

# Nuclear Reaction from a Structure Point of View

G. Blanchon

CEA,DAM,DIF F-91297 Arpajon, France

Ecole Internationale de Physique Subatomique de Lyon,  
9-13 Novembre 2015

Scattering

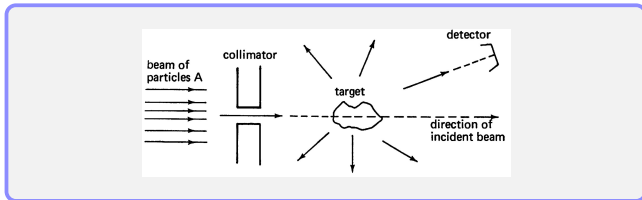
Green's functions

Nuclear Structure Method

## NUCLEON SCATTERING

## Reminder on cross section

- ▶ Consider a beam of particles hitting a thin sheet of material
- ▶  $N_i = J_i S$  incident particles hit the surface per second
- ▶  $N_c$  outgoing particles counted per second (only count particles belonging to an outgoing channel  $c$ . For instance elastic channel: detection of a particle with the same energy than the incident particle)
- ▶ Probability  $P_c$  of reaction:  $P_c = \frac{N_c}{N_i} = \frac{N_c}{J_i S}$



- ▶ The cross section  $\sigma_c$  is an effective area associated to one target nucleus, that provides a measure of the probability of reaction in the channel  $c$ .
- ▶  $\Sigma_c = \sigma_c N_t$  ( $N_t = nSdx$  number of target nuclei) is the portion of the surface  $S$  which, when hit by the incident particle, will lead to the reaction channel  $c$ .

$$P_c = \frac{\Sigma_c}{S} = \frac{N_c}{J_i S}, \quad \sigma_c = \frac{N_c}{N_t} \frac{1}{J_i} = \frac{\text{reaction rate}}{\text{incident flux}}$$

## ► Problem

- Nucleon scattering from a target nucleus is a many-body problem with  $A$  bound nucleons and a scattered one: very difficult...
- Many body problem approximated by a two-body problem

$$\left( \frac{\hbar^2}{2\mu} \nabla^2 + V(\mathbf{r}) \right) \phi(\mathbf{r}) = E\phi(\mathbf{r})$$

with  $V(\mathbf{r})$  a one-body effective potential

## ► Requirements

- $V$  should describe the direct reaction in a nuclear collision and should give the energy averaged scattering amplitude
- $V$  should take into account in an effective way all the inelastic channels

## ► Solution

- Complex one-body potential:  $V(\mathbf{r}) = U(\mathbf{r}) + iW(\mathbf{r})$
- Real part: simple refraction of the incident wave
- Imaginary part models flux loss during the elastic scattering process

Probability current:

$$\mathbf{j}(\mathbf{r}) = -i \frac{\hbar}{2\mu} (\phi^*(\mathbf{r}) \nabla \phi(\mathbf{r}) - \phi(\mathbf{r}) \nabla \phi^*(\mathbf{r}))$$

Schrödinger Equation:

$$\left( \frac{\hbar^2}{2\mu} \nabla^2 + (U(r) + iW(r)) \right) \phi(\mathbf{r}) = E\phi(\mathbf{r})$$

$\phi^*(\mathbf{r}) \times \{S.E.\} - \phi(\mathbf{r}) \{S.E.\}^*$ :

$$\text{Flux variation: } \nabla \cdot \mathbf{j} = \frac{i}{\hbar} (V^* - V(r)) |\phi(r)|^2 = \frac{2}{\hbar} W(r) |\phi(r)|^2$$

Negative imaginary potential: flux absorption

# Schrödinger equation with a spherical potential

$$H|\psi\rangle = (T + V)|\psi\rangle = E|\psi\rangle$$
$$\int \langle \mathbf{r} | (T + V) | \mathbf{r}' \rangle \langle \mathbf{r}' | \psi \rangle d\mathbf{r}' = E \langle \mathbf{r} | \psi \rangle$$

## Kinetic part

$$T = \frac{\mathbf{p}^2}{2m}$$
$$\langle \mathbf{r} | \mathbf{p}^2 | \mathbf{r}' \rangle = \int \langle \mathbf{r} | \mathbf{p}^2 | \mathbf{p} \rangle \langle \mathbf{p} | \mathbf{r}' \rangle d\mathbf{p}$$
$$= \int \langle \mathbf{r} | \mathbf{p} \rangle \mathbf{p}^2 \langle \mathbf{p} | \mathbf{r}' \rangle d\mathbf{p}$$
$$= \frac{1}{(2\pi\hbar)^3} \int \mathbf{p}^2 e^{i\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')} d\mathbf{p}$$
$$= -\hbar^2 \delta''(\mathbf{r}-\mathbf{r}')$$
$$\langle \mathbf{r} | T | \psi \rangle = -\frac{\hbar^2}{2m} \Delta \psi(\mathbf{r})$$

## Potential part

$$\langle \mathbf{r} | V | \psi \rangle = \int d\mathbf{r}' \langle \mathbf{r} | V | \mathbf{r}' \rangle \langle \mathbf{r}' | \psi \rangle$$
$$\langle \mathbf{r} | V | \mathbf{r}' \rangle \equiv V(\mathbf{r}, \mathbf{r}')$$

## Local potential

$$V(\mathbf{r}, \mathbf{r}') = V(r) \delta(\mathbf{r}, \mathbf{r}')$$

# Schrödinger equation with a spherical potential

$$-\frac{\hbar^2}{2m}\Delta\psi(\mathbf{r}) + \int d\mathbf{r}' V(\mathbf{r}, \mathbf{r}')\psi(\mathbf{r}') = E\psi(\mathbf{r})$$

Spherical coordinates,

$$\left. \begin{aligned} \Delta &\equiv p_r^2 + \frac{l^2}{r^2} \\ p_r^2 &= -\hbar^2 \frac{1}{r} \frac{d^2}{dr^2} r \end{aligned} \right\} \langle \mathbf{r} | T | \psi \rangle = \left[ -\frac{\hbar^2}{2m} \frac{1}{r} \frac{d^2}{dr^2} r + \frac{l^2}{2mr^2} \right] \psi(\mathbf{r})$$

Using the following multipole expansions and projecting on  $|ljm\rangle$

$$\psi(\mathbf{r}) = \sum_{ljm} \frac{u_{ljm}(r)}{r} \mathcal{Y}_{jl}^m(\hat{\mathbf{r}}) \quad \text{and} \quad \nu_{ljm}(r, r') = \iint d\hat{\mathbf{r}} d\hat{\mathbf{r}}' \mathcal{Y}_{jl}^m(\hat{\mathbf{r}}) V(\mathbf{r}, \mathbf{r}') \mathcal{Y}_{jl}^{m\dagger}(\hat{\mathbf{r}}')$$

Integro-differential Schrödinger equation

$$-\frac{\hbar^2}{2m} \left[ \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} \right] u_{ljm}(r) + \int dr' r \nu_{ljm}(r, r') r' u_{ljm}(r') = E u_{ljm}(r)$$



## Phase shift determination

## Integro-differential Schrödinger equation

$$-\frac{\hbar^2}{2m} \left[ \frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} \right] u_{ljm}(r) + \int dr' r \nu_{ljm}(r, r') r' u_{ljm}(r') = E u_{ljm}(r)$$

Equations can be expressed on a radial mesh with  $h$  the step. The potential is negligible at  $R_{max} = h \times N$ .

$$\begin{aligned} u(r) &\longrightarrow u_i \\ \frac{d^2}{dr^2} u(r) &\longrightarrow \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} \\ \nu(r, r') &\longrightarrow \nu_{ij} \end{aligned}$$

Schrödinger equation reads

$$\left[ \begin{pmatrix} -2 & 1 & & & & & & & \\ 1 & -2 & 1 & & & & & & \\ & & \ddots & \ddots & \ddots & & & & \\ & & & 1 & -2 & 1 & & & \\ & & & & 1 & -2 & 1 & & \\ & & & & & & & \ddots & \ddots & \ddots \\ & & & & & & & & & M_{N,N} \end{pmatrix} + \begin{pmatrix} M_{1,1} & \cdots & & & & & & & \\ \vdots & \ddots & & & & & & & \\ & & \ddots & & & & & & \\ & & & \ddots & & & & & \\ & & & & \ddots & & & & \\ & & & & & \ddots & & & \\ & & & & & & \ddots & & \\ & & & & & & & \ddots & \\ & & & & & & & & \ddots & \\ & & & & & & & & & M_{N,N} \end{pmatrix} \right] \begin{pmatrix} u_1 \\ \vdots \\ u_N \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ -1 \end{pmatrix}$$

Conditions at the limits:  $u_0 = 0$ ,  $u_{N+1} = 1$ ,  $M_{i,N+1} = 0$

$$\sum_k \mathcal{M}_{i,k} u_k = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ -1 \end{pmatrix}$$

Solution merges from matrix inversion

$$u_j = -(\mathcal{M}^{-1})_{j,N}$$

Solution can further be re-injected into Schrödinger equation with better precision and iterated until the needed precision is obtained.

## Connection to asymptotic solutions

$$u_{lj}(r) \underset{r \rightarrow +\infty}{=} C [\cos(\delta_{lj}) j_l(kr) - \sin(\delta_{lj}) n_l(kr)]$$

avec  $k^2 = -(2m/\hbar^2) \times E$

with  $j_l$ ,  $n_l$  Bessel and Neumann spherical functions.

## Normalisation by a Dirac in energy

$$C = \sqrt{\frac{1}{\pi} \frac{2m}{\hbar^2 k}}$$

## Phase shift is obtained from

$$\frac{u'_N}{u_N} = \frac{\cos(\delta_{lj}) j'_l(kR_{max}) - \sin(\delta_{lj}) n'_l(kR_{max})}{\cos(\delta_{lj}) j_l(kR_{max}) - \sin(\delta_{lj}) n_l(kR_{max})}$$

# Phase shift determination

## Connection to asymptotic solutions

$$u_{lj}(r) \underset{r \rightarrow +\infty}{=} C [\cos(\delta_{lj}) j_l(kr) - \sin(\delta_{lj}) n_l(kr)]$$

avec  $k^2 = -(2m/\hbar^2) \times E$

with  $j_l$ ,  $n_l$  Bessel and Neumann spherical functions.

## Normalisation by a Dirac in energy

$$C = \sqrt{\frac{1}{\pi} \frac{2m}{\hbar^2 k}}$$

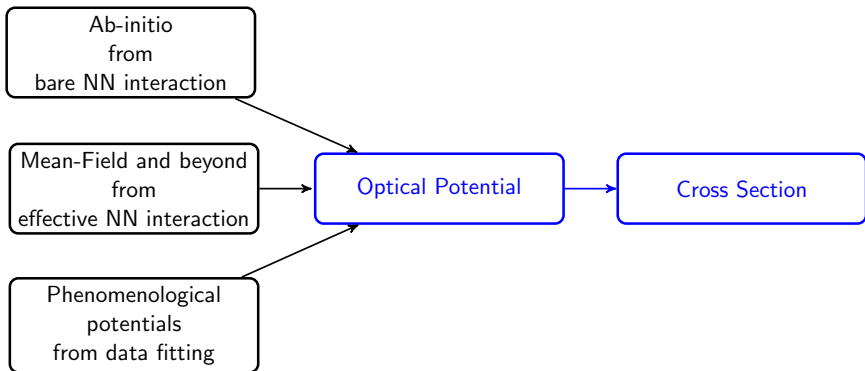
## Phase shift

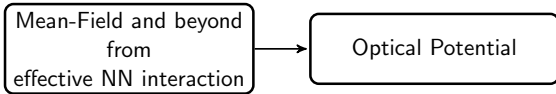
$$\tan(\delta_{lj}) = \frac{u_N j_l'(kR_{max}) - u_N' j_l(kR_{max})}{u_N n_l'(kR_{max}) - u_N' n_l(kR_{max})}$$

# From optical potential to reaction observables

Cross Section (without spin)

$$\sigma_{el} = \frac{\pi}{k^2} \sum_{\ell} |1 - S_{\ell}|^2 \quad \text{with} \quad S_{\ell} = e^{i2\delta_{\ell}}$$





### Goals

- ▶ Build an optical potential from an effective NN interaction
- ▶ Consistent use of the effective NN interaction
- ▶ Self-consistency

### Tools

- ▶ Green's functions formalism
- ▶ Gogny D1S phenomenological effective interaction

## EFFECTIVE NN INTERACTION

## Pros

- ▶ Phenomenological account of short range correlations
- ▶ Simple shape
- ▶ Energy independent
- ▶ Extended reach of EDF approaches

## Cons

- ▶ Simple shape
- ▶ Validity out of the parametrization range
- ▶ Loss of the contact with more fundamental theories



# Skyrme and Gogny interactions

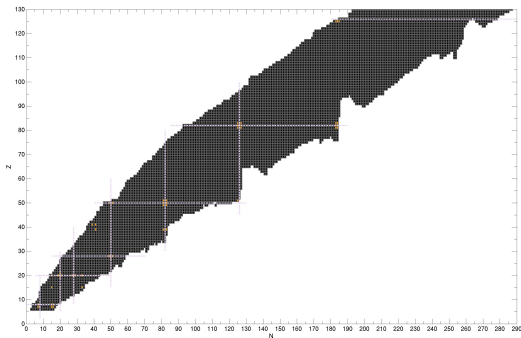
Skyrme interaction

Zero-range interaction

Gogny interaction

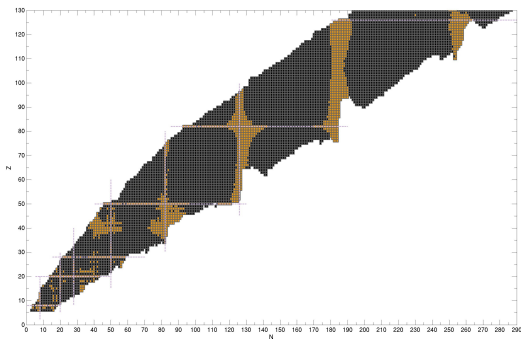
Finite-range interaction  
(Brink and Boeker)

## Spherical Hartree-Fock ( $\sim 30$ nuclei)



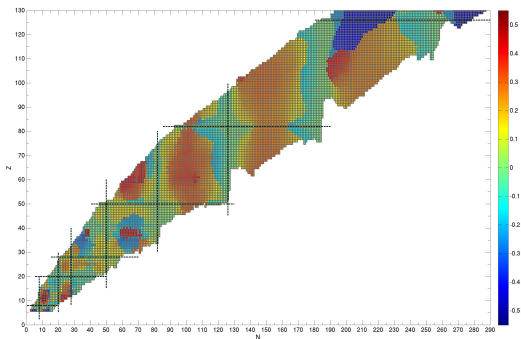
*Calculations with Gogny D1S interaction (S. Hilaire and J.P. Ebran)*

## Spherical Hartree-Fock-Bogoliubov ( $\sim 300$ nuclei)



*Calculations with Gogny D1S interaction (S. Hilaire and J.P. Ebran)*

## Axially-deformed Hartree-Fock-Bogoliubov ( $\sim 6000$ nuclei)



*Calculations with Gogny D1S interaction (S. Hilaire and J.P. Ebran)*

## GREEN'S FUNCTIONS

## Definitions

The state  $|\alpha, t_0\rangle$  of a particle with quantum numbers  $\alpha$  at time  $t_0$  evolves in

$$|\alpha, t_0; t\rangle = e^{-\frac{i}{\hbar}H(t-t_0)}|\alpha, t_0\rangle$$

at a time  $t$  ( $t > t_0$ ) and for a time-independent Hamiltonian.

$$\begin{aligned}\psi(\mathbf{r}, t) &= \langle \mathbf{r} | \alpha, t_0; t \rangle = \langle \mathbf{r} | e^{-\frac{i}{\hbar}H(t-t_0)} | \alpha, t_0 \rangle \\ &= \int d\mathbf{r}' \langle \mathbf{r} | e^{-\frac{i}{\hbar}H(t-t_0)} | \mathbf{r}' \rangle \langle \mathbf{r}' | \alpha, t_0 \rangle \\ &= i\hbar \int d\mathbf{r}' G(\mathbf{r}, \mathbf{r}'; t - t_0) \psi(\mathbf{r}', t_0)\end{aligned}$$

where  $G$  is referred to as

Propagator or Green's Function

$$G(\mathbf{r}, \mathbf{r}'; t - t_0) = -\frac{i}{\hbar} \langle \mathbf{r} | e^{-\frac{i}{\hbar}H(t-t_0)} | \mathbf{r}' \rangle$$

## Propagator or Green's Function

$$G(\mathbf{r}, \mathbf{r}'; t - t_0) = -\frac{i}{\hbar} \langle \mathbf{r} | e^{-\frac{i}{\hbar} H(t-t_0)} | \mathbf{r}' \rangle$$

$$\psi(\mathbf{r}, t) = i\hbar \int d\mathbf{r}' G(\mathbf{r}, \mathbf{r}'; t - t_0) \psi(\mathbf{r}', t_0)$$

The wave function at  $\mathbf{r}$  and  $t$  is determined by the wave function at the original time  $t_0$ , receiving contributions from all  $\mathbf{r}'$  weighted by the amplitude  $G$ .

## Second quantization

$\psi^\dagger(\mathbf{r}, t)$  creates a particle at  $(\mathbf{r}, t)$   
 $\psi(\mathbf{r}, t)$  annihilates a particle at  $(\mathbf{r}, t)$

Bose-Einstein statistics (-)/Fermi-Dirac statistics (+)

$$\left[ \psi^\dagger(\mathbf{r}, t), \psi^\dagger(\mathbf{r}', t) \right]_{\pm} = 0$$

$$\left[ \psi^\dagger(\mathbf{r}, t), \psi(\mathbf{r}', t) \right]_{\pm} = 0$$

$$\left[ \psi(\mathbf{r}, t), \psi^\dagger(\mathbf{r}', t) \right]_{\pm} = \delta(\mathbf{r} - \mathbf{r}')$$



$$\begin{aligned} G(\mathbf{r}, \mathbf{r}'; t - t_0) &= -\frac{i}{\hbar} \langle \mathbf{r} | e^{-\frac{i}{\hbar} H(t-t_0)} | \mathbf{r}' \rangle = -\frac{i}{\hbar} \langle 0 | a_{\mathbf{r}} e^{-\frac{i}{\hbar} H(t-t_0)} a_{\mathbf{r}'}^\dagger | 0 \rangle \\ &= -\frac{i}{\hbar} \sum_{nn'} \langle 0 | a_{\mathbf{r}} | n \rangle \langle n | e^{-\frac{i}{\hbar} H(t-t_0)} | n' \rangle \langle n' | a_{\mathbf{r}'}^\dagger | 0 \rangle \end{aligned}$$

### One-body propagator in second quantization

$$G(1, 1') = -i \langle 0 | \mathcal{T}(\psi(1)\psi^\dagger(1')) | 0 \rangle$$

$\mathcal{T}$  is the time ordering operator and  $1 \equiv \mathbf{r}_1, t_1$

$$\begin{aligned} \text{Ex: } \mathcal{T}(\psi(1)\psi^\dagger(1')) &= \psi(1)\psi^\dagger(1') \quad \text{if } t_1 > t_1' \\ &= -\psi^\dagger(1')\psi(1) \quad \text{if } t_1 < t_1' \end{aligned}$$

$$\begin{aligned} G(\mathbf{r}, \mathbf{r}'; t - t_0) &= -\frac{i}{\hbar} \langle \mathbf{r} | e^{-\frac{i}{\hbar} H(t-t_0)} | \mathbf{r}' \rangle = -\frac{i}{\hbar} \langle 0 | a_{\mathbf{r}} e^{-\frac{i}{\hbar} H(t-t_0)} a_{\mathbf{r}'}^\dagger | 0 \rangle \\ &= -\frac{i}{\hbar} \sum_{nn'} \langle 0 | a_{\mathbf{r}} | n \rangle \langle n | e^{-\frac{i}{\hbar} H(t-t_0)} | n' \rangle \langle n' | a_{\mathbf{r}'}^\dagger | 0 \rangle \end{aligned}$$

One-body propagator in second quantization

$$G(1, 1') = -i \langle 0 | \mathcal{T}(\psi(1)\psi^\dagger(1')) | 0 \rangle$$

$\mathcal{T}$  is the time ordering operator and  $1 \equiv \mathbf{r}_1, t_1$

Particle propagator  $t_1 > t_1'$

$$G_1(1, 1') = i \langle 0 | \psi(1)\psi^\dagger(1') | 0 \rangle$$

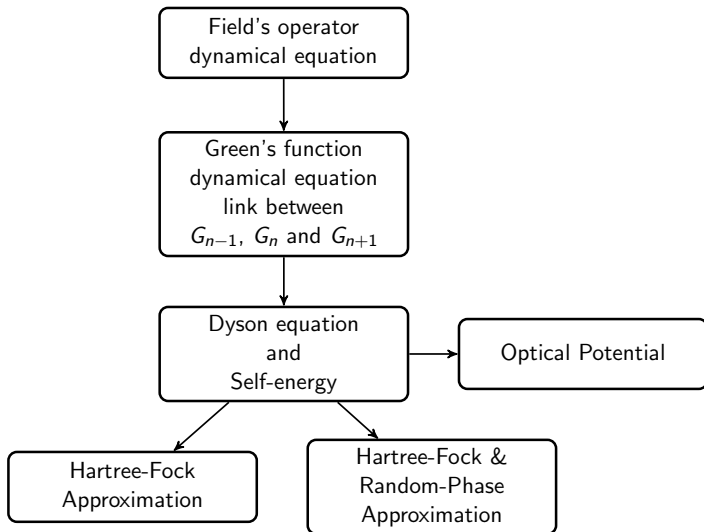
Hole propagator  $t_1 < t_1'$

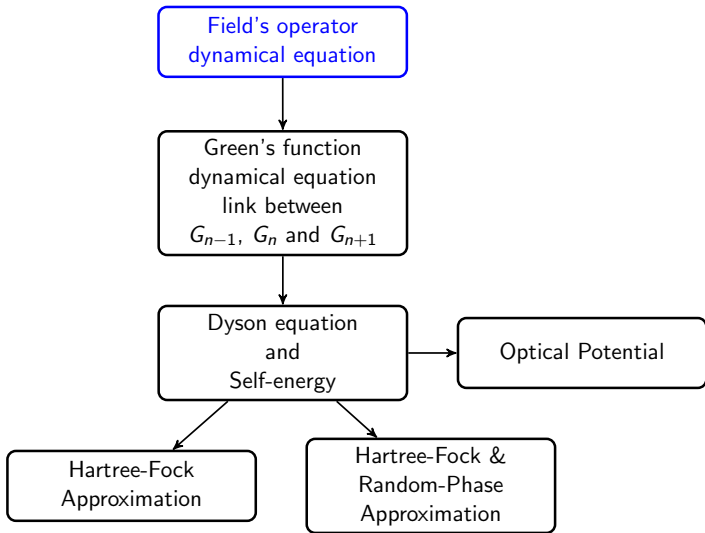
$$G_1(1, 1') = -i \langle 0 | \psi^\dagger(1')\psi(1) | 0 \rangle$$

### n-body Green's function

$$G_n = (-i)^n \langle 0 | \mathcal{T} \{ \psi(1) \dots \psi(n) \psi^\dagger(n') \dots \psi^\dagger(1') \} | 0 \rangle$$

Green's functions are average value  
of  
creation and annihilation operators





# Field's operator dynamical equation

Heisenberg picture

{ Time-dependent operators  
Time-independent state vectors

Schrödinger picture

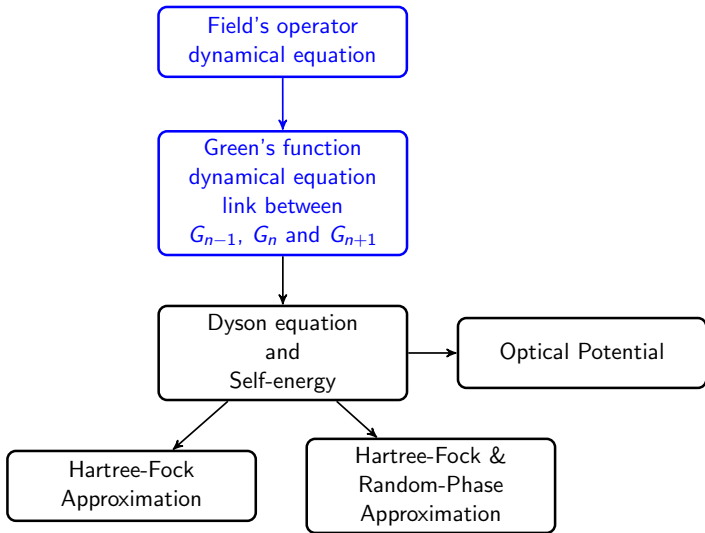
{ Time-independent operators  
Time-dependent state vectors

$$\langle \psi'_S(t) | \hat{O}_S | \psi_S(t) \rangle = \langle \psi'_H | \underbrace{e^{i\hat{H}t/\hbar} \hat{O}_S e^{-i\hat{H}t/\hbar}}_{\hat{O}_H(t)} | \psi_H \rangle$$

$$i\hbar \frac{\partial \hat{O}_H(t)}{\partial t} = e^{i\hat{H}t/\hbar} [\hat{O}_S, \hat{H}] e^{-i\hat{H}t/\hbar} = [\hat{O}_H(t), \hat{H}]$$

Equation of motion for an operator  $\hat{O}_H(t)$  in Heisenberg picture

$$i\hbar \frac{\partial \hat{O}_H(t)}{\partial t} = [\hat{O}_H(t), H]$$



# Green's function dynamical equation: one-body case

Equation of motion  
for an operator  $\hat{O}_H(t)$   
in Heisenberg picture

$$i\hbar \frac{\partial \hat{O}_H(t)}{\partial t} = [\hat{O}_H(t), H]$$

Hamiltonian in second quantization

$$H = T + V$$

$$T = \frac{\hbar^2}{2m} \int \psi^\dagger(x) \Delta \psi(x) dx$$

$$V = \frac{1}{2} \int \psi^\dagger(x) \psi^\dagger(x') v(x, x') \psi(x') \psi(x) dx dx'$$

$$i \frac{\partial \psi(x)}{\partial t} = -\frac{1}{2m} \Delta \psi(x) + \int dx'' v(x, x'') \psi^\dagger(x'') \psi(x'') \psi(x)$$



$$i \frac{\partial \psi(x)}{\partial t} = -\frac{1}{2m} \Delta \psi(x) + \int dx'' v(x, x'') \psi^\dagger(x'') \psi(x'') \psi(x)$$

$\times \psi^\dagger(x')$  from the right  
and applying  $T$

Keeping in mind the definition...

**One-body Green's function**

$$G(1, 1') = -i \langle 0 | \mathcal{T} (\psi(1) \psi^\dagger(1')) | 0 \rangle$$

$$i \langle 0 | \mathcal{T} \left( \frac{\partial}{\partial t} \psi(x) \psi^\dagger(x') \right) | 0 \rangle = -\frac{1}{2m} \langle 0 | \mathcal{T} (\Delta \psi(x) \psi^\dagger(x')) | 0 \rangle \\ + \int dx'' v(x, x'') \langle 0 | \mathcal{T} (\psi^\dagger(x'') \psi(x'') \psi(x) \psi^\dagger(x')) | 0 \rangle$$

$\mathcal{T}$  commutes with  $\Delta$

$\Delta G_1(x, x')$

$$i \langle 0 | \underbrace{\mathcal{T} \left( \frac{\partial}{\partial t} \psi(x) \psi^\dagger(x') \right)}_{\text{blue bracket}} | 0 \rangle = -\frac{1}{2m} \langle 0 | \underbrace{\mathcal{T} \left( \Delta \psi(x) \psi^\dagger(x') \right)}_{\text{blue bracket}} | 0 \rangle$$

$$+ \int dx'' v(x, x'') \langle 0 | \underbrace{\mathcal{T} \left( \psi^\dagger(x'') \psi(x'') \psi(x) \psi^\dagger(x') \right)}_{\text{red bracket}} | 0 \rangle$$

$\mathcal{T}$  doesn't commute with  $\frac{\partial}{\partial t}$

Two-body Green's function

$$\mathcal{T}(\psi(x)\psi^\dagger(x')) = \theta(t - t')\psi(x)\psi^\dagger(x') - \theta(t' - t)\psi^\dagger(x')\psi(x)$$

$$\frac{\partial}{\partial t} \left\{ \mathcal{T}(\psi(x)\psi^\dagger(x')) \right\} = \delta(x - x') + \mathcal{T} \left( \frac{\partial}{\partial t} \psi(x)\psi^\dagger(x') \right)$$

$$\frac{\partial}{\partial t} G_1(x, x') = \delta(x - x') + \langle 0 | \mathcal{T} \left( \frac{\partial}{\partial t} \psi(x)\psi^\dagger(x') \right) | 0 \rangle$$

$G_2(x''x; x''_+x')$

$$\left(i\frac{\partial}{\partial t} + \frac{1}{2m}\Delta\right) G_1(x, x') = \delta(x - x') - i \int dx'' v(x, x'') G_2(x''; x; x'_+ x')$$

Definition of the free propagator

$$\left(i\frac{\partial}{\partial t} + \frac{1}{2m}\Delta\right) G_0(x, x') = \delta(x - x')$$

$$\begin{aligned} \left(i\frac{\partial}{\partial t} + \frac{1}{2m}\Delta\right) G_1(x, x') &= \left(i\frac{\partial}{\partial t} + \frac{1}{2m}\Delta\right) G_0(x, x') \\ &\quad - i \int dx'' dx''' \left(i\frac{\partial}{\partial t} + \frac{1}{2m}\Delta\right) G_0(x, x''') v(x''', x'') G_2(x''; x; x'_+ x') \end{aligned}$$

$$\left(i\frac{\partial}{\partial t} + \frac{1}{2m}\Delta\right) G_1(x, x') = \delta(x - x') - i \int dx'' dx''' \delta(x - x''') v(x''', x'') G_2(x'' x; x'_+ x')$$

Definition of the free propagator

$$\left(i\frac{\partial}{\partial t} + \frac{1}{2m}\Delta\right) G_0(x, x') = \delta(x - x')$$

$$\left(i\frac{\partial}{\partial t} + \frac{1}{2m}\Delta\right) G_1(x, x') = \left(i\frac{\partial}{\partial t} + \frac{1}{2m}\Delta\right) G_0(x, x') - i \int dx'' dx''' \left(i\frac{\partial}{\partial t} + \frac{1}{2m}\Delta\right) G_0(x, x''') v(x''', x'') G_2(x'' x; x'_+ x')$$

### Dynamical equation for $G_1$

$$G_1(1, 1') = G_0(1, 1') - i \int d2d3 G_0(1, 2) v(2, 3) G_2(23; 1'3^+)$$

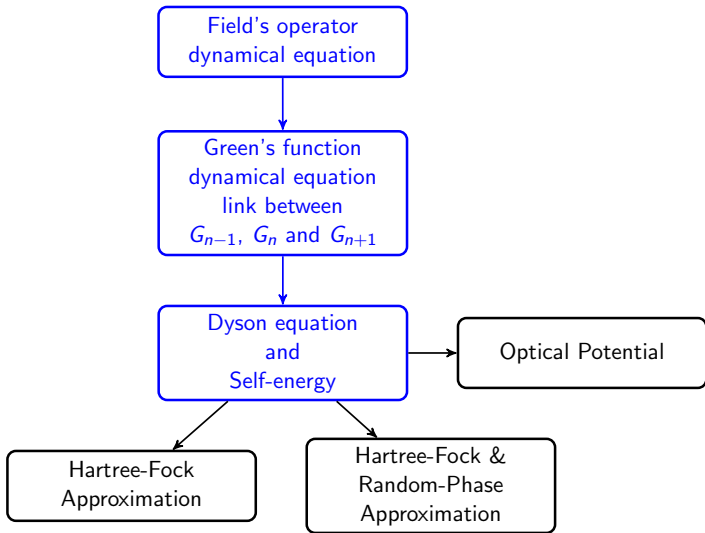
The dynamical equation for the one-body Green's function connects  $G_0$ ,  $G_1$  and  $G_2$ .

### Dynamical equation for $G_n$

$$\left( i \frac{\partial}{\partial t_1} + \frac{1}{2m} \Delta_1 \right) G_n(1\dots n; 1' \dots n') = \{ G_{n-1}(2\dots n; 2' \dots n') \delta(1 - 1') \}_{sym} - i \int dm v(1, m) G_{n+1}(1\dots n, m; 1' \dots n' m^+)$$

where  $\{ \}_{sym}$  stands for the summation of the terms where  $1'$  is replaced by  $2', \dots, n'$  with a  $\pm$  signe corresponding to the parity of the permutation

*(For the complete demo, see Fetter & Walecka...).*



### Dynamical equation for $G_1$

$$G_1(1, 1') = G_0(1, 1') - i \int d2d3 G_0(1, 2) v(2, 3) G_2(23; 1'3^+)$$

### Dyson equation

$$G_1(1, 1') = G_0(1, 1') + \int d2d3 G_0(1, 2) \underbrace{\Sigma(2, 3)}_{\text{Self-energy}} G_1(3, 1')$$

### Self-energy

$$\int d3 \Sigma(2, 3) G_1(3, 1') = -i \int d3 v(2, 3) G_2(23, 1'3^+)$$



Dynamical equation for  $G_1$ 

$$G_1(1, 1') = G_0(1, 1') - i \int d2d3 G_0(1, 2) v(2, 3) G_2(23; 1'3^+)$$

## Dyson equation

$$G_1(1, 1') = G_0(1, 1') + \int d2d3 G_0(1, 2) \underbrace{\Sigma(2, 3)}_{\text{Self-energy}} G_1(3, 1')$$

## Self-energy

$$\int d1'd3 \Sigma(2, 3) G_1(3, 1') G_1^{-1}(1', 4) = -i \int d1'd3 v(2, 3) G_2(23, 1'3^+) G_1^{-1}(1', 4)$$

Dynamical equation for  $G_1$ 

$$G_1(1, 1') = G_0(1, 1') - i \int d2d3 G_0(1, 2) v(2, 3) G_2(23; 1'3^+)$$

## Dyson equation

$$G_1(1, 1') = G_0(1, 1') + \int d2d3 G_0(1, 2) \underbrace{\Sigma(2, 3)}_{\text{Self-energy}} G_1(3, 1')$$

## Self-energy

$$\int d1' d3 \underbrace{\Sigma(2, 3) G_1(3, 1') G_1^{-1}(1', 4)}_{\delta(3,4)} = -i \int d1' d3 v(2, 3) G_2(23, 1'3^+) G_1^{-1}(1', 4)$$

Dynamical equation for  $G_1$ 

$$G_1(1, 1') = G_0(1, 1') - i \int d2d3 G_0(1, 2) v(2, 3) G_2(23; 1'3^+)$$

## Dyson equation

$$G_1(1, 1') = G_0(1, 1') + \int d2d3 G_0(1, 2) \underbrace{\Sigma(2, 3)}_{\text{Self-energy}} G_1(3, 1')$$

## Self-energy

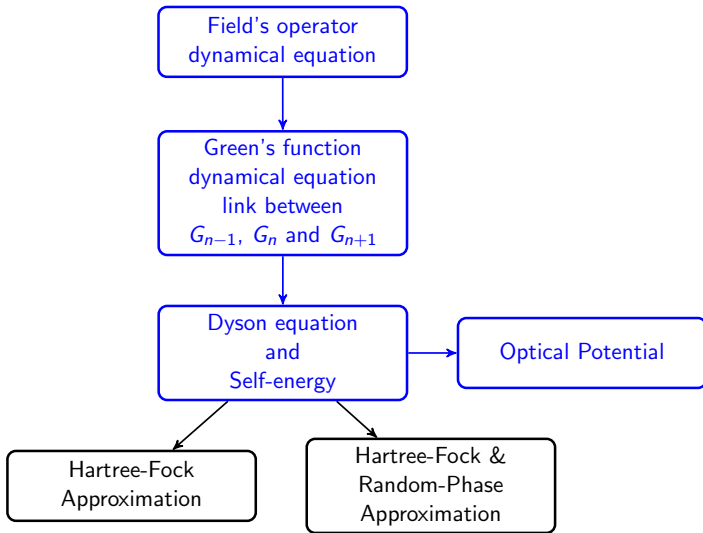
$$\Sigma(2, 3) = -i \int d4d5 v(2, 4) G_2(24, 54^+) G_1^{-1}(5, 3)$$

## Self-energy

$$\Sigma(2, 3) = -i \int d4d5v(2, 4)G_2(24, 54^+)G_1^{-1}(5, 3)$$

- ▶ Self-energy is exactly determined starting from a two-body interaction.
- ▶  $G_2$  is connected to  $G_1$  and  $G_3$  and so on...

Need for approximations



### Dyson equation

$$G_1(1, 1') = G_0(1, 1') - \int d2d3 G_0(1, 2) \Sigma(2, 3) G_1(3, 1')$$

## Dyson equation

$$G_1(1, 1') = G_0(1, 1') - \int d2d3 G_0(1, 2) \Sigma(2, 3) G_1(3, 1')$$

$$\left( \frac{\partial}{\partial t} + \frac{1}{2m} \Delta \right) \mapsto \text{Dyson equation}$$

$$\left( \frac{\partial}{\partial t} + \frac{1}{2m} \Delta \right) G_1(x, x') = \delta(x, x') - \int dx'' \Sigma(x, x'') G_1(x'', x')$$

## Dyson equation

$$G_1(1, 1') = G_0(1, 1') - \int d2d3 G_0(1, 2) \Sigma(2, 3) G_1(3, 1')$$

$$\left( \frac{\partial}{\partial t} + \frac{1}{2m} \Delta \right) \mapsto \text{Dyson equation}$$

$$\left( \frac{\partial}{\partial t} + \frac{1}{2m} \Delta \right) G_1(x, x') = \delta(x, x') - \int dx'' \Sigma(x, x'') G_1(x'', x')$$

$$\text{FT} \left[ \left( \frac{\partial}{\partial t} + \frac{1}{2m} \Delta \right) \mapsto \text{Dyson equation} \right]$$

$$\left( \varepsilon - \frac{p^2}{2m} \right) G_1(\mathbf{r}, \mathbf{r}'; \varepsilon) = \delta(\mathbf{r}, \mathbf{r}') - \int d\mathbf{r}'' \Sigma(\mathbf{r}, \mathbf{r}''; \varepsilon) G_1(\mathbf{r}'', \mathbf{r}'; \varepsilon)$$



FT  $\left[ \left( \frac{\partial}{\partial t} + \frac{1}{2m} \Delta \right) \mapsto \text{Dyson equation} \right]$

$$\left( \varepsilon - \frac{p^2}{2m} \right) G_1(\mathbf{r}, \mathbf{r}'; \varepsilon) = \delta(\mathbf{r}, \mathbf{r}') - \int d\mathbf{r}'' \Sigma(\mathbf{r}, \mathbf{r}''; \varepsilon) G_1(\mathbf{r}'', \mathbf{r}'; \varepsilon)$$

### One-body Green's function

$$G_1(x, x') = -i \langle 0 | \mathcal{T}(\psi(x) \psi^\dagger(x')) | 0 \rangle$$

### Field's operators

$$\psi^\dagger(x) = \sum_{\lambda} \phi_{\lambda}^*(\mathbf{r}) a_{\lambda}^{\dagger}(t)$$

$$\psi(x) = \sum_{\lambda} \phi_{\lambda}(\mathbf{r}) a_{\lambda}(t)$$

FT  $\left[ \left( \frac{\partial}{\partial t} + \frac{1}{2m} \Delta \right) \mapsto \text{Dyson equation} \right]$

$$\left( \varepsilon - \frac{p^2}{2m} \right) G_1(\mathbf{r}, \mathbf{r}'; \varepsilon) = \delta(\mathbf{r}, \mathbf{r}') - \int d\mathbf{r}'' \Sigma(\mathbf{r}, \mathbf{r}''; \varepsilon) G_1(\mathbf{r}'', \mathbf{r}'; \varepsilon)$$

### One-body Green's function

$$G_1(x, x') = \sum_{\lambda\lambda'} \phi_\lambda(\mathbf{r}) \phi_{\lambda'}^*(\mathbf{r}') G_{\lambda\lambda'}(t-t')$$

### Field's operators

$$\psi^\dagger(x) = \sum_{\lambda} \phi_{\lambda}^*(\mathbf{r}) a_{\lambda}^\dagger(t)$$

$$\psi(x) = \sum_{\lambda} \phi_{\lambda}(\mathbf{r}) a_{\lambda}(t)$$

FT  $\left[ \left( \frac{\partial}{\partial t} + \frac{1}{2m} \Delta \right) \mapsto \text{Dyson equation} \right]$

$$\left( \varepsilon - \frac{p^2}{2m} \right) G_1(\mathbf{r}, \mathbf{r}'; \varepsilon) = \delta(\mathbf{r}, \mathbf{r}') - \int d\mathbf{r}'' \Sigma(\mathbf{r}, \mathbf{r}''; \varepsilon) G_1(\mathbf{r}'', \mathbf{r}'; \varepsilon)$$

FT( $G_1$ )

$$G_1(\mathbf{r}, \mathbf{r}'; \varepsilon) = \sum_{\lambda\lambda'} \phi_\lambda(\mathbf{r}) \phi_{\lambda'}^*(\mathbf{r}') G_{\lambda\lambda'}(\varepsilon)$$

Field's operators

$$\psi^\dagger(x) = \sum_{\lambda} \phi_{\lambda}^*(\mathbf{r}) a_{\lambda}^{\dagger}(t)$$

$$\psi(x) = \sum_{\lambda} \phi_{\lambda}(\mathbf{r}) a_{\lambda}(t)$$

FT  $\left[ \left( \frac{\partial}{\partial t} + \frac{1}{2m} \Delta \right) \mapsto \text{Dyson equation} \right]$

$$\left( \varepsilon - \frac{p^2}{2m} \right) \sum_{\lambda\lambda'} \phi_{\lambda}(\mathbf{r}) \phi_{\lambda'}^*(\mathbf{r}') G_{\lambda\lambda'}(\varepsilon) = \delta(\mathbf{r}, \mathbf{r}') - \int d\mathbf{r}'' \Sigma(\mathbf{r}, \mathbf{r}''; \varepsilon) \sum_{\lambda\lambda'} \phi_{\lambda}(\mathbf{r}) \phi_{\lambda'}^*(\mathbf{r}') G_{\lambda\lambda'}(\varepsilon)$$

FT( $G_1$ )

$$G_1(\mathbf{r}, \mathbf{r}'; \varepsilon) = \sum_{\lambda\lambda'} \phi_{\lambda}(\mathbf{r}) \phi_{\lambda'}^*(\mathbf{r}') G_{\lambda\lambda'}(\varepsilon)$$

Field's operators

$$\psi^{\dagger}(x) = \sum_{\lambda} \phi_{\lambda}^*(\mathbf{r}) a_{\lambda}^{\dagger}(t)$$

$$\psi(x) = \sum_{\lambda} \phi_{\lambda}(\mathbf{r}) a_{\lambda}(t)$$

$$\text{FT} \left[ \left( \frac{\partial}{\partial t} + \frac{1}{2m} \Delta \right) \mapsto \text{Dyson equation} \right]$$

$$\left( \varepsilon - \frac{p^2}{2m} \right) \sum_{\lambda\lambda'} \phi_{\lambda}(\mathbf{r}) \phi_{\lambda'}^*(\mathbf{r}') G_{\lambda\lambda'}(\varepsilon) = \delta(\mathbf{r}, \mathbf{r}') \\ - \int d\mathbf{r}'' \Sigma(\mathbf{r}, \mathbf{r}''; \varepsilon) \sum_{\lambda\lambda'} \phi_{\lambda}(\mathbf{r}) \phi_{\lambda'}^*(\mathbf{r}') G_{\lambda\lambda'}(\varepsilon)$$

$$\int d\mathbf{r} d\mathbf{r}' \phi_{\lambda_3}^*(\mathbf{r}) \phi_{\lambda_4}(\mathbf{r}') \text{FT} \left[ \left( \frac{\partial}{\partial t} + \frac{1}{2m} \Delta \right) \mapsto \text{Dyson equation} \right]$$

$$\sum_{\lambda_1} \left\{ \varepsilon \delta_{\lambda_1 \lambda_3} - \int d\mathbf{r} \phi_{\lambda_3}^*(\mathbf{r}) \frac{p^2}{2m} \phi_{\lambda_1}(\mathbf{r}) \right. \\ \left. + \int d\mathbf{r} \phi_{\lambda_3}^*(\mathbf{r}) \int d\mathbf{r}'' \Sigma(\mathbf{r}, \mathbf{r}''; \varepsilon) \phi_{\lambda_1}(\mathbf{r}'') \right\} G_{\lambda_1 \lambda_4}(\varepsilon) = \delta_{\lambda_3 \lambda_4}$$

$$\int dr dr' \phi_{\lambda_3}^*(\mathbf{r}) \phi_{\lambda_4}(\mathbf{r}') \text{FT} \left[ \left( \frac{\partial}{\partial t} + \frac{1}{2m} \Delta \right) \mapsto \text{Dyson equation} \right]$$

$$\sum_{\lambda_1} \left\{ \varepsilon \delta_{\lambda_1 \lambda_3} - \int d\mathbf{r} \phi_{\lambda_3}^*(\mathbf{r}) \frac{p^2}{2m} \phi_{\lambda_1}(\mathbf{r}) + \int d\mathbf{r} \phi_{\lambda_3}^*(\mathbf{r}) \int d\mathbf{r}'' \Sigma(\mathbf{r}, \mathbf{r}''; \varepsilon) \phi_{\lambda_1}(\mathbf{r}'') \right\} G_{\lambda_1 \lambda_4}(\varepsilon) = \delta_{\lambda_3 \lambda_4}$$

Let's consider a set of wave functions  $\phi_\lambda$  that diagonalizes it

$$[\varepsilon - E_\lambda(\varepsilon)] G_{\lambda \lambda'}(\varepsilon) = \delta_{\lambda \lambda'}$$

hence

$$\langle \lambda_3 | \frac{p^2}{2m} + \int d\mathbf{r}'' \Sigma(\mathbf{r}, \mathbf{r}''; \varepsilon) | \lambda_1 \rangle = E_{\lambda_1}(\varepsilon) \delta_{\lambda_3 \lambda_1}$$

The set of wave functions  $\phi_\lambda$  obeys

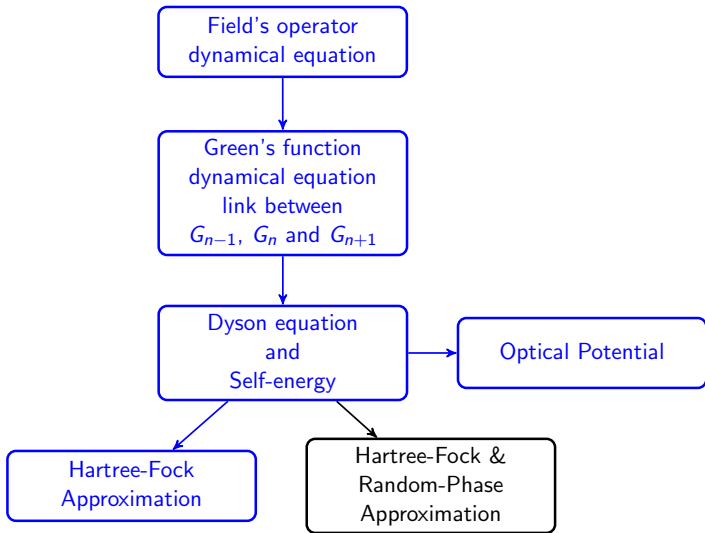
$$\frac{p^2}{2m} \phi_\lambda(\mathbf{r}) + \int d\mathbf{r}'' \Sigma(\mathbf{r}, \mathbf{r}''; \varepsilon) \phi_\lambda(\mathbf{r}'') = E_\lambda(\varepsilon) \phi_\lambda(\mathbf{r})$$

### Schrödinger equation

$$\frac{p^2}{2m} \phi_\lambda(\mathbf{r}, \varepsilon) + \int d\mathbf{r}' \Sigma(\mathbf{r}, \mathbf{r}'; \varepsilon) \phi_\lambda(\mathbf{r}', \varepsilon) = E(\varepsilon) \phi_\lambda(\mathbf{r}, \varepsilon)$$

$\phi$ 's are the wave functions of a particle experiencing a potential  $\Sigma$  which is non-local and energy dependent

Optical potential is connected to the Fourier transform of Self-energy itself connected to the two-body interaction.

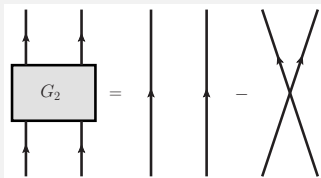




Dynamical equation for  $G_1$ 

$$G_1(1, 1') = G_0(1, 1') - i \int d2d3 G_0(1, 2)v(2, 3)G_2(23, 1'3^+)$$

## Hartree-Fock approximation



1. Two-body correlations are neglected
2.  $G_2$  becomes an antisymmetrized product of  $G_1$ 's

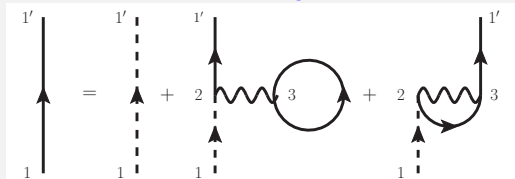
Dynamical equation for  $G_1$  within HF approximation

$$G_1^{HF}(1, 1') = G_0(1, 1') - i \int d2d3 G_0(1, 2)v(2, 3) \left( G_1^{HF}(2, 1') \right. \\ \left. G_1^{HF}(3, 3^+) - G_1^{HF}(2, 3^+)G_1^{HF}(3, 1') \right)$$

Dynamical equation for  $G_1$  within HF approximation

$$G_1^{HF}(1, 1') = G_0(1, 1') - i \int d2d3 G_0(1, 2) v(2, 3) \left( G_1^{HF}(2, 1') \right. \\ \left. G_1^{HF}(3, 3^+) - G_1^{HF}(2, 3^+) G_1^{HF}(3, 1') \right)$$

## Hartree-Fock Diagrammatic



Infinite sum of 'bubbles' and 'oysters'

### Exact Self-energy

$$\Sigma(2, 3) = -i \int d4d5v(2, 4)G_2(24, 54^+)G_1^{-1}(5, 3)$$

### Self-energy at the HF approximation

$$\Sigma^{HF}(2, 3) = -i \int d4d5v(2, 4) (G_1(2, 5)G_1(4, 4^+) - G_1(2, 4^+)G_1(4, 5)) G_1^{-1}(5, 3)$$

### Exact Self-energy

$$\Sigma(2, 3) = -i \int d4d5v(2, 4)G_2(24, 54^+)G_1^{-1}(5, 3)$$

### Self-energy at the HF approximation

$$\Sigma^{HF}(2, 3) = -i \int d4d5v(2, 4) (G_1(2, 5)G_1(4, 4^+) - G_1(2, 4^+)G_1(4, 5)) G_1^{-1}(5, 3)$$

## Exact Self-energy

$$\Sigma(2, 3) = -i \int d4d5v(2, 4)G_2(24, 54^+)G_1^{-1}(5, 3)$$

## Self-energy at the HF approximation

$$\Sigma^{HF}(2, 3) = -i \int d4v(2, 4) (\delta(2, 3)G_1(4, 4^+) - G_1(2, 4^+)\delta(4, 3))$$

### Exact Self-energy

$$\Sigma(2, 3) = -i \int d4d5 v(2, 4) G_2(24, 54^+) G_1^{-1}(5, 3)$$

### Self-energy at the HF approximation

$$\Sigma^{HF}(2, 3) = -i \int d4 v(2, 4) \delta(2, 3) G_1(4, 4^+) + i v(2, 3) G_1(2, 3)$$

### Exact Self-energy

$$\Sigma(2, 3) = -i \int d4d5v(2, 4)G_2(24, 54^+)G_1^{-1}(5, 3)$$

### Self-energy at the HF approximation

$$\Sigma^{HF}(2, 3) = -i \int d4v(2, 4)\delta(2, 3)G_1(4, 4^+) + i v(2, 3)G_1(2, 3)$$

### Schrödinger equation

$$\frac{p^2}{2m}\phi_\lambda(\mathbf{r}, \varepsilon) + \int d\mathbf{r}' \underbrace{\Sigma^{HF}(\mathbf{r}, \mathbf{r}'; \varepsilon)}_{\text{FT of Self-energy}} \phi_\lambda(\mathbf{r}', \varepsilon) = E(\varepsilon)\phi_\lambda(\mathbf{r}, \varepsilon)$$

## Self-energy at the HF approximation

$$\Sigma^{HF}(2, 3) = -i \int d4 v(2, 4) \delta(2, 3) G_1(4, 4^+) + i v(2, 3) G_1(2, 3)$$

## One-body Green's function

$$G_1(x, x') = \sum_{\lambda\lambda'} \phi_\lambda(\mathbf{r}) \phi_{\lambda'}^*(\mathbf{r}') G_{\lambda\lambda'}(t-t')$$

## Occupation numbers

$$G_{\lambda\lambda}(t-t' = +0) = -i(1 - m_\lambda)$$

$$G_{\lambda\lambda}(t-t' = -0) = i m_\lambda$$

$$m_\lambda = \langle \psi_0 | a_\lambda^\dagger a_\lambda | \psi_0 \rangle$$

Fourier transform of  $\Sigma^{HF}$  with  $v(x, x') = v(\mathbf{r} - \mathbf{r}') \delta(t - t')$

$$\begin{aligned} \Sigma^{HF}(\mathbf{r}, \mathbf{r}''; \varepsilon) &= \delta(\mathbf{r}, \mathbf{r}'') \int d\mathbf{r}' v(\mathbf{r}, \mathbf{r}') \sum_{\lambda} m_\lambda \phi_\lambda^*(\mathbf{r}') \phi_\lambda(\mathbf{r}') \\ &\quad - v(\mathbf{r}, \mathbf{r}'') \sum_{\lambda} m_\lambda \phi_\lambda^*(\mathbf{r}) \phi_\lambda(\mathbf{r}'') \\ &= \delta(\mathbf{r}, \mathbf{r}'') \int d\mathbf{r}' v(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}') - v(\mathbf{r}, \mathbf{r}'') \rho(\mathbf{r}, \mathbf{r}'') \end{aligned}$$

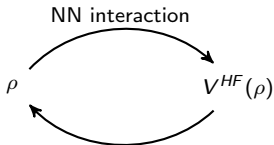


## Schrödinger equation

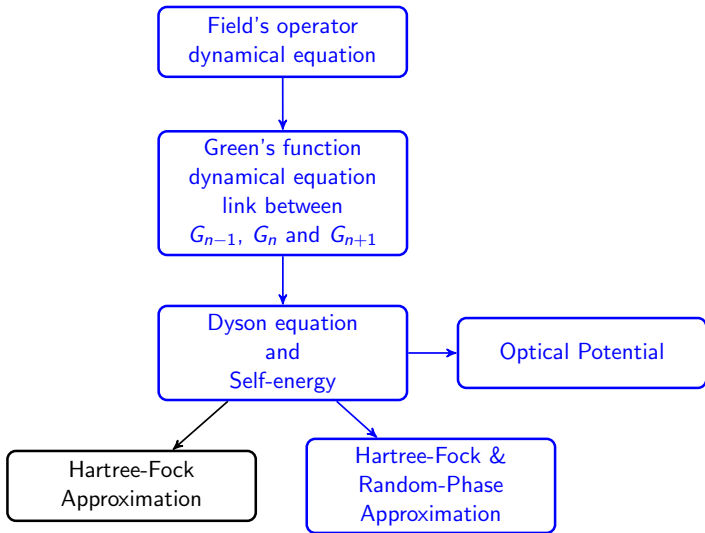
$$\frac{p^2}{2m} \phi_\lambda(\mathbf{r}, \varepsilon) + \int d\mathbf{r}' V^{HF}(\mathbf{r}, \mathbf{r}'; \varepsilon) \phi_\lambda(\mathbf{r}', \varepsilon) = E(\varepsilon) \phi_\lambda(\mathbf{r}, \varepsilon)$$

## HF potential

$$V^{HF}(\mathbf{r}, \mathbf{r}''; \varepsilon) = \delta(\mathbf{r}, \mathbf{r}'') \int d\mathbf{r}' v(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}') - v(\mathbf{r}, \mathbf{r}'') \rho(\mathbf{r}, \mathbf{r}'')$$



Schrödinger equation



## SOME CONSIDERATIONS ABOUT $G_2$

### n-body Green's function

$$G_n = (-i)^n \langle 0 | \mathcal{T} \{ \psi(1) \dots \psi(n) \psi^\dagger(n') \dots \psi^\dagger(1') \} | 0 \rangle$$

## Two-body Green's function

$$G_2(12; 1'2') = -\langle 0 | \mathcal{T} \{ \psi(1)\psi(2)\psi^\dagger(2')\psi^\dagger(1') \} | 0 \rangle$$

Different meanings according to times relative order

2p-propagator

$$t_1, t_2 > t_1', t_2'$$

$(A + 2)$ -particle  
system

2h-propagator

$$t_1, t_2 < t_1', t_2'$$

$(A - 2)$ -particle  
system

ph-propagator

$$t_1, t_2' < t_2, t_1'$$

$$t_2, t_1' < t_1, t_2'$$

Excited states of the  
 $A$ -particle system

## Two-body Green's function

$$G_2(12; 1'2') = -\langle 0 | \psi(1)\psi(2)\psi^\dagger(2')\psi^\dagger(1') | 0 \rangle$$

2p-propagator

$$t_1, t_2 > t_1', t_2'$$

(A + 2)-particle  
system

2h-propagator

$$t_1, t_2 < t_1', t_2'$$

(A - 2)-particle  
system

ph-propagator

$$t_1, t_2' < t_2, t_1'$$

$$t_2, t_1' < t_1, t_2'$$

Excited states of the  
A-particle system

## Two-body Green's function

$$G_2(12; 1'2') = -\langle 0 | \psi^\dagger(2') \psi^\dagger(1') \psi(1) \psi(2) | 0 \rangle$$



2p-propagator

$$t_1, t_2 > t_1', t_2'$$

(A + 2)-particle  
system

2h-propagator

$$t_1, t_2 < t_1', t_2'$$

(A - 2)-particle  
system

ph-propagator

$$t_1, t_2' < t_2, t_1'$$

$$t_2, t_1' < t_1, t_2'$$

Excited states of the  
A-particle system

## Two-body Green's function

$$G_2(12; 1'2') = -\langle 0 | \psi^\dagger(2') \psi(1) \psi(2) \psi^\dagger(1') | 0 \rangle$$

2p-propagator

$$t_1, t_2 > t_1', t_2'$$

(A + 2)-particle  
system

2h-propagator

$$t_1, t_2 < t_1', t_2'$$

(A - 2)-particle  
system

ph-propagator

$$t_1, t_2' < t_2, t_1'$$

$$t_2, t_1' < t_1, t_2'$$

Excited states of the  
A-particle system



## Two-body Green's function

$$G_2(12; 1'2') = -\langle 0 | \mathcal{T} \{ \psi(1)\psi(2)\psi^\dagger(2')\psi^\dagger(1') \} | 0 \rangle$$

### Field's operators

$$\psi^\dagger(x) = \sum_{\lambda} \phi_{\lambda}^*(\mathbf{r}) a_{\lambda}^{\dagger}(t)$$

$$\psi(x) = \sum_{\lambda} \phi_{\lambda}(\mathbf{r}) a_{\lambda}(t)$$

### Two-body Green's function in ' $\lambda$ -representation'

$$G_2(x_1 x_2; x_1' x_2') = \sum_{\substack{\lambda_1 \lambda_2 \\ \lambda_1' \lambda_2'}} \phi_{\lambda_1}(\mathbf{r}_1) \phi_{\lambda_2}(\mathbf{r}_2) G_{\lambda_1 \lambda_2, \lambda_1' \lambda_2'}(t_1 t_2; t_1' t_2') \phi_{\lambda_1'}^*(\mathbf{r}'_1) \phi_{\lambda_2'}^*(\mathbf{r}'_2)$$

with

$$G_{\lambda_1 \lambda_2, \lambda_1' \lambda_2'}(t_1 t_2; t_1' t_2') = -\langle 0 | \mathcal{T} (a_{\lambda_1}(t_1) a_{\lambda_2}(t_2) a_{\lambda_2'}^{\dagger}(t_2') a_{\lambda_1'}^{\dagger}(t_1')) | 0 \rangle$$

Two-body Green's function in ' $\lambda$ -representation'

$$G_{\lambda_1 \lambda_2, \lambda_1', \lambda_2'}(t_1 t_2; t_1' t_2') = -\langle 0 | \mathcal{T}(a_{\lambda_1}(t_1) a_{\lambda_2}(t_2) a_{\lambda_2'}^\dagger(t_2') a_{\lambda_1'}^\dagger(t_1')) | 0 \rangle$$

pp/hh-propagator

$$t_1 = t_2 = t \\ t_1' = t_2' = t'$$

Heisenberg operator

$$a_\lambda(t) = e^{i\hat{H}t/\hbar} a_\lambda e^{-i\hat{H}t/\hbar}$$

## Two-body Green's function pp/hh

$$G_{\lambda_1 \lambda_2, \lambda_1', \lambda_2'}(t, t') = -\langle 0 | \mathcal{T}(a_{\lambda_1}(t) a_{\lambda_2}(t) a_{\lambda_2'}^\dagger(t') a_{\lambda_1'}^\dagger(t')) | 0 \rangle$$

## Two-body Green's function in ' $\lambda$ -representation'

$$G_{\lambda_1 \lambda_2, \lambda_1', \lambda_2'}(t_1 t_2; t_1' t_2') = -\langle 0 | \mathcal{T}(a_{\lambda_1}(t_1) a_{\lambda_2}(t_2) a_{\lambda_2'}^\dagger(t_2') a_{\lambda_1'}^\dagger(t_1')) | 0 \rangle$$

pp/hh-propagator

$$t_1 = t_2 = t$$

$$t_1' = t_2' = t'$$

Heisenberg operator

$$a_\lambda(t) = e^{i\hat{H}t/\hbar} a_\lambda e^{-i\hat{H}t/\hbar}$$

## Two-body Green's function pp/hh

$$G_{\lambda_1 \lambda_2, \lambda_1', \lambda_2'}(t, t') = -\langle 0 | a_{\lambda_1}(t) a_{\lambda_2}(t) a_{\lambda_2'}^\dagger(t') a_{\lambda_1'}^\dagger(t') | 0 \rangle \quad t' < t$$

$$= -\langle 0 | a_{\lambda_2'}^\dagger(t') a_{\lambda_1'}^\dagger(t') a_{\lambda_1}(t) a_{\lambda_2}(t) | 0 \rangle \quad t' > t$$

## Two-body Green's function in ' $\lambda$ -representation'

$$G_{\lambda_1 \lambda_2, \lambda_1', \lambda_2'}(t_1 t_2; t_1' t_2') = -\langle 0 | \mathcal{T}(a_{\lambda_1}(t_1) a_{\lambda_2}(t_2) a_{\lambda_2'}^\dagger(t_2') a_{\lambda_1'}^\dagger(t_1')) | 0 \rangle$$

pp/hh-propagator

$$t_1 = t_2 = t$$

$$t_1' = t_2' = t'$$

Heisenberg operator

$$a_\lambda(t) = e^{i\hat{H}t/\hbar} a_\lambda e^{-i\hat{H}t/\hbar}$$

## Two-body Green's function pp/hh ( $\hbar = 1$ )

$$G_{\lambda_1 \lambda_2, \lambda_1', \lambda_2'}(t, t') = -\langle 0 | e^{i\hat{H}t} a_{\lambda_1} a_{\lambda_2} e^{-i\hat{H}t} e^{i\hat{H}t'} a_{\lambda_2'}^\dagger a_{\lambda_1'}^\dagger e^{-i\hat{H}t'} | 0 \rangle \quad t' < t$$

$$= -\langle 0 | e^{i\hat{H}t'} a_{\lambda_1'}^\dagger a_{\lambda_2'}^\dagger e^{-i\hat{H}t'} e^{i\hat{H}t} a_{\lambda_1} a_{\lambda_2} e^{-i\hat{H}t} | 0 \rangle \quad t' > t$$

## Two-body Green's function in ' $\lambda$ -representation'

$$G_{\lambda_1 \lambda_2, \lambda_1', \lambda_2'}(t_1 t_2; t_1' t_2') = -\langle 0 | \mathcal{T}(a_{\lambda_1}(t_1) a_{\lambda_2}(t_2) a_{\lambda_2'}^\dagger(t_2') a_{\lambda_1'}^\dagger(t_1')) | 0 \rangle$$

pp/hh-propagator

$$t_1 = t_2 = t$$

$$t_1' = t_2' = t'$$

Heisenberg operator

$$a_\lambda(t) = e^{i\hat{H}t/\hbar} a_\lambda e^{-i\hat{H}t/\hbar}$$

## Two-body Green's function pp/hh ( $\hbar = 1$ )

$$G_{\lambda_1 \lambda_2, \lambda_1', \lambda_2'}(t, t') = -e^{iE_0(t-t')} \langle 0 | a_{\lambda_1} a_{\lambda_2} e^{-i\hat{H}(t-t')} a_{\lambda_2'}^\dagger a_{\lambda_1'}^\dagger | 0 \rangle \quad t' < t$$

$$= -e^{-iE_0(t-t')} \langle 0 | a_{\lambda_2'}^\dagger a_{\lambda_1'}^\dagger e^{-i\hat{H}(t'-t)} a_{\lambda_1} a_{\lambda_2} | 0 \rangle \quad t' > t$$

Two-body Green's function pp/hh ( $\hbar = 1$ )

$$\begin{aligned}
 G_{\lambda_1 \lambda_2, \lambda_1', \lambda_2'}(t, t') &= -e^{iE_0(t-t')} \langle 0 | a_{\lambda_1} a_{\lambda_2} e^{-i\hat{H}(t-t')} a_{\lambda_2'}^\dagger a_{\lambda_1'}^\dagger | 0 \rangle & t' < t \\
 &= -e^{-iE_0(t-t')} \langle 0 | a_{\lambda_2'}^\dagger a_{\lambda_1'}^\dagger e^{-i\hat{H}(t'-t)} a_{\lambda_1} a_{\lambda_2} | 0 \rangle & t' > t
 \end{aligned}$$

$$\begin{aligned}
 G_{\lambda_1 \lambda_2, \lambda_1', \lambda_2'}(t, t') &\stackrel{t' < t}{=} - \sum_n e^{iE_0(t-t')} \langle 0 | a_{\lambda_1} a_{\lambda_2} | \psi_n \rangle \langle \psi_n | e^{-i\hat{H}(t-t')} a_{\lambda_2'}^\dagger a_{\lambda_1'}^\dagger | 0 \rangle \\
 &\stackrel{t' > t}{=} - \sum_m e^{-iE_0(t-t')} \langle 0 | a_{\lambda_2'}^\dagger a_{\lambda_1'}^\dagger | \psi_m \rangle \langle \psi_m | e^{-i\hat{H}(t'-t)} a_{\lambda_1} a_{\lambda_2} | 0 \rangle
 \end{aligned}$$

Assuming,

 $\psi_n$  state of (N+2)-system

$$E_n = E_n(N+2) - E_0(N)$$

 $\psi_m$  state of (N-2)-system

$$E_m = E_m(N-2) - E_0(N)$$

Two-body Green's function pp/hh ( $\hbar = 1$ )

$$\begin{aligned}
 G_{\lambda_1 \lambda_2, \lambda_1', \lambda_2'}(t, t') &= -e^{iE_0(t-t')} \langle 0 | a_{\lambda_1} a_{\lambda_2} e^{-i\hat{H}(t-t')} a_{\lambda_2'}^\dagger a_{\lambda_1'}^\dagger | 0 \rangle & t' < t \\
 &= -e^{-iE_0(t-t')} \langle 0 | a_{\lambda_2'}^\dagger a_{\lambda_1'}^\dagger e^{-i\hat{H}(t'-t)} a_{\lambda_1} a_{\lambda_2} | 0 \rangle & t' > t
 \end{aligned}$$

$$\begin{aligned}
 G_{\lambda_1 \lambda_2, \lambda_1', \lambda_2'}(t, t') &\stackrel{t' < t}{=} - \sum_n e^{-iE_n(t-t')} \langle 0 | a_{\lambda_1} a_{\lambda_2} | \psi_n \rangle \langle \psi_n | a_{\lambda_2'}^\dagger a_{\lambda_1'}^\dagger | 0 \rangle \\
 &\stackrel{t' > t}{=} - \sum_m e^{iE_m(t-t')} \langle 0 | a_{\lambda_2'}^\dagger a_{\lambda_1'}^\dagger | \psi_m \rangle \langle \psi_m | a_{\lambda_1} a_{\lambda_2} | 0 \rangle
 \end{aligned}$$

Assuming,

$\psi_n$  state of (N+2)-system  
 $E_n = E_n(N+2) - E_0(N)$

$\psi_m$  state of (N-2)-system  
 $E_m = E_m(N-2) - E_0(N)$

Two-body Green's function pp/hh ( $\hbar = 1$ )

$$\begin{aligned}
 G_{\lambda_1 \lambda_2, \lambda_1', \lambda_2'}(t, t') &= -e^{iE_0(t-t')} \langle 0 | a_{\lambda_1} a_{\lambda_2} e^{-i\hat{H}(t-t')} a_{\lambda_2'}^\dagger a_{\lambda_1'}^\dagger | 0 \rangle & t' < t \\
 &= -e^{-iE_0(t-t')} \langle 0 | a_{\lambda_2'}^\dagger a_{\lambda_1'}^\dagger e^{-i\hat{H}(t'-t)} a_{\lambda_1} a_{\lambda_2} | 0 \rangle & t' > t
 \end{aligned}$$

$$\begin{aligned}
 G_{\lambda_1 \lambda_2, \lambda_1', \lambda_2'}(t, t') &\stackrel{t' < t}{=} - \sum_n e^{-iE_n(t-t')} X_{\lambda_1 \lambda_2}^{(n)*} X_{\lambda_1' \lambda_2'}^{(n)} \\
 &\stackrel{t' > t}{=} - \sum_m e^{iE_m(t-t')} Y_{\lambda_1', \lambda_2'}^{(m)*} Y_{\lambda_1 \lambda_2}^{(m)}
 \end{aligned}$$

## pp/hh-Amplitudes

$$\begin{aligned}
 X_{ab}^{(n)} &= \langle \psi_n | a_a^\dagger a_b^\dagger | 0 \rangle \\
 Y_{ab}^{(m)} &= \langle \psi_m | a_a a_b | 0 \rangle
 \end{aligned}$$

## Assuming,

$\psi_n$  state of (N+2)-system  
 $E_n = E_n(N+2) - E_0(N)$

$\psi_m$  state of (N-2)-system  
 $E_m = E_m(N-2) - E_0(N)$



## Two-body Green's function pp/hh

$$\begin{aligned}
 G_{\lambda_1 \lambda_2, \lambda_1', \lambda_2'}(t, t') & \stackrel{t' < t}{=} - \sum_n e^{-iE_n(t-t')} X_{\lambda_1 \lambda_2}^{(n)*} X_{\lambda_1' \lambda_2'}^{(n)} \\
 & \stackrel{t' > t}{=} - \sum_m e^{iE_m(t-t')} Y_{\lambda_1', \lambda_2'}^{(m)*} Y_{\lambda_1 \lambda_2}^{(m)}
 \end{aligned}$$

## FT(Two-body Green's function) pp/hh

$$G_{\lambda_1 \lambda_2, \lambda_1', \lambda_2'}(\omega) = -i \sum_{n(N+2)} \frac{X_{\lambda_1 \lambda_2}^{(n)*} X_{\lambda_1' \lambda_2'}^{(n)}}{\omega - E_n + i\eta} + i \sum_{m(N-2)} \frac{Y_{\lambda_1', \lambda_2'}^{(m)*} Y_{\lambda_1 \lambda_2}^{(m)}}{\omega + E_m - i\eta}$$

Useful results for the following...

FT(Two-body Green's function) pp/hh

$$G_{\lambda_1 \lambda_2, \lambda_1' \lambda_2'}(\omega) = -i \sum_{n(N+2)} \frac{X_{\lambda_1 \lambda_2}^{(n)*} X_{\lambda_1' \lambda_2'}^{(n)}}{\omega - E_n + i\eta} + i \sum_{m(N-2)} \frac{Y_{\lambda_1' \lambda_2'}^{(m)*} Y_{\lambda_1 \lambda_2}^{(m)}}{\omega + E_m - i\eta}$$

FT(Two-body Green's function) ph/hp

$$G_{\lambda_1 \lambda_2, \lambda_1' \lambda_2'}(\omega) = -i \sum_n \frac{\chi_{\lambda_1' \lambda_1}^{(n)*} \chi_{\lambda_2 \lambda_2'}^{(n)}}{\omega - E_n + i\eta} + i \sum_n \frac{\chi_{\lambda_2' \lambda_2}^{(n)*} \chi_{\lambda_1 \lambda_1'}^{(n)}}{\omega + E_n - i\eta}$$

ph/hp-Amplitudes & Energy

$$\chi_{ab}^{(n)} = \langle \psi_n | a_a a_b^\dagger | 0 \rangle$$

$$E_n = E_n(N) - E_0(N)$$

ph/hp-propagator

$$t_1 = t_1' + 0$$

$$t_2 = t_2' + 0$$

SLOW CONVERGENCE OF PERTURBATION SERIE  
BUILT ON TOP OF  $G_0$



LET'S BUILT ONE ON TOP OF  $G_1$

Let's get rid of  $G_0$  from...

Dynamical equations for  $G_2$

$$G_2(12; 1'2') = G_0(1, 1')G_1(2, 2') - G_0(1, 2')G_1(2, 1') \\ - i \int d3d4 G_0(1, 3)v(3, 4)G_3(324; 1'2'4^+)$$

Let's get rid of  $G_0$  from...

Dynamical equations for  $G_2$

$$G_2(12; 1'2') = G_0(1, 1')G_1(2, 2') - G_0(1, 2')G_1(2, 1') \\ - i \int d3d4 G_0(1, 3)v(3, 4)G_3(324; 1'2'4^+)$$

$$\int d1 G_0^{-1}(5, 1) G_2(12, 1'2')$$

$$\int d1 G_0^{-1}(5, 1) G_2(12; 1'2') = \int d1 G_0^{-1}(5, 1) G_0(1, 1') G_1(2, 2') \\ - \int d1 G_0^{-1}(5, 1) G_0(1, 2') G_1(2, 1') \\ - i \int d3d4 d1 G_0^{-1}(5, 1) G_0(1, 3) v(3, 4) G_3(324; 1'2'4^+)$$

Let's get rid of  $G_0$  from...

Dynamical equations for  $G_2$

$$G_2(12; 1'2') = G_0(1, 1')G_1(2, 2') - G_0(1, 2')G_1(2, 1') \\ - i \int d3d4 G_0(1, 3)v(3, 4)G_3(324; 1'2'4^+)$$

$$\int d1 G_0^{-1}(5, 1)G_2(12, 1'2')$$

$$\int d1 G_0^{-1}(5, 1)G_2(12; 1'2') = \delta(5, 1')G_1(2, 2') \\ - \delta(5, 2')G_1(2, 1') \\ - i \int d3d4 \delta(5, 3)v(3, 4)G_3(324; 1'2'4^+)$$

And determine  $G_0^{-1}$

Dynamical equations for  $G_1$

$$G_1(1, 1') = G_0(1, 1') - i \int d3d4 G_0(1, 3) v(3, 4) G_2(34, 1'4^+)$$

$$\int d1d1' G_0^{-1}(5, 1) G_1(1, 1') G_1^{-1}(1', 6)$$

$$\begin{aligned} \int d1d1' G_0^{-1}(5, 1) G_1(1, 1') G_1^{-1}(1', 6) &= \int d1d1' G_0^{-1}(5, 1) G_0(1, 1') G_1^{-1}(1', 6) \\ &\quad - i \int d3d4 d1d1' G_0^{-1}(5, 1) G_0(1, 3) v(3, 4) G_2(34, 1'4^+) G_1^{-1}(1', 6) \end{aligned}$$

And determine  $G_0^{-1}$

Dynamical equations for  $G_1$

$$G_1(1, 1') = G_0(1, 1') - i \int d3d4 G_0(1, 3) v(3, 4) G_2(34, 1'4^+)$$

$$\int d1d1' G_0^{-1}(5, 1) G_1(1, 1') G_1^{-1}(1', 6)$$

$$\begin{aligned} \int d1 G_0^{-1}(5, 1) \delta(1, 6) &= \int d1' \delta(5, 1') G_1^{-1}(1', 6) \\ &\quad - i \int d3d4d1' \delta(5, 3) v(3, 4) G_2(34, 1'4^+) G_1^{-1}(1', 6) \end{aligned}$$



And determine  $G_0^{-1}$

Dynamical equations for  $G_1$

$$G_1(1, 1') = G_0(1, 1') - i \int d3d4 G_0(1, 3) v(3, 4) G_2(34, 1'4^+)$$

$$\int d1d1' G_0^{-1}(5, 1) G_1(1, 1') G_1^{-1}(1', 6)$$

$$G_0^{-1}(5, 6) = G_1^{-1}(5, 6) - i \int d4d1' v(5, 4) G_2(54, 1'4^+) G_1^{-1}(1', 6)$$

$$\int d1 G_0^{-1}(5, 1) G_2(12, 1'2')$$

$$\int d1 G_0^{-1}(5, 1) G_2(12; 1'2') = \delta(5, 1') G_1(2, 2') - \delta(5, 2') G_1(2, 1') \\ - i \int d3 d4 \delta(5, 3) v(3, 4) G_3(324; 1'2'4^+)$$

$$\int d1 d1' G_0^{-1}(5, 1) G_1(1, 1') G_1^{-1}(1', 6)$$

$$G_0^{-1}(5, 6) = G_1^{-1}(5, 6) - i \int d4 d1' v(5, 4) G_2(54, 1'4^+) G_1^{-1}(1', 6)$$

$$\int d1 G_0^{-1}(5, 1) G_2(12, 1'2') \longleftarrow G_0^{-1}(5, 1)$$

$$\int d1 G_1^{-1}(5, 1) G_2(12; 1'2') = \delta(5, 1') G_1(2, 2') - \delta(5, 2') G_1(2, 1') \\ - i \int d4 v(5, 4) G_3(524; 1'2'4^+) \\ + i \int d1 d3 d4 v(5, 4) G_2(54, 34^+) G_1^{-1}(3, 1) G_2(12; 1'2')$$

$$\int d1 G_0^{-1}(5, 1) G_2(12, 1'2') \leftarrow G_0^{-1}(5, 1)$$

$$\begin{aligned} \int d1 G_1^{-1}(5, 1) G_2(12; 1'2') &= \delta(5, 1') G_1(2, 2') - \delta(5, 2') G_1(2, 1') \\ &\quad - i \int d4 v(5, 4) G_3(524; 1'2'4^+) \\ &\quad + i \int d1 d3 d4 v(5, 4) G_2(54, 34^+) G_1^{-1}(3, 1) G_2(12; 1'2') \end{aligned}$$

$$\int d1 d5 G_1(7, 5) G_0^{-1}(5, 1) G_2(12, 1'2')$$

$$\begin{aligned} \int d1 d5 G_1(7, 5) G_1^{-1}(5, 1) G_2(12; 1'2') &= \int d5 G_1(7, 5) \delta(5, 1') G_1(2, 2') \\ &\quad - \int d5 G_1(7, 5) \delta(5, 2') G_1(2, 1') \\ &\quad - i \int d4 d5 G_1(7, 5) v(5, 4) G_3(524; 1'2'4^+) \\ &\quad + i \int d1 d3 d4 d5 G_1(7, 5) v(5, 4) G_2(54, 34^+) G_1^{-1}(3, 1) G_2(12; 1'2') \end{aligned}$$

$$\int d1 G_0^{-1}(5, 1) G_2(12, 1'2') \longleftarrow G_0^{-1}(5, 1)$$

$$\begin{aligned} \int d1 G_1^{-1}(5, 1) G_2(12; 1'2') &= \delta(5, 1') G_1(2, 2') - \delta(5, 2') G_1(2, 1') \\ &\quad - i \int d4 v(5, 4) G_3(524; 1'2'4^+) \\ &\quad + i \int d1 d3 d4 v(5, 4) G_2(54, 34^+) G_1^{-1}(3, 1) G_2(12; 1'2') \end{aligned}$$

$$\int d1 d5 G_1(7, 5) G_0^{-1}(5, 1) G_2(12, 1'2')$$

$$\begin{aligned} \int d1 d5 G_1(7, 5) G_1^{-1}(5, 1) G_2(12; 1'2') &= \int d5 G_1(7, 5) \delta(5, 1') G_1(2, 2') \\ &\quad - \int d5 G_1(7, 5) \delta(5, 2') G_1(2, 1') \\ &\quad - i \int d4 d5 G_1(7, 5) v(5, 4) G_3(524; 1'2'4^+) \\ &\quad + i \int d1 d3 d4 d5 G_1(7, 5) v(5, 4) G_2(54, 34^+) G_1^{-1}(3, 1) G_2(12; 1'2') \end{aligned}$$

$$\int d1 G_0^{-1}(5, 1) G_2(12, 1'2') \leftarrow G_0^{-1}(5, 1)$$

$$\begin{aligned} \int d1 G_1^{-1}(5, 1) G_2(12; 1'2') &= \delta(5, 1') G_1(2, 2') - \delta(5, 2') G_1(2, 1') \\ &\quad - i \int d4 v(5, 4) G_3(524; 1'2'4^+) \\ &\quad + i \int d1 d3 d4 v(5, 4) G_2(54, 34^+) G_1^{-1}(3, 1) G_2(12; 1'2') \end{aligned}$$

$$\int d1 d5 G_1(7, 5) G_0^{-1}(5, 1) G_2(12, 1'2')$$

$$\begin{aligned} \int d1 \delta(7, 1) G_2(12; 1'2') &= G_1(7, 1') G_1(2, 2') \\ &\quad - G_1(7, 2') G_1(2, 1') \\ &\quad - i \int d4 d5 G_1(7, 5) v(5, 4) G_3(524; 1'2'4^+) \\ &\quad + i \int d1 d3 d4 d5 G_1(7, 5) v(5, 4) G_2(54, 34^+) G_1^{-1}(3, 1) G_2(12; 1'2') \end{aligned}$$

$$\int d1 G_0^{-1}(5, 1) G_2(12, 1'2') \leftarrow G_0^{-1}(5, 1)$$

$$\begin{aligned} \int d1 G_1^{-1}(5, 1) G_2(12; 1'2') &= \delta(5, 1') G_1(2, 2') - \delta(5, 2') G_1(2, 1') \\ &\quad - i \int d4 v(5, 4) G_3(524; 1'2'4^+) \\ &\quad + i \int d1 d3 d4 v(5, 4) G_2(54, 34^+) G_1^{-1}(3, 1) G_2(12; 1'2') \end{aligned}$$

$$\int d1 d5 G_1(7, 5) G_0^{-1}(5, 1) G_2(12, 1'2')$$

$$\begin{aligned} G_2(72; 1'2') &= G_1(7, 1') G_1(2, 2') \\ &\quad - G_1(7, 2') G_1(2, 1') \\ &\quad - i \int d4 d5 G_1(7, 5) v(5, 4) G_3(524; 1'2'4^+) \\ &\quad + i \int d1 d3 d4 d5 G_1(7, 5) v(5, 4) G_2(54, 34^+) G_1^{-1}(3, 1) G_2(12; 1'2') \end{aligned}$$

Finally, we get

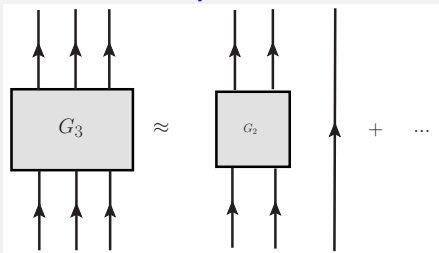
$G_2$  as a function  $G_1$ ,  $G_2$  and  $G_3$

$$\begin{aligned}
 G_2(72; 1'2') &= G_1(7, 1')G_1(2, 2') - G_1(7, 2')G_1(2, 1') \\
 &\quad - i \int d4d5 G_1(7, 5)v(5, 4) \{ G_3(524; 1'2'4^+) \\
 &\quad \quad - \int d1d3 G_2(54, 34^+)G_1^{-1}(3, 1)G_2(12; 1'2') \}
 \end{aligned}$$

We find the Hartree-Fock terms corrected by higher order terms

Need for an approximation to deal with  $G_3$

$G_3$  approximated as the antisymmetrized sum of  $G_1 G_2$  products



We neglect interaction between the correlated pair of particles and the third particle



$G_3$  approximated as the antisymmetrized sum of  $G_1 G_2$  products

$$\begin{aligned}
 G_3(123, 1'2'3') &\approx G_1(1, 1')G_2(23; 2'3') + G_1(2, 2')G_2(13; 1'3') \\
 &+ G_1(3, 3')G_2(12; 1'2') - G_1(1, 2')G_2(23; 1'3') \\
 &- G_1(1, 3')G_2(23; 2'1') - G_1(2, 1')G_2(13; 2'3') \\
 &- G_1(2, 3')G_2(13; 1'2') - G_1(3, 1')G_2(12; 2'3') \\
 &- G_1(3, 2')G_2(12; 1'3') - 2G_3^{(0)}(123; 1'2'3')
 \end{aligned}$$

$G_3^{(0)}$  is the free contribution to  $G_3$

$$\begin{aligned}
 G_3^{(0)}(123, 1'2'3') &= G_1(1, 1')G_1(2, 2')G_1(3, 3') - G_1(1, 1')G_1(2, 3')G_1(3, 2') \\
 &- G_1(1, 2')G_1(2, 1')G_1(3, 3') + G_1(1, 2')G_1(2, 3')G_1(3, 1') \\
 &- G_1(1, 3')G_1(2, 2')G_1(3, 1') + G_1(1, 3')G_1(2, 1')G_1(3, 2')
 \end{aligned}$$

Now we have an approximation for  $G_3$ , we deal with...

$G_2$  as a function  $G_1$ ,  $G_2$  and  $G_3$

$$\begin{aligned}
 G_2(72; 1'2') &= G_1(7, 1')G_1(2, 2') - G_1(7, 2')G_1(2, 1') \\
 &\quad - i \int d4d5 G_1(7, 5)v(5, 4) \{ G_3(524; 1'2'4^+) \\
 &\quad \quad \quad - \int d1d3 G_2(54, 34^+) G_1^{-1}(3, 1) G_2(12; 1'2') \}
 \end{aligned}$$

$$- \int d1d3 G_2(54, 34^+) G_1^{-1}(3, 1) G_2(12; 1'2') ?$$

$$- \int d1d3G_2(54, 34^+)G_1^{-1}(3, 1)G_2(12; 1'2')$$

$$\int d1G_1^{-1}(5, 1)G_2(12; 1'2') = \delta(5, 1')G_1(2, 2') - \delta(5, 2')G_1(2, 1')$$

$$- i \int d4v(5, 4)G_3(524; 1'2'4^+)$$

$$+ i \int d1d3d4v(5, 4)G_2(54, 34^+)G_1^{-1}(3, 1)G_2(12; 1'2')$$

$$\begin{aligned} & - \int d1d3G_2(54, 34^+)G_1^{-1}(3, 1)G_2(12; 1'2') \\ \int d1d5G_2(64, 54^+)G_1^{-1}(5, 1)G_2(12; 1'2') & = \int d5G_2(64, 54^+)\delta(5, 1')G_1(2, 2') \\ & - \int d5G_2(64, 54^+)\delta(5, 2')G_1(2, 1') \\ & - i \int d4d5G_2(64, 54^+)v(5, 4)G_3(524; 1'2'4^+) \\ & + i \int d1d3d4d5G_2(64, 54^+)v(5, 4)G_2(54, 34^+)G_1^{-1}(3, 1)G_2(12; 1'2') \end{aligned}$$

$$\begin{aligned} & - \int d1d3G_2(54, 34^+)G_1^{-1}(3, 1)G_2(12; 1'2') \\ \int d1d5G_2(64, 54^+)G_1^{-1}(5, 1)G_2(12; 1'2') & = G_2(64, 1'4^+)G_1(2, 2') \\ & - G_2(64, 2'4^+)G_1(2, 1') \\ & - i \int d4d5G_2(64, 54^+)v(5, 4)G_3(524; 1'2'4^+) \\ + i \int d1d3d4d5G_2(64, 54^+)v(5, 4)G_2(54, 34^+)G_1^{-1}(3, 1)G_2(12; 1'2') \end{aligned}$$

$$- \int d1d3G_2(54, 34^+)G_1^{-1}(3, 1)G_2(12; 1'2')$$

$$\int d1d5G_2(64, 54^+)G_1^{-1}(5, 1)G_2(12; 1'2') = G_2(64, 1'4^+)G_1(2, 2')$$

$$- G_2(64, 2'4^+)G_1(2, 1')$$

$$- i \int d4d5G_2(64, 54^+)v(5, 4)G_3(524; 1'2'4^+)$$

$$+ i \int d1d3d4d5G_2(64, 54^+)v(5, 4)G_2(54, 34^+)G_1^{-1}(3, 1)G_2(12; 1'2')$$

Once again we neglect correlations between  $G_1$  and  $G_2$  and between two  $G_2$ 's.

$$- \int d1d3G_2(54, 34^+)G_1^{-1}(3, 1)G_2(12; 1'2')$$

$$\int d1d5G_2(64, 54^+)G_1^{-1}(5, 1)G_2(12; 1'2') \approx G_2(64, 1'4^+)G_1(2, 2')$$

$$- G_2(64, 2'4^+)G_1(2, 1')$$

$G_2$  as a function  $G_1$ ,  $G_2$  and  $G_3$ 

$$\begin{aligned}
 G_2(72; 1'2') &= G_1(7, 1')G_1(2, 2') - G_1(7, 2')G_1(2, 1') \\
 &\quad - i \int d4d5 G_1(7, 5)v(5, 4) \{ G_3(524; 1'2'4^+) \\
 &\quad \quad \quad - \int d1d3 G_2(54, 34^+) G_1^{-1}(3, 1) G_2(12; 1'2') \}
 \end{aligned}$$

## Approximation #1

$$\begin{aligned}
 G_3(123, 1'2'3') &\approx G_1(1, 1')G_2(23; 2'3') + G_1(2, 2')G_2(13; 1'3') \\
 &\quad + G_1(3, 3')G_2(12; 1'2') - G_1(1, 2')G_2(23; 1'3') \\
 &\quad - G_1(1, 3')G_2(23; 2'1') - G_1(2, 1')G_2(13; 2'3') \\
 &\quad - G_1(2, 3')G_2(13; 1'2') - G_1(3, 1')G_2(12; 2'3') \\
 &\quad - G_1(3, 2')G_2(12; 1'3') - 2G_3^{(0)}(123; 1'2'3')
 \end{aligned}$$

## Approximation #2

$$\begin{aligned}
 \int d1d5 G_2(64, 54^+) G_1^{-1}(5, 1) G_2(12; 1'2') &\approx G_2(64, 1'4^+) G_1(2, 2') \\
 &\quad - G_2(64, 2'4^+) G_1(2, 1')
 \end{aligned}$$

### Approximated version of $G_2$

$$\begin{aligned}
 G_2(12; 1'2') &= G_1(1, 1')G_1(2, 2') - G_1(1, 2')G_1(2, 1') \\
 &- i \int d3d4 G_1(1, 3)v(3, 4) [G_1(3, 1')G_2(24; 2'4^+) \\
 &+ G_1(2, 2')G_2(34; 1'4^+) - G_1(3, 2')G_2(24; 1'4^+) \\
 &- G_1(3, 4)G_2(24; 2'1') - G_1(2, 1')G_2(34; 2'4^+) \\
 &- G_1(2, 4)G_2(34, 1'2') - G_1(4, 1')G_2(23; 2'4) \\
 &- G_1(4, 2')G_2(32; 1'4) - 2G_3^{(0)}(324; 1'2'4^+)]
 \end{aligned}$$

Neglecting correlations between  $G_1$  and  $G_2$  and between two  $G_2$ 's.



ph-propagator ( $G_2$  with  $t_1 = t_{1'} + 0$  and  $t_2 = t_{2'} + 0$ )

## Two-body Green's function

$$G_2(12; 1'2') = -\langle 0 | \mathcal{T} \{ \psi(1)\psi(2)\psi^\dagger(2')\psi^\dagger(1') \} | 0 \rangle$$

## Approximated version of $G_2$

$$\begin{aligned} G_2(12; 1'2') &= G_1(1, 1')G_1(2, 2') - G_1(1, 2')G_1(2, 1') \\ &- i \int d3d4 G_1(1, 3)v(3, 4) [G_1(3, 1')G_2(24; 2'4^+) \\ &+ G_1(2, 2')G_2(34; 1'4^+) - G_1(3, 2')G_2(24; 1'4^+) \\ &- G_1(3, 4)G_2(24; 2'1') - G_1(2, 1')G_2(34; 2'4^+) \\ &- G_1(2, 4)G_2(34; 1'2') - G_1(4, 1')G_2(23; 2'4) \\ &- G_1(4, 2')G_2(32; 1'4) - 2G_3^{(0)}(324; 1'2'4^+)] \end{aligned}$$

# ph-propagator and RPA equations

ph-propagator ( $G_2$  with  $t_1 = t_1' + 0$  and  $t_2 = t_2' + 0$ )

## Two-body Green's function

$$G_2(12; 1'2') = -\langle 0 | \mathcal{T} \{ \psi(1)\psi(2)\psi^\dagger(2')\psi^\dagger(1') \} | 0 \rangle$$

## Approximated version of $G_2$

$$\begin{aligned} G_2(12; 1'2') &= G_1(1, 1')G_1(2, 2') - G_1(1, 2')G_1(2, 1') \\ &- i \int d^3d^4 G_1(1, 3)v(3, 4) [G_1(3, 1')G_2(24; 2'4^+) \\ &+ G_1(2, 2')G_2(34; 1'4^+) - G_1(3, 2')G_2(24; 1'4^+) \\ &- G_1(3, 4)G_2(24; 2'1') - G_1(2, 1')G_2(34; 2'4^+) \\ &- G_1(2, 4)G_2(34, 1'2') - G_1(4, 1')G_2(23; 2'4) \\ &- G_1(4, 2')G_2(32; 1'4) - 2G_3^{(0)}(324; 1'2'4^+)] \end{aligned}$$

with  $v(3, 4) = v(r_3, r_4)\delta(t_3, t_4)$ .

ph-propagator ( $G_2$  with  $t_1 = t_{1'} + 0$  and  $t_2 = t_{2'} + 0$ )

Two-body Green's function

$$G_2(12; 1'2') = -\langle 0 | \mathcal{T} \{ \psi(1) \psi(2) \psi^\dagger(2') \psi^\dagger(1') \} | 0 \rangle$$

ph- $G_2$

$$\begin{aligned} G_2(1^+2^+; 1'2') &= G_1(1^+, 1') G_1(2^+, 2') - G_1(1, 2') G_1(2, 1') \\ &- i \int d3d4 G_1(1, 3) v(3, 4) [G_1(3, 1') G_2(24; 2'4^+) \\ &- G_1(4, 1') G_2(23; 2'4)] \end{aligned}$$

with  $v(3, 4) = v(r_3, r_4) \delta(t_3, t_4)$ .

Now we have isolated ph-contributions

FT(Two-body Green's function) ph/hp in ' $\lambda$ -representation'

$$G_{\lambda_1 \lambda_2, \lambda_1' \lambda_2'}(\omega) = -i \sum_n \frac{\chi_{\lambda_1' \lambda_1}^{(n)*} \chi_{\lambda_2 \lambda_2'}^{(n)}}{\omega - E_n + i\eta} + i \sum_n \frac{\chi_{\lambda_2' \lambda_2}^{(n)*} \chi_{\lambda_1 \lambda_1'}^{(n)}}{\omega + E_n - i\eta}$$

ph- $G_2$

$$\begin{aligned} G_2(1^+ 2^+; 1' 2') &= G_1(1^+, 1') G_1(2^+, 2') - G_1(1, 2') G_1(2, 1') \\ &- i \int d^3d_4 G_1(1, 3) v(3, 4) [G_1(3, 1') G_2(24; 2' 4^+) \\ &- G_1(4, 1') G_2(23; 2' 4)] \end{aligned}$$

with  $v(3, 4) = v(r_3, r_4) \delta(t_3, t_4)$ .

Now we have isolated ph-contributions

FT(Two-body Green's function) ph/hp in ' $\lambda$ -representation'

$$G_{\lambda_1\lambda_2,\lambda_1',\lambda_2'}(\omega) = -i \sum_n \frac{\chi_{\lambda_1'\lambda_1}^{(n)*} \chi_{\lambda_2\lambda_2'}^{(n)}}{\omega - E_n + i\eta} + i \sum_n \frac{\chi_{\lambda_2'\lambda_2}^{(n)*} \chi_{\lambda_1\lambda_1'}^{(n)}}{\omega + E_n - i\eta}$$

ph- $G_2$  in ' $\lambda$ -representation'

$$\begin{aligned} G_{\lambda_1\lambda_2,\lambda_1',\lambda_2'}(t_1 - t_2) &= G_{\lambda_1}(+0)G_{\lambda_2}(+0)\delta_{\lambda_1\lambda_1'}\delta_{\lambda_2\lambda_2'} \\ &- G_{\lambda_1}(t_1 - t_2)G_{\lambda_2}(t_2 - t_1)\delta_{\lambda_1\lambda_2'}\delta_{\lambda_2\lambda_1'} \\ &+ i \sum_{\lambda_3\lambda_4} \int_{-\infty}^{+\infty} dt' G_{\lambda_1}(t_1, t')G_{\lambda_1'}(t', t_1) \\ &\times \langle \lambda_1\lambda_3 | v(3, 4) | \lambda_4\lambda_1' \rangle_A G_{\lambda_3\lambda_2;\lambda_4\lambda_2'}(t' - t_2) \end{aligned}$$

with  $v(3, 4) = v(r_3, r_4)\delta(t_3, t_4)$ .

Let's redefine ...

$$G''_{\lambda_1 \lambda_{1'}, \lambda_2 \lambda_{2'}}(t_1 - t_2) = G_{\lambda_1 \lambda_2, \lambda_{1'} \lambda_{2'}}(t_1 - t_2)$$

Thus

$G'' = ph - G_2$  in ' $\lambda$ -representation'

$$\begin{aligned} G''_{\lambda_1 \lambda_{1'}, \lambda_2 \lambda_{2'}}(t_1 - t_2) &= -G_{\lambda_1}(t_1 - t_2) G_{\lambda_2}(t_2 - t_1) \delta_{\lambda_1 \lambda_2} \delta_{\lambda_2 \lambda_{1'}} \\ &+ i \sum_{\lambda_3 \lambda_4} \int_{-\infty}^{+\infty} dt' G_{\lambda_1}(t_1, t') G_{\lambda_{1'}}(t', t_1) \\ &\times \langle \lambda_1 \lambda_3 | \nu(3, 4) | \lambda_4 \lambda_{1'} \rangle_A G''_{\lambda_3 \lambda_2; \lambda_4 \lambda_{2'}}(t' - t_2) \end{aligned}$$

FT(Two-body Green's function) ph/hp in ' $\lambda$ -representation'

$$G_{\lambda_1 \lambda_2, \lambda_1' \lambda_2'}(\omega) = -i \sum_n \frac{\chi_{\lambda_1' \lambda_1}^{(n)*} \chi_{\lambda_2 \lambda_2'}^{(n)}}{\omega - E_n + i\eta} + i \sum_n \frac{\chi_{\lambda_2' \lambda_2}^{(n)*} \chi_{\lambda_1 \lambda_1'}^{(n)}}{\omega + E_n - i\eta}$$

$G'' = ph - G_2$  in ' $\lambda$ -representation'

$$\begin{aligned} G''_{\lambda_1 \lambda_1', \lambda_2 \lambda_2'}(t_1 - t_2) &= -G_{\lambda_1}(t_1 - t_2) G_{\lambda_2}(t_2 - t_1) \delta_{\lambda_1 \lambda_2'} \delta_{\lambda_2 \lambda_1'} \\ &+ i \sum_{\lambda_3 \lambda_4} \int_{-\infty}^{+\infty} dt' G_{\lambda_1}(t_1, t') G_{\lambda_1'}(t', t_1) \\ &\times \langle \lambda_1 \lambda_3 | v(3, 4) | \lambda_4 \lambda_1' \rangle_A G''_{\lambda_3 \lambda_2; \lambda_4 \lambda_2'}(t' - t_2) \end{aligned}$$

FT(Two-body Green's function) ph/hp in ' $\lambda$ -representation'

$$G_{\lambda_1 \lambda_2, \lambda_1', \lambda_2'}(\omega) = -i \sum_n \frac{\chi_{\lambda_1', \lambda_1}^{(n)*} \chi_{\lambda_2 \lambda_2'}^{(n)}}{\omega - E_n + i\eta} + i \sum_n \frac{\chi_{\lambda_2', \lambda_2}^{(n)*} \chi_{\lambda_1 \lambda_1'}^{(n)}}{\omega + E_n - i\eta}$$

$G'' = ph - G_2$  in ' $\lambda$ -representation'

$$\sum_n \left( \frac{\chi_{i'i}^{(n)*} \chi_{j'j}^{(n)}}{\omega - E_n + i\eta} - \frac{\chi_{ii'}^{(n)} \chi_{j'j'}^{(n)*}}{\omega + E_n - i\eta} \right) = \frac{(1 - m_i)m_{i'} - m_i(1 - m_{i'})}{\omega - \varepsilon_i + \varepsilon_{i'} + i\eta}$$

$$\left( \delta_{ij} \delta_{i'j'} + \sum_{nkl} \langle il | v | i'k \rangle \left[ \frac{\chi_{lk}^{(n)*} \chi_{j'j}^{(n)}}{\omega - E_n + i\eta} - \frac{\chi_{kl}^{(n)} \chi_{j'j'}^{(n)*}}{\omega + E_n - i\eta} \right] \right)$$



FT(Two-body Green's function) ph/hp in ' $\lambda$ -representation'

$$G_{\lambda_1 \lambda_2, \lambda_1' \lambda_2'}(\omega) = -i \sum_n \frac{\chi_{\lambda_1' \lambda_1}^{(n)*} \chi_{\lambda_2 \lambda_2'}^{(n)}}{\omega - E_n + i\eta} + i \sum_n \frac{\chi_{\lambda_2' \lambda_2}^{(n)*} \chi_{\lambda_1 \lambda_1'}^{(n)}}{\omega + E_n - i\eta}$$

ph RPA equations

$$(E_n - \varepsilon_i + \varepsilon_{i'}) \chi_{i'i}^{(n)} - \sum_{kk'} \langle ik' | v | i' k \rangle A \chi_{kk'}^{(n)} - \sum_{kk'} \langle ik | v | i' k' \rangle A \chi_{kk'}^{(n)} = 0$$

$$(E_n - \varepsilon_i + \varepsilon_{i'}) \chi_{ii'}^{(n)} + \sum_{kk'} \langle ik | v | i' k' \rangle A \chi_{k'k}^{(n)} + \sum_{kk'} \langle ik' | v | i' k \rangle A \chi_{kk'}^{(n)} = 0$$

## ph RPA equations

$$(E_n - \varepsilon_i + \varepsilon_{i'})\chi_{i'i}^{(n)} - \sum_{kk'} \langle ik' | v | i' k \rangle_A \chi_{kk'}^{(n)} - \sum_{kk'} \langle ik | v | i' k' \rangle_A \chi_{kk'}^{(n)} = 0$$

$$(E_n - \varepsilon_i + \varepsilon_{i'})\chi_{ii'}^{(n)} + \sum_{kk'} \langle ik | v | i' k' \rangle_A \chi_{k'k}^{(n)} + \sum_{kk'} \langle ik' | v | i' k \rangle_A \chi_{kk'}^{(n)} = 0$$

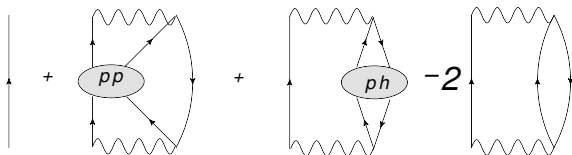
$E_n$  excited energy of the target nucleus  
 $\chi$ 's 'occupation' of each ph pair

### Exact Self-energy

$$\Sigma(2, 3) = -i \int d4d5v(2, 4)G_2(24, 54^+)G_1^{-1}(5, 3)$$

## Self-energy at the HF+RPA approximation

$$\begin{aligned} \Sigma_1(1, 1') &= \Sigma_{HF}(1, 1') + \Sigma_{pp}(1, 1') + \Sigma_{ph}(1, 1') - 2\Sigma^{(2)}(1, 1') \\ \Sigma_{HF}(1, 1') &= iv(1, 1')G_1^{HF}(1, 1') - i\delta(1, 1') \int d2v(1, 2)G_1^{HF}(2; 2^+) \\ \Sigma_{pp}(1, 1') &= \int d3d4v(1, 3)G_1^{HF}(4, 3)G_2(13; 1'4)v(4, 1') \\ \Sigma_{ph}(1, 1') &= - \int d3d4v(1, 3) \left[ G_1^{HF}(1, 1')G_2(34; 3^+4^+) \right. \\ &\quad - G_1^{HF}(1, 4)G_2(43; 1'3^+) - G_1^{HF}(3, 1')G_2(41; 4^+3) \\ &\quad \left. - G_1^{HF}(3, 4)G_2(14; 1'3) \right] v(4, 1') \end{aligned}$$



## Schrödinger equation

$$\frac{p^2}{2m}\phi_\lambda(\mathbf{r}, \varepsilon) + \int d\mathbf{r}' V^{HF}(\mathbf{r}, \mathbf{r}'; \varepsilon)\phi_\lambda(\mathbf{r}', \varepsilon) = E(\varepsilon)\phi_\lambda(\mathbf{r}, \varepsilon)$$

## HF potential

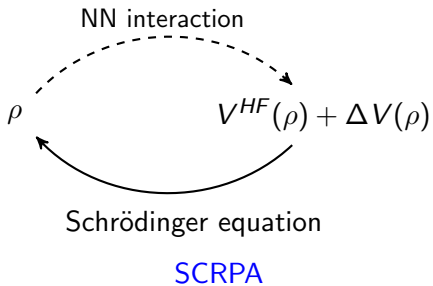
$$V^{HF}(\mathbf{r}, \mathbf{r}''; \varepsilon) = \delta(\mathbf{r}, \mathbf{r}'') \int d\mathbf{r}' v(\mathbf{r}, \mathbf{r}')\rho(\mathbf{r}') - v(\mathbf{r}, \mathbf{r}'')\rho(\mathbf{r}, \mathbf{r}'')$$

## RPA potential

$$\begin{aligned} V^{RPA}(\mathbf{r}, \mathbf{r}', E) &= \lim_{\eta \rightarrow 0^+} \sum_{N \neq 0, ijkl} \sum_{\lambda} \chi_{ij}^{(N)} \chi_{kl}^{(N)} \\ &\times \left( \frac{n_\lambda}{E - \epsilon_\lambda + E_N - i\eta} + \frac{1 - n_\lambda}{E - \epsilon_\lambda - E_N + i\eta} \right) \\ &\times F_{ij\lambda}(\mathbf{r}) F_{kl\lambda}^*(\mathbf{r}') \end{aligned}$$

with

$$F_{ij\lambda}(\mathbf{r}) = \int d^3\mathbf{r}_1 \phi_i^*(\mathbf{r}_1) v(\mathbf{r}, \mathbf{r}_1) [1 - P] \phi_\lambda(\mathbf{r}) \phi_j(\mathbf{r}_1)$$



The optical potential as a possible connection between different levels of phenomenology

- ▶ Phenomenological optical potential
- ▶ Potentials based on phenomenological effective NN interaction (Gogny, Skyrme...)
- ▶ Ab-initio potentials based on phenomenological bare NN interaction

The optical potential as a possible connection between different levels of phenomenology

- ▶ Phenomenological optical potential
- ▶ Potentials based on phenomenological effective NN interaction (Gogny, Skyrme...)
- ▶ Ab-initio potentials based on phenomenological bare NN interaction

Possibility of fruitful exchanges between those communities



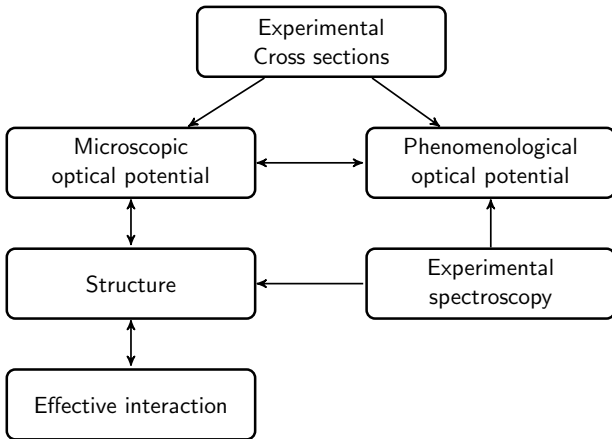
- ▶ Nuclear matter method (50 MeV - 1 GeV)
- ▶ Resonating Group Method / No Core Shell Model (light nuclei and weak energy)
- ▶ Green's function Monte Carlo (light nuclei and weak energy)
- ▶ Self-consistent Green's function (doubly magic nuclei)
- ▶ Gorkov-SCGF (around doubly magic nuclei)
- ▶ Coupled cluster (doubly magic nuclei)

# Potential based on effective interaction

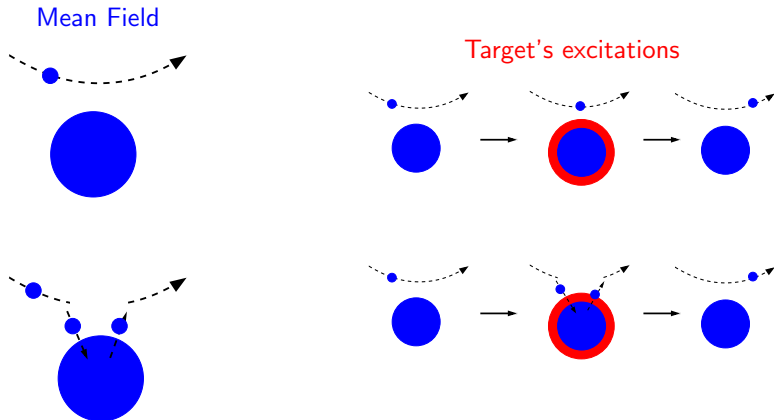
- ▶ Nuclear Structure Method developed by N. Vinh Mau
- ▶ Recent interest (Orsay, Hanoï, Japan, Milano, China, Bruyères, Russia)

- ▶ Precision required for the evaluations
- ▶ Contrained by numerous calculations using reaction codes:  
TALYS, EMPIRE
- ▶ Predictivity outside the range parametrization
- ▶ Parametrization of non local dispersive potentials
- ▶ Issues induced by localisation procedures : effet Perey,  
dépendance spurieuse en énergie

## NUCLEAR STRUCTURE METHOD FOR SCATTERING



$$V = V^{HF} + \Delta V^{RPA}$$



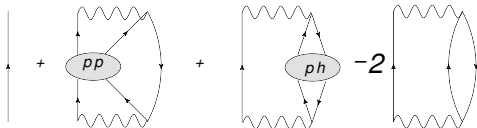
(N. Vinh Mau, *Theory of nuclear structure* (IAEA, Vienna) p. 931 (1970),

G. Blanchon, M. Dupuis, H.F. Arellano et N. Vinh Mau, *PRC* 91, 014612 (2015))

## Optical potential

$$V = V^{HF} + V^{PP} + V^{RPA} - 2V^{(2)}$$

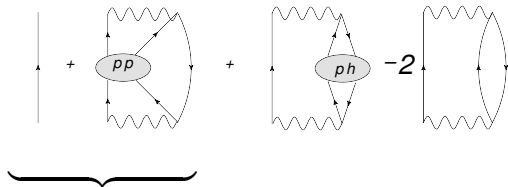
Bare  
Interaction



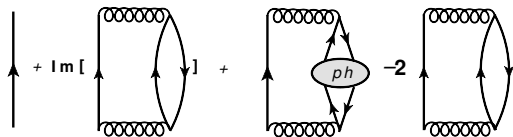
## Optical potential

$$V = V^{HF} + V^{PP} + V^{RPA} - 2V^{(2)}$$

Bare  
Interaction



Effective  
Interaction

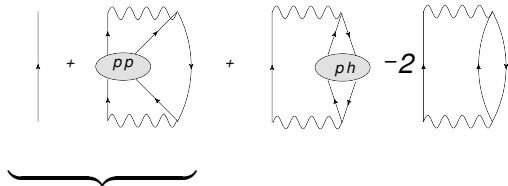




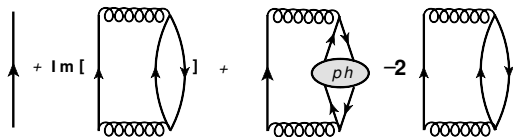
## Optical potential

$$V = V^{HF} + V^{PP} + V^{RPA} - 2V^{(2)}$$

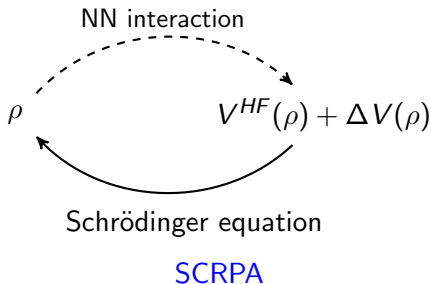
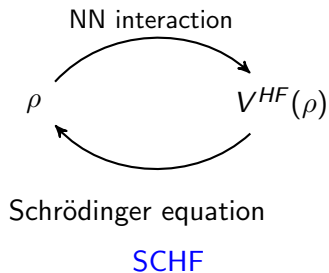
Bare  
Interaction



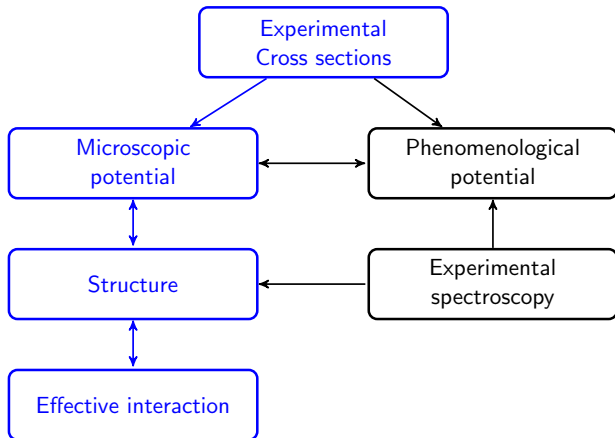
Gogny  
Interaction



# Self-consistency



# Elastic scattering $n/p + {}^{40}\text{Ca}$

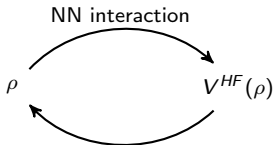


## Schrödinger equation

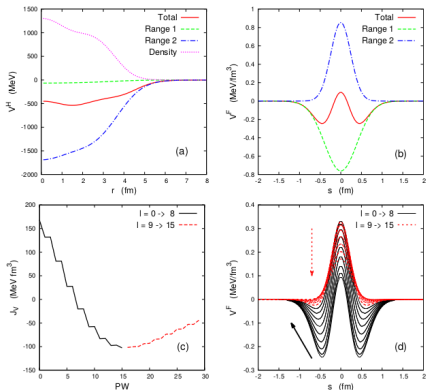
$$\frac{p^2}{2m} \phi_\lambda(\mathbf{r}, \varepsilon) + \int d\mathbf{r}' V^{HF}(\mathbf{r}, \mathbf{r}'; \varepsilon) \phi_\lambda(\mathbf{r}', \varepsilon) = E(\varepsilon) \phi_\lambda(\mathbf{r}, \varepsilon)$$

## HF potential

$$V^{HF}(\mathbf{r}, \mathbf{r}''; \varepsilon) = \delta(\mathbf{r}, \mathbf{r}'') \int d\mathbf{r}' v(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}') - v(\mathbf{r}, \mathbf{r}'') \rho(\mathbf{r}, \mathbf{r}'')$$

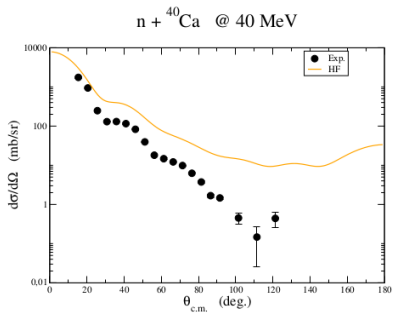
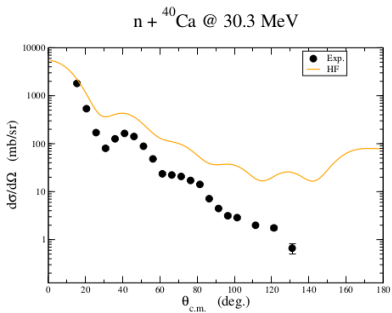


Schrödinger equation

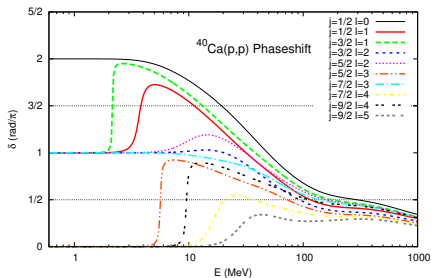
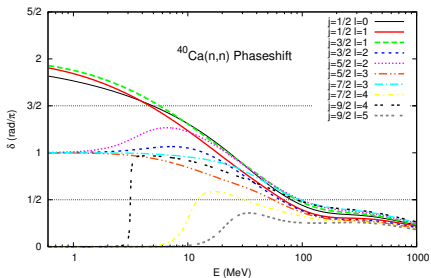


**Fig. 15.** Contributions for  $n + {}^{40}\text{Ca}$  to: (a) to the Hartree local potential ( $V^H$ ): Total (solid line), first range of D1S (dashed line), second range of D1S (dash-dotted line) and density term (dotted line). (b) First partial wave of the nonlocal Fock term at  $r = r' = 4.3$  fm: Total (solid line), first range of D1S (dashed line) and second range of D1S (dash-dotted line). (c) Volume integral of the Fock potential as a function of partial wave: Negative slope (solid line), positive slope (dashed line). (d) Same as (c) for the Fock components nonlocality at  $r = r' = 4.3$  fm.

# HF cross section

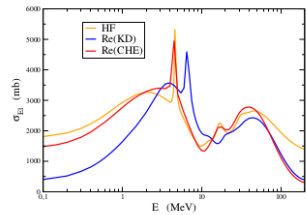
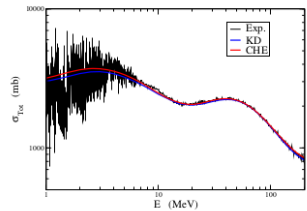


# HF phaseshift $n/p+^{40}\text{Ca}$

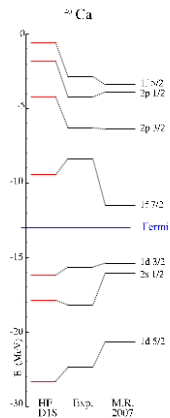


- ▶ Single particle resonances when  $\delta = n\pi/2$  ( $n$  impair).
- ▶ Exact treatment of the intermediate wave  $\phi_\lambda$ .
- ▶ Strong impact on  $\Delta V_{RPA}$
- ▶ Levinson theorem and total cross section

Total cross section  $n+^{40}\text{Ca}$



Bound states HF/D1S Exp. CHE



►  $V^{HF}$  gives the main contribution to the real part of the potential

(B. Morillon and P. Romain, *Phys. Rev. C* 70, 014601 (2004).) → dispersive potential

(A. J. Koning and J. P. Delaroche, *Nuclear Physics A* 713, 231 (2003).)



# ph-RPA potential

$$\Delta V_{RPA} = \text{Im} [V^{(2)}] + V^{RPA} - 2V^{(2)}$$

$$V^{RPA}(\mathbf{r}, \mathbf{r}', E) = \lim_{\eta \rightarrow 0^+} \sum_{N \neq 0} \sum_{ijkl} \chi_{ij}^{(N)} \chi_{kl}^{(N)} \times \left( \frac{n_\lambda}{E - \epsilon_\lambda + E_N - i\Gamma(E_N)} + \frac{1 - n_\lambda}{E - \epsilon_\lambda - E_N + i\Gamma(E_N)} \right) F_{ij\lambda}(\mathbf{r}) F_{kl\lambda}^*(\mathbf{r}')$$



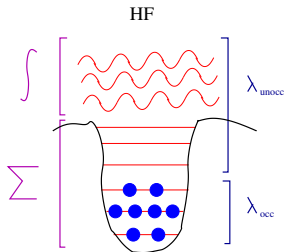
with

$$F_{ij\lambda}(\mathbf{r}) = \int d^3\mathbf{r}_1 \phi_i^*(\mathbf{r}_1) v(\mathbf{r}, \mathbf{r}_1) [1 - P] \phi_\lambda(\mathbf{r}) \phi_j(\mathbf{r}_1)$$

- ▶  $\phi$  are HF wave functions.
- ▶ Bound as well as continuum states are taken into account for the intermediate state  $\phi_\lambda$ .
- ▶ Target excitations are obtained from the spherical RPA/D1S code.

*Blaizot, et al., NPA 265, 315 (1976).*

*Berger, et al., Comp. Phys. Com. 63, 365 (1991).*



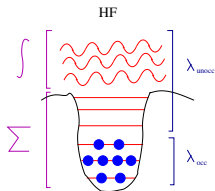
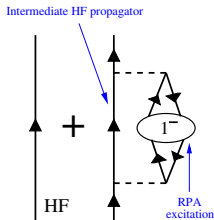
Uncorrelated particle-hole potential

$$V^{(2)}(\mathbf{r}, \mathbf{r}', E) = \frac{1}{2} \sum_{ij} \sum_{\lambda}^f \left( \frac{n_i(1-n_j)n_{\lambda}}{E - \epsilon_{\lambda} + E_{ij} - i\Gamma(E_{ij})} + \frac{n_j(1-n_i)(1-n_{\lambda})}{E - \epsilon_{\lambda} - E_{ij} + i\Gamma(E_{ij})} \right) F_{ij\lambda}(\mathbf{r}) F_{kl\lambda}^*(\mathbf{r}')$$

with  $E_{ij} = \epsilon_i - \epsilon_j$ .

# Coupling to a single excited state

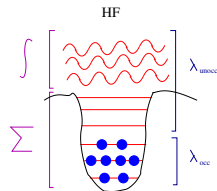
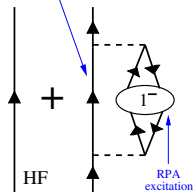
- ▶  $p+^{40}\text{Ca}$  scattering
- ▶ Potential:  $V^{HF} + \text{Im}(V^{RPA})$
- ▶ Coupling to the first  $1^-$  state of  $^{40}\text{Ca}$  with  $E_{1^-} = 9.7$  MeV



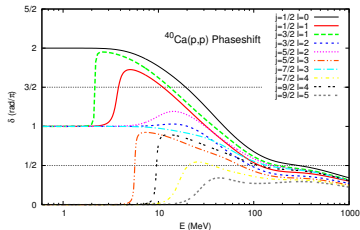
# Coupling to a single excited state

- ▶  $p+^{40}\text{Ca}$  scattering
- ▶ Potential:  $V^{HF} + \text{Im}(V^{RPA})$
- ▶ Coupling to the first  $1^-$  state of  $^{40}\text{Ca}$  with  $E_{1^-} = 9.7$  MeV

Intermediate HF propagator

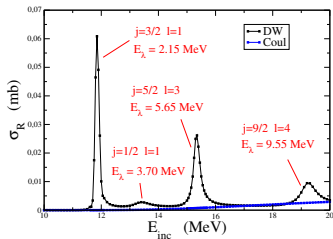


- ▶ HF phaseshift



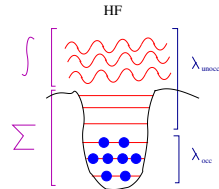
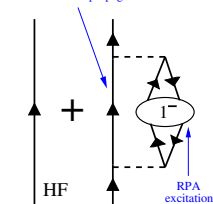
# Coupling to a single excited state

- ▶  $p+^{40}\text{Ca}$  scattering
- ▶ Potential:  $V^{HF} + \text{Im}(V^{RPA})$
- ▶ Coupling to the first  $1^-$  state of  $^{40}\text{Ca}$  with  $E_{1^-} = 9.7 \text{ MeV}$

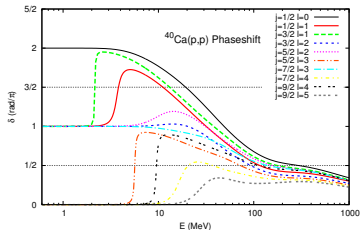


- ▶ Importance of the intermediate single particle resonances
- ▶ Strong impact on reaction cross section

Intermediate HF propagator

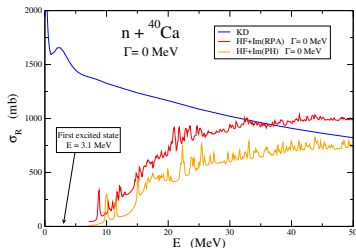


- ▶ HF phaseshift



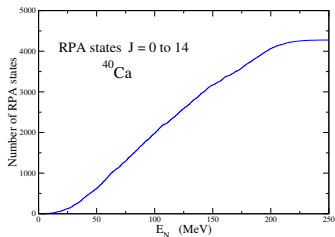
# Effect of HF intermediate propagator

- ▶  $\sigma_R$  from  $V_{HF} + \text{Im}(V_{RPA})$
- ▶  $\sigma_R$  from  $V_{HF} + \text{Im}(V_{PH})$



→ Effect of the HF resonances  
on  $\text{Im}(V_{RPA})$

- ▶ Zero width calculation:
  - ▶  $\sigma_R = 0$  for incident energies below the energy of the first excited state of the target nucleus
- ▶  ${}^{40}\text{Ca}$  RPA states  $J = 0 \rightarrow 8$



$$S = \langle S \rangle + \widehat{S}$$

Averaged cross section

$$\langle \sigma_E \rangle = \frac{\pi}{k^2} \langle |1 - S|^2 \rangle$$

$$\langle \sigma_R \rangle = \frac{\pi}{k^2} \langle 1 - |S|^2 \rangle$$

$$\langle \sigma_T \rangle = \frac{\pi}{k^2} \langle 1 - \text{Re}[S] \rangle$$

Averaged potential

$$\bar{\sigma}_E = \frac{\pi}{k^2} |1 - \langle S \rangle|^2$$

$$\bar{\sigma}_R = \frac{\pi}{k^2} (1 - |\langle S \rangle|^2)$$

$$\bar{\sigma}_T = \frac{\pi}{k^2} (1 - \text{Re}[\langle S \rangle])$$

$$\langle \sigma_E \rangle = \bar{\sigma}_E + \sigma_{CE}$$

$$\langle \sigma_R \rangle = \bar{\sigma}_R - \sigma_{CE}$$

$$\langle \sigma_T \rangle = \bar{\sigma}_T$$

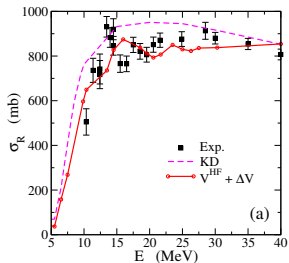
Compound elastic

$$\sigma_{CE} = \frac{\pi}{k^2} \langle |\widehat{S}|^2 \rangle$$

- ▶ TALYS: Hauser-Feshbach/ Koning-Delaroche
- ▶ particularly relevant for neutron scattering below 10 MeV

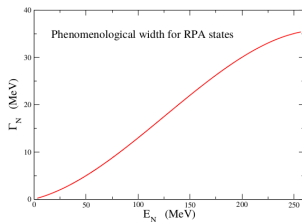
# Integral cross sections $n/p + {}^{40}\text{Ca}$

## ► $p + {}^{40}\text{Ca}$

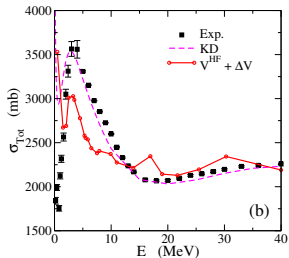


► Coupling to 4500 excited states of the target ( $J = 0$  à 14) given by a RPA code projected on oscillator basis.

► Use of phenomenological width for the excited states of the target.



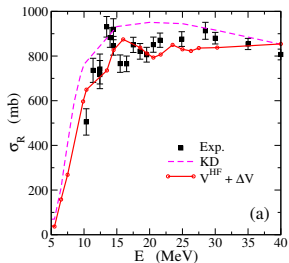
## ► $n + {}^{40}\text{Ca}$



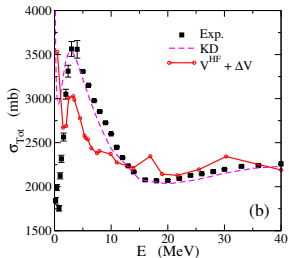


# Integral cross sections $n/p + {}^{40}\text{Ca}$

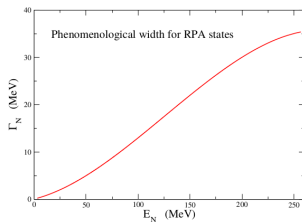
## ► $p + {}^{40}\text{Ca}$



## ► $n + {}^{40}\text{Ca}$

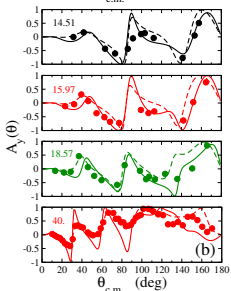
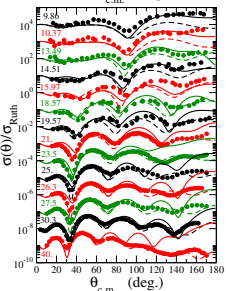
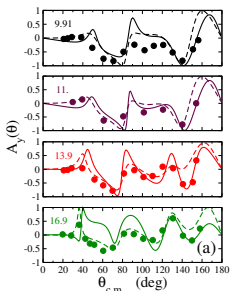
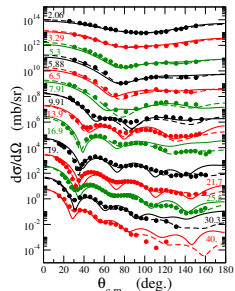


- Coupling to 4500 excited states of the target ( $J = 0$  à 14) given by a RPA code projected on oscillator basis.
- Use of phenomenological width for the excited states of the target.



- In the future we would like a microscopic determination of energy widths and shifts: 2p-2h coupling

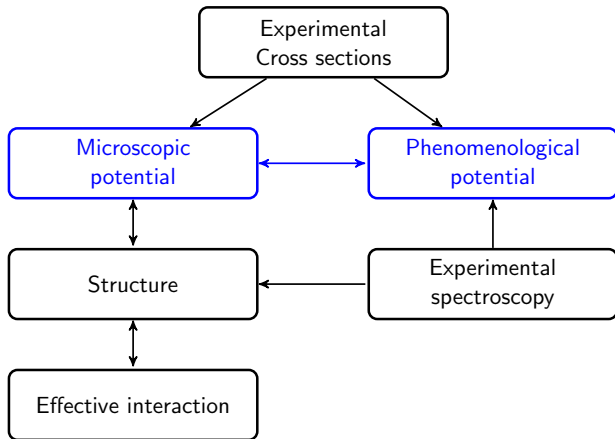
# Cross section and Analysing powers $n/p+^{40}\text{Ca}$



NSM (full line)  
Koning-Delaroche (dashed line)

- ▶ Good agreement with cross section data below 30 MeV.
- ▶ In terms of energy regime, NSM is complementary to g-matrix approaches.
- ▶ Good agreement with analysing powers data: correct behaviour of the "spin-orbit" term of the potential.
- ▶ Effective interaction fitted with structure data + fission barriers

# Microscopic and phenomenological potentials



# Potential for $n + {}^{40}\text{Ca}$ @ 10 MeV

- ▶ NSM potential
- ▶ Non local dispersive potential fitted on all the available data for  ${}^{40}\text{Ca}$

$$v_{ij}(r, r') = \iint d\hat{\mathbf{r}} d\hat{\mathbf{r}}' \mathcal{Y}_{ij}^m(\hat{\mathbf{r}}) V(\mathbf{r}, \mathbf{r}') \mathcal{Y}_{ij}^{m\dagger}(\hat{\mathbf{r}}')$$

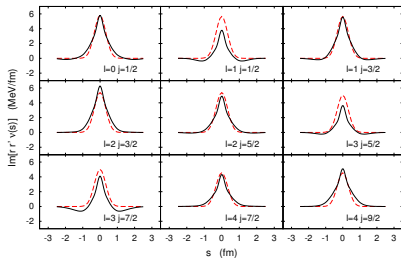
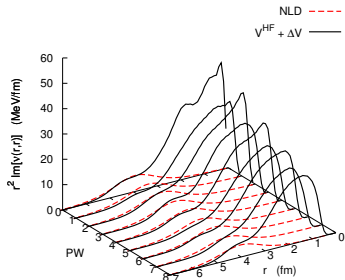
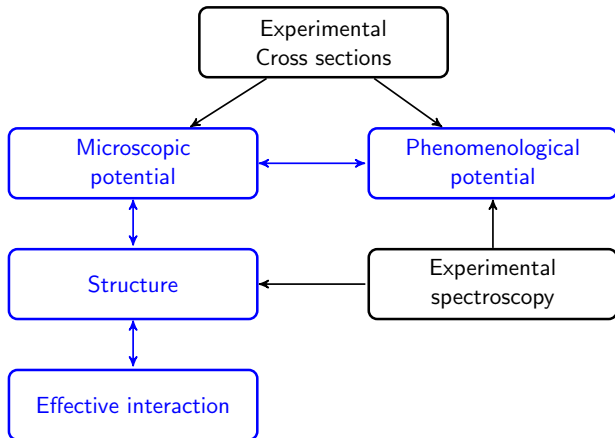


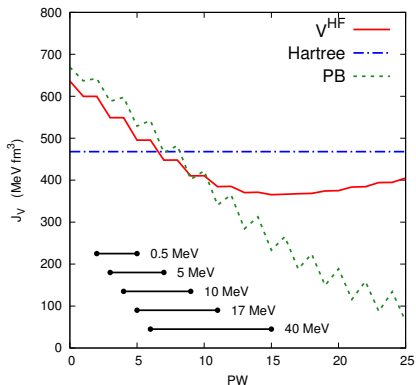
Figure:  $s = |\mathbf{r} - \mathbf{r}'|$

M.H. Mahzoon, R.J. Charity, W.H. Dickhoff, H. Dussan, S.J. Waldecker, *Phys. Rev. Lett.* 112, 162503 (2014)

# Phenomenological potential and effective interaction

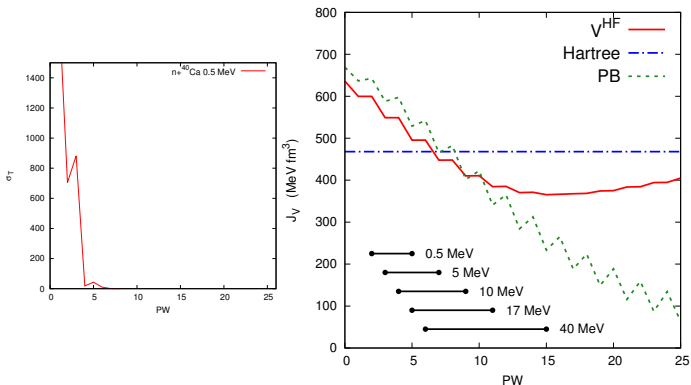


Volume integral: 
$$J_V^{lj} = \frac{-4\pi}{A} \int dr r^2 \int dr' r'^2 v_{lj}(r, r')$$



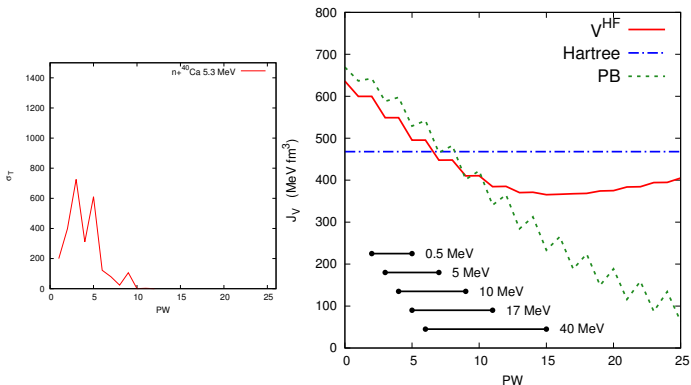
- Perey Buck optical potential with gaussian non locality and energy independent.

Volume integral: 
$$J_V^{lj} = \frac{-4\pi}{A} \int dr r^2 \int dr' r'^2 v_{lj}(r, r')$$



- Pery Buck optical potential with gaussian non locality and energy independent.

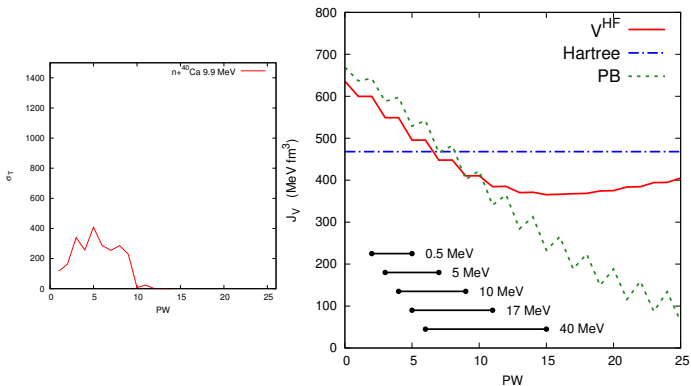
Volume integral: 
$$J_V^{lj} = \frac{-4\pi}{A} \int dr r^2 \int dr' r'^2 v_{lj}(r, r')$$



- Perey Buck optical potential with gaussian non locality and energy independent.

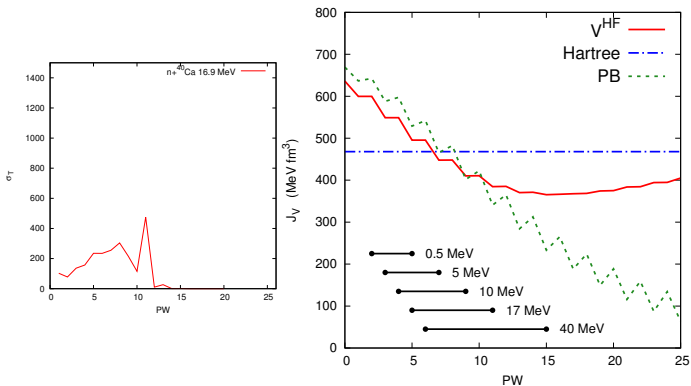


Volume integral: 
$$J_V^{lj} = \frac{-4\pi}{A} \int dr r^2 \int dr' r'^2 v_{lj}(r, r')$$



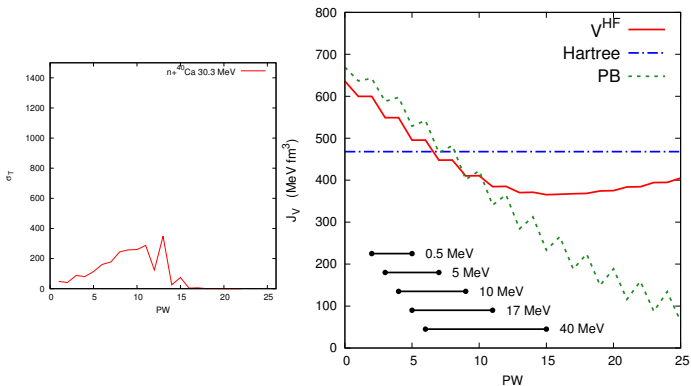
- Perey Buck optical potential with gaussian non locality and energy independent.

Volume integral: 
$$J_V^{lj} = \frac{-4\pi}{A} \int dr r^2 \int dr' r'^2 v_{lj}(r, r')$$



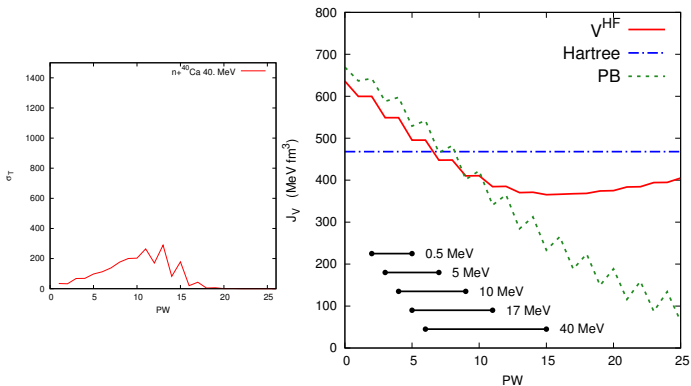
- Perey Buck optical potential with gaussian non locality and energy independent.

Volume integral: 
$$J_V^{lj} = \frac{-4\pi}{A} \int dr r^2 \int dr' r'^2 v_{lj}(r, r')$$



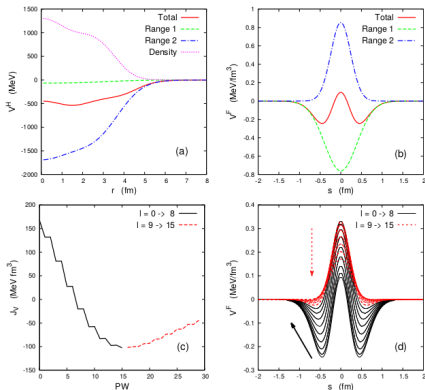
- Perey Buck optical potential with gaussian non locality and energy independent.

Volume integral:  $J_V^{lj} = \frac{-4\pi}{A} \int dr r^2 \int dr' r'^2 v_{lj}(r, r')$



- Perey Buck optical potential with gaussian non locality and energy independent.

# HF potential shape



**Fig. 15.** Contributions for  $n + {}^{40}\text{Ca}$  to: (a) to the Hartree local potential ( $V^H$ ): Total (solid line), first range of D1S (dashed line), second range of D1S (dash-dotted line) and density term (dotted line). (b) First partial wave of the nonlocal Fock term at  $r = r' = 4.3$  fm: Total (solid line), first range of D1S (dashed line) and second range of D1S (dash-dotted line). (c) Volume integral of the Fock potential as a function of partial wave: Negative slope (solid line), positive slope (dashed line). (d) Same as (c) for the Fock components nonlocality at  $r = r' = 4.3$  fm.

- ▶ *Quelques applications du formalisme des fonctions de Green à l'étude des noyaux*,  
N. Vinh Mau
- ▶ *Quantum Theory of Many-Particle Systems*,  
Fetter and Walecka.
- ▶ *A Guide to Feynman Diagrams in the Many-Body Problem*,  
Mattuck.
- ▶ *Quantum Statistical Mechanics: Green's Function Methods in Equilibrium and Non-Equilibrium Problems*,  
Kadanoff.
- ▶ *The nuclear many-body problem*,  
Ring and Schuck.