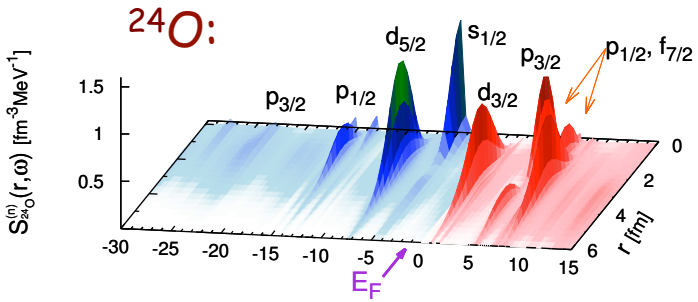
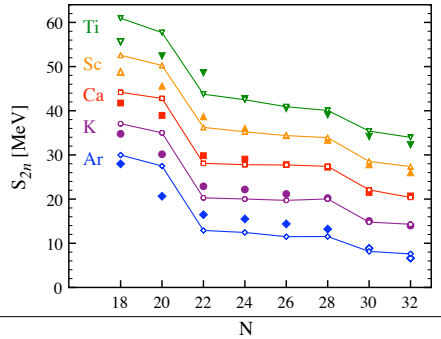
TALENT Course no. 2: Many-Body Methods for Nuclear Physics

Self-consistent Green's function in Finite Nucleai and related things…

Carlo Barbieri — University of Surrey





Expectation values

Take the Hamiltonian,

$$H = \sum_{\alpha\beta} t_{\alpha\beta}\, c^\dagger_\alpha c_\beta + \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta}\, c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma$$

(or any 1- and 2-body operators). The g.s. expectation values are:

$$\langle \Psi_0^N | H | \Psi_0^N \rangle = \sum_{\alpha\beta} t_{\alpha\beta} \langle \Psi_0^N | c^\dagger_\alpha c_\beta | \Psi_0^N \rangle + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta\gamma\delta} \langle \Psi_0^N | c^\dagger_\alpha c^\dagger_\beta c_\delta c_\gamma | \Psi_0^N \rangle$$

$$= \sum_{\alpha\beta} t_{\alpha\beta}\, \rho_{\beta\alpha} + \frac{1}{4} \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta,\gamma\delta}\, \Gamma_{\gamma\delta,\alpha\beta}$$

one-body density matrix

two-body density matrix

Expectation values

The one-body density matrix (and hence expectation values) is extracted easily from $g_{\alpha\beta}$

$$\rho_{\alpha\beta} = \langle \Psi_0^N | c_\beta^\dagger c_\alpha | \Psi_0^N \rangle = -\, i\hbar \lim_{t' \to t^+} g_{\alpha\beta}(t, t')$$

$$= + \int d\omega \; S^h_{\alpha\beta}(\omega)$$

Hence:

$$\langle \Psi_0^N | O | \Psi_0^N \rangle = -\sum_{\alpha\beta} \int d\omega \; o_{\alpha\beta} \; S^h_{\beta\alpha}(\omega)$$

$$= \pm i\hbar \lim_{t' \to t^+} \sum_{\alpha\beta} o_{\alpha\beta} \; g_{\beta\alpha}(t, t')$$

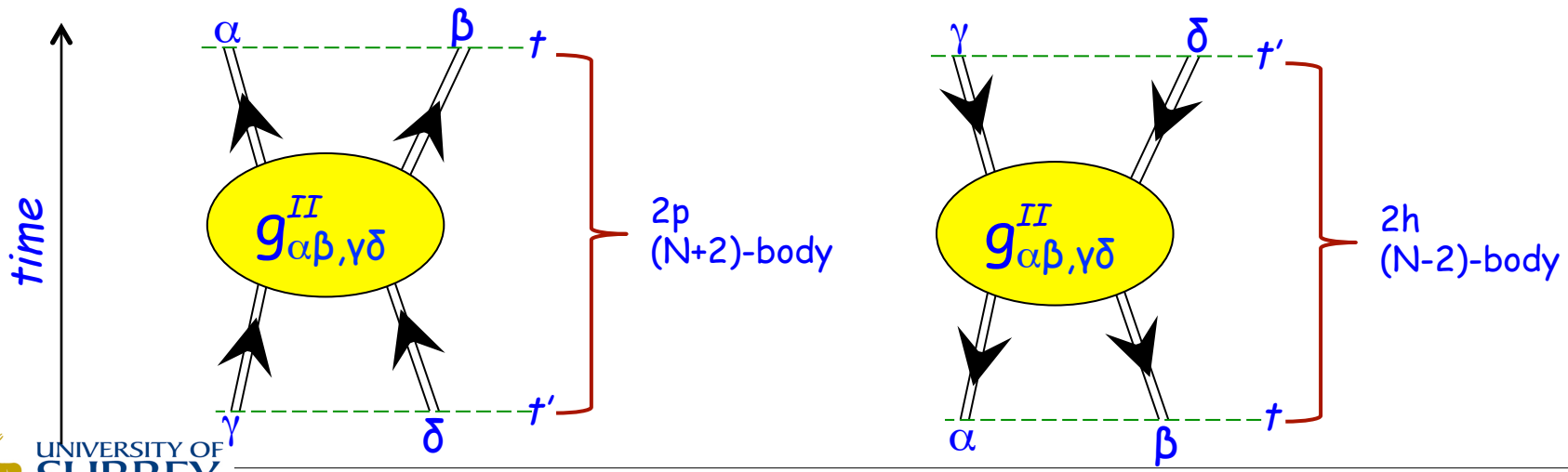
Two-particle/two-hole propagator

Two-body density matrices and matrix elements require a particular ordering of the 4-points Green's function.

$$g^{4-pt}_{\alpha\beta,\gamma\delta}(t_1,t_2;t'_1,t'_2) = -\frac{i}{\hbar}\langle\Psi_0^N|T[c_\beta(t_2)c_\alpha(t_1)c^\dagger_\gamma(t'_1)c^\dagger_\delta(t'_2)]|\Psi_0^N\rangle$$

Define the two-particle/two-hole propagator:

$$g^{II}_{\alpha\beta,\gamma\delta}(t,t') = -\frac{i}{\hbar}\langle\Psi_0^N|T[c_\beta(t)c_\alpha(t)c^\dagger_\gamma(t')c^\dagger_\delta(t')]|\Psi_0^N\rangle$$



Two-particle/two-hole propagator

- Representations of $g^{II}_{\alpha\beta,\gamma\delta}$:

$$g^{II}_{\alpha\beta,\gamma\delta}(\omega) = \sum_n \frac{\langle \Psi_0^N | c_\beta c_\alpha | \Psi_n^{N+2} \rangle \, \langle \Psi^{N+2_n} | c_\gamma^\dagger c_\delta^\dagger | \Psi_0^N \rangle}{\omega - (E_n^{N+2} - E_0^N) + i\eta}$$

← *two-particles (g^{pp})*

$$- \sum_k \frac{\langle \Psi_0^N | c_\gamma^\dagger c_\delta^\dagger | \Psi_k^{N-2} \rangle \, \langle \Psi_k^{N-2} | c_\beta c_\alpha | \Psi_0^N \rangle}{\omega - \left(E_0^N - E_k^{N-2}\right) - i\eta}$$

← *two-holes (g^{hh})*

$$\begin{aligned} S^{pp}_{\alpha\beta,\gamma\delta}(\omega) &= -\frac{1}{\pi} \, \mathrm{Im} \, g^{pp}_{\alpha\beta,\gamma\delta}(\omega) \\ &= \sum_n \langle \Psi_0^N | c_\beta c_\alpha | \Psi_n^{N+2} \rangle \langle \Psi_n^{N+2} | c_\gamma^\dagger c_\delta^\dagger | \Psi_0^N \rangle \, \delta\left(\hbar\omega - (E_n^{N+2} - E_0^N)\right) \\ S^{hh}_{\alpha\beta,\gamma\delta}(\omega) &= \frac{1}{\pi} \, \mathrm{Im} \, g^{hh}_{\alpha\beta,\gamma\delta}(\omega) \\ &= -\sum_k \langle \Psi_0^N | c_\gamma^\dagger c_\delta^\dagger | \Psi_k^{N-2} \rangle \langle \Psi_k^{N-2} | c_\beta c_\alpha | \Psi_0^N \rangle \, \delta\left(\hbar\omega - (E_0^N - E_k^{N-2})\right) \end{aligned}$$

Expectation values

Hence—for *2-body* matrix elements:

$$\Gamma_{\alpha\beta,\gamma\delta} = \langle \Psi^N | c^\dagger_\gamma c^\dagger_\delta c_\beta c_\alpha | \Psi^N \rangle = -\frac{1}{4} \int d\omega S^{hh}_{\alpha\beta,\gamma\delta}(\omega)$$

$$\begin{aligned} \langle \Psi^N_0 | V | \Psi^N_0 \rangle &= -\sum_{\alpha\beta\gamma\delta} \int d\omega v_{\alpha\beta,\gamma\delta} S^{hh}_{\gamma\delta,\alpha\beta}(\omega) \\ &= +i\hbar \lim_{t' \to t^+} \sum_{\alpha\beta} v_{\alpha\beta,\gamma\delta} g^{II}_{\gamma\delta,\alpha\beta}(t,t') \end{aligned}$$

"Some Magic"

Let's consider the full Hamiltonian:

$$H = \hat{T} + \hat{V} + \hat{W}$$

$$= \sum_{\alpha\beta} t_{\alpha\beta}\, a^{\dagger}_{\alpha} a_{\beta} + \frac{1}{4} \sum_{\substack{\alpha\beta \\ \gamma\delta}} v_{\alpha\beta,\gamma\delta}\, a^{\dagger}_{\alpha} a^{\dagger}_{\beta} a_{\delta} a_{\gamma} +$$

$$+ \frac{1}{36} \sum_{\substack{\alpha\beta\gamma \\ \mu\nu\lambda}} w_{\alpha\beta\gamma,\mu\nu\lambda}\, a^{\dagger}_{\alpha} a^{\dagger}_{\beta} a^{\dagger}_{\gamma} a_{\lambda} a_{\nu} a_{\mu}$$

T : one-body part of the Hamiltoninan (for nuclei, it's just the kinetic energy)

V, W: the two- and three-body interactions ($v_{\alpha\beta,\gamma\delta}$ and $w_{\alpha\beta\gamma,\mu\nu\lambda}$, their <u>properly antisymmetrized</u> matrix elements)

Second quantization excercise

Use $i\hbar \dfrac{d\,a(t)}{dt} = [a, H]$ to prove the following relations:

$$i\hbar \frac{d a_\alpha(t)}{dt} = \sum_\beta t_{\alpha\beta}\, a_\beta(t) + \frac{1}{2}\sum_{\beta\gamma\delta} v_{\alpha\beta\gamma\delta}\, a^\dagger_\beta(t)\, a_\delta(t)\, a_\gamma(t)$$

$$+ \frac{1}{12}\sum_{\substack{\beta\gamma \\ \mu\nu\lambda}} w_{\alpha\beta\gamma,\mu\nu\lambda}\, a^\dagger_\beta(t)\, a^\dagger_\gamma(t)\, a_\lambda(t)\, a_\nu(t)\, a_\mu(t)$$

$$i\hbar \frac{d a^\dagger_\gamma(t)}{dt} = \sum_\alpha t_{\alpha\gamma}\, a^\dagger_\alpha(t) + \frac{1}{2}\sum_{\substack{\alpha\beta \\ \delta}} v_{\alpha\beta,\gamma\delta}\, a^\dagger_\alpha(t)\, a^\dagger_\beta(t)\, a_\delta(t)$$

$$+ \frac{1}{12}\sum_{\substack{\alpha\beta\delta \\ \nu\lambda}} w_{\alpha\beta\delta,\gamma\nu\lambda}\, a^\dagger_\alpha(t)\, a^\dagger_\beta(t)\, a^\dagger_\delta(t)\, a_\lambda(t)\, a_\nu(t)$$

"Some Magic"

By using the equation of motion, one can take the derivative of the propagator:

$$(i\hbar)^2 \frac{d}{dt} g_{\alpha\xi}(t,t') = \langle \Psi_0^A | T\left[i\hbar \frac{dQ_\alpha(t)}{dt} Q_\xi^\dagger(t') \right] | \Psi_0^A \rangle$$

$$= \langle \Psi_0^A | T\Big[Q_\xi^\dagger(t')\, t_{\alpha\beta}\, Q_\beta(t) \; +$$

$$+ 2\, Q_\xi^\dagger(t') \frac{V_{\alpha\beta\gamma\delta}}{4} Q_\beta^\dagger(t) Q_\delta(t) Q_\gamma(t) \; +$$

$$+ 3\, Q_\xi^\dagger(t') \frac{W_{\alpha\beta\gamma\mu\nu\lambda}}{36} Q_\beta^\dagger(t) Q_\gamma^\dagger(t) Q_\lambda(t) Q_\nu(t) Q_\mu(t) \Big] | \Psi_0^A \rangle$$

By taking the time ordering for $t' \rightarrow t^{+0}$ one gets the expectation values *of both T, V and W!*

"Some Magic"

...thus:

$$(-i\hbar) \lim_{t' \to t^+} \sum_\alpha \left\{ i\hbar \frac{d}{dt} g_{\alpha\alpha}(t,t') \right\} = \langle \hat{T} \rangle + 2\langle \hat{V} \rangle + 3\langle \hat{W} \rangle$$

which leads to the (Galitski-Migdal-Boffi)-Koltun sum rule:

$$\frac{-i\hbar}{2} \lim_{\tau \to 0^-} \mathrm{Tr} \left\{ i\hbar \frac{d}{d\tau} g(\tau) + \hat{T} g(\tau) \right\} = E_0^A + \frac{1}{2} \langle \hat{W} \rangle$$

$$\frac{-i\hbar}{3} \lim_{\tau \to 0^-} \mathrm{Tr} \left\{ i\hbar \frac{d}{d\tau} g(\tau) + 2\hat{T} g(\tau) \right\} = E_0^A - \frac{1}{3} \langle \hat{V} \rangle$$

With <u>only two body</u> interactions, $g_{\alpha\beta}(t,t')$ is sufficient to obtain the total energy!

Unperturbed propagator

- Take a system of non interacting fermions

$$H_0 = \sum_\alpha \varepsilon_\alpha \, c_\alpha^\dagger c_\alpha \qquad\qquad |\Phi_0^N\rangle = \prod_{i=1}^{N} c_i^\dagger |0\rangle$$

- The unperturbed propagator is:

$$\left(i\hbar \frac{d}{dt} c_\alpha(t) = e^{iH_0 t/\hbar} \, [c_\alpha, H] \, e^{-iH_0 t/\hbar} \right)$$

$$g_{\alpha\beta}^{(0)}(t,t') = -\frac{i}{\hbar} \langle \Phi_0^N | T[c_\alpha(t) c_\beta^\dagger(t')] | \Phi_0^N \rangle$$

- or

$$\begin{aligned} g_{\alpha\beta}^{(0)}(t-t') &= -\frac{i}{\hbar}\theta(t-t') \langle \Phi_0^N | c_\alpha e^{-i(H_0 - E_0^N)(t-t')/\hbar} c_\beta^\dagger | \Phi_0^N \rangle \\ &\quad + \frac{i}{\hbar}\theta(t'-t) \langle \Phi_0^N | c_\beta^\dagger e^{i(H_0 - E_0^N)(t-t')/\hbar} c_\alpha | \Phi_0^N \rangle \end{aligned}$$

Unperturbed propagator

The completeness for states with N±1 particles includes:

$$|\Phi_n^{N+1}\rangle = c_n^\dagger |\Phi_0^N\rangle \qquad E_n^{N+1} = E_0^N + \varepsilon_n$$

$$|\Phi_k^{N-1}\rangle = c_k |\Phi_0^N\rangle \qquad E_k^{N-1} = E_0^N - \varepsilon_k$$

...states with more p-h excitations are *not* connected to $|\Phi_0^N\rangle$ by single $c_\alpha / c_\beta^\dagger$ operators

Thus, for example:

$$\langle \Phi_k^{N-1} | c_\alpha | \Phi_0^N \rangle = \begin{cases} 1 \text{ for } \alpha \text{ in } |\Phi_0^N\rangle \\ 0 \text{ for } \alpha \text{ not in } |\Phi_0^N\rangle \end{cases}$$

$$\begin{aligned} g_{\alpha\beta}^{(0)}(t-t') &= -\frac{i}{\hbar}\theta(t-t')\langle \Phi_0^N | c_\alpha e^{-i(H_0 - E_0^N)(t-t')/\hbar} c_\beta^\dagger | \Phi_0^N \rangle \\ &\quad + \frac{i}{\hbar}\theta(t'-t)\langle \Phi_0^N | c_\beta^\dagger e^{i(H_0 - E_0^N)(t-t')/\hbar} c_\alpha | \Phi_0^N \rangle \end{aligned}$$

Unperturbed propagator

Thus, the unperturbed propagator for a set of non interacting fermions is written as,

$$g^{(0)}_{\alpha\beta}(t-t') = -\frac{i}{\hbar}\delta_{\alpha\beta}\left\{\theta(t-t')\delta_{\alpha\notin F}e^{-i\varepsilon_\alpha(t-t')/\hbar} - \theta(t'-t)\delta_{\alpha\in F}e^{i\varepsilon_\alpha(t-t')/\hbar}\right\}$$

And in Lehmann representation:

$$g^{(0)}_{\alpha\beta}(\omega) = \sum_{n=N+1}^{\infty}\frac{\delta_{\alpha\,\beta}\delta_{\alpha\,n}}{\hbar\omega-\varepsilon_n+i\eta} + \sum_{k=1}^{N}\frac{\delta_{\alpha\,\beta}\delta_{\alpha\,k}}{\hbar\omega-\varepsilon_k-i\eta}$$

Unperturbed propagator

If one chooses a different basis {α'}, then

$$g^{(0)}_{\alpha'\beta'}(t-t') = -\frac{i}{\hbar}\left\{\theta(t-t')\sum_{n=N+1}^{\infty}(\mathcal{X}^n_{\alpha'})^*\,\mathcal{X}^n_{\beta'}e^{-i\varepsilon_n(t-t')/\hbar} - \theta(t'-t)\sum_{k=1}^{N}\mathcal{Y}^k_{\alpha'}\,(\mathcal{Y}^k_{\beta'})^* e^{i\varepsilon_k(t-t')/\hbar}\right\}$$

$$g^{(0)}_{\alpha'\beta'}(\omega) = \sum_{n=N+1}^{\infty}\frac{(\mathcal{X}^n_{\alpha'})^*\,\mathcal{X}^n_{\beta'}}{\hbar\omega-\varepsilon_n+i\eta} + \sum_{k=1}^{N}\frac{\mathcal{Y}^k_{\alpha'}\,(\mathcal{Y}^k_{\beta'})^*}{\hbar\omega-\varepsilon_k-i\eta}$$

where:

$$\begin{cases}\mathcal{X}^n_\beta = \langle n|c^\dagger_\alpha|0\rangle \\ \mathcal{Y}^n_\beta = \langle 0|c_\alpha|k\rangle\end{cases}$$

In a general basis the propagator maintain its poles (excitation energies) but it is no longer diagonal!

Unperturbed propagator

$g^{(0)}_{\alpha\beta}(t-t')$ has an inverse operator:

$$
\begin{aligned}
& i\hbar\frac{\partial}{\partial t}g^{(0)}_{\alpha\beta}(t-t') \\
&= \delta_{\alpha\beta}\delta(t-t') - \frac{i}{\hbar}\delta_{\alpha\beta}\left\{\theta(t-t')\delta_{\alpha\notin F}\varepsilon_\alpha e^{-i\varepsilon_\alpha(t-t')/\hbar} - \theta(t'-t)\delta_{\alpha\in F}\varepsilon_\alpha e^{i\varepsilon_\alpha(t-t')/\hbar}\right\} \\
&= \delta_{\alpha\beta}\delta(t-t') + \varepsilon_\alpha g^{(0)}_{\alpha\beta}(t-t')
\end{aligned}
$$

Thus:

$$
g^{(0)\,-1}_{\alpha\beta}(t,t_1) = \delta_{\alpha\beta}\delta(t-t_1)\left\{i\hbar\frac{\partial}{\partial t_1} - \varepsilon_\alpha\right\}
$$

$$
\sum_\gamma \int dt_1\; g^{(0)\,-1}_{\alpha\gamma}(t,t_1)g^{(0)}_{\gamma\beta}(t_1,t') \;=\; \delta_{\alpha\beta}\delta(t-t')
$$

$$
\sum_\gamma \int dt_1\; g^{(0)}_{\alpha\gamma}(t,t_1)g^{(0)\,-1}_{\gamma\beta}(t_1,t') \;=\; \left\{-i\hbar\frac{\partial}{\partial t'} - \varepsilon_\alpha\right\}g^{(0)}_{\alpha\beta}(t-t') = \delta_{\alpha\beta}\delta(t-t')
$$

Unperturbed $g^{4\text{-}pt}$ propagator

The 4-points unperturbed propagator is:

$$g^{(0)\,4-pt}_{\alpha\beta,\gamma\delta}(t_\alpha,t_\beta;t_\gamma,t_\delta) = -\frac{i}{\hbar}\langle\Phi_0^N|T[c_\beta(t_\beta)c_\alpha(t_\alpha)c^\dagger_\gamma(t_\gamma)c^\dagger_\delta(t_\delta)]|\Phi_0^N\rangle$$

By Wick theorem, one has:

$$g^{(0)\,4-pt}_{\alpha\beta,\gamma\delta}(t_\alpha,t_\beta;t_\gamma,t_\delta) = i\hbar\left[g^{(0)}_{\alpha\gamma}(t_\alpha,t_\gamma)g^{(0)}_{\beta\delta}(t_\beta,t_\delta) - g^{(0)}_{\beta\gamma}(t_\beta,t_\gamma)g^{(0)}_{\alpha\delta}(t_\alpha,t_\delta)\right]$$

Equation of motion for $g_{\alpha\beta}$

Take the Hamiltonian,

$$H = H_0 + V - U$$

$$H_0 = \sum_{\alpha} \varepsilon_\alpha \, c_\alpha^\dagger c_\alpha \qquad U = \sum_{\alpha\beta} u_{\alpha\beta} \, c_\alpha^\dagger c_\beta \qquad V = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} v_{\alpha\beta,\gamma\delta} \, c_\alpha^\dagger c_\beta^\dagger c_\delta c_\gamma$$

Equation of motion for the operator:

$$i\hbar \frac{d}{dt} c_\alpha(t) = e^{iHt/\hbar} \, [c_\alpha, H] \, e^{-iHt/\hbar}$$

$$[c_\zeta, H] = \varepsilon_\zeta c_\zeta - \sum_{\beta} u_{\zeta\beta} \, c_\beta + \frac{1}{2} \sum_{\beta\gamma\delta} v_{\zeta\beta,\gamma\delta} \, c_\beta^\dagger c_\delta c_\gamma$$

→ derivative creates an additional ph excitation weighted by V

Equation of motion for $g_{\alpha\beta}$

$$g_{\alpha\beta}(t,t') = -\frac{i}{\hbar}\langle\Psi_0^N|T[c_\alpha(t)c_\beta^\dagger(t')]|\Psi_0^N\rangle$$

Take the derivative w.r.t. time t :

$$i\hbar\frac{\partial}{\partial t}g_{\alpha\beta}(t,t') = \delta(t-t')\langle\Psi_0^N|\{c_\alpha(t),c_\beta^\dagger(t')\}|\Psi_0^N\rangle + \langle\Psi_0^N|T\left[\frac{\partial c_\alpha(t)}{\partial t}c_\beta^\dagger(t')\right]|\Psi_0^N\rangle$$

$$i\hbar\frac{\partial}{\partial t}g_{\alpha\beta}(t-t') = \delta(t-t')\delta_{\alpha\beta} + \varepsilon_\alpha g_{\alpha\beta}(t-t') - \sum_\gamma u_{\alpha\gamma}\, g_{\gamma\beta}(t-t') - \frac{i}{\hbar}\sum_{\lambda\mu\nu} v_{\alpha\lambda,\mu\nu}\,\frac{1}{2}\,\langle\Psi_0^N|\,T[c_\lambda^\dagger(t)c_\nu(t)c_\mu(t)c_\beta^\dagger(t')]|\Psi_0^N\rangle$$

Equation of motion for $g_{\alpha\beta}$

$$\left\{ i\hbar \frac{\partial}{\partial t} g_{\alpha\beta}(t-t') \; - \; \varepsilon_\alpha \right\} g_{\alpha\beta}(t-t') = g_\alpha^{(0)\,-1}(t) g_{\alpha\beta}(t-t') \quad =$$

$$\delta(t-t')\delta_{\alpha\beta} \; - \; \sum_\gamma u_{\alpha\gamma} \, g_{\gamma\beta}(t-t')$$

$$+ \frac{1}{2} \sum_{\lambda\mu\nu} v_{\alpha\lambda,\mu\nu} \, \langle \Psi_0^N | \, T[c_\lambda^\dagger(t) c_\nu(t) c_\mu(t) c_\beta^\dagger(t')] | \Psi_0^N \rangle$$

Apply $g^{(0)}{}_{\alpha\beta}(t-t')$:

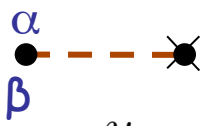
$$g_{\alpha\beta}(t-t') \;=\; g_{\alpha\beta}^{(0)}(t-t') \; - \; \sum_{\gamma\delta} \int dt_\gamma \, g_{\alpha\gamma}^{(0)}(t-t_\gamma) \, u_{\gamma\delta} \, g_{\delta\beta}(t_\gamma - t')$$

$$-\frac{i}{\hbar} \sum_{\gamma\lambda\mu\nu} \int dt_\gamma \, g_{\alpha\gamma}^{(0)}(t-t_\gamma) \, v_{\gamma\lambda,\mu\nu} \frac{1}{2} \, \langle \Psi_0^N | \, T[c_\lambda^\dagger(t_\gamma) c_\nu(t_\gamma) c_\mu(t_\gamma) c_\beta^\dagger(t')] | \Psi_0^N \rangle$$

Equation of motion for $g_{\alpha\beta}$

Feynman diagram conventions:

$g_{\alpha\beta}(t-t') =$

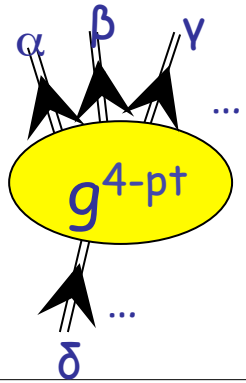
$u_{\alpha\beta},\ t_{\alpha\beta} =$ 

$u_{\alpha\beta}\ c^{\dagger}_{\alpha} c_{\beta}$

$g^{(0)}{}_{\alpha\beta}(t-t') =$

$v_{\alpha\beta,\gamma\delta} =$

$v_{\zeta\beta,\gamma\delta}\ c^{\dagger}_{\beta} c_{\delta} c_{\gamma}$

$g^{(0)}{}_{\alpha\beta\gamma\delta\ldots}(t_1,t_2,t_3,t_4) =$ 

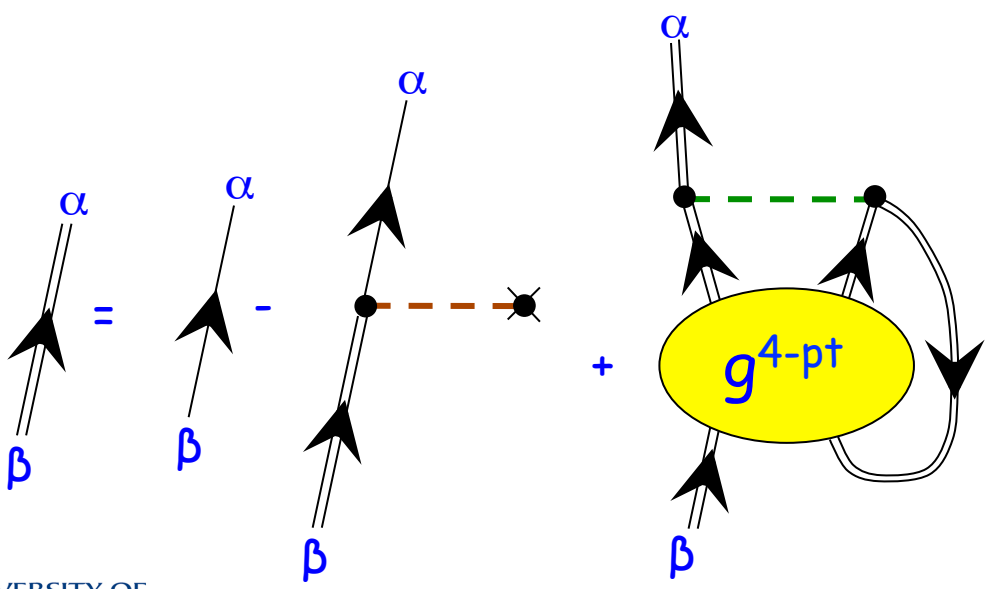
Equation of motion for $g_{\alpha\beta}$

The EOM for g is:

$$g_{\alpha\beta}(t-t') = g^{(0)}_{\alpha\beta}(t-t') - \sum_{\gamma\delta}\int dt_\gamma\, g^{(0)}_{\alpha\gamma}(t-t_\gamma)\, u_{\gamma\delta}\, g_{\delta\beta}(t_\gamma - t')$$

$$-\frac{i}{\hbar}\sum_{\gamma\lambda\mu\nu}\int dt_\gamma\, g^{(0)}_{\alpha\gamma}(t-t_\gamma)\, v_{\gamma\lambda,\mu\nu}\frac{1}{2}\,\langle\Psi^N_0|\, T[c^\dagger_\lambda(t_\gamma)c_\nu(t_\gamma)c_\mu(t_\gamma)c^\dagger_\beta(t')]|\Psi^N_0\rangle$$

Equivalent diagram:



→Expansion is in terms of g
→ EOM breaks a leg into three ➔ thus a GF with 2 more points
→ hierarchy of equartions!

4-points vertex

The 4-pt Green's function,

$$g^{(0)\,4-pt}_{\alpha\beta,\gamma\delta}(t_\alpha,t_\beta;t_\gamma,t_\delta) = -\frac{i}{\hbar}\langle\Phi_0^N|T[c_\beta(t_\beta)c_\alpha(t_\alpha)c^\dagger_\gamma(t_\gamma)c^\dagger_\delta(t_\delta)]|\Phi_0^N\rangle$$

can be expanded as:

non-interacting but fully correlated 1-body propagators

$$g^{(0)\,4-pt}_{\alpha\beta,\gamma\delta}(t_\alpha,t_\beta;t_\gamma,t_\delta) = i\hbar\left[g_{\alpha\gamma}(t_\alpha,t_\gamma)g_{\beta\delta}(t_\beta,t_\delta) - g_{\beta\gamma}(t_\beta,t_\gamma)g_{\alpha\delta}(t_\alpha,t_\delta)\right]$$

$$+\ (i\hbar)^2\int dt_1\int dt_2\int dt_3\int dt_4\sum_{\alpha'\beta'\gamma'\delta'} g_{\alpha\alpha'}(t_\alpha,t_1)g_{\beta\beta'}(t_\beta,t_2)$$

$$\times\ \Gamma_{\alpha'\beta',\gamma'\delta'}(t_1,t_2;t_3,t_4)\ g_{\gamma'\gamma}(t_3,t_\gamma)g_{\delta'\delta}(t_4,t_\delta)$$

two-particle interactions

4-points vertex

The 4-pt Green's function,

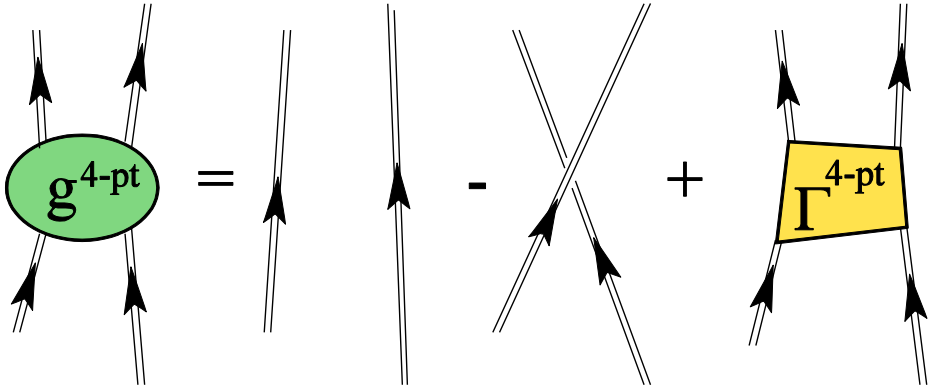
$$g^{(0)\,4-pt}_{\alpha\beta,\gamma\delta}(t_\alpha,t_\beta;t_\gamma,t_\delta) = -\frac{i}{\hbar}\langle\Phi_0^N|T[c_\beta(t_\beta)c_\alpha(t_\alpha)c^\dagger_\gamma(t_\gamma)c^\dagger_\delta(t_\delta)]|\Phi_0^N\rangle$$

can be expanded as:

$$g^{(0)\,4-pt}_{\alpha\beta,\gamma\delta}(t_\alpha,t_\beta;t_\gamma,t_\delta) = \; i\hbar\left[g_{\alpha\gamma}(t_\alpha,t_\gamma)g_{\beta\delta}(t_\beta,t_\delta) - g_{\beta\gamma}(t_\beta,t_\gamma)g_{\alpha\delta}(t_\alpha,t_\delta)\right]$$
$$+\; (i\hbar)^2\, g_{\alpha\alpha'}(t_\alpha,t_1)g_{\beta\beta'}(t_\beta,t_2)\,\Gamma_{\alpha'\beta',\gamma'\delta'}(t_1,t_2;t_3,t_4)\,g_{\gamma'\gamma}(t_3,t_\gamma)g_{\delta'\delta}(t_4,t_\delta)$$

CONVENTION: repeated indices are summed and times are integrated

corresponding diagram:



Dyson equation

The EOM for g(t-t') is:

$$g_{\alpha\beta}(t-t') = g^{(0)}_{\alpha\beta}(t-t') - \sum_{\gamma\delta}\int dt_\gamma\, g^{(0)}_{\alpha\gamma}(t-t_\gamma)\, u_{\gamma\delta}\, g_{\delta\beta}(t_\gamma - t') + \sum_{\gamma\lambda\mu\nu}\int dt_\gamma\, g^{(0)}_{\alpha\gamma}(t-t_\gamma)\, v_{\gamma\lambda,\mu\nu}\frac{1}{2} g^{2p1h-1p}_{\mu\nu\lambda,\beta}(t-t')$$

where:

$$g^{2p1h-1p}_{\mu\nu\lambda,\beta}(t-t') = -\frac{i}{\hbar}\langle\Psi^N_0|\, T[c^\dagger_\lambda(t)c_\nu(t)c_\mu(t)c^\dagger_\beta(t')]|\Psi^N_0\rangle = -g^{4-pt}_{\mu\nu,\beta\lambda}(t^-,t,t',t^+)$$

is a particular 2-times ordering of the 4-point GF.

Substitute the expansion of $g^{4\text{-pt}}$ in terms of non interacting propagators and $\Gamma^{4\text{-pt}}$

Dyson equation

$$v_{\gamma\lambda,\mu\nu}\frac{1}{2}g^{2p1h-1p}_{\mu\nu\lambda,\beta}(t-t')$$

where: $g^{2p1h\text{-}1p}(t\text{-}t') \approx \underbrace{[g\ g - g\ g]} + g\ g\ \Gamma\ g\ g$

$$v_{\gamma\lambda,\mu\nu}\frac{1}{2}(-i\hbar)\left[g_{\mu\beta}(t^-,t')g_{\nu\lambda}(t,t^+) - g_{\nu\beta}(t,t')g_{\mu\lambda}(t^-,t^+)\right]$$
$$= v_{\gamma\lambda,\mu\nu}\,(-i\hbar)g_{\nu\lambda}(t,t^+)\ g_{\mu\beta}(t^-,t')$$
$$= v_{\gamma\lambda,\mu\nu}\ \rho_{\nu\lambda}\ g_{\mu\beta}(t^-,t')$$

→ $$\Sigma^{HF}_{\alpha\beta} = \sum_{\mu\nu} v_{\alpha\mu,\beta\nu}\rho_{\nu\mu} = \sum_{\mu\nu} v_{\alpha\mu,\beta\nu}\langle\Phi^N_0|c^\dagger_\mu c_\nu|\Psi^N_0\rangle$$

this *extends* the Hartree-Fock potential to a fully correlated density

$$\rho_{\alpha\beta} = \langle\Psi^N_0|c^\dagger_\beta c_\alpha|\Psi^N_0\rangle = \pm i\hbar\ \lim_{t'\to t^+}\ g_{\alpha\beta}(t,t')$$

Dyson equation

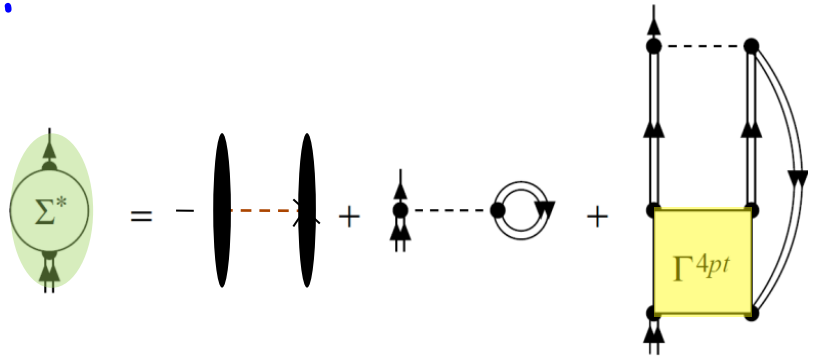
Dyson equation:

$$g_{\alpha\beta}(t-t') \;=\; g^{(0)}_{\alpha\beta}(t-t') \;+\; g^{(0)}_{\alpha\gamma}(t-t_\gamma)\,\Sigma^\star_{\gamma\delta}(t_\gamma,t_\delta)\,g_{\delta\beta}(t_\gamma-t')$$

Irreducible self-energy:

$$\begin{aligned}\Sigma^\star_{\alpha\beta}(t,t') \;=\; & -u_{\alpha\beta}\delta(t-t') \;+\; v_{\alpha\delta,\beta\gamma}\,\rho_{\gamma\delta}\,\delta(t-t') \\ & -(i\hbar)^2\frac{1}{2}v_{\alpha\lambda,\mu\nu}\,g_{\mu\mu'}(t-t_\mu)g_{\nu\nu'}(t-t_\nu) \\ & \times g_{\lambda'\lambda}(t_\lambda-t)\,\Gamma_{\mu'\nu',\beta\lambda'}(t_\mu,t_\nu;t',t_\lambda)\end{aligned}$$

diagrammatically:

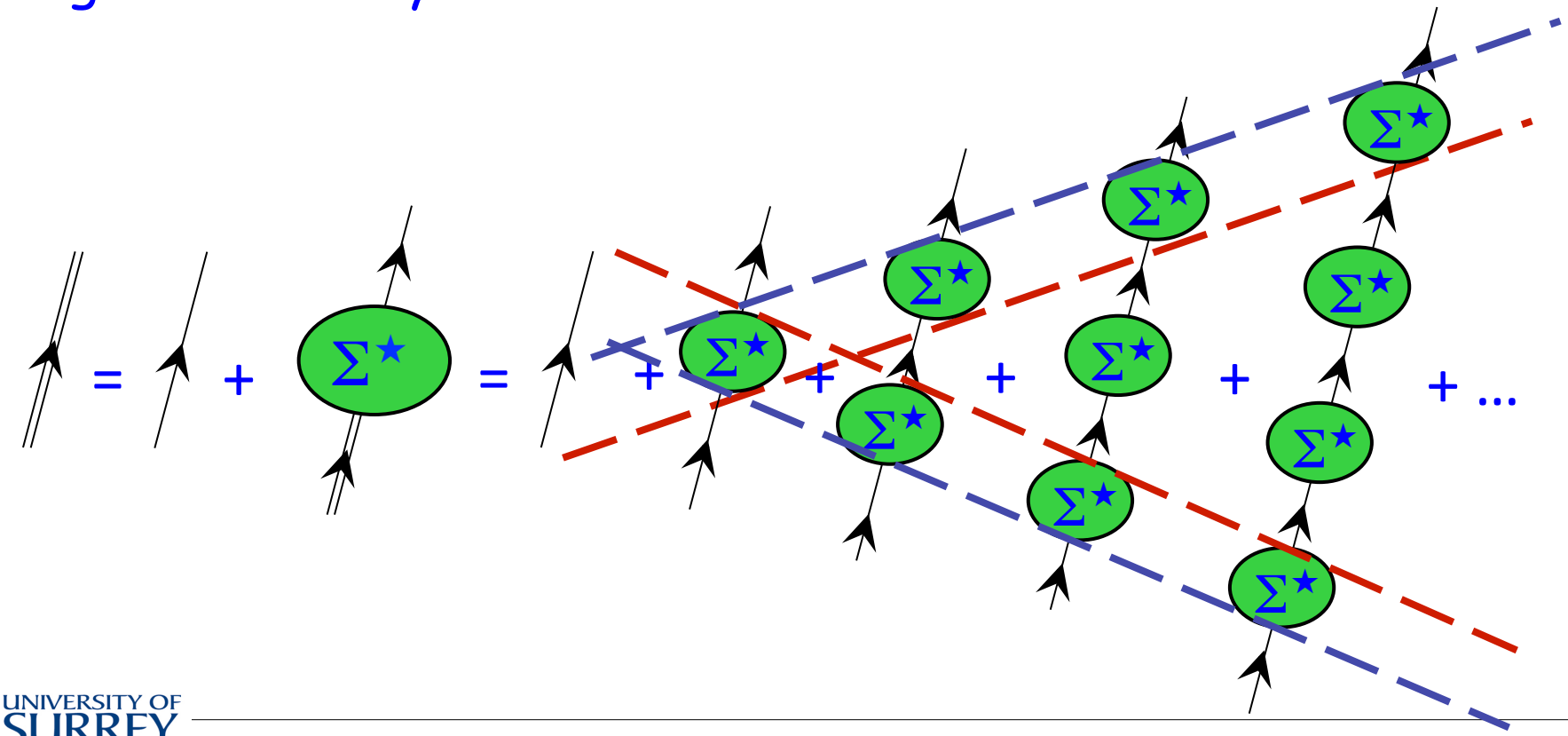


Dyson equation

Dyson equation:

$$g_{\alpha\beta}(t-t') \;=\; g^{(0)}_{\alpha\beta}(t-t') \;+\; g^{(0)}_{\alpha\gamma}(t-t_\gamma)\,\Sigma^{\star}_{\gamma\delta}(t_\gamma,t_\delta)\,g_{\delta\beta}(t_\gamma-t')$$

Diagrammatically:



Dyson equation

The reducible self-energy sums $\Sigma^{\star}_{\alpha\beta}$ to all orders,

$$\Sigma_{\alpha\beta}(t,t') = \Sigma^{\star}_{\alpha\beta}(t,t') + \Sigma^{\star}_{\alpha\gamma}(t,t_\gamma)\, g^{(0)}_{\gamma\delta}(t_\gamma,t_\delta)\, \Sigma_{\delta\beta}(t_\gamma - t')$$

Then:

$$g_{\alpha\beta}(t-t') = g^{(0)}_{\alpha\beta}(t-t') + g^{(0)}_{\alpha\gamma}(t-t_\gamma)\, \Sigma_{\gamma\delta}(t_\gamma,t_\delta)\, g^{(0)}_{\delta\beta}(t_\gamma - t')$$

Conservation laws

There exist two-different forms of the Dyson equation:

$$
\begin{aligned}
g_{\alpha\beta}(t-t') &= g^{(0)}_{\alpha\beta}(t-t') + g^{(0)}_{\alpha\gamma}(t-t_\gamma)\,\Sigma^{A,\star}_{\gamma\delta}(t_\gamma,t_\delta)\,g_{\delta\beta}(t_\gamma-t') \\
\Sigma^{A,\star}_{\alpha\beta}(t,t') &= -u_{\alpha\beta}\delta(t-t') + v_{\alpha\delta,\beta\gamma}\,\rho_{\gamma\delta}\,\delta(t-t') \\
&\quad -(i\hbar)^2\frac{1}{2}v_{\alpha\lambda,\mu\nu}\,g_{\mu\mu'}(t-t_\mu)g_{\nu\nu'}(t-t_\nu) \\
&\quad \times g_{\lambda'\lambda}(t_\lambda-t)\,\Gamma_{\mu'\nu',\beta\lambda'}(t_\mu,t_\nu;t',t_\lambda)
\end{aligned}
$$

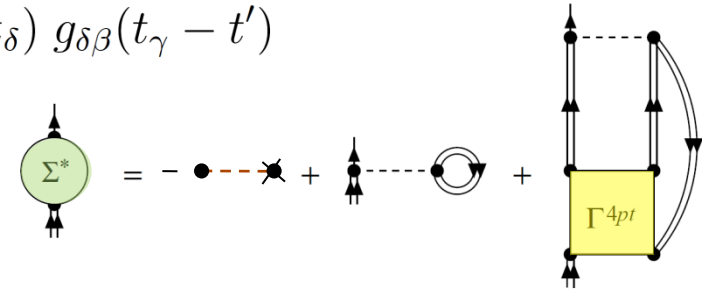
$$
\begin{aligned}
g_{\alpha\beta}(t-t') &= g^{(0)}_{\alpha\beta}(t-t') + g_{\alpha\gamma}(t-t_\gamma)\,\Sigma^{B,\star}_{\gamma\delta}(t_\gamma,t_\delta)\,g^{(0)}_{\delta\beta}(t_\gamma-t') \\
\Sigma^{B,\star}_{\alpha\beta}(t,t') &= -u_{\alpha\beta}\delta(t-t') + v_{\alpha\delta,\beta\gamma}\,\rho_{\gamma\delta}\,\delta(t-t') \\
&\quad -(i\hbar)^2\frac{1}{2}\Gamma_{\alpha\lambda',\mu'\nu'}(t,t_\lambda;t_\mu,t_\nu)\,g_{\lambda\lambda'}(t'-t_\lambda) \\
&\quad \times g_{\mu'\mu}(t_\mu-t')g_{\nu'\nu}(t_\nu-t')\,v_{\mu\nu,\beta\lambda}
\end{aligned}
$$

➔ One usually chooses an approximation for Γ and then builds an approximation of $\Sigma^{\star}_{\alpha\beta}$!!!!

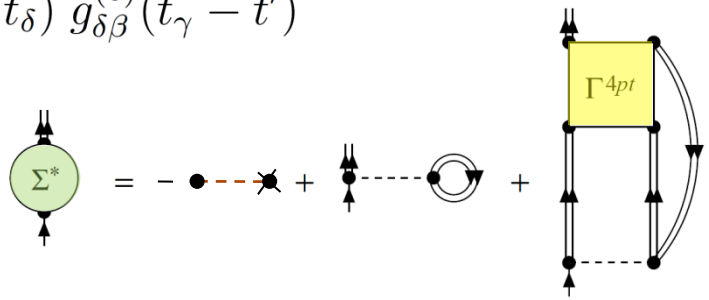
Conservation laws

There exist two-different forms of the Dyson equation:

$$g_{\alpha\beta}(t-t') \;=\; g^{(0)}_{\alpha\beta}(t-t') \;+\; g^{(0)}_{\alpha\gamma}(t-t_\gamma)\,\Sigma^{A,\star}_{\gamma\delta}(t_\gamma,t_\delta)\,g_{\delta\beta}(t_\gamma-t')$$



$$g_{\alpha\beta}(t-t') \;=\; g^{(0)}_{\alpha\beta}(t-t') \;+\; g_{\alpha\gamma}(t-t_\gamma)\,\Sigma^{B,\star}_{\gamma\delta}(t_\gamma,t_\delta)\,g^{(0)}_{\delta\beta}(t_\gamma-t')$$



➔ One usually chooses an approximation for Γ and then builds an approximation of $\Sigma^{\star}_{\alpha\beta}$!!!!

Conservation laws

Theorem (Baym, Kadanoff 1961):

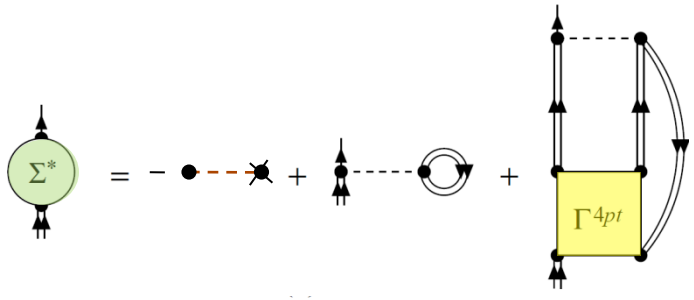
Assume that the propagator $g_{\alpha\beta}(t-t')$ solves both forms of the Dyson equation (that means $\Sigma^{A,\star}_{\alpha\beta} = \Sigma^{B,\star}_{\alpha\beta}$) and $\Gamma_{\alpha\beta,\gamma\delta} = \Gamma_{\beta\alpha,\delta\gamma}$. Then <N>, <P>, <L> and <E> calculated with $g_{\alpha\beta}(t-t')$ are all conserved:

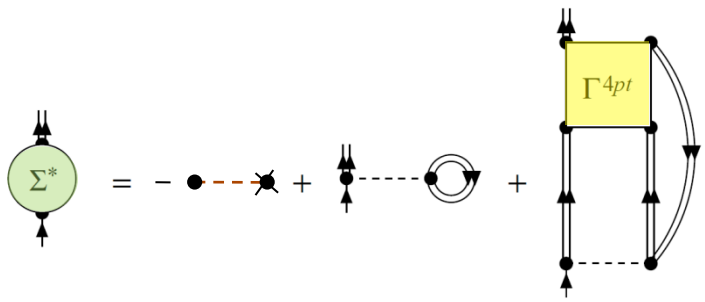
$$\frac{d\langle N(t)\rangle}{dt} = 0 \qquad \frac{d\langle \mathbf{P}(t)\rangle}{dt} = 0 \qquad \frac{d\langle \mathbf{J}(t)\rangle}{dt} = 0 \qquad \frac{d\langle E(t)\rangle}{dt} = 0$$

[G. Baym and L. P. Kadanoff, Phys. Rev. 124, 287 (1961);

Dyson equation

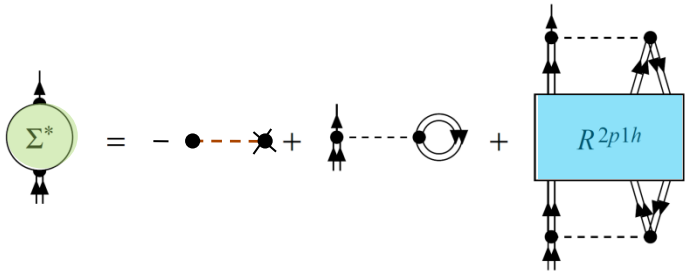
Different forms for the self-energy





← if $\Gamma^{4\text{-pt}}$ is approximated in such a way that these two are equivalent, then conservation laws are fulfilled.

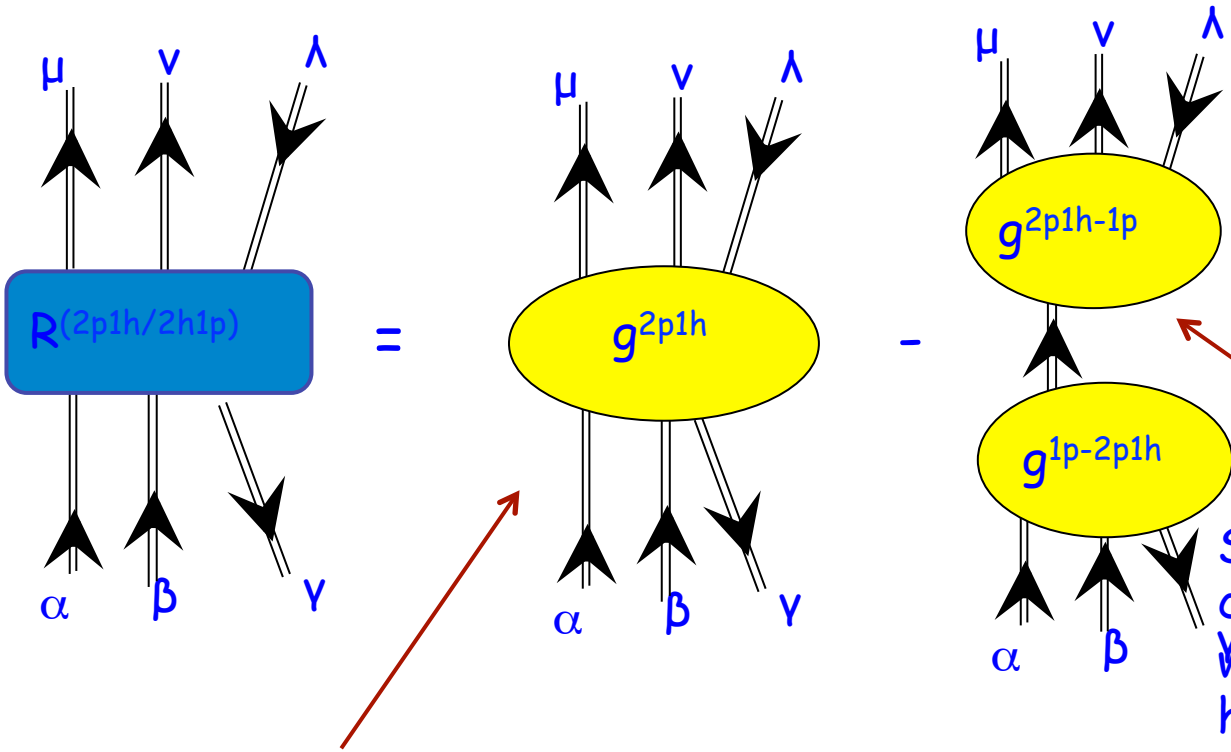
←The exact $\Gamma^{4\text{-pt}}$ depends of 4 times variables



← R^{2p1h} is specialized to two-times only!

Irreducible 2p1h/2h1p propagator

Graphic representation of the 2p1h/2h1p irreducible propagator R(ω):



Propagation of 3 excitations

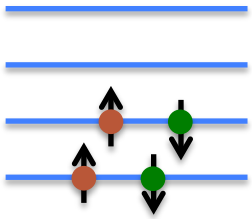
Subtract the contribution in which a particle-hole anihilate each other → The Dyson equation will account for it!

Application to the paring model:

In order to make sense of the equation written so far, we will start solving the Dyson Eq. for our pairing model.

To do this, we will exploit perturbation theory to calculate the self-energy. Thus, we start from our unperturbed solution for the ground state:

$$|\Phi_0\rangle \equiv |$$



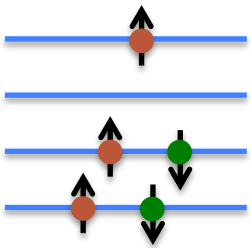
$$\rangle = \hat{P}^{\dagger}_{p=1}\,\hat{P}^{\dagger}_{p=0}|0\rangle$$

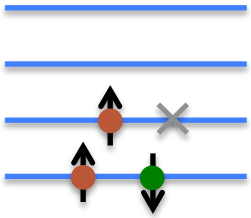
…starting from here, we will develop the static and dynamic contributions to the self-energy. For now we will to the first at 1st order and the latter at 2nd order.

Green's function theory is a prticle attached/particle removed theory, so we will be looking at 3-body and 5-body states. This means that the total spin of the intermediate states |A-1> and |A+1> is non zero and there will be one unpaired particle. We will only look at cases when *all other nucleons are paired*.

Application to the paring model:

To calculate **<u>the self energy at first order</u>** in perturbations theory we can simple take the expectation value among the :

$$|\Phi^a;\uparrow\rangle \equiv |$$  $$\rangle = a^\dagger_{a\uparrow}|\Phi_0\rangle = a^\dagger_{a\uparrow}\hat{P}^\dagger_1\,\hat{P}^\dagger_0|0\rangle$$

$$|\Phi^j;\uparrow\rangle \equiv |$$  $$\rangle = a_{j\downarrow}|\Phi_0\rangle = a_{j\downarrow}\hat{P}^\dagger_1\,\hat{P}^\dagger_0|0\rangle$$

The 1st order self-energy $\Sigma^{(1)}_{\alpha\,\beta}$ (with $\alpha = i, j, k, \ldots, a, b, \ldots = 0\uparrow,\ 0\downarrow,\ 1\uparrow,\ 1\downarrow,\ 2\uparrow, \ldots$) is simply the perturbing interaction H_1:

$$\Sigma^{(1)}_{a\,b} = \langle\Phi^a; S_z|H_1|\Phi^b; S'_z\rangle\ ,$$

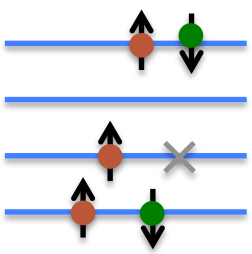
$$\Sigma^{(1)}_{a\,j} = \langle\Phi^a; S_z|H_1|\Phi^j; S'_z\rangle\ ,$$ etc....

Application to the paring model:

The $\Sigma^{(1)}_{\alpha\,\beta}$ is **static**, i.e. **energy independent**. It will have other contributions at higher orders in perturbation theory. But we don't worry about this because we can calculate the exact one (i.e. no PT at all). We will see this later, for now let's just stick to $\Sigma^{(1)}_{\alpha\,\beta}$ here, which is the first contribution. This is good enough for now.

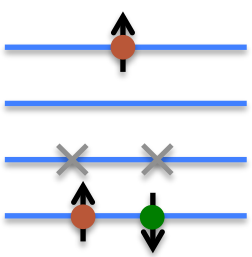
At **second order**, the interaction H1 can create/annihilate additional extra pairs, leading to an **energy dependent** contribution to the self energy. For this we will need 2p1h/2h1pintermediate states as follows:

$$|\Phi_i^{ab};\uparrow\rangle \equiv |$$



$$\rangle = a_i a_a^\dagger a_b^\dagger |\Phi_0\rangle = a_{i\downarrow} \hat{P}^\dagger_{a=b}\, \hat{P}^\dagger_1\, \hat{P}^\dagger_0 |0\rangle$$

$$|\Phi_{ij}^{a}\uparrow\rangle \equiv |$$



$$\rangle = a_a^\dagger a_i a_j |\Phi_0\rangle = a^\dagger_{a\uparrow} \hat{P}_{i=j}\, \hat{P}^\dagger_1\, \hat{P}^\dagger_0 |0\rangle$$

Application to the paring model:

The **energy dependent second order self-energy** is then as follows as follows:

$$\Sigma^{(2)}_{\alpha\beta}(\omega) = \sum_{a\,b\,i} \langle \Phi^{\alpha} | H_1 | \Phi^{ab}_{i} \rangle \frac{1}{\omega - (\varepsilon^{(0)+}_{a} + \varepsilon^{(0)+}_{b} - \varepsilon^{(0)-}_{j}) + i\eta} \langle \Phi^{ab}_{i} | H_1 | \Phi^{\beta} \rangle$$

$$+ \sum_{a\,i\,j} \langle \Phi^{\alpha} | H_1 | \Phi^{a}_{ij} \rangle \frac{1}{\omega - (\varepsilon^{(0)-}_{i} + \varepsilon^{(0)-}_{j} - \varepsilon^{(0)+}_{a}) - i\eta} \langle \Phi^{a}_{ij} | H_1 | \Phi^{\beta} \rangle$$

The above equations define a first approximation of the self energy:

$$\Sigma^{\star}_{\alpha\beta}(\omega) = \Sigma^{(1)}_{\alpha\beta} + \Sigma^{(2)}_{\alpha\beta}(\omega)$$

The dyson equation in energy domain is then written as follows (with implicit summations):

$$g_{\alpha\beta}(\omega) = g^{(0)}_{\alpha\beta}(\omega) \; + g^{(0)}_{\alpha\gamma}(\omega) \; \Sigma^{\star}_{\gamma\delta}(\omega) \; g_{\delta\beta}(\omega)$$

Gorkov equations

[V. Somà, T. Duguet, CB, Pys. Rev. C84, 046317 (2011)]

$$\sum_b \begin{pmatrix} t_{ab} - \mu_{ab} + \Sigma^{11}_{ab}(\omega) & \Sigma^{12}_{ab}(\omega) \\ \Sigma^{21}_{ab}(\omega) & -t_{ab} + \mu_{ab} + \Sigma^{22}_{ab}(\omega) \end{pmatrix}\Bigg|_{\omega_k} \begin{pmatrix} \mathcal{U}^k_b \\ \mathcal{V}^k_b \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k_a \\ \mathcal{V}^k_a \end{pmatrix}$$

$$\Downarrow$$

$$\boxed{\begin{pmatrix} T - \mu + \Lambda & \tilde{h} & \mathcal{C} & -\mathcal{D}^\dagger \\ \tilde{h}^\dagger & -T + \mu - \Lambda & -\mathcal{D}^\dagger & \mathcal{C} \\ \mathcal{C}^\dagger & -\mathcal{D} & E & 0 \\ -\mathcal{D} & \mathcal{C}^\dagger & 0 & -E \end{pmatrix} \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix}}$$

Energy *independent* eigenvalue problem

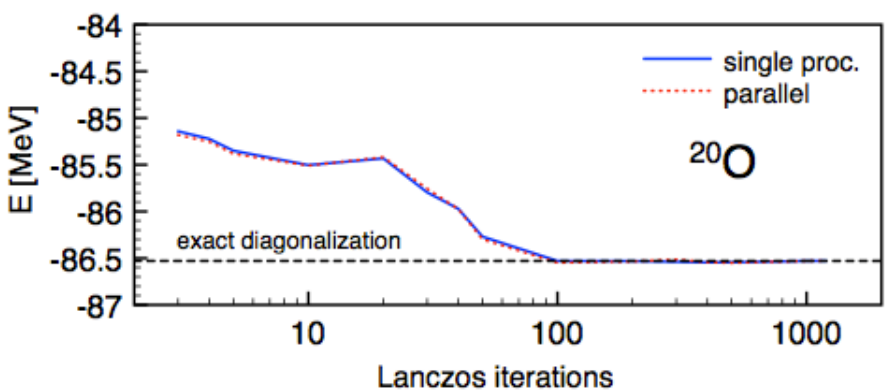
with the normalization condition $\sum_a \left[\left|\mathcal{U}^k_a\right|^2 + \left|\mathcal{V}^k_a\right|^2 \right] + \sum_{k_1 k_2 k_3} \left[\left|\mathcal{W}^{k_1 k_2 k_3}_k\right|^2 + \left|\mathcal{Z}^{k_1 k_2 k_3}_k\right|^2 \right] = 1$

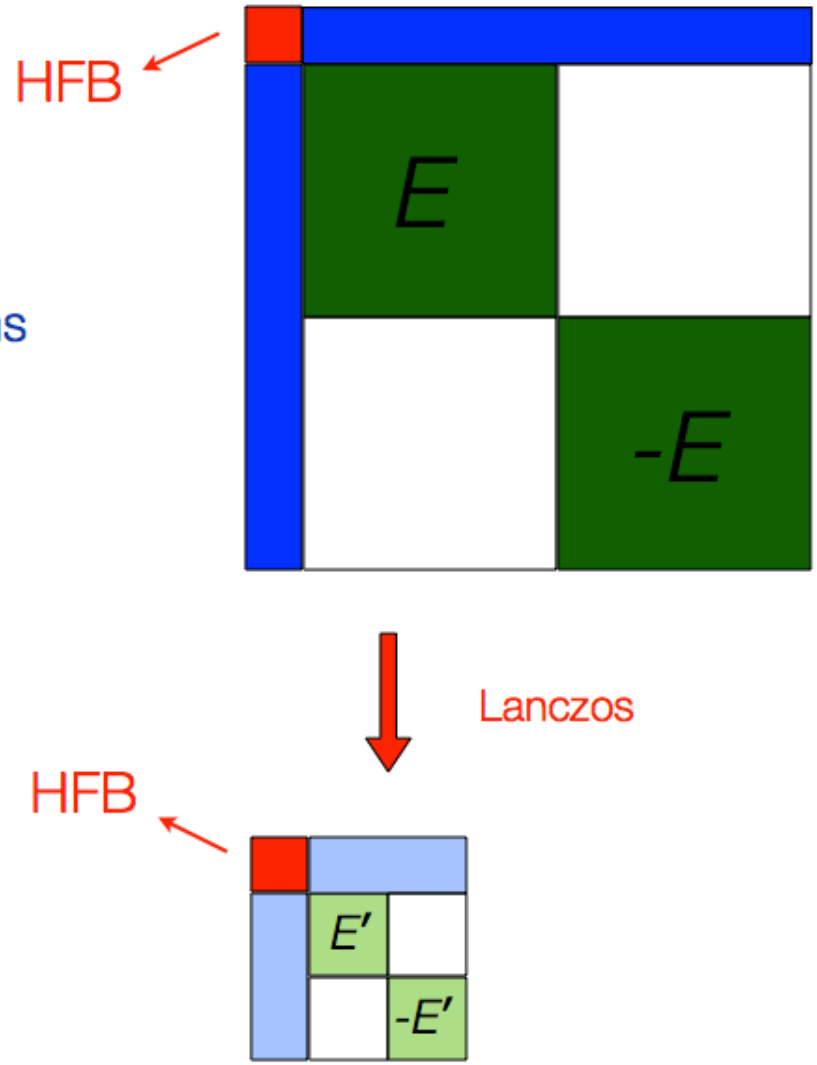
Lanczos reduction of self-energy

V. Somà, CB, T. Duguet, , Phys. Rev. C **89**, 024323 (2014)

$$\begin{pmatrix} T-\mu+\Lambda & \tilde{h} & \mathcal{C} & -\mathcal{D}^\dagger \\ \tilde{h}^\dagger & -T+\mu-\Lambda & -\mathcal{D}^\dagger & \mathcal{C} \\ \mathcal{C}^\dagger & -\mathcal{D} & E & 0 \\ -\mathcal{D} & \mathcal{C}^\dagger & 0 & -E \end{pmatrix} \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix}$$

- Conserves moments of spectral functions
- Equivalent to exact diagonalization for $N_L \rightarrow$ dim(E)





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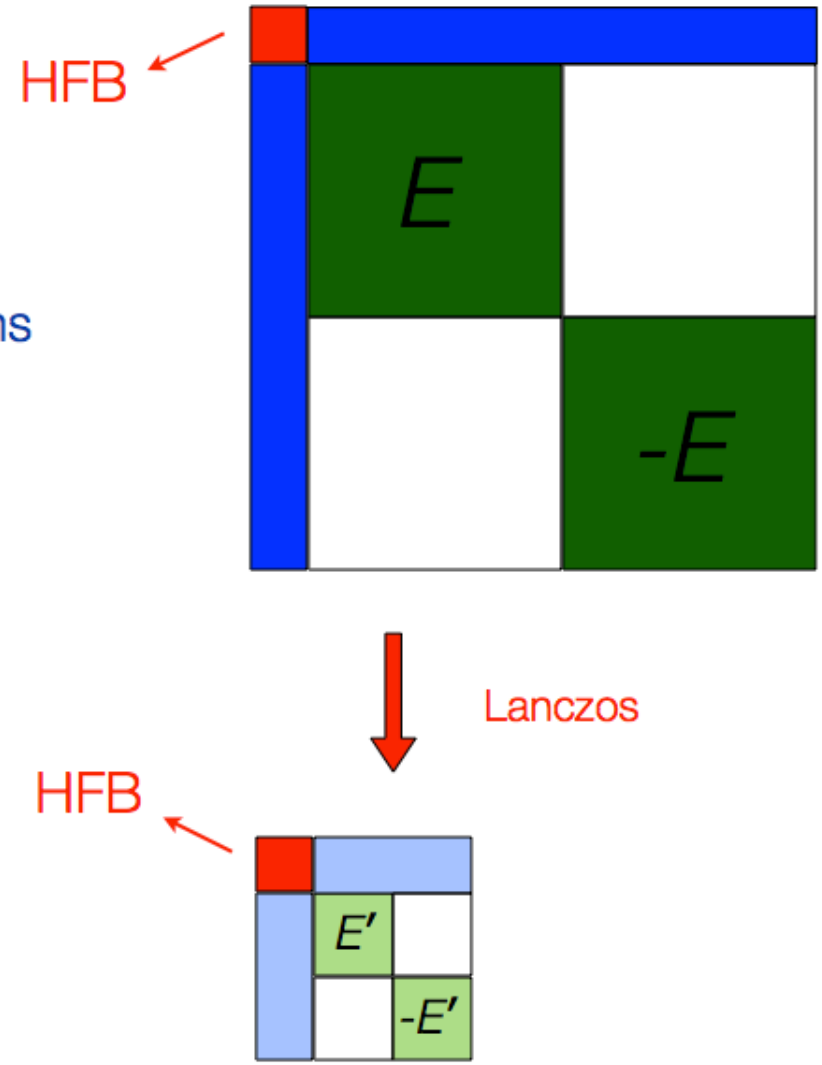
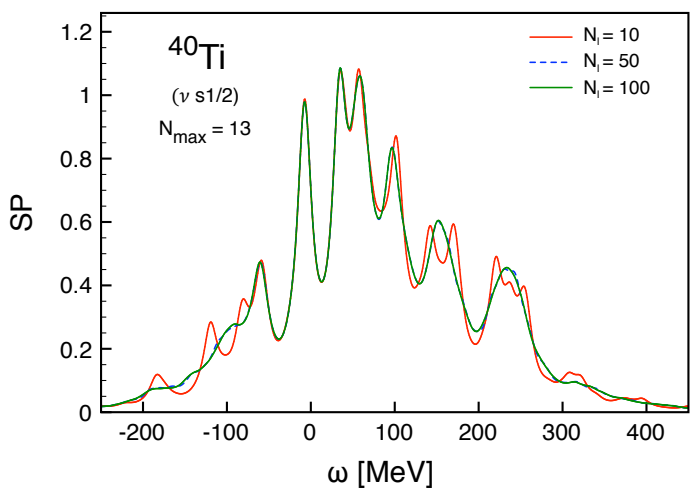


Spectral strength

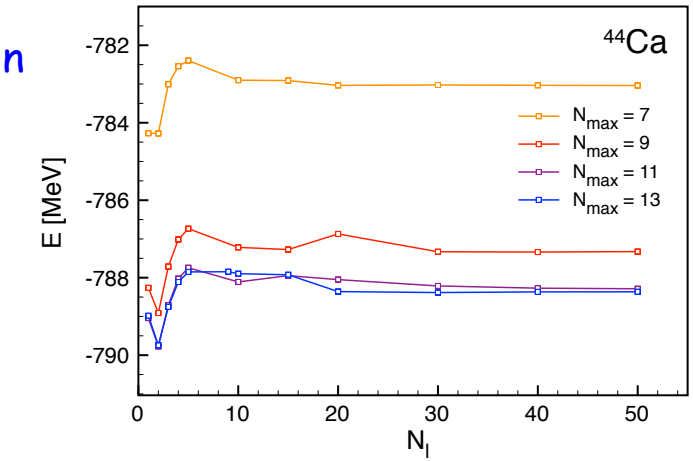


Testing Krylov projection

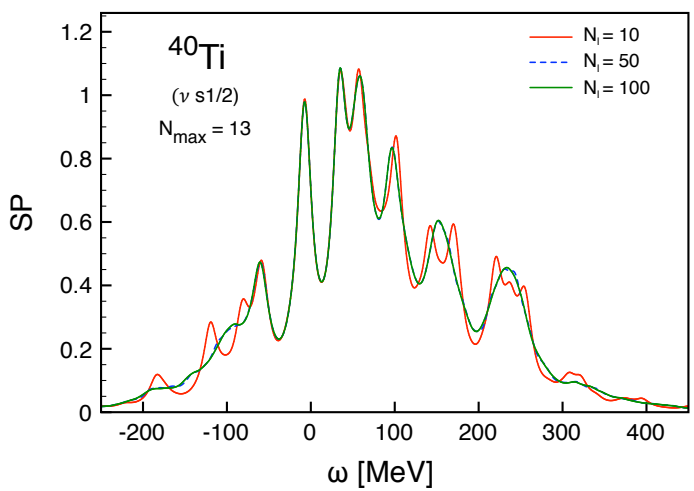
V. Somà, CB, T. Duguet, , Phys. Rev. C **89**, 024323 (2014)

- Energy and spectra independent of the projection
- Same behavior for all model spaces

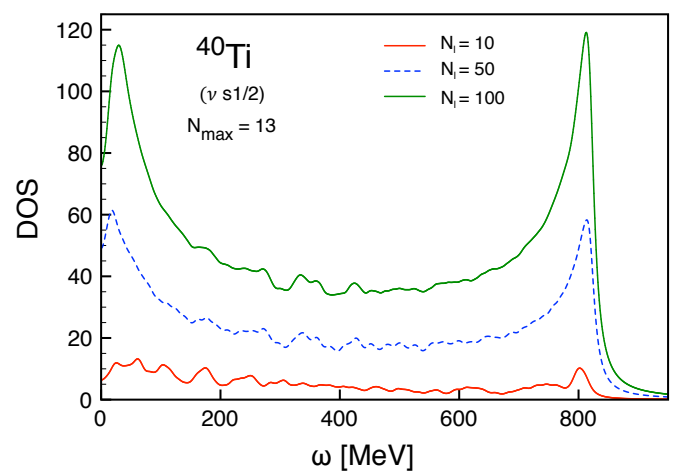
Favourable scaling



Spectral strength



Deinsity of states



Gorkov Green's functions and equations

[V. Somà, T. Duguet, CB, Pys. Rev. C84, 046317 (2011)]

✺ Set of 4 Green's functions

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

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

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

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

[Gorkov 1958]

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

Gorkov equations

$$\mathbf{\Sigma}^\star_{ab}(\omega) \equiv \begin{pmatrix} \Sigma^{\star\,11}_{ab}(\omega) & \Sigma^{\star\,12}_{ab}(\omega) \\ \Sigma^{\star\,21}_{ab}(\omega) & \Sigma^{\star\,22}_{ab}(\omega) \end{pmatrix}$$

$$\mathbf{\Sigma}^\star_{ab}(\omega) \equiv \mathbf{\Sigma}_{ab}(\omega) - \mathbf{U}_{ab}$$

Espressions for 1st & 2nd order diagrams

[V. Somà, T. Duguet, CB, Phys. Rev. C84, 046317 (2011)]

Gorkov equations

[V. Somà, T. Duguet, CB, Pys. Rev. C84, 046317 (2011)]

$$\sum_b \begin{pmatrix} t_{ab} - \mu_{ab} + \Sigma^{11}_{ab}(\omega) & \Sigma^{12}_{ab}(\omega) \\ \Sigma^{21}_{ab}(\omega) & -t_{ab} + \mu_{ab} + \Sigma^{22}_{ab}(\omega) \end{pmatrix}\Bigg|_{\omega_k} \begin{pmatrix} \mathcal{U}^k_b \\ \mathcal{V}^k_b \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k_a \\ \mathcal{V}^k_a \end{pmatrix}$$

$$\Downarrow$$

$$\boxed{\begin{pmatrix} T - \mu + \Lambda & \tilde{h} & \mathcal{C} & -\mathcal{D}^\dagger \\ \tilde{h}^\dagger & -T + \mu - \Lambda & -\mathcal{D}^\dagger & \mathcal{C} \\ \mathcal{C}^\dagger & -\mathcal{D} & E & 0 \\ -\mathcal{D} & \mathcal{C}^\dagger & 0 & -E \end{pmatrix} \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix} = \omega_k \begin{pmatrix} \mathcal{U}^k \\ \mathcal{V}^k \\ \mathcal{W}_k \\ \mathcal{Z}_k \end{pmatrix}}$$

Energy *independent* eigenvalue problem

with the normalization condition $\sum_a \left[\left|\mathcal{U}^k_a\right|^2 + \left|\mathcal{V}^k_a\right|^2 \right] + \sum_{k_1 k_2 k_3} \left[\left|\mathcal{W}^{k_1 k_2 k_3}_k\right|^2 + \left|\mathcal{Z}^{k_1 k_2 k_3}_k\right|^2 \right] = 1$