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

Self-consistent Green's function in Finite Nuclei and related things…
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Lecture II

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:

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

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

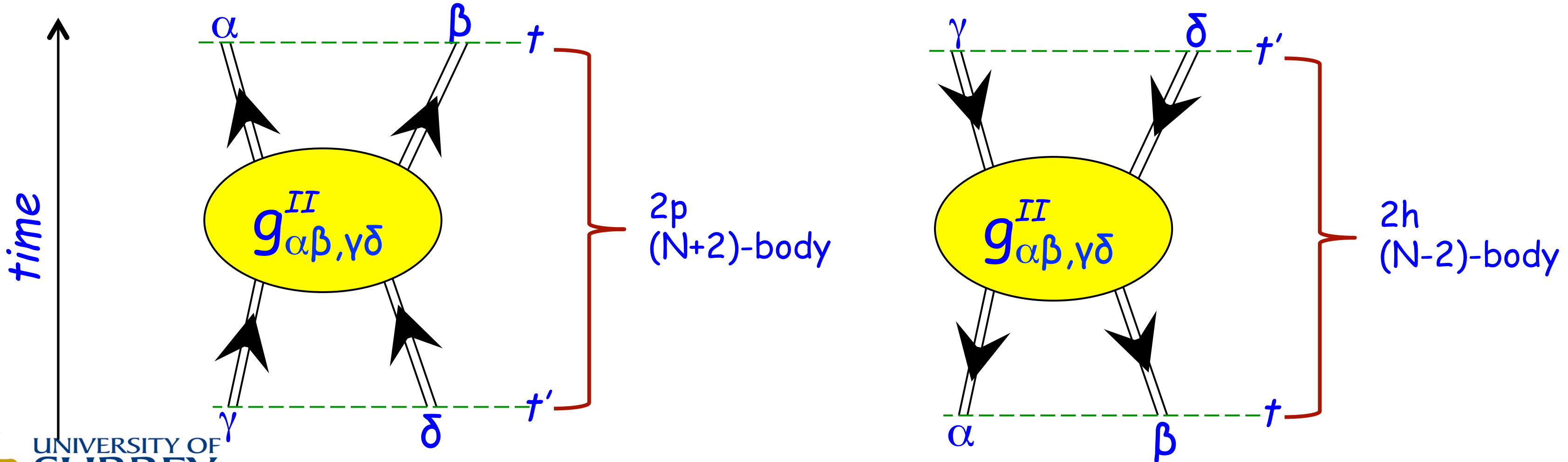
Two-particle/two-hole propagator

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

$$g^{4-pt}_{\alpha\beta,\gamma\delta}(t_1,t_2;t'_1,t'_2) = -\frac{i}{\hbar}\langle\Psi^N_0|T[c_\beta(t_2)c_\alpha(t_1)c^\dagger_\gamma(t'_1)c^\dagger_\delta(t'_2)]|\Psi^N_0\rangle$$

Define the two-particle/two-hole propagator:

$$g^{II}_{\alpha\beta,\gamma\delta}(t,t') = -\frac{i}{\hbar}\langle\Psi^N_0|T[c_\beta(t)c_\alpha(t)c^\dagger_\gamma(t')c^\dagger_\delta(t')]|\Psi^N_0\rangle$$



Two-particle/two-hole propagator

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

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

$$- \sum_k \frac{\langle\Psi_0^N|c^\dagger_\gamma c^\dagger_\delta|\Psi_k^{N-2}\rangle\ \langle\Psi_k^{N-2}|c_\beta c_\alpha|\Psi_0^N\rangle}{\omega-\left(E_0^N-E_k^{N-2}\right)-i\eta}$$ ← *two-holes (g^{hh})*

$$S^{pp}_{\alpha\beta,\gamma\delta}(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\ g^{pp}_{\alpha\beta,\gamma\delta}(\omega)$$

$$= \sum_n \langle\Psi_0^N|c_\beta c_\alpha|\Psi_n^{N+2}\rangle\langle\Psi_n^{N+2}|c^\dagger_\gamma c^\dagger_\delta|\Psi_0^N\rangle\ \delta\left(\hbar\omega-(E_n^{N+2}-E_0^N)\right)$$

$$S^{hh}_{\alpha\beta,\gamma\delta}(\omega) = \frac{1}{\pi}\,\mathrm{Im}\ g^{hh}_{\alpha\beta,\gamma\delta}(\omega)$$

$$= -\sum_k \langle\Psi_0^N|c^\dagger_\gamma c^\dagger_\delta|\Psi_k^{N-2}\rangle\langle\Psi_k^{N-2}|c_\beta c_\alpha|\Psi_0^N\rangle\ \delta\left(\hbar\omega-(E_0^N-E_k^{N-2})\right)$$

Expectation values

Hence—for *2-body* matrix elements:

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

$$\begin{aligned} \langle \Psi_0^N | V | \Psi_0^N \rangle &= -\sum_{\alpha\beta\gamma\delta} \int d\omega v_{\alpha\beta,\gamma\delta} S^{hh}_{\gamma\delta,\alpha\beta}(\omega) \\ &= +i\hbar \lim_{t' \to t^+} \sum_{\alpha\beta} v_{\alpha\beta,\gamma\delta} g^{II}_{\gamma\delta,\alpha\beta}(t,t') \end{aligned}$$

"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 properly antisymmetrized matrix elements)

Second quantization excercise

Use $i\hbar \frac{d a(t)}{dt} = [a, H]$ 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:

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

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

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

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

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

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

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

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

- or

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

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:

$\langle \Phi_k^{N-1} | c_\alpha | \Phi_0^N \rangle$ = 1 for α in $|\Phi_0^N\rangle$; 0 for α not in $|\Phi_0^N\rangle$

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

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:

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

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

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

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

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

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

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

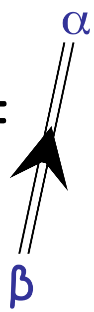
$$g_{\alpha\beta}(t-t') \;\;=\;\; g_{\alpha\beta}^{(0)}(t-t') \;-\; \sum_{\gamma\delta} \int dt_\gamma \; g_{\alpha\gamma}^{(0)}(t-t_\gamma)\; u_{\gamma\delta}\; g_{\delta\beta}(t_\gamma - t')$$

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

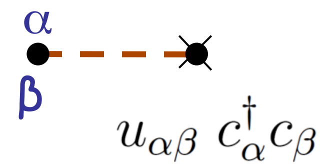
Equation of motion for $g_{\alpha\beta}$

Feynman diagram conventions:

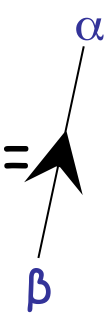
$g_{\alpha\beta}(t-t') =$



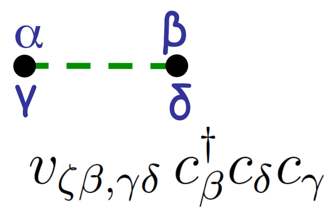
$u_{\alpha\beta},\ t_{\alpha\beta} =$



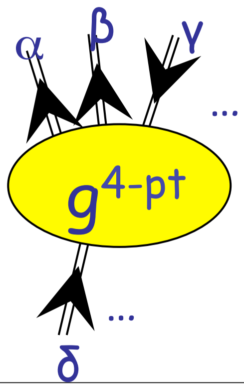
$g^{(0)}{}_{\alpha\beta}(t-t') =$



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



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



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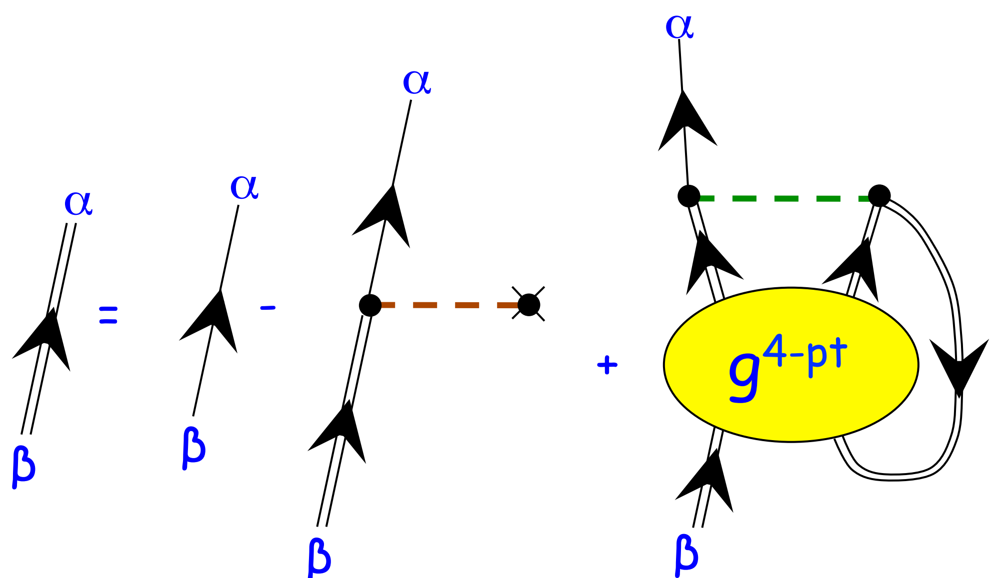
Equation of motion for $g_{\alpha\beta}$

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 equations!

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,

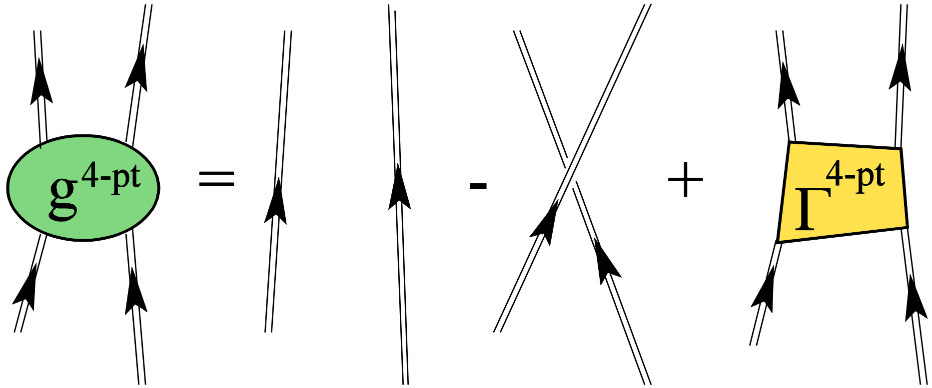
$$g^{(0)\,4-pt}_{\alpha\beta,\gamma\delta}(t_\alpha,t_\beta;t_\gamma,t_\delta) = -\frac{i}{\hbar}\langle\Phi_0^N|T[c_\beta(t_\beta)c_\alpha(t_\alpha)c^\dagger_\gamma(t_\gamma)c^\dagger_\delta(t_\delta)]|\Phi_0^N\rangle$$

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

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

$$= \quad v_{\gamma\lambda,\mu\nu}\,(-i\hbar)g_{\nu\lambda}(t,t^+)\;g_{\mu\beta}(t^-,t')$$

$$= \quad v_{\gamma\lambda,\mu\nu}\;\rho_{\nu\lambda}\,g_{\mu\beta}(t^-,t')$$

→
$$\Sigma^{HF}_{\alpha\beta} = \sum_{\mu\nu} v_{\alpha\mu,\beta\nu}\rho_{\nu\mu}$$
$$= \sum_{\mu\nu} v_{\alpha\mu,\beta\nu}\langle\Phi_0^N|c^\dagger_\mu c_\nu|\Psi_0^N\rangle$$

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

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

Dyson equation

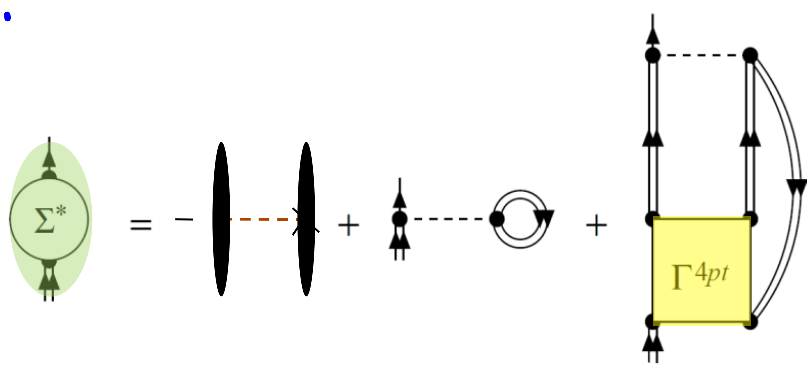
Dyson equation:

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

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:

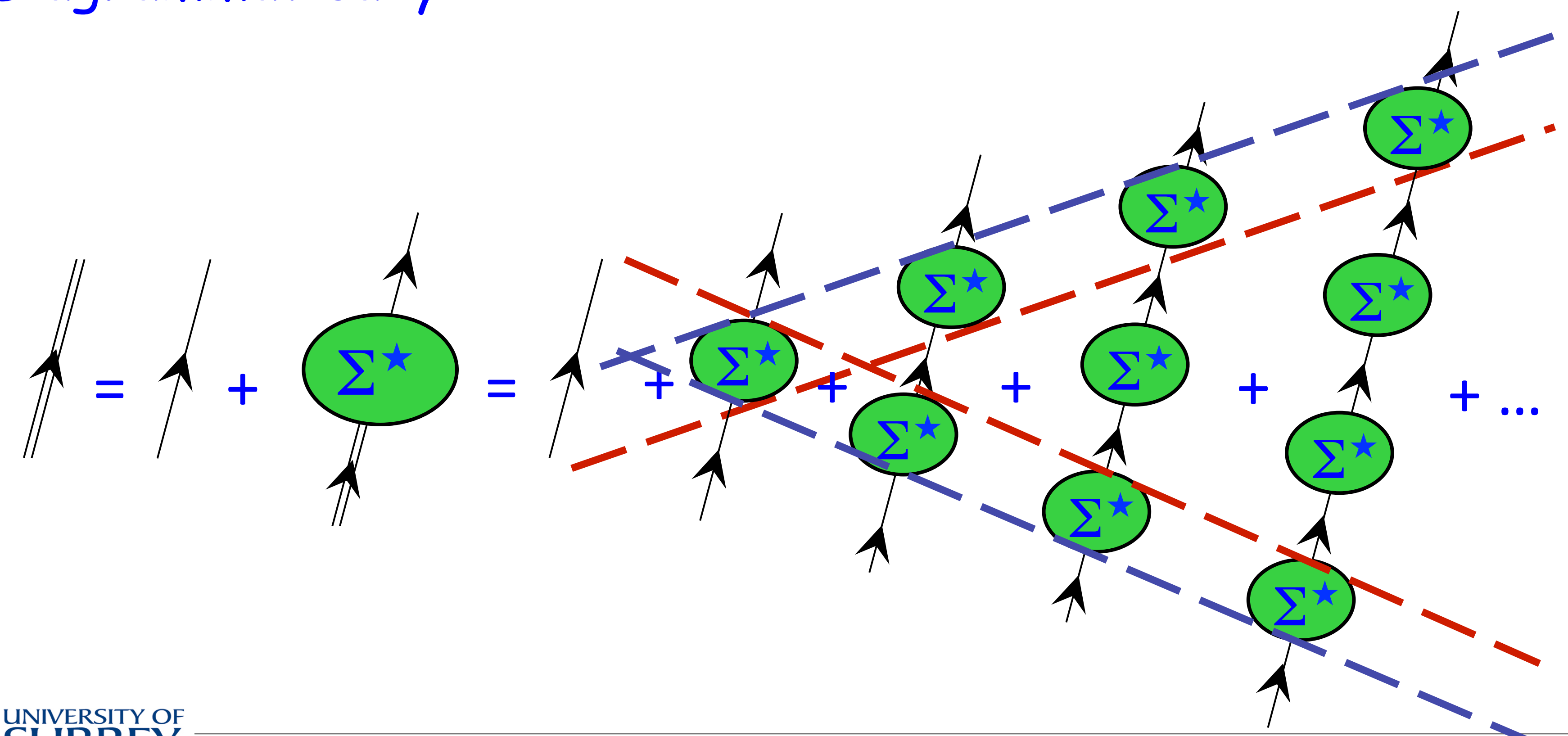


Dyson equation

Dyson equation:

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

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:

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

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

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

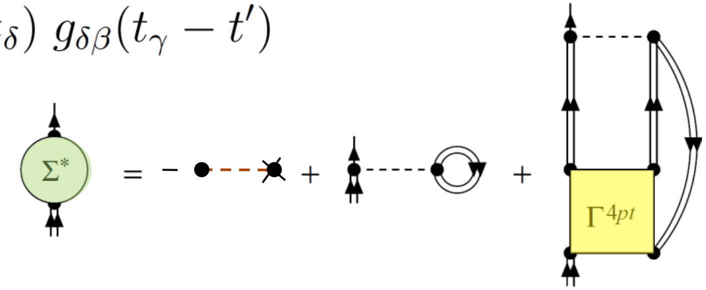
$$\begin{aligned}\Sigma^{B,\star}_{\alpha\beta}(t,t') = &-u_{\alpha\beta}\delta(t-t') + v_{\alpha\delta,\beta\gamma}\,\rho_{\gamma\delta}\,\delta(t-t')\\ &-(i\hbar)^2\frac{1}{2}\Gamma_{\alpha\lambda',\mu'\nu'}(t,t_\lambda;t_\mu,t_\nu)\,g_{\lambda\lambda'}(t'-t_\lambda)\\ &\times g_{\mu'\mu}(t_\mu-t')g_{\nu'\nu}(t_\nu-t')\,v_{\mu\nu,\beta\lambda}\end{aligned}$$

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

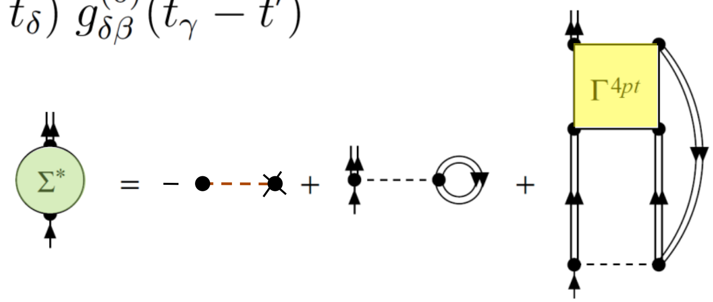
Conservation laws

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):

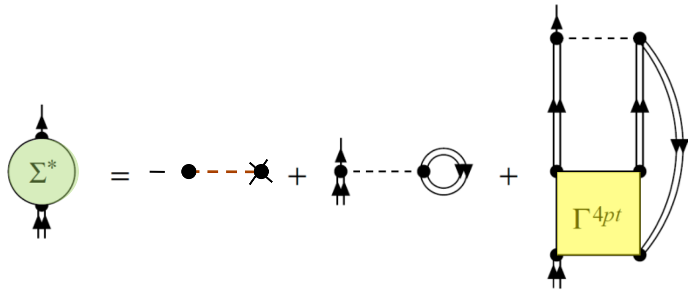
Assume that the propagator $g_{\alpha\beta}(t-t')$ solves both forms of the Dyson equation (that means $\Sigma^{A,\star}_{\alpha\beta} = \Sigma^{B,\star}_{\alpha\beta}$) and $\Gamma_{\alpha\beta,\gamma\delta} = \Gamma_{\beta\alpha,\delta\gamma}$. Then <N>, <P>, <L> and <E> calculated with $g_{\alpha\beta}(t-t')$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

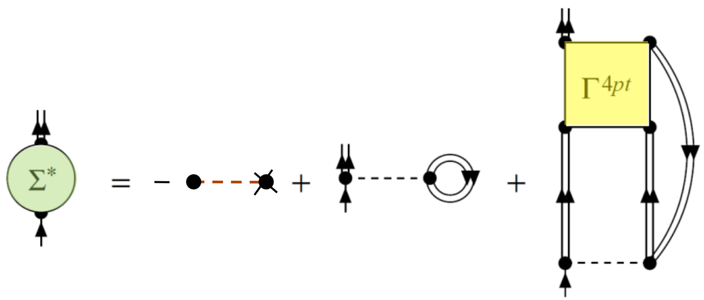
$$\frac{d\langle N(t)\rangle}{dt} = 0 \qquad \frac{d\langle \mathbf{P}(t)\rangle}{dt} = 0 \qquad \frac{d\langle \mathbf{J}(t)\rangle}{dt} = 0 \qquad \frac{d\langle E(t)\rangle}{dt} = 0$$

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

Dyson equation

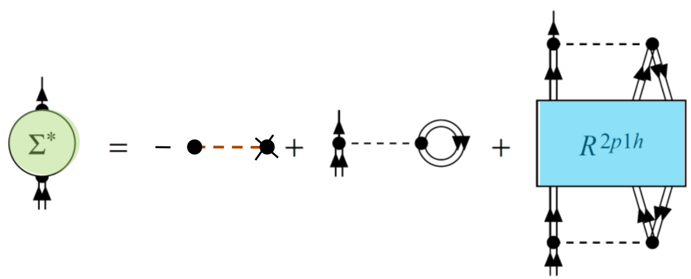
Different forms for the self-energy





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

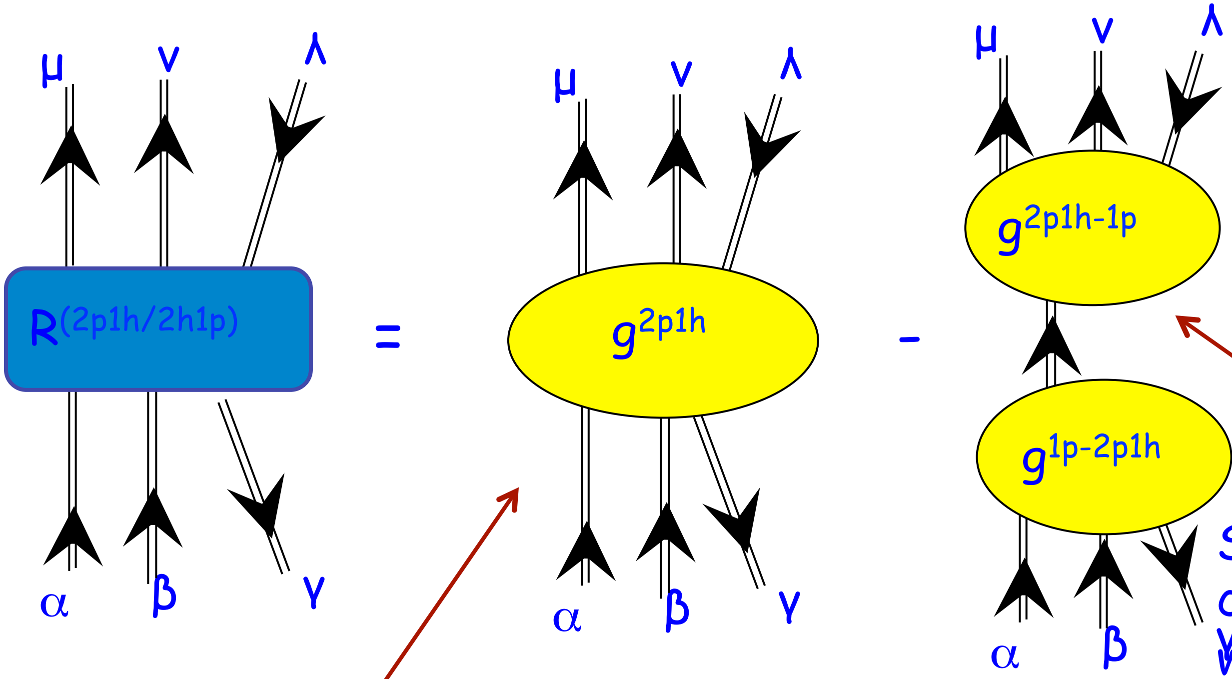
←The exact $\Gamma^{4\text{-pt}}$ depends of 4 times variables



← 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!