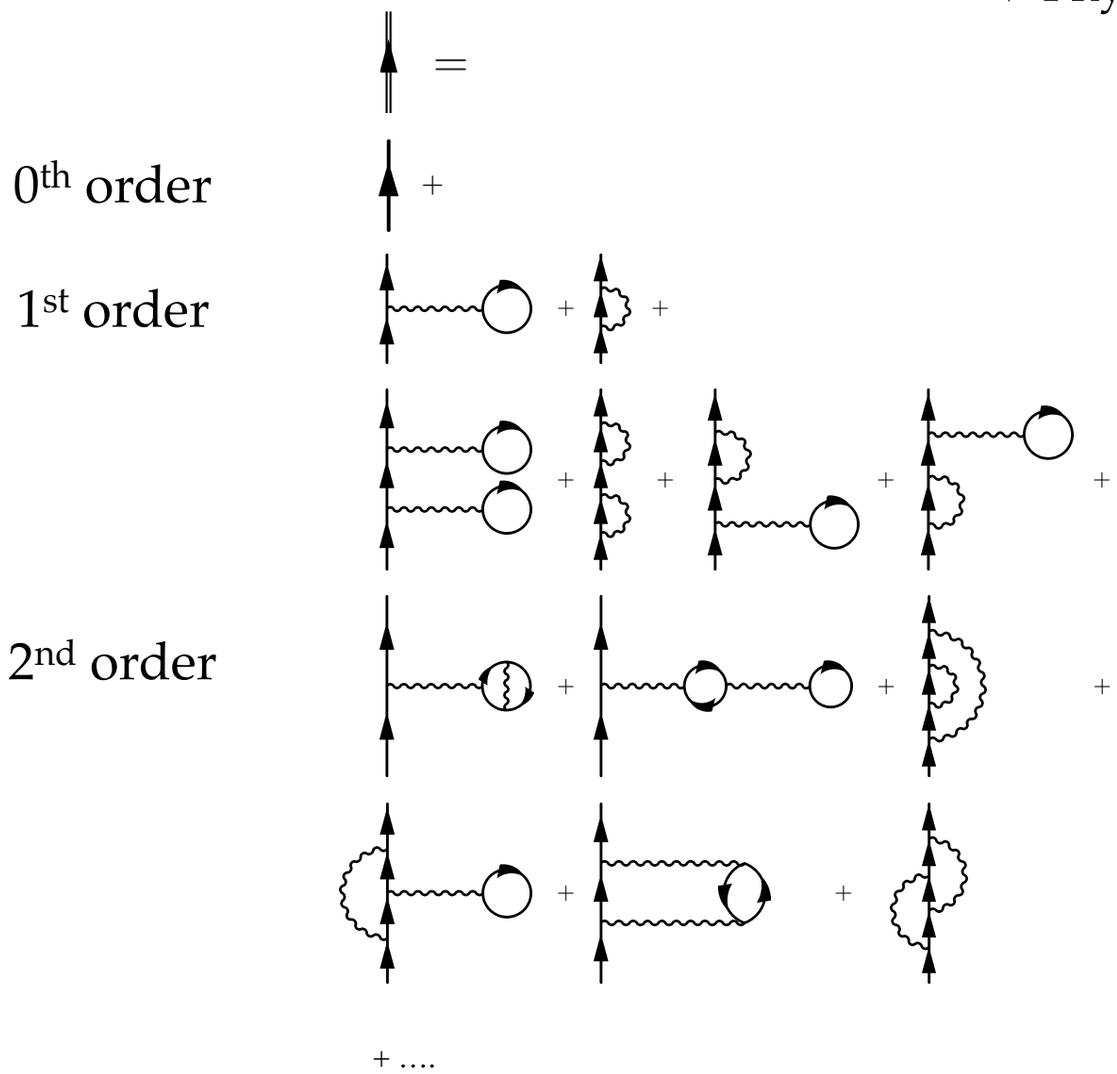
Introduce exact / unperturbed propagators and interaction lines



in $$G = \sum_{n} \sum_{\text{connected}} \underbrace{G^{(0)} \cdots G^{(0)} \cdots}_{2n+1 \text{ propagators}} \underbrace{v \cdots v \cdots}_{n \text{ interactions}}$$

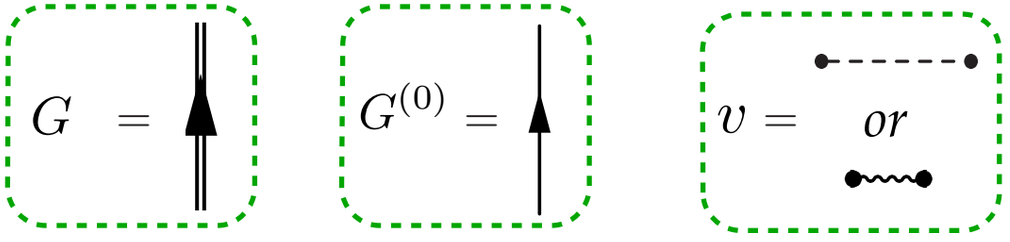
and write down the expansion for G

- ✓ All topologically different diagrams contribute at a given order
- ✓ Physical processes can be associated to Feynman diagrams



Diagrammatic expansion

Introduce unperturbed / exact propagators and interaction lines



in $$G = \sum_{n} \sum_{\text{connected}} \underbrace{G^{(0)} \cdots G^{(0)} \cdots}_{2n+1 \text{ propagators}} \underbrace{v \cdots v \cdots}_{n \text{ interactions}}$$

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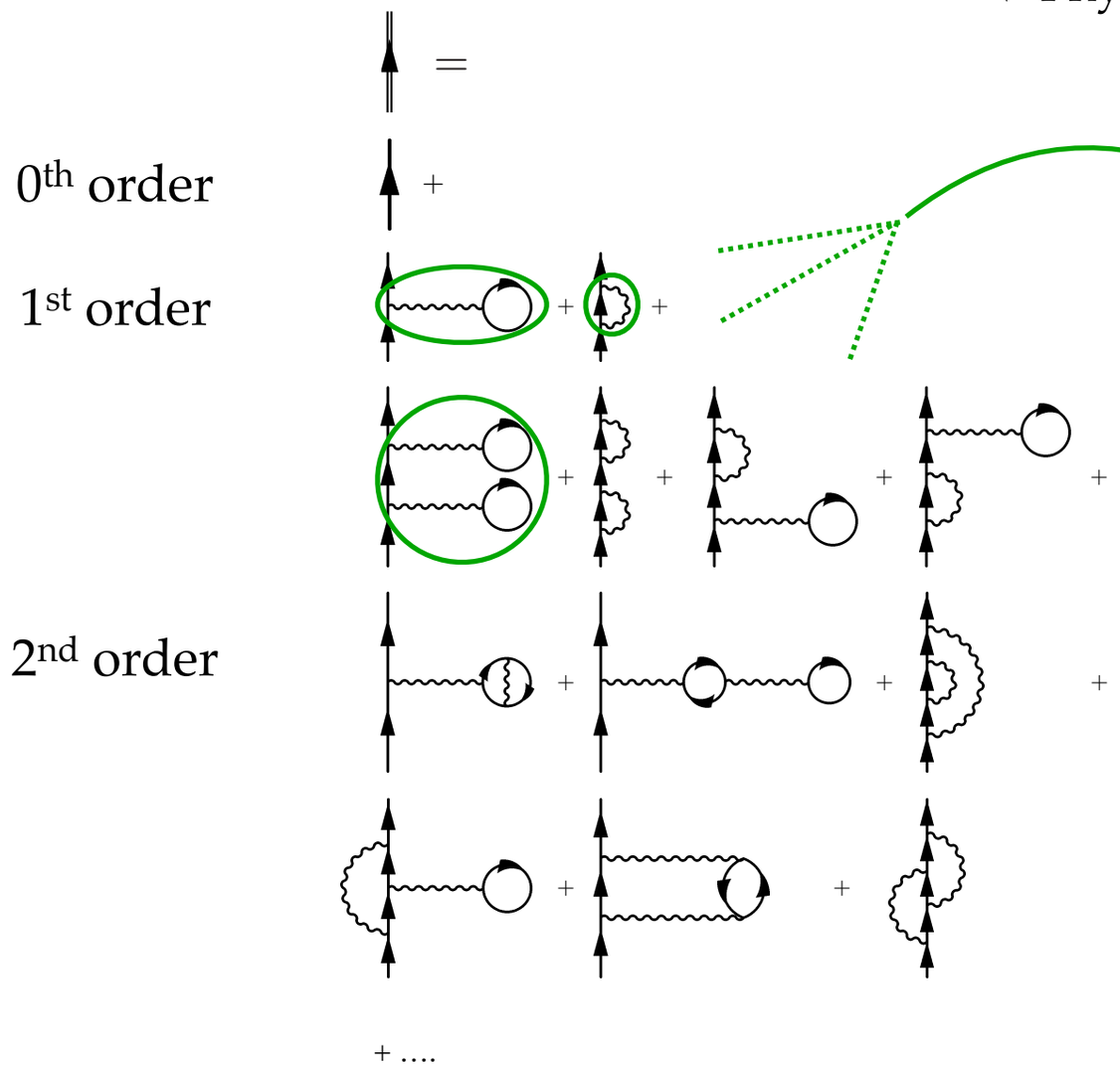
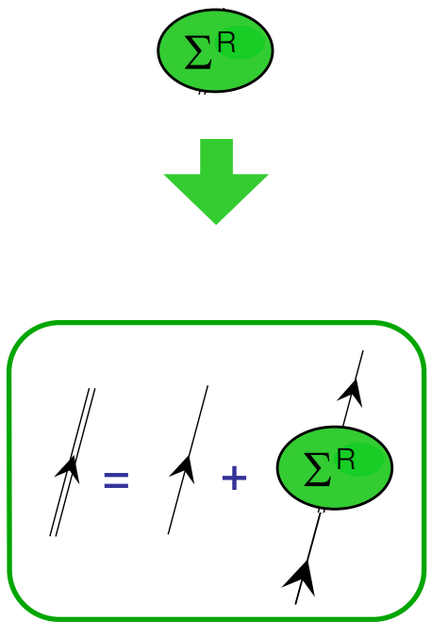
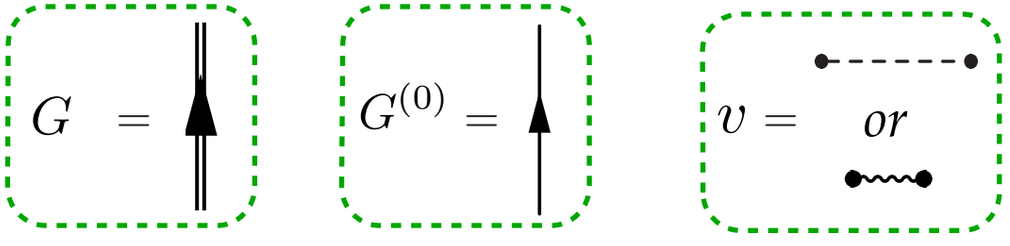


Define **reducible** self-energy
(all diagrams without external legs)



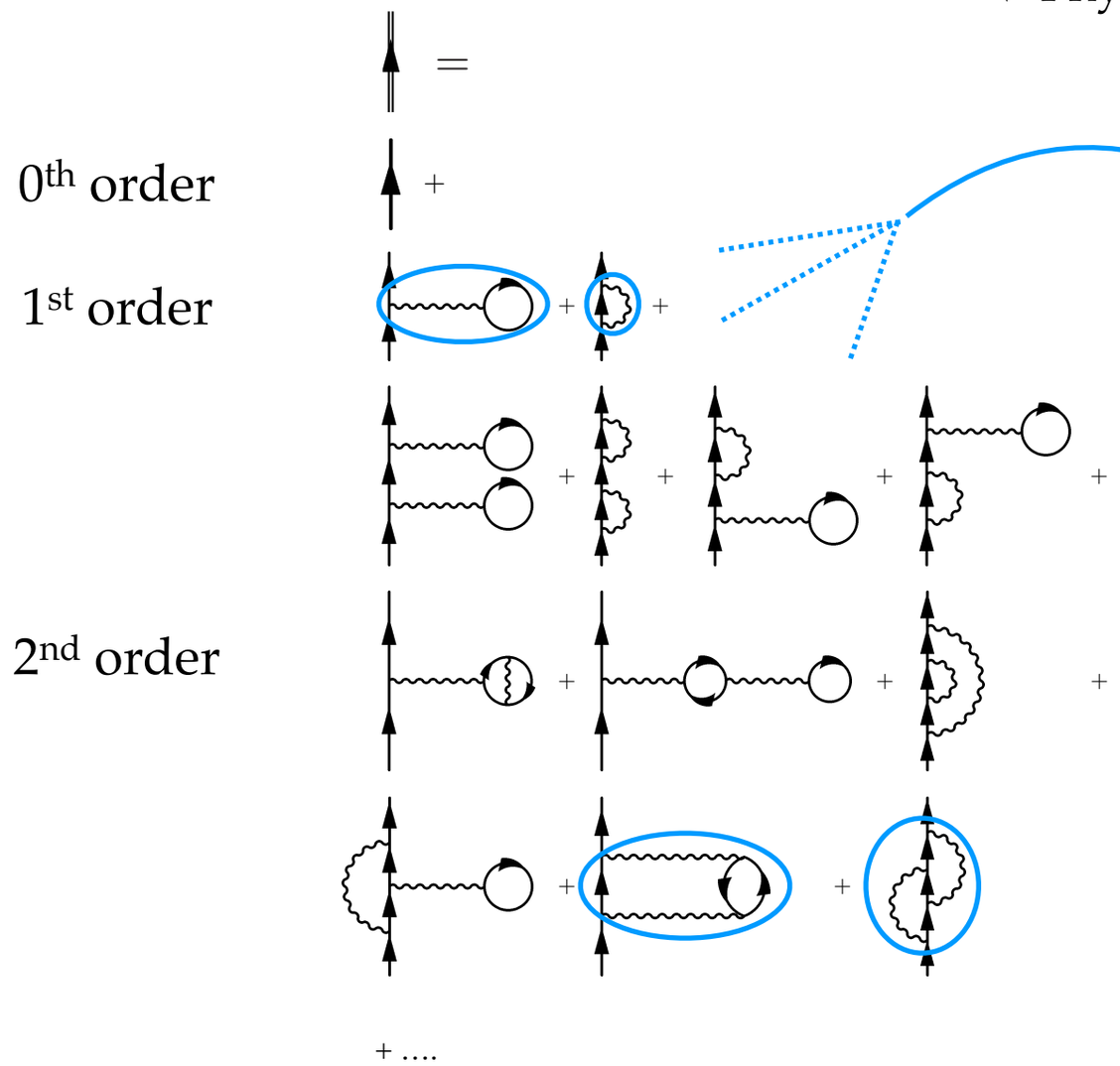
Diagrammatic expansion

Introduce unperturbed / exact propagators and interaction lines



in $$G = \sum_{n} \sum_{\text{connected}} \underbrace{G^{(0)} \cdots G^{(0)} \cdots}_{2n+1 \text{ propagators}} \underbrace{v \cdots v \cdots}_{n \text{ interactions}}$$

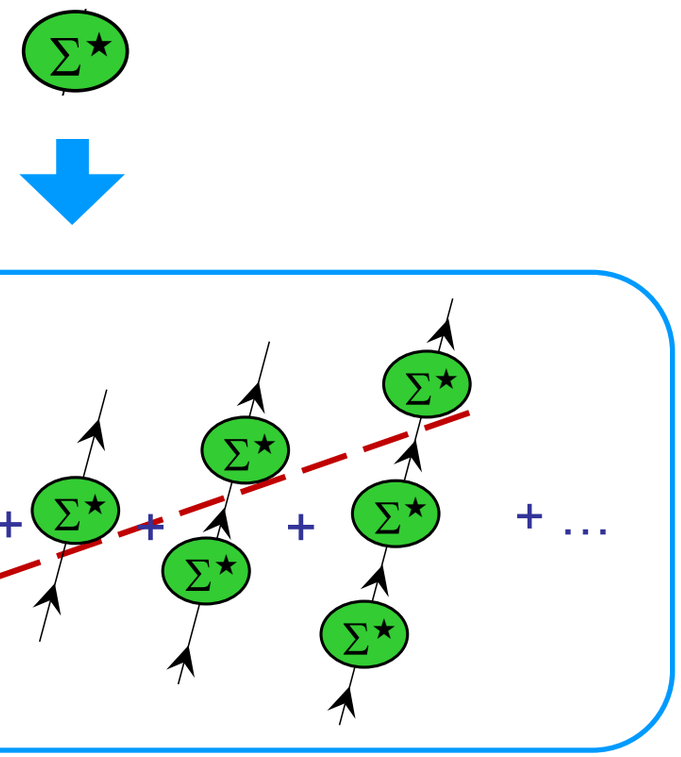
and write down the expansion for G



✓ All topologically different diagrams contribute at a given order

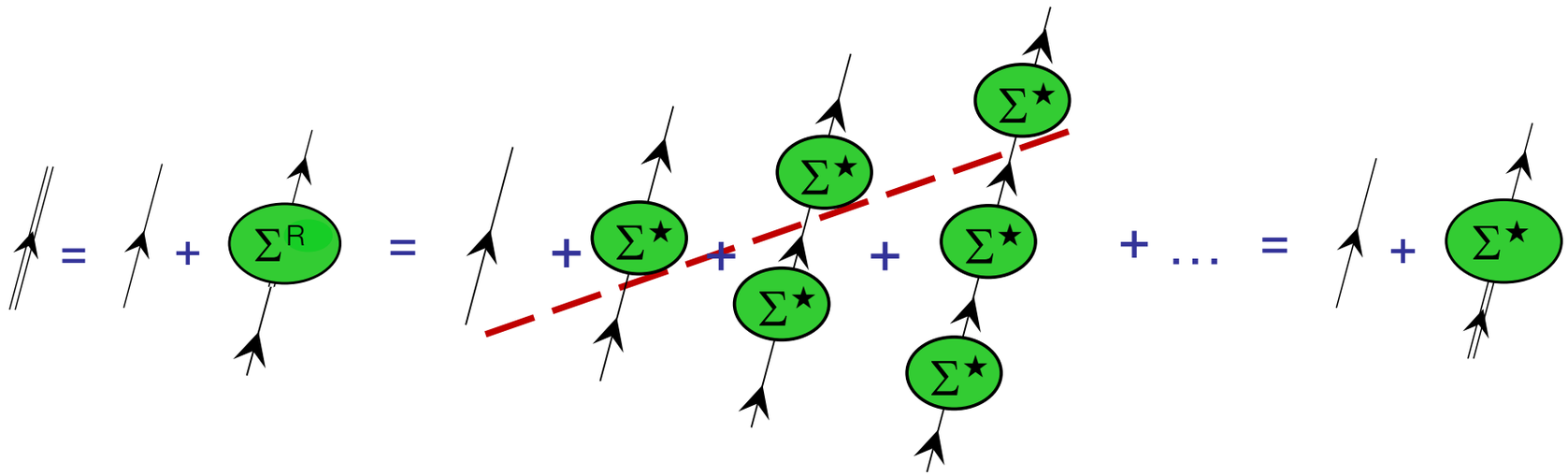
✓ Physical processes can be associated to Feynman diagrams

Define **irreducible** self-energy



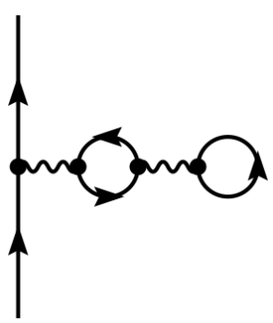
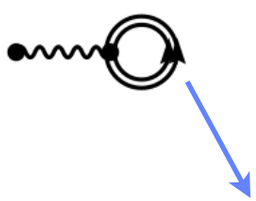
Dyson equation

One finds again the Dyson equation $$G(1,2) = G^{(0)}(1,2) + \int d3\, d4\, G^{(0)}(1,3)\, \Sigma^*(3,4)\, G(4,2)$$



Partial sums *or* skeleton vs. composed diagrams

➟ Self-energy can be built with **dressed** propagation lines;
one then keeps only **skeleton** diagrams ➟ self-consistency

E.g.  will be generated by the self-energy term 

dressed propagator

Dyson equation

Dyson equation is exact

$$G(1,2) = G^{(0)}(1,2) + \int d3\, d4\, G^{(0)}(1,3)\, \Sigma^*(3,4)\, G(4,2)$$

…the game is now to choose a suitable approximation for the self-energy.

Having in mind the (composed irreducible) self-energy expansion,
one can choose to select only certain general classes of diagrams:

1) With **polarisation** parts inserted in interaction lines

   ➟ *dressed* or *effective* or *renormalised* interactions

2) With **self-energy** parts inserted in propagator lines

   ➟ *dressed* or *renormalised* propagators

3) With (**irreducible) vertex** parts inserted in place of a vertex

   ➟ *dressed* vertices

Φ-functional

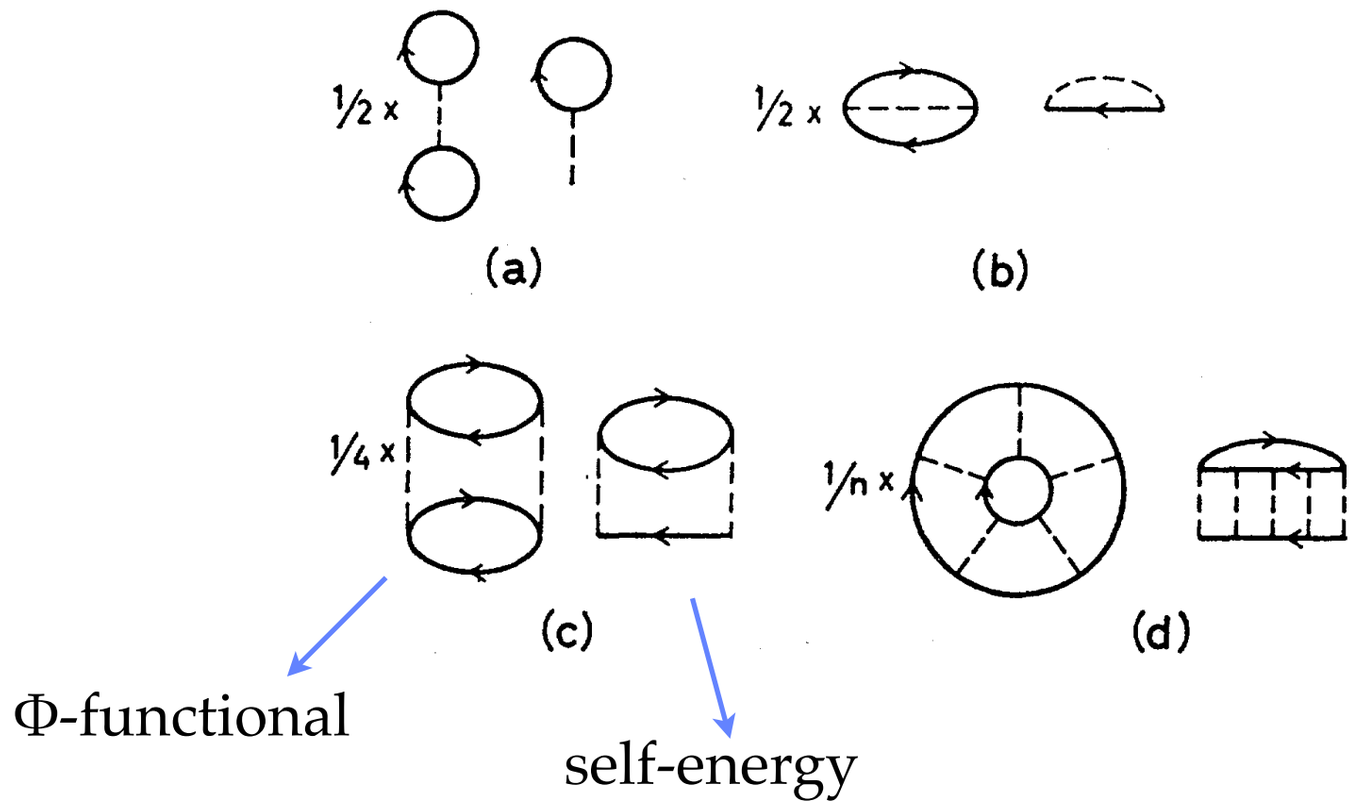
There exists a class of self-energy approximations that automatically fulfil basic conservation laws (number of particles, momentum, energy…).

The condition is the existence of a functional Φ of G and v, such that

$$\Sigma(1,2) = \frac{\delta\,\Phi[G,v]}{\delta\,G(1,2)}$$

[Baym & Kadanoff 1961, 1962]

Common approximations like Hartree, Fock, 2nd order, T-matrix are **Φ-derivable**



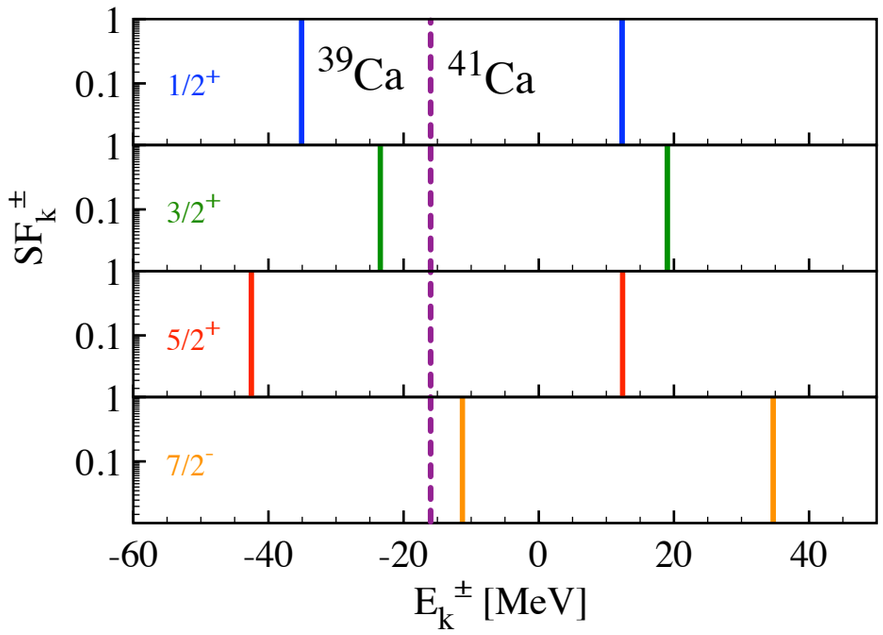
Approximations to the exact self-energy

Hartree - Fock

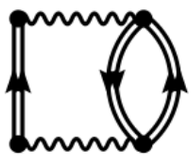
- ➟ *Hartree*: particles in a common potential, contains unphysical self-interaction
- ➟ *Fock*: removes self-interaction
- ➟ Account for **static** correlations

SCGF calculations in nuclei

[Somà *et al.* unpublished]

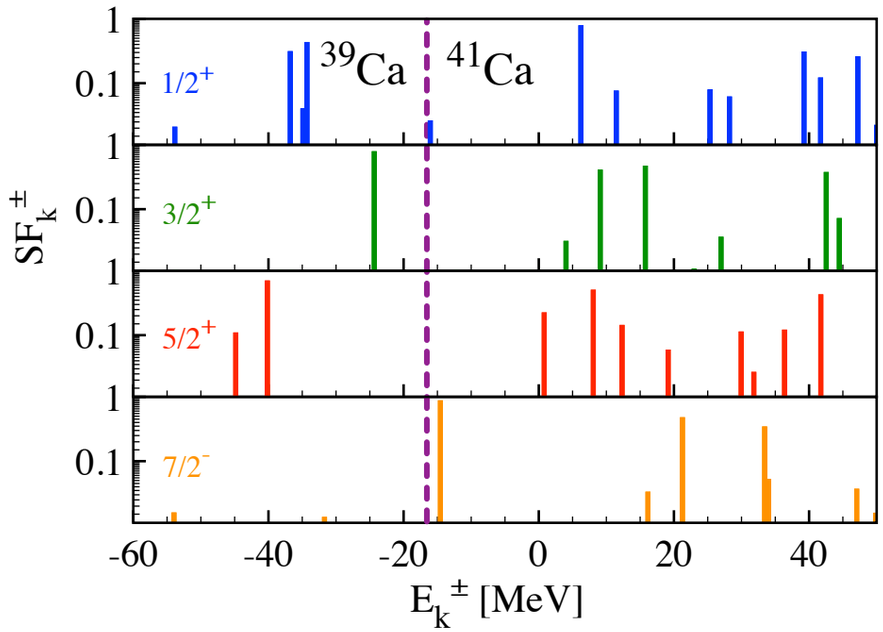


2nd order



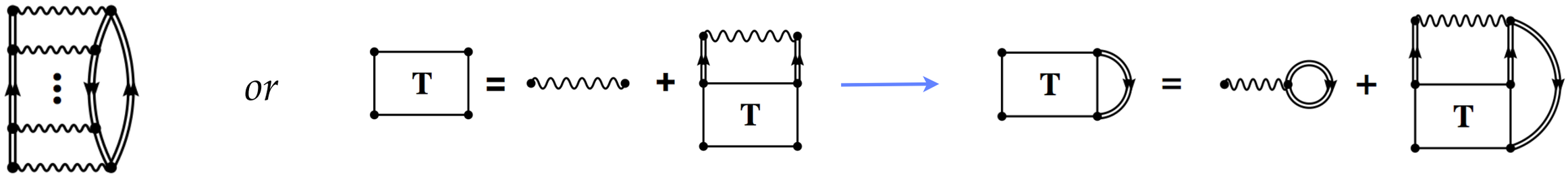
+ exchange

- ➟ Next term in the renormalisation of the propagator
- ➟ Introduces leading **dynamical** correlation



Approximations to the exact self-energy

pp/hh T-matrix or **ladder**



+ exchanges

[Galitskii 1958; …]

➟ Contains an infinite number of diagrams

➟ Resums contributions relevant at low-density and in strongly-interacting systems

➟ Quality decreases at high density as screening becomes important

Electronic systems

➟ Works well at low densities, i.e. close to completely filled or empty bands

➟ Extensively used in Hubbard models

Nuclear systems

➟ Treats the repulsive short-range part of nuclear interactions

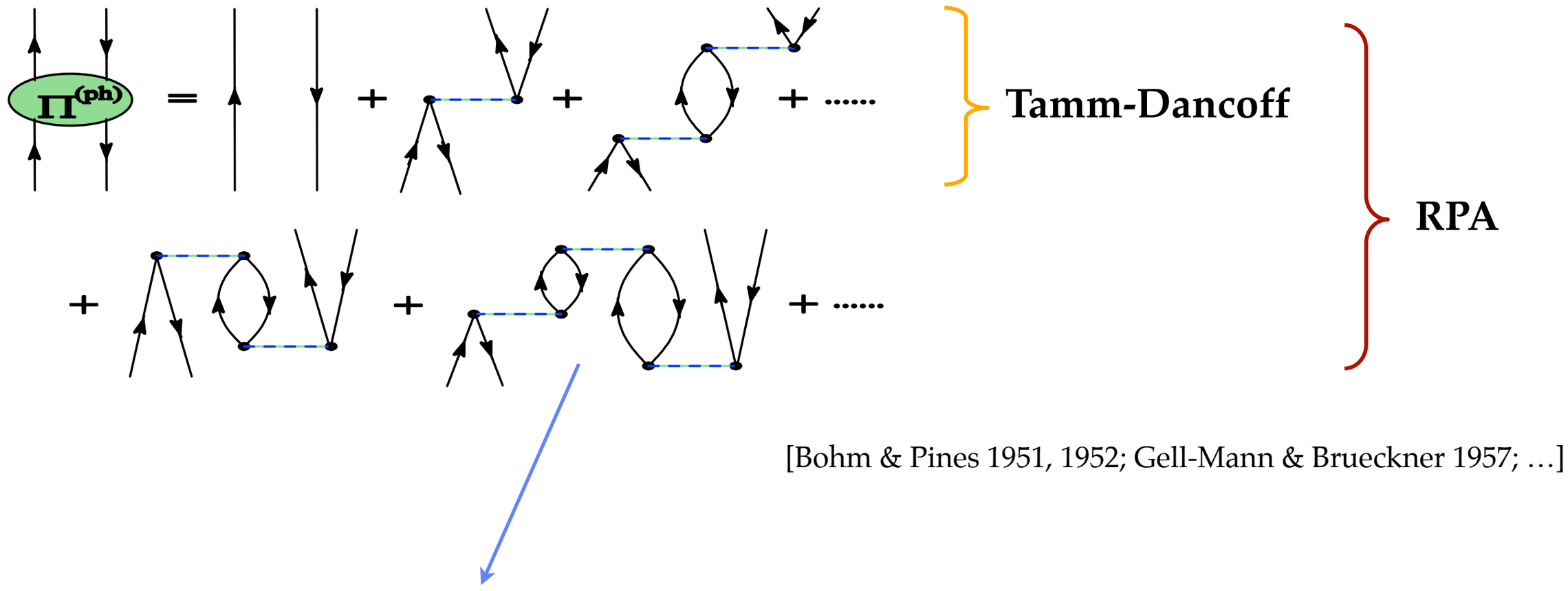
➟ Method of choice for nuclear matter (self-consistency obligatory for high densities)

➟ Applications to finite nuclei very demanding

Approximations to the exact self-energy

Random Phase Approximation (RPA) or **ring ladder** or **ph ladder**

➟ Expansion for the *polarisation* propagator



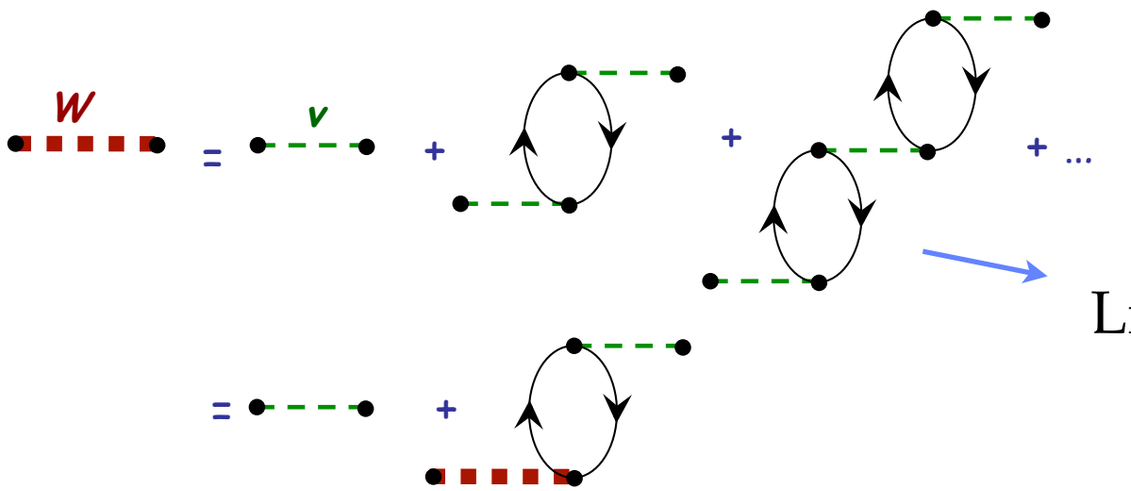
[Bohm & Pines 1951, 1952; Gell-Mann & Brueckner 1957; …]

In RPA Pauli correlations are partially **neglected**, but one assumes that missing corrections cancel each other **randomly**.

Approximations to the exact self-energy

GW

RPA can be applied to resum an interaction (typically electron-electron) in the medium

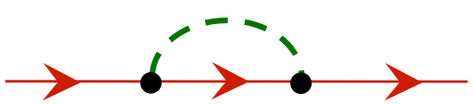


Lindhard function $\Pi^{(0)}(\mathbf{q},\omega)$

$$W(\mathbf{q},\omega) = v(\mathbf{q}) + v(\mathbf{q})\,\Pi^{(0)}(\mathbf{q},\omega)\,W(\mathbf{q},\omega) \quad \Rightarrow \quad \Sigma^{GW}(\mathbf{k},\omega) = i\int \frac{d\omega'}{2\pi}\int \frac{d\mathbf{k}'}{(2\pi)^3}\,G(\mathbf{k}-\mathbf{k}',\omega-\omega')\,W(\mathbf{k}',\omega')$$

- Accounts for screening effects
- For electrons only Fock term in *GW* (Hartree → constant electrostatic repulsion)
- Different degrees of self-consistency

G⁰W⁰



GW⁰

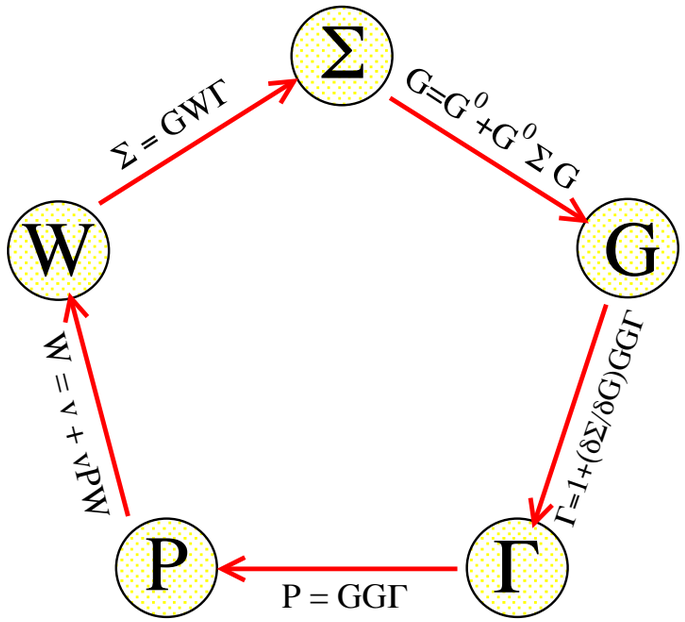
GW

Approximations to the exact self-energy

GW

GW approximation can be formally derived from **Hedin** pentagon of equations

[Hedin 1965]



[figure from F. Sottile, PhD thesis 2003]

Σ =self-energy

G = single-particle GF

Γ = vertex function

P = polarisability

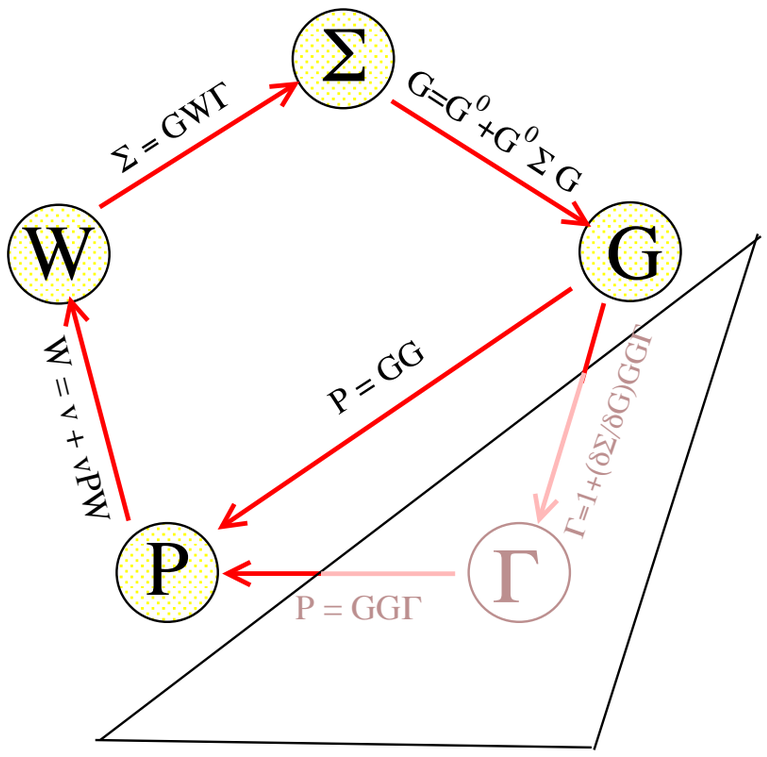
W = screened interaction

Approximations to the exact self-energy

GW

GW approximation can be formally derived from **Hedin** pentagon of equations

[Hedin 1965]



[figure from F. Sottile, PhD thesis 2003]

$$\Gamma^{GWA}(1,2,3) = \delta(1,2)\delta(1,3)$$

G^0W^0

$$P^0(1,2) = -iG^0(1,2)G^0(2,1^+)$$

$$W^0(1,2) = v(1,2) + \int d(34)v(1^+,3)P^0(3,4)W^0(4,2)$$

$$\Sigma(1,2) = iG^0(1,2)W^0(1^+,2)$$

GW

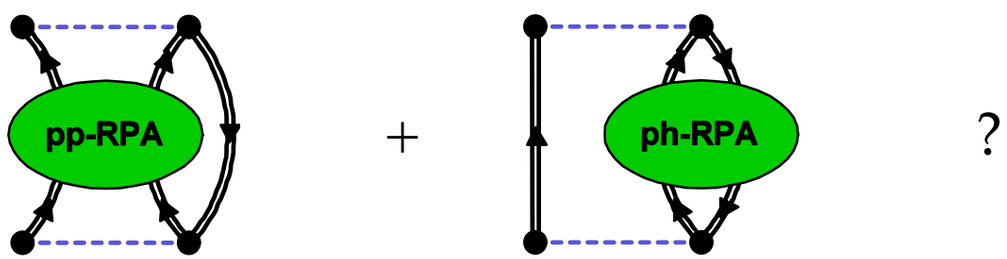
Iterate all three + Dyson equation

➟ Works well in the high-density regime where screening is important

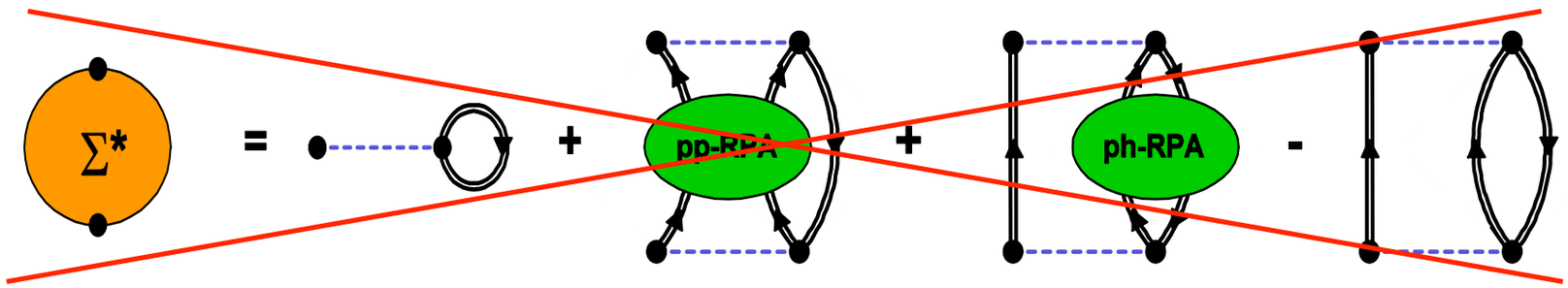
Approximations to the exact self-energy

How to go beyond **ladder**-type or ***GW*** resummations?

To extend the domain of applicability one has to **combine different correlation channels**



Simply summing the two would not work



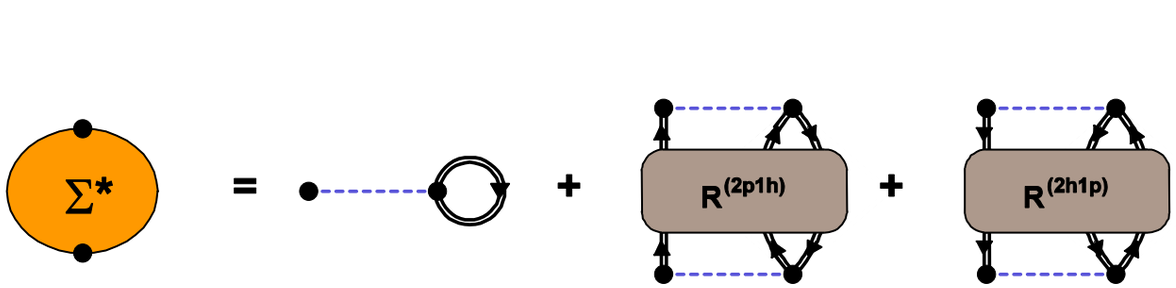
➟ interference terms missing

➟ double-counting of second-order diagram

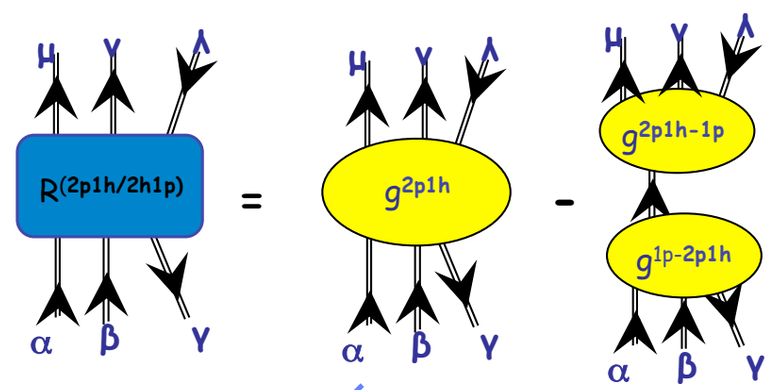
↘ avoided by starting ladders from 3rd order only ➟ FLEX [Brickers *et al.* 1989]

Approximations to the exact self-energy

In general, one needs to consider the full 2p1h / 2h1p propagator *R*



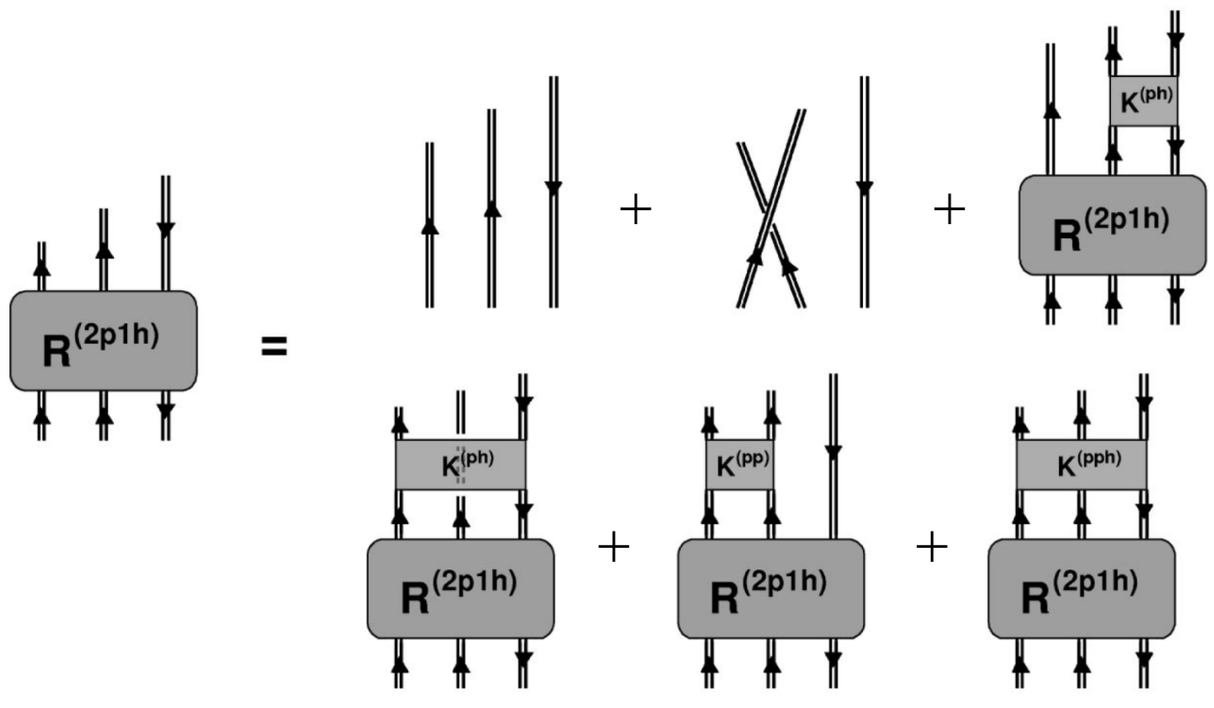
where



propagation of three excitations

Dyson equation takes care of this

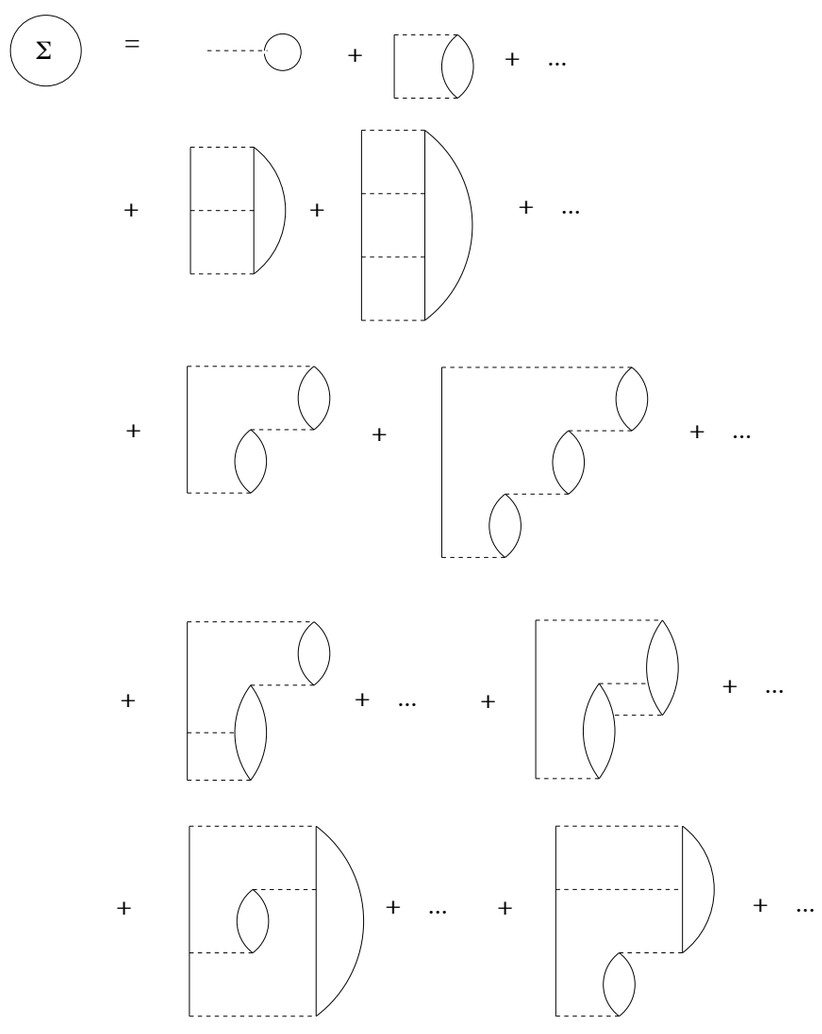
R obeys the following (Bethe-Salpeter) equation



Approximations to the exact self-energy

Parquet theory [Diatlov *et al.* 1957; Jackson *et al.* 1982; Bergli & Hjorth-Jensen 2010]

➟ Couples pp/hh and ph ladders on equal footing

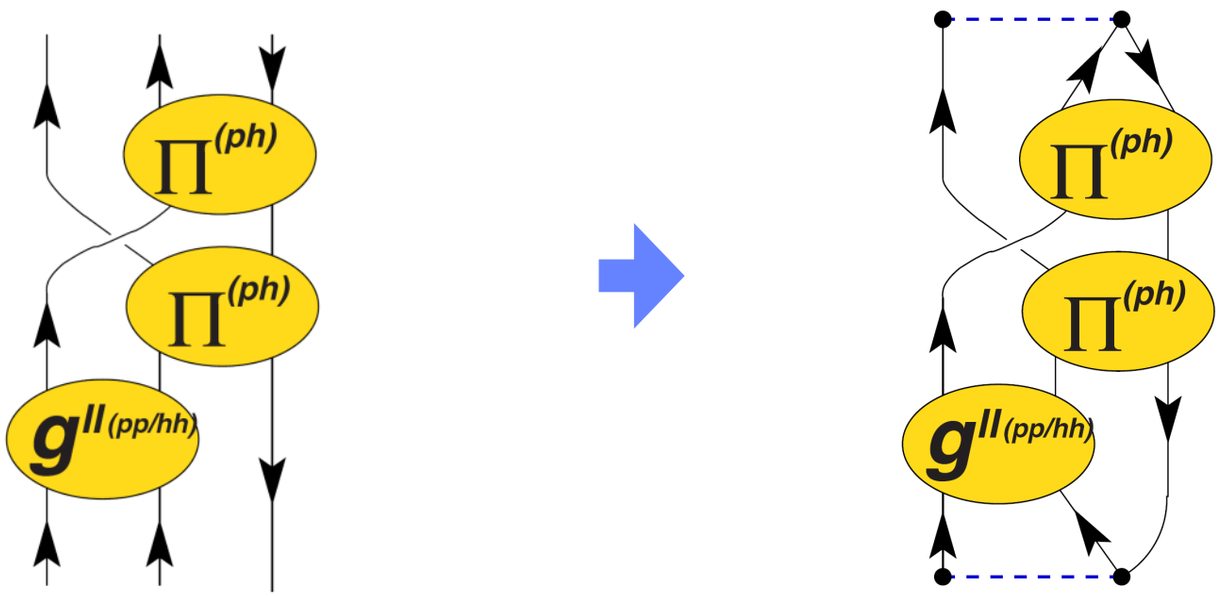


✓ Mainly proof-of-principle applications

Approximations to the exact self-energy

Faddeev RPA (F-RPA) [Barbieri & Dickhoff 2001; Barbieri, Van Neck & Dickhoff 2007]

- Strategy is to solve each pp/hh and ph channel separately, then couple to a third line and mix the corresponding amplitudes
- All-order summation through a set of **Faddeev equations**

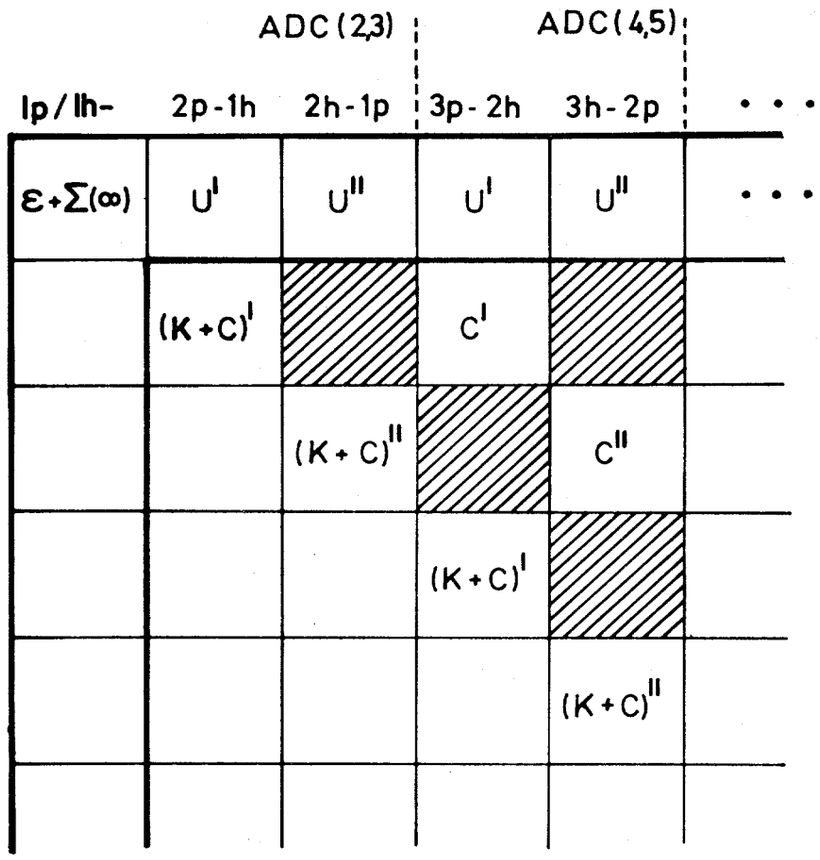


✓ Realistic applications to nuclei, atoms and molecules

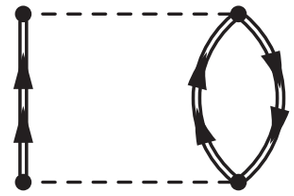
Approximations to the exact self-energy

Algebraic Diagrammatic Construction (ADC) [Schirmer, Cederbaum & Walter 1983]

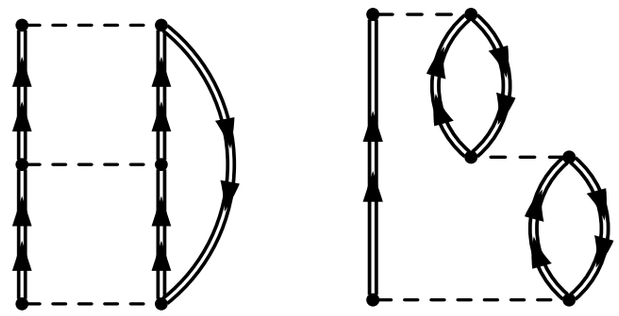
- ➟ Exact summation of the self-energy reformulated into a simple algebraic form
- ➟ ADC(n) includes complete n-th order (dressed) perturbation theory diagrams for G
- ➟ Results in Hermitian eigenvalue problems within limited spaces of $N\pm1$ systems



ADC(2)



ADC(3)



✓ Realistic applications to nuclei, atoms and molecules

Approximations to the exact self-energy

Unified ladder-GW approach [Romaniello, Bechstedt & Reining 2012]

➟ Re-express the self-energy as

$$\Sigma(11') = v_H(1)\delta(11') + \Sigma_x(11') + iv_c(1^+2) \times G(13)\Xi(35;1'4)L(42;52^+),$$

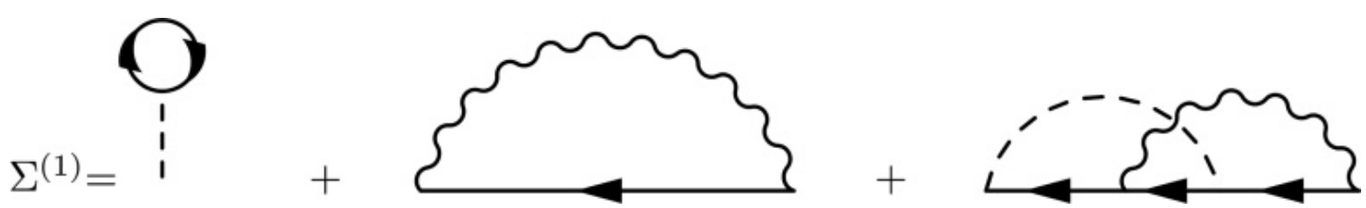
Effective interaction — Response

➟ Keeping $\Xi = v$c leads to GW scheme

➟ Keeping $L = GG$ leads to T-matrix scheme

➟ Link between T-matrix and Hedin equations

➟ Derivation of a **screened T-matrix**

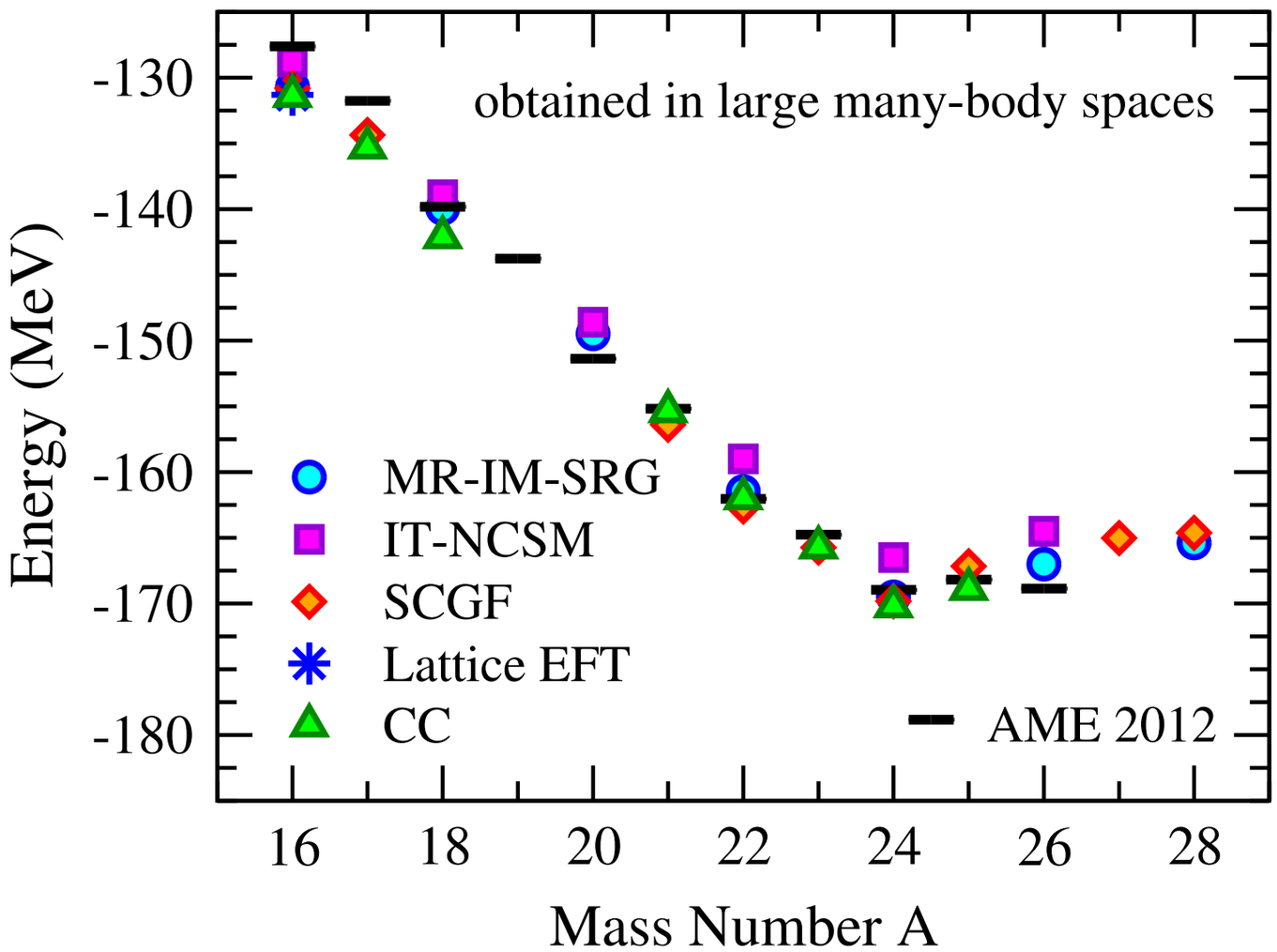


Hartree — GW — SOSEX

✓ First applications promising

Oxygen benchmark

Several ab initio methods recently addressed the oxygen chain



[Hergert *et al.* 2013]

[Cipollone *et al.* 2013] **[ADC(3)]**

[Jansen *et al.* 2014]

➡ Same input Hamiltonian (NN+3N)

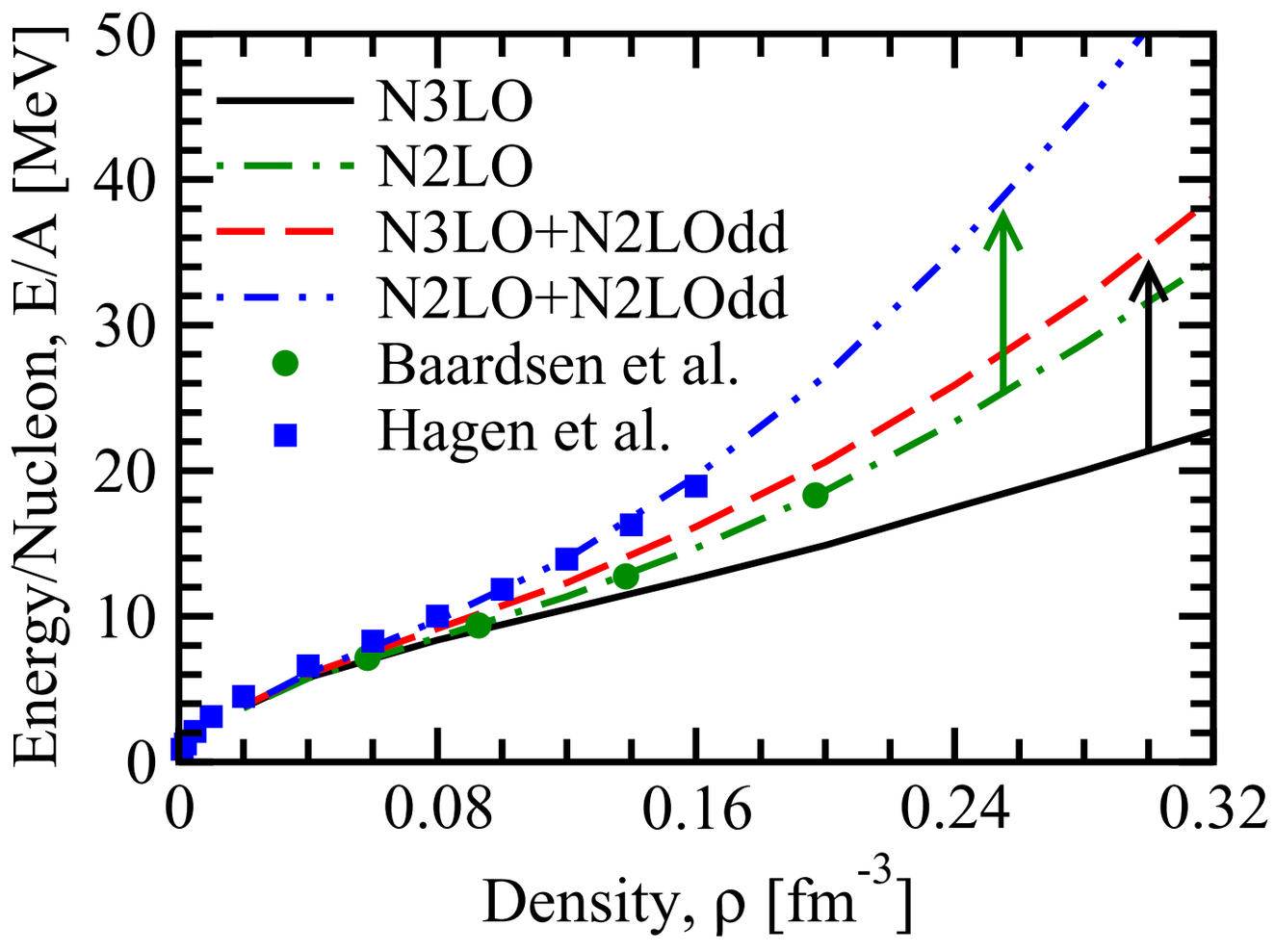
➡ Good agreement between all methods

Nuclear matter benchmark

Infinite matter: **self-consistent *T*-matrix**.

➟ Excellent agreement with CCSD calculations

Equation of state of neutron matter



[Carbone, Rios & Polls 2014]

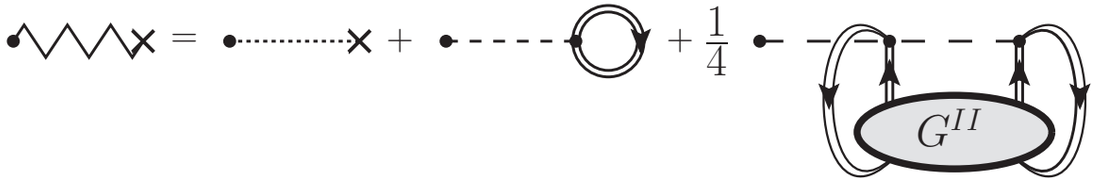
Three-body forces

In nuclear physics, treatment of **many-body interactions** is required.

Green's function formalism was recently extended to account for **three-body forces.**

[Carbone, Cipollone, Barbieri, Rios, Polls 2013]

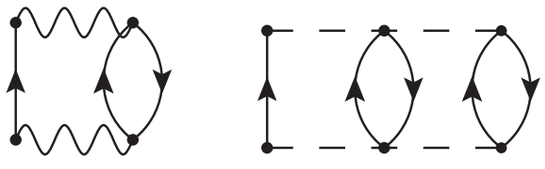
➟ Introduction of one- and two-body effective interactions allows to substantially reduce the number of diagrams



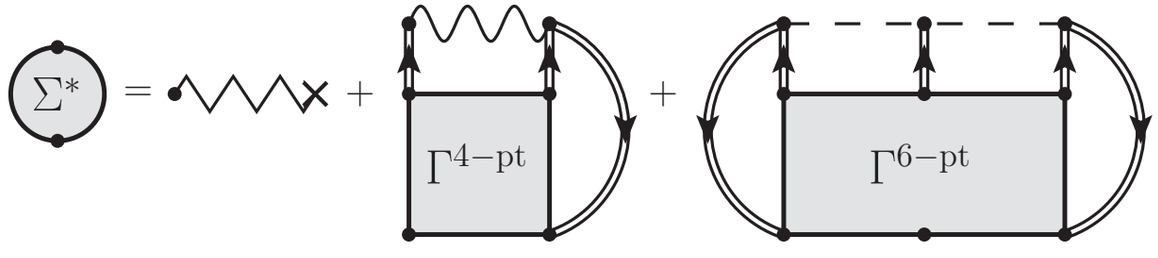
effective 1-body

effective 2-body

E.g. at 2nd order



In general



With these, re-work out all previous slides!

Anomalous Green's functions: Gorkov theory

Standard expansion schemes fail when **pairing correlations** are essential.

It is possible to formulate the expansion around a symmetry-breaking reference, e.g. a **Bogoliubov vacuum.**

- ➟ Remains a **single-reference** method
- ➟ Symmetry must be eventually restored (see Duguet's talk)

General idea: start from an auxiliary many-body state $|\Psi_0\rangle \equiv \sum_A^{\text{even}} c_A \, |\psi_0^A\rangle$

and consequently define a set of 4 one-body propagators [Gorkov 1958]

$$i\,G^{11}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{a_a(t)a_b^\dagger(t')\right\}|\Psi_0\rangle \quad \equiv$$

$$i\,G^{21}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{\bar{a}_a^\dagger(t)a_b^\dagger(t')\right\}|\Psi_0\rangle \quad \equiv$$

$$i\,G^{12}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{a_a(t)\bar{a}_b(t')\right\}|\Psi_0\rangle \quad \equiv$$

$$i\,G^{22}_{ab}(t,t') \equiv \langle\Psi_0|T\left\{\bar{a}_a^\dagger(t)\bar{a}_b(t')\right\}|\Psi_0\rangle \quad \equiv$$

With these, re-work out all previous slides!

More GFs

Solution of Dyson equation

Due to the presence of poles in G often problematic. However, it can be transformed into an **energy-dependent** eigenvalue equation, which can be further recast into an **energy-independent** eigenvalue equation (no poles now!).

Self-consistency

Not always dressed propagators are used in Σ, i.e. not always Dyson equation is iterated self-consistently.

- ➟ Effects/benefits/drawbacks of self-consistency
- ➟ Dependence on G^0?
- ➟ Connection with conservation laws?
- ➟ Consistency between renormalisations of G, Γ and W?

Generalisations

- ➟ Finite temperature GFs
- ➟ Non-equilibrium GFs
- ➟ …