An brief introduction to Green’s functions

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AUSSOIS

The many-body problem

- Many-body Schrödinger equation

$$\hat{H}\Psi(\mathbf{r}_1, ..., \mathbf{r}_N) = E\Psi(\mathbf{r}_1, ..., \mathbf{r}_N)$$

$$\hat{H} = -\frac{1}{2}\sum_i \nabla_i^2 + \frac{1}{2}\sum_{i\neq j}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_i v(\mathbf{r}_i)$$

(NB: Born-Oppenheimer approximation)

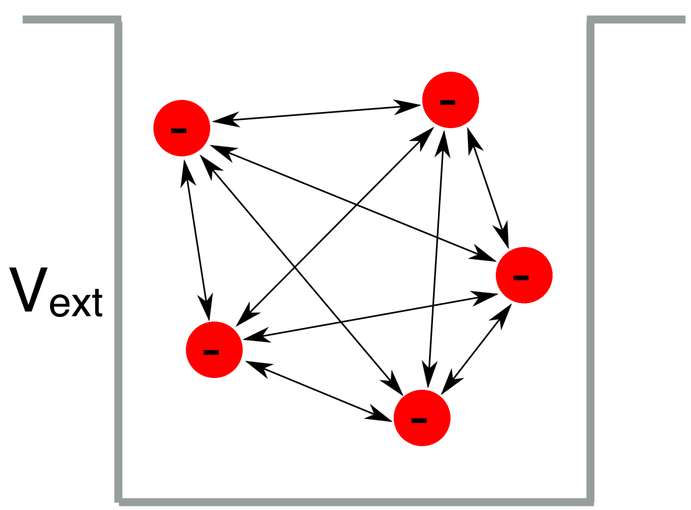
- Many-body wavefunction and observables

$$\Psi(\mathbf{r}_1, ..., \mathbf{r}_N) \longrightarrow \langle\Psi|\,\hat{O}\,|\Psi\rangle$$

Theoretical Background

- **Wave-function based approaches**

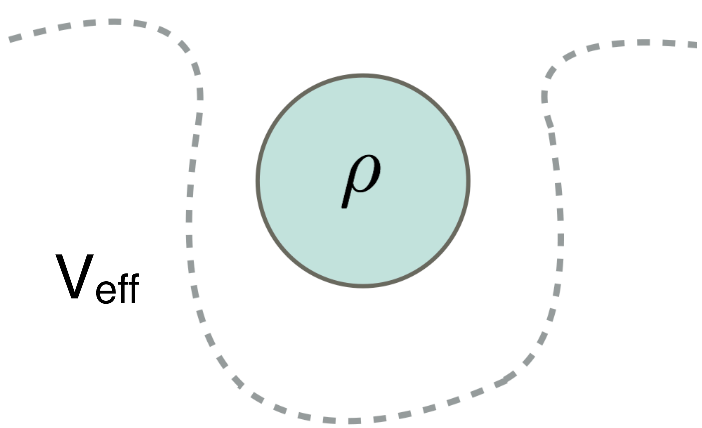
Key quantity: many-body wavefunction



Observable $= \langle \Psi | \hat{O} | \Psi \rangle$

- **Reduced quantity based approaches**

Key quantity: Simpler physical quantity, e.g. the density

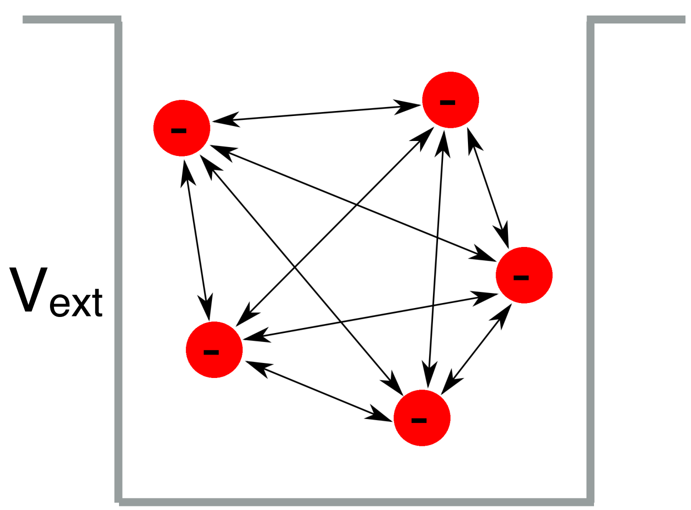


Observable $= \mathrm{F}[\rho]$

Theoretical Background

- **Wave-function based approaches**
- **Reduced quantity based approaches**

Key quantity: many-body wavefunction



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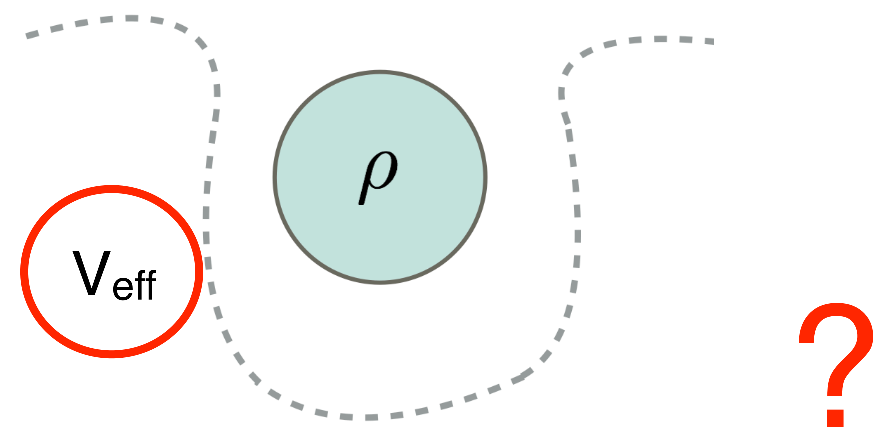

Observable $= \mathrm{F}[\rho]$

Theoretical Background

- **Reduced quantities**

density	$\rho(\mathbf{r})$	Density Functional Theory
current-density	$\mathbf{j}(\mathbf{r})$	Current-Density Functional Theory
1-body density matrix	$\gamma(\mathbf{r},\mathbf{r}')$	Reduced Density Matrix Functional Theory
1-body Green's function	$G(\mathbf{x},\mathbf{x}';\omega)$	Many-Body Perturbation theory

…

Theoretical Background

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Program of the lecture

- GFs in maths
- GFs in physics
- GFs in quantum mechanics
- 1-GF: Dyson equation and self-energy
- 2-GF
- Higher-order GF

Mr George Green

- British Mathematician and Physicist
- An Essay on the Application of Mathematical Analysis to the Theories of Electricity and Magnetism (Green, 1828)
- One year of formal schooling as a child, between the ages of 8 and 9

England, 1793-1841

Memorial stone in Westminster Abbey

Green's mill in Sneinton

Figures from Wikipedia

Green's functions in maths : solving differential equations

differential equation $\hat{D}_x f(x) = F(x)$

$\hat{D}_x$ is a differential operator, e.g. $d^2/dt^2 + c$

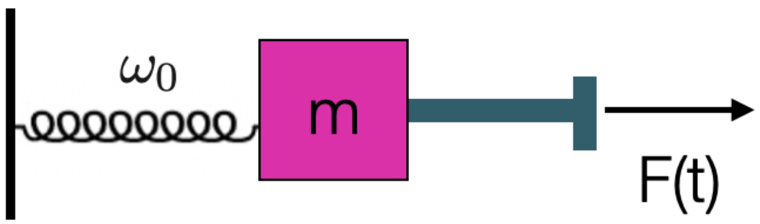
$F(x)$ is the inhomogeneous term, e.g. a force

The solution $f(x)$ can be expressed in terms of the Green's function $G(x, y)$

$$\hat{D}_x G(x, y) = \delta(x - y)$$

solution $f(x) = \int dy G(x, y) F(y)$

Green's functions in physics : Harmonic oscillator



$$\underbrace{\frac{d^2x}{dt^2} + \omega_0^2 x}_{\hat{D}_t f(t)} = \underbrace{f_0 \sin \omega t}_{F(t)}$$

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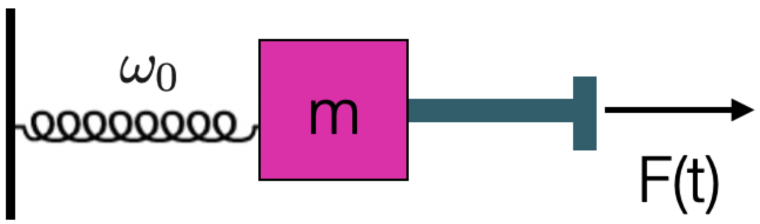

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GF $$\frac{d^2G_0(t)}{dt^2} + \omega_0^2 G_0(t) = \delta(t) \longrightarrow G_0(t) = \theta(t)\frac{1}{\omega_0}\sin \omega_0 t$$

solution $$x(t) = \int dt' G_0(t-t')F(t')$$

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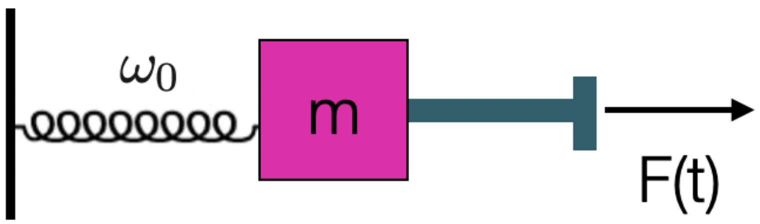

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FT

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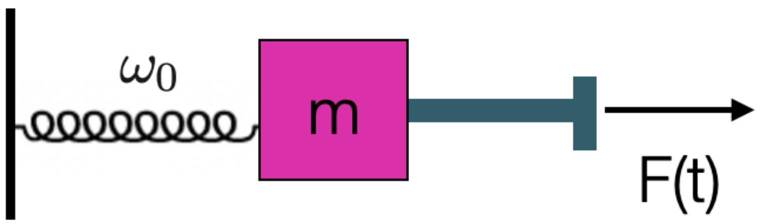

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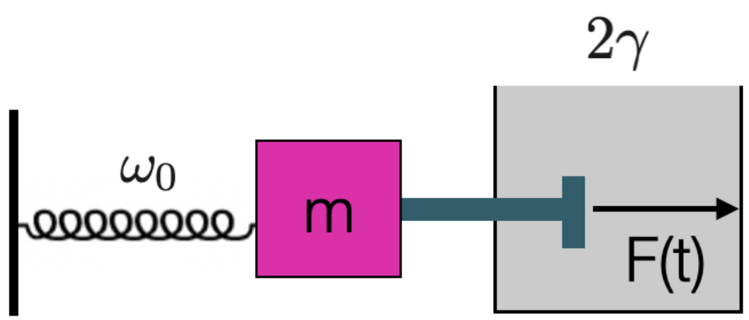
$G_0(\omega)$ has poles at the natural frequency

Green's functions in physics : Harmonic oscillator in a medium



$$\frac{d^2x}{dt^2} + 2\gamma\frac{dx}{dt} + \omega_0^2 x = f_0 \sin\omega t$$

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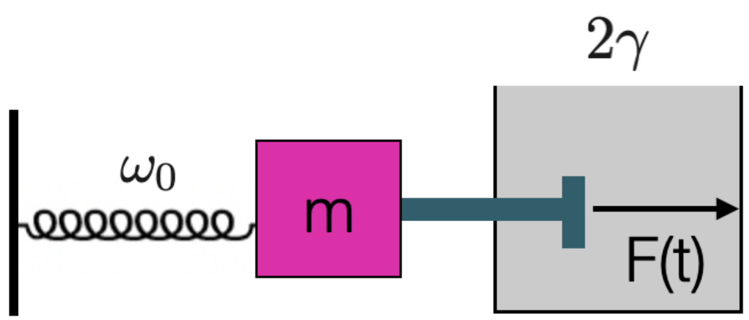

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$$G(\omega) = \frac{1}{\omega_0^2 - \omega^2 - 2i\omega\gamma}$$

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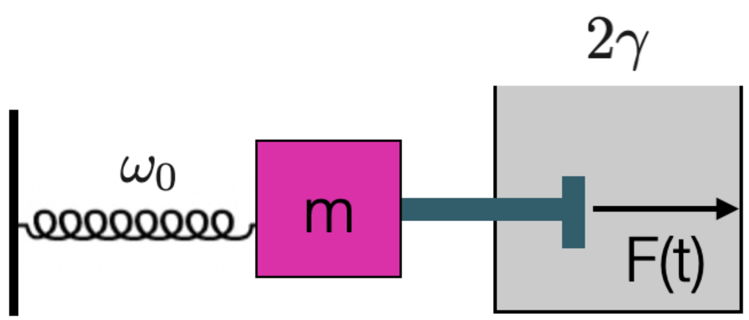

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$4\omega\gamma$

spectral function $$A(\omega) = -\frac{1}{2\pi i}\left[G^*(\omega) - G(\omega)\right] = \frac{1}{\pi}\frac{\frac{1}{2}\Gamma(\omega)}{(\omega_0^2-\omega^2)^2 + \frac{1}{4}\Gamma^2(\omega)}$$

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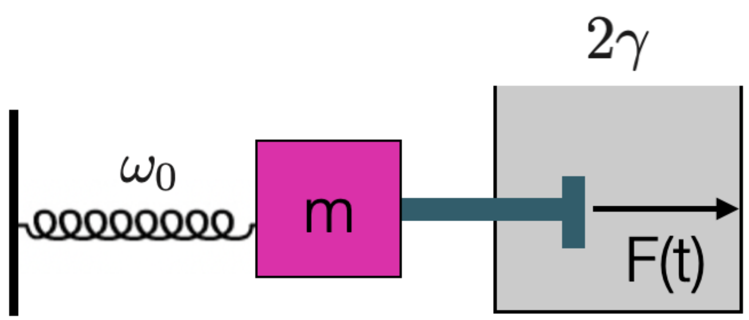

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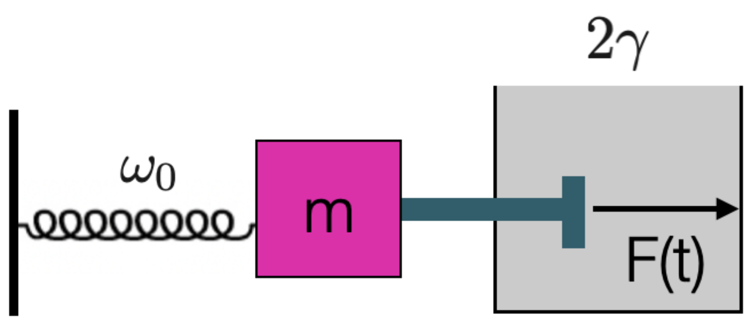

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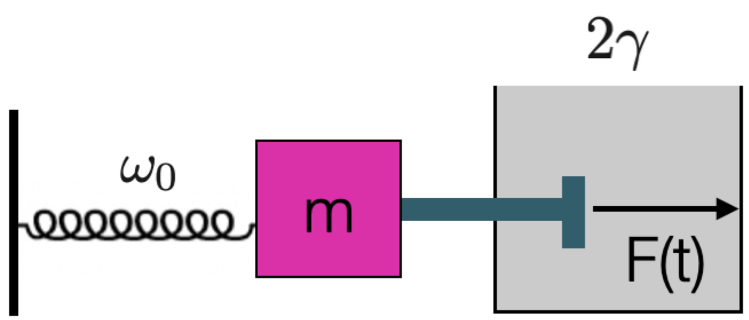
$$G(\omega) = \frac{1}{[G_0(\omega)]^{-1} - \Sigma(\omega)}$$

$2i\omega\gamma$

Green's functions in physics : Harmonic oscillator in a medium



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Dyson equation

$$G(\omega) = \frac{1}{[G_0(\omega)]^{-1} - \Sigma(\omega)} = G_0(\omega) + G_0(\omega)\Sigma(\omega)G(\omega)$$

self-energy

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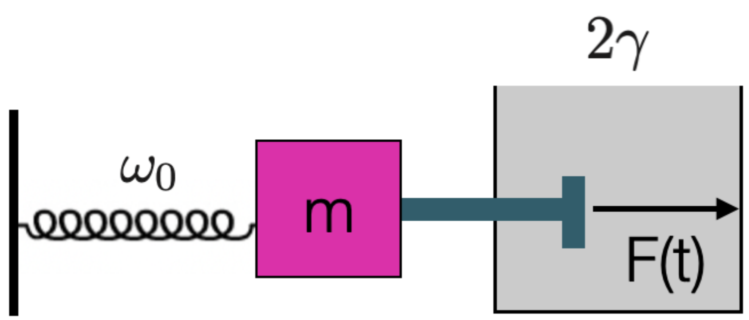

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$$\overbrace{=}^{\text{small }\gamma} G_0(\omega) + G_0(\omega)\Sigma(\omega)G_0(\omega) + G_0(\omega)\Sigma(\omega)G_0(\omega)\Sigma(\omega)G_0(\omega) + \ldots$$

Green's functions in Quantum mechanics

$$\hat{D}_t = i\partial/\partial t + \hat{L}$$

$$\hat{L}|\phi_n\rangle = \lambda_n|\phi_n\rangle$$ self-adjoint

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$$(z \neq \{\lambda_n\} \in \sigma_d)$$

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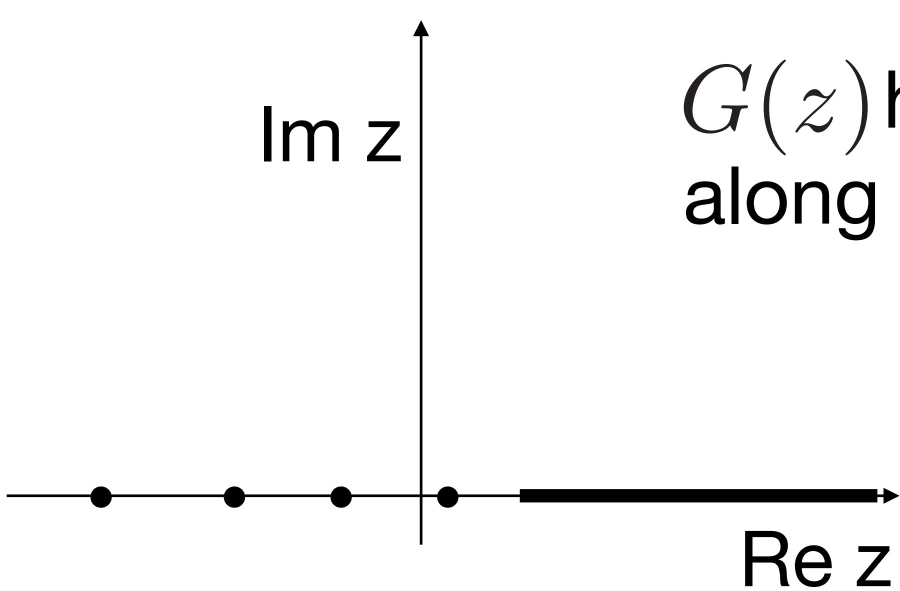

$G(z)$ has discrete poles and a branchcut along the real axis and it is analytic elsewhere

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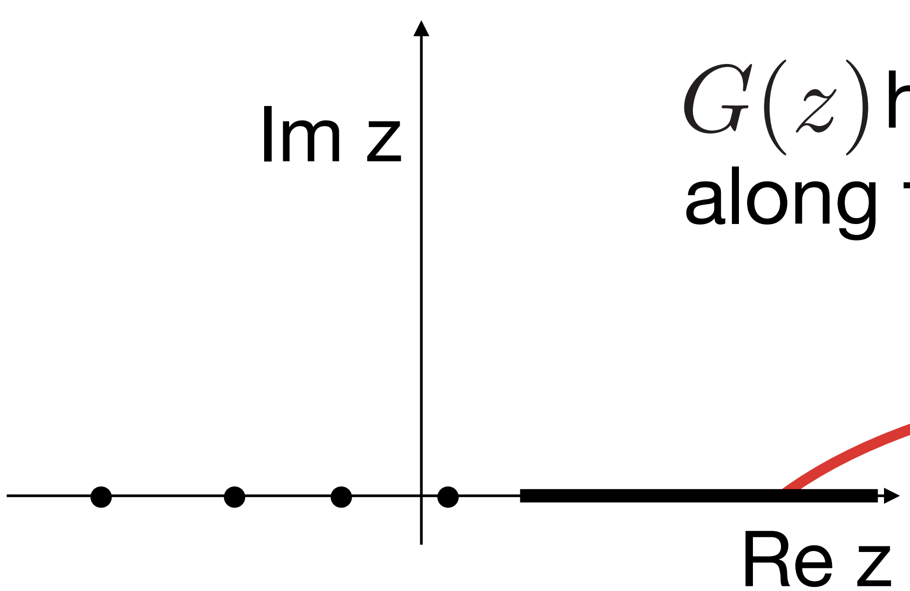

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$$G^{\pm} = \lim_{\eta \to 0} G(z \pm i\eta)$$

$$A(\omega) = -\frac{1}{2\pi i}[G^{+}(z) - G^{-}(z)]$$

Green's functions in Quantum mechanics

many-body
Schrödinger eq.

$$[z - \hat{H}^{\text{tot}}]G^{\text{tot}}(z) = 1$$

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working only with a few-body GF: downfolding

$$[z - \hat{h}^{\rm eff}(z)]G^{\rm S}(z) = 1$$

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$$\begin{pmatrix} \hat{H}^{\mathrm{S}} & \hat{H}^{\mathrm{SR}} \\ \hat{H}^{\mathrm{RS}} & \hat{H}^{\mathrm{R}} \end{pmatrix} \times \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix} = z \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}$$

$$\phi_2 = -(\hat{H}^R - z)^{-1}\hat{H}^{RS}\phi_1 \longrightarrow \left[\hat{H}^S - \hat{H}^{SR}(\hat{H}^R - z)^{-1}\hat{H}^{RS}\right]\phi_1 = z\phi_1$$

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$\Sigma_s(z)$

Notation

- Zero temperature, equilibrium, BOA, non-relativistic

many-body Hamiltonian

$$\hat{H} = \int d\mathbf{x}\hat{\psi}^\dagger(\mathbf{x})h(\mathbf{r})\hat{\psi}(\mathbf{x}) + \frac{1}{2}\int\int d\mathbf{x}d\mathbf{x}'\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}')\hat{\psi}(\mathbf{x}')\hat{\psi}(\mathbf{x})v_c(\mathbf{x},\mathbf{x}')$$

- Combined space-spin-time indices

$$(1^+) = (\mathbf{x}_1, t_1^+) \text{ with } t_1^+ = t_1 + \delta \; (\delta \to 0^+)$$

- Implicit integration

integration over indices not present on the left-hand side of an equation is implicit

$$G(1,2) = G_0(1,2) + G_0(1,3)\Sigma(3,4)G(4,2)$$

- Atomic units

$$\hbar = m_e = e = 4\pi\epsilon_0 = 1$$

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$$= -\frac{\nabla^2_{\mathbf{r}}}{2} + v_{ext}(\mathbf{r})$$

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Survival kit: second quantisation

Fermions

Ψ has to be antisymmetric with respect to the interchange of the coordinates of two electrons

$$\Psi(\mathbf{x}_1, ..., \mathbf{x}_i, ..., \mathbf{x}_j, ..., \mathbf{x}_N) = -\Psi(\mathbf{x}_1, ..., \mathbf{x}_j, ..., \mathbf{x}_i, ..., \mathbf{x}_N)$$

All (antisymmetric) states of a N-particle system belong to the Hilbert space $\mathcal{H}_a^{(N)}$
They form a complete set ($\sum_k |\Psi_k\rangle\langle\Psi_k| = \mathbb{1}$), and can always be taken orthonormal ($\langle\Psi_k|\Psi_l\rangle = \delta_{kl}$)

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closure relation

A collection of all Hilbert space with arbitrary number of particles define a Fock space

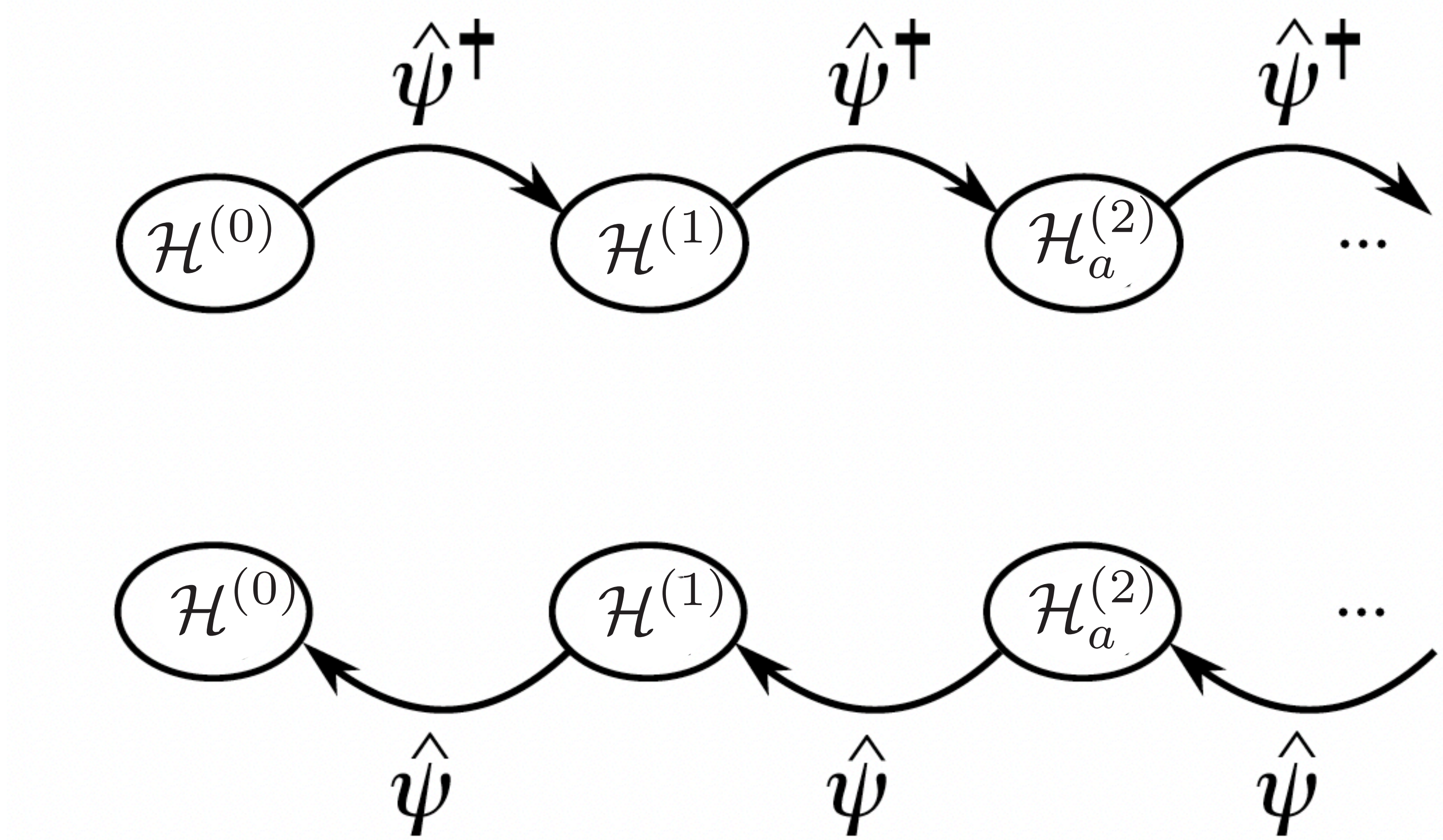
$$\mathcal{F} = \mathcal{H}^{(0)} \oplus \mathcal{H}^{(1)} \oplus \mathcal{H}_a^{(2)} \oplus ... \mathcal{H}_a^{(N)} \oplus ...$$

closure relation $\sum_k \sum_M |\Psi_k^M\rangle\langle\Psi_k^M| = \mathbb{1}$

orthonormal relation $\langle\Psi_k^M|\Psi_l^N\rangle = \delta_{kl}\delta_{MN}$

Survival kit: second quantisation

- **Field operators/creation and annihilation operators**



$$\{\hat{\psi}(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x}')\} = \delta(\mathbf{x} - \mathbf{x}')$$

$$\{\hat{\psi}(\mathbf{x}), \hat{\psi}(\mathbf{x}')\} = \{\hat{\psi}^\dagger(\mathbf{x}), \hat{\psi}^\dagger(\mathbf{x}')\} = 0$$

expansion in a one-particle basis set →

$$\hat{\psi}^\dagger(\mathbf{x}) = \sum_i \phi_i^*(\mathbf{x})\hat{c}_i^\dagger$$

$$\hat{\psi}(\mathbf{x}) = \sum_i \phi_i(\mathbf{x})\hat{c}_i$$

$$\{\hat{c}_i, \hat{c}_j^\dagger\} = \delta_{ij}$$

$$\{\hat{c}_i, \hat{c}_j\} = \{\hat{c}_i^\dagger, \hat{c}_j^\dagger\} = 0$$

Survival kit: second quantisation

Hamiltonian in first quantisation

$$\hat{H} = -\frac{1}{2}\sum_i \nabla_i^2 + \sum_i v(\mathbf{r}_i) + \frac{1}{2}\sum_{i\neq j}\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$

Hamiltonian in second quantisation

$$\hat{H} = \int d\mathbf{x}\hat{\psi}^\dagger(\mathbf{x})\left[-\frac{\nabla_\mathbf{r}^2}{2} + v(\mathbf{r})\right]\hat{\psi}(\mathbf{x}) + \frac{1}{2}\int d\mathbf{x}d\mathbf{x}'\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}')\frac{1}{|\mathbf{r}-\mathbf{r}'|}\hat{\psi}(\mathbf{x}')\hat{\psi}(\mathbf{x})$$

Survival kit: evolution operator

Evolution operator

The time evolution operator maps a wavefunction at time t_0 into a wavefunction at time t

$$|\Psi(t)\rangle = \hat{U}(t,t_0)|\Psi(t_0)\rangle$$

$$i\frac{\partial \hat{U}(t,t_0)}{\partial t} = \hat{H}(t)\hat{U}(t,t_0)$$

$\hat{H}$ time independent

$$\hat{U}(t,t_0) = e^{-i\hat{H}(t-t_0)}$$

Survival kit: pictures

Pictures

$\hat{A}(t)$ being a general time-dependent operator, unitary at each *t*

$$\hat{A}^\dagger(t)\hat{A}(t) = 1 = \hat{A}(t)\hat{A}^\dagger(t)$$

The expectation value $\langle \hat{O} \rangle = \langle \Psi | \hat{O} | \Psi \rangle$ can be written as

$$\langle \hat{O} \rangle = \langle \Psi | \hat{A}^\dagger(t)\hat{A}(t)\hat{O}\hat{A}^\dagger(t)\hat{A}(t) | \Psi \rangle = \langle \hat{A}(t)\Psi | \hat{A}(t)\hat{O}\hat{A}^\dagger(t) | \hat{A}(t)\Psi \rangle$$

$$|\Psi_A(t)\rangle \equiv |\hat{A}(t)\Psi\rangle$$

$$\hat{O}_A(t) \equiv \hat{A}(t)\hat{O}\hat{A}^\dagger(t)$$

$$\langle \Psi | \hat{O} | \Psi \rangle = \langle \Psi_A | \hat{O}_A | \Psi_A \rangle$$

picture transformation

Survival kit: pictures

- **Schrödinger picture:** $\hat{A}(t) = 1$

Operators and wavefunctions have their natural time dependence

- **Heisenberg picture:** $\hat{A}(t) = \hat{U}_S^\dagger(t, t_0) = \hat{U}_S(t_0, t)$

$$|\Psi_H(t)\rangle = \hat{U}_s(t_0, t)|\Psi_S(t_0)\rangle = |\Psi_S(t_0)\rangle = constant$$

$$\hat{O}_H(t) = \hat{U}_S^\dagger(t, t_0)\hat{O}_S(t)\hat{U}_S(t, t_0)$$

$\hat{H}_S$ time independent

$$\hat{O}_H(t) = e^{i\hat{H}_s t}\hat{O}_S(t)e^{-i\hat{H}_s t}$$

time evolution

$$\mathrm{i}\frac{d\hat{O}_H(t)}{dt} = \mathrm{i}\left[\frac{\partial\hat{O}}{\partial t}\right]_H + \left[\hat{O}_H, \hat{H}_H\right]$$

n-body Green's functions

n-body Green's function

$$G^{(n)}(1,2,...,n;1',2',...,n') \equiv (-\mathrm{i})^n \frac{\langle\Psi_0|\hat{T}[\hat{\psi}_H(1)...\hat{\psi}_H(n)\hat{\psi}^\dagger_H(n')...\hat{\psi}^\dagger_H(1')]\;|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}$$

field operators in the Heisenberg picture

$$\hat{\psi}_H(1) = e^{i\hat{H}t_1}\hat{\psi}(\mathbf{x}_1)e^{-i\hat{H}t_1}$$

time-ordering operator $\hat{T}$

ground-state many-body wavefunction $|\Psi_0\rangle$

1-body Green's function

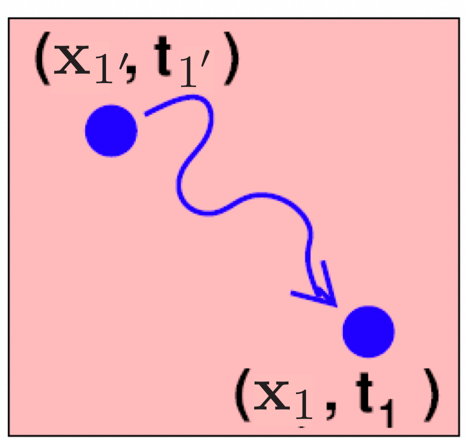
1-body Green's function

$$G(1,1') = -i\langle\Psi_0|\hat{T}[\hat{\psi}_H(1)\hat{\psi}_H^\dagger(1')]|\Psi_0\rangle$$

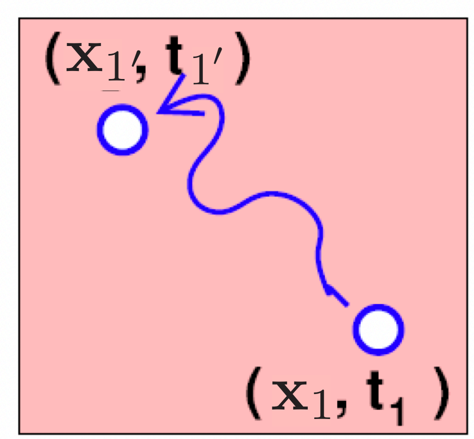
time-ordering operator

$$\hat{T}[\hat{\psi}_H(1)\hat{\psi}_H^\dagger(1')] = \begin{cases} \hat{\psi}_H(1)\hat{\psi}_H^\dagger(1') & \text{for } t_1 > t_{1'} \\ -\hat{\psi}_H^\dagger(1')\hat{\psi}_H(1) & \text{for } t_{1'} > t_1 \end{cases}$$

$$G(1,1') = -\mathrm{i}\Theta(t_1 - t_{1'})\,\langle\Psi_0|\,\hat{\psi}_H(1)\hat{\psi}_H^\dagger(1')\,|\Psi_0\rangle + \mathrm{i}\Theta(t_{1'} - t_1)\,\langle\Psi_0|\,\hat{\psi}_H^\dagger(1')\hat{\psi}_H(1)\,|\Psi_0\rangle$$



propagation of an electron



propagation of a hole

1-body Green's function

1-body Green's function

$$G(1,1') = -i\langle\Psi_0|\hat{T}[\hat{\psi}_H(1)\hat{\psi}^\dagger_H(1')]|\Psi_0\rangle$$

time-ordering operator

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greater G $$G^>(1,1') = -\mathrm{i}\langle\Psi_0|\hat{\psi}_H(1)\hat{\psi}^\dagger_H(1')|\Psi_0\rangle$$

lesser G $$G^<(1,1') = \mathrm{i}\langle\Psi_0|\hat{\psi}^\dagger_H(1')\hat{\psi}_H(1)|\Psi_0\rangle$$

retarded G $$G^R(1,1') = -\mathrm{i}\left[G^>(1,1') - G^<(1,1')\right]\Theta(t_1 - t_{1'})$$

advanced G $$G^A(1,1') = \mathrm{i}\left[G^>(1,1') - G^<(1,1')\right]\Theta(t_{1'} - t_1)$$

1-body Green's function

Lehmann representation of 1-GF

$$G(1,1') = -\mathrm{i}\Theta(t_1 - t_{1'}) \langle \Psi_0 | \hat{\psi}_H(1) \hat{\psi}_H^\dagger(1') | \Psi_0 \rangle + \mathrm{i}\Theta(t_{1'} - t_1) \langle \Psi_0 | \hat{\psi}_H^\dagger(1') \hat{\psi}_H(1) | \Psi_0 \rangle$$

Insert the resolution of identity $\sum_k \sum_M |\Psi_k^M\rangle\langle\Psi_k^M|$ in Fock space

Fourier transform to frequency using the relation $\int_{-\infty}^{\infty} dt \left[\Theta(\pm t) e^{-\mathrm{i}\alpha t}\right] e^{\mathrm{i}\omega t} = \lim_{\eta\to 0^+} \frac{\pm \mathrm{i}}{\omega - \alpha \pm \mathrm{i}\eta}$

$$G(\mathbf{x},\mathbf{x}';\omega) = \lim_{\eta\to 0^+} \left[\sum_m \frac{B_m^A(\mathbf{x},\mathbf{x}')}{\omega - (E_m^{N+1} - E_0^N) + \mathrm{i}\eta} + \sum_n \frac{B_n^R(\mathbf{x},\mathbf{x}')}{\omega - (E_0^N - E_n^{N-1}) - \mathrm{i}\eta} \right]$$

1-body Green's function

Lehmann representation of 1-GF

$$G(1,1') = -\mathrm{i}\Theta(t_1 - t_{1'}) \langle \Psi_0 | \hat{\psi}_H(1)\hat{\psi}_H^\dagger(1') | \Psi_0 \rangle + \mathrm{i}\Theta(t_{1'} - t_1) \langle \Psi_0 | \hat{\psi}_H^\dagger(1')\hat{\psi}_H(1) | \Psi_0 \rangle$$

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ground-state energy of the *N*-electron system

1-body Green's function

Lehmann representation of 1-GF

$$G(1,1') = -\mathrm{i}\Theta(t_1-t_{1'})\langle\Psi_0|\hat{\psi}_H(1)\hat{\psi}^\dagger_H(1')|\Psi_0\rangle + \mathrm{i}\Theta(t_{1'}-t_1)\langle\Psi_0|\hat{\psi}^\dagger_H(1')\hat{\psi}_H(1)|\Psi_0\rangle$$

Insert the resolution of identity $\sum_k \sum_M |\Psi_k^M\rangle\langle\Psi_k^M|$ in Fock space

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$$G(\mathbf{x},\mathbf{x}';\omega) = \lim_{\eta\to 0^+}\left[\sum_m \frac{B_m^A(\mathbf{x},\mathbf{x}')}{\omega-(E_m^{N+1}-E_0^N)+\mathrm{i}\eta} + \sum_n \frac{B_n^R(\mathbf{x},\mathbf{x}')}{\omega-(E_0^N-E_n^{N-1})-\mathrm{i}\eta}\right]$$

ground-state energy of the *N*-electron system

(ground/excited)-state energies of the ($N\pm1$)-electron system

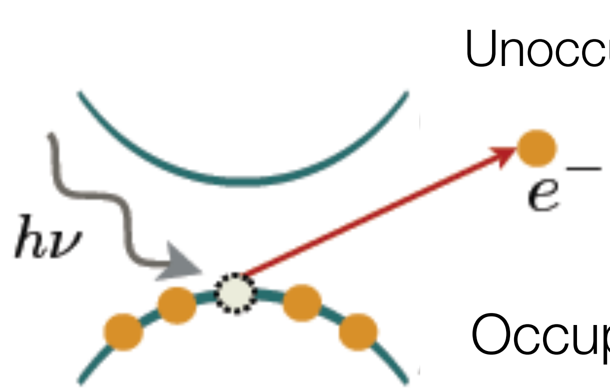
1-body Green's function

Link to photoemission spectra

$$G(\mathbf{x},\mathbf{x}';\omega) = \lim_{\eta\to 0^+}\left[\sum_m \frac{B_m^A(\mathbf{x},\mathbf{x}')}{\omega-(E_m^{N+1}-E_0^N)+i\eta}+\sum_n \frac{B_n^R(\mathbf{x},\mathbf{x}')}{\omega-(E_0^N-E_n^{N-1})-i\eta}\right]$$

ground-state energy of the *N*-electron system

(ground/excited)-state energies of the ($N\pm 1$)-electron system



direct photoemission : N ⟶ N-1

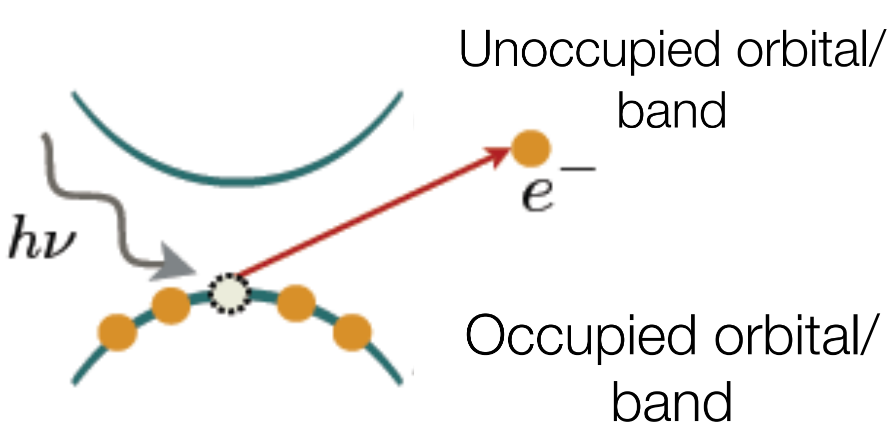
1-body Green's function

Link to photoemission spectra

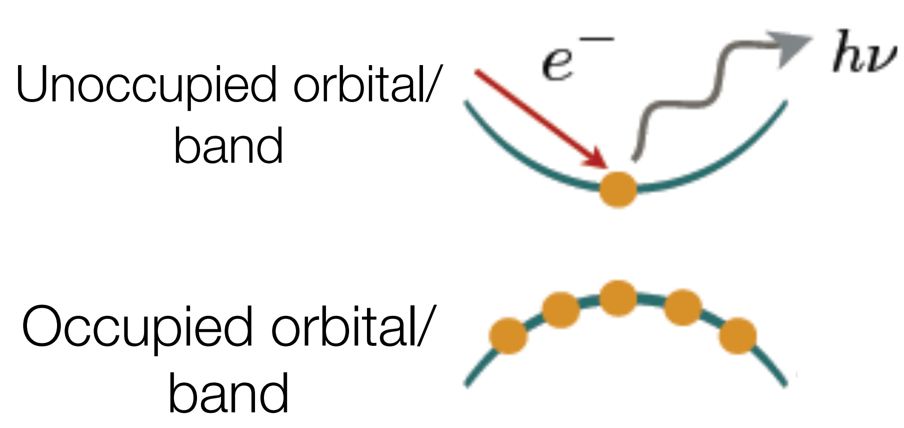
$$G(\mathbf{x},\mathbf{x}';\omega) = \lim_{\eta\to 0^+}\left[\sum_m \frac{B_m^A(\mathbf{x},\mathbf{x}')}{\omega - (E_m^{N+1} - E_0^N) + i\eta} + \sum_n \frac{B_n^R(\mathbf{x},\mathbf{x}')}{\omega - (E_0^N - E_n^{N-1}) - i\eta}\right]$$

ground-state energy of the *N*-electron system

(ground/excited)-state energies of the ($N \pm 1$)-electron system



direct photoemission : N⟶ N-1



inverse photoemission : N⟶ N+1

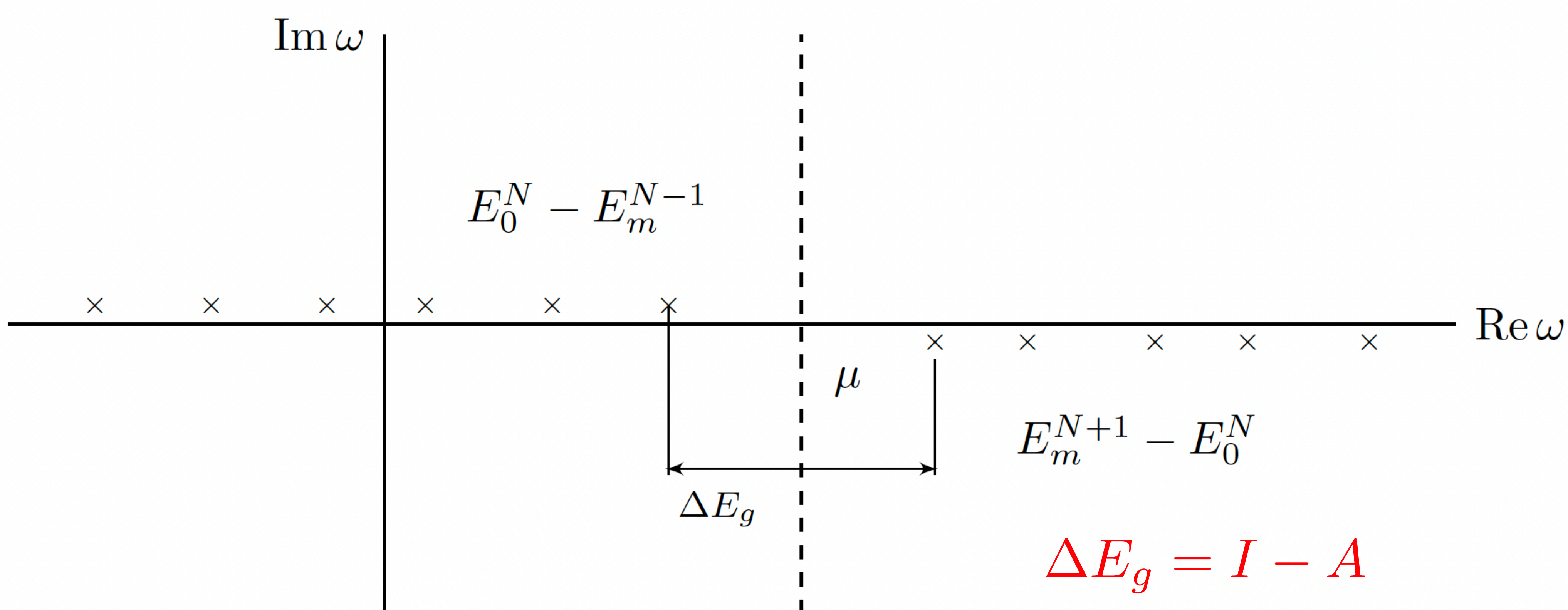
1-body Green's function

Link to photoemission spectra

$$G(\mathbf{x},\mathbf{x}';\omega) = \lim_{\eta\to 0^+}\left[\sum_m \frac{B_m^A(\mathbf{x},\mathbf{x}')}{\omega - (E_m^{N+1} - E_0^N) + i\eta} + \sum_n \frac{B_n^R(\mathbf{x},\mathbf{x}')}{\omega - (E_0^N - E_n^{N-1}) - i\eta}\right]$$

ground-state energy of the *N*-electron system

(ground/excited)-state energies of the ($N\pm 1$)-electron system



$$\Delta E_g = I - A$$

Polar structure of G

1-body Green's function

Link to photoemission spectra

$$G(\mathbf{x},\mathbf{x}';\omega) = \lim_{\eta\to 0^+}\left[\sum_m \frac{B_m^A(\mathbf{x},\mathbf{x}')}{\omega-(E_m^{N+1}-E_0^N)+\mathrm{i}\eta} + \sum_n \frac{B_n^R(\mathbf{x},\mathbf{x}')}{\omega-(E_0^N-E_n^{N-1})-\mathrm{i}\eta}\right]$$

$$B_m^A(\mathbf{x},\mathbf{x}') = \langle\Psi_0^N|\hat{\psi}(\mathbf{x})|\Psi_m^{N+1}\rangle\langle\Psi_m^{N+1}|\hat{\psi}^\dagger(\mathbf{x}')|\Psi_0^N\rangle$$

$$B_n^R(\mathbf{x},\mathbf{x}') = \langle\Psi_0^N|\hat{\psi}^\dagger(\mathbf{x}')|\Psi_n^{N-1}\rangle\langle\Psi_n^{N-1}|\hat{\psi}(\mathbf{x})|\Psi_0^N\rangle$$

1-body Green's function

- **Link to photoemission spectra**

$$G(\mathbf{x},\mathbf{x}';\omega) = \lim_{\eta\to 0^+}\left[\sum_m \frac{B_m^A(\mathbf{x},\mathbf{x}')}{\omega-(E_m^{N+1}-E_0^N)+\mathrm{i}\eta} + \sum_n \frac{B_n^R(\mathbf{x},\mathbf{x}')}{\omega-(E_0^N-E_n^{N-1})-\mathrm{i}\eta}\right]$$

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$$B_n^R(\mathbf{x},\mathbf{x}') = \langle\Psi_0^N|\hat{\psi}^\dagger(\mathbf{x}')|\Psi_n^{N-1}\rangle\langle\Psi_n^{N-1}|\hat{\psi}(\mathbf{x})|\Psi_0^N\rangle$$

ground-state many-body wavefunction of the *N*-electron system

1-body Green's function

Link to photoemission spectra

$$G(\mathbf{x},\mathbf{x}';\omega) = \lim_{\eta\to 0^+}\left[\sum_m \frac{B_m^A(\mathbf{x},\mathbf{x}')}{\omega-(E_m^{N+1}-E_0^N)+\mathrm{i}\eta} + \sum_n \frac{B_n^R(\mathbf{x},\mathbf{x}')}{\omega-(E_0^N-E_n^{N-1})-\mathrm{i}\eta}\right]$$

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ground-state many-body wavefunction of the *N*-electron system

(ground/excited)-state many-body wavefunction of the ($N\pm1$)-electron system

1-body Green's function

Link to photoemission spectra

$$G(\mathbf{x},\mathbf{x}';\omega) = \lim_{\eta\to 0^+}\left[\sum_m \frac{B_m^A(\mathbf{x},\mathbf{x}')}{\omega-(E_m^{N+1}-E_0^N)+i\eta} + \sum_n \frac{B_n^R(\mathbf{x},\mathbf{x}')}{\omega-(E_0^N-E_n^{N-1})-i\eta}\right]$$

$$B_m^A(\mathbf{x},\mathbf{x}') = \overbrace{\langle\Psi_0^N|\hat{\psi}(\mathbf{x})|\Psi_m^{N+1}\rangle}^{f_m(\mathbf{x})}\overbrace{\langle\Psi_m^{N+1}|\hat{\psi}^\dagger(\mathbf{x}')|\Psi_0^N\rangle}^{f_m^*(\mathbf{x}')}$$

$$B_n^R(\mathbf{x},\mathbf{x}') = \overbrace{\langle\Psi_0^N|\hat{\psi}^\dagger(\mathbf{x}')|\Psi_n^{N-1}\rangle}^{g_n(\mathbf{x}')}\overbrace{\langle\Psi_n^{N-1}|\hat{\psi}(\mathbf{x})|\Psi_0^N\rangle}^{g_n^*(\mathbf{x})}$$

Feynman-Dyson amplitudes f_m, g_n

$$\sum_m f_m(x_1)f_m^*(x_{1'}) + \sum_n g_n(x_1)g_n^*(x_{1'}) = \delta(x_1 - x_{1'})$$

1-body Green's function

Link to photoemission spectra

$$G(\mathbf{x},\mathbf{x}';\omega) = \lim_{\eta\to 0^+}\left[\sum_m \frac{B_m^A(\mathbf{x},\mathbf{x}')}{\omega - (E_m^{N+1} - E_0^N) + \mathrm{i}\eta} + \sum_n \frac{B_n^R(\mathbf{x},\mathbf{x}')}{\omega - (E_0^N - E_n^{N-1}) - \mathrm{i}\eta}\right]$$

noninteracting G

$$G_0(\mathbf{x},\mathbf{x}';\omega) = \sum_i \frac{\phi_i(\mathbf{x})\phi_i^*(\mathbf{x}')}{\omega - \epsilon_i^0 + \mathrm{sgn}(\epsilon_i^0 - \mu)\mathrm{i}\eta}$$

1-body Green's function

- **Spectral function**

$$A(\mathbf{x},\mathbf{x}';\omega) = -\frac{1}{2\pi i}[G^R(\mathbf{x},\mathbf{x}';\omega) - G^A(\mathbf{x},\mathbf{x}';\omega)] = \frac{1}{\pi}\text{sgn}(\mu-\omega)\Im G(\mathbf{x},\mathbf{x}';\omega)$$

$$= \sum_m B_m^A(\mathbf{x},\mathbf{x}')\delta(\omega - (E_m^{N+1} - E_0^N)) + \sum_n B_n^R(\mathbf{x},\mathbf{x}')\delta(\omega - (E_n^{N-1} - E_0^N))$$

1-body Green's function

- Spectral function

$$A(\mathbf{x},\mathbf{x}';\omega) = -\frac{1}{2\pi i}[G^R(\mathbf{x},\mathbf{x}';\omega) - G^A(\mathbf{x},\mathbf{x}';\omega)] = \frac{1}{\pi}\mathrm{sgn}(\mu-\omega)\Im G(\mathbf{x},\mathbf{x}';\omega)$$

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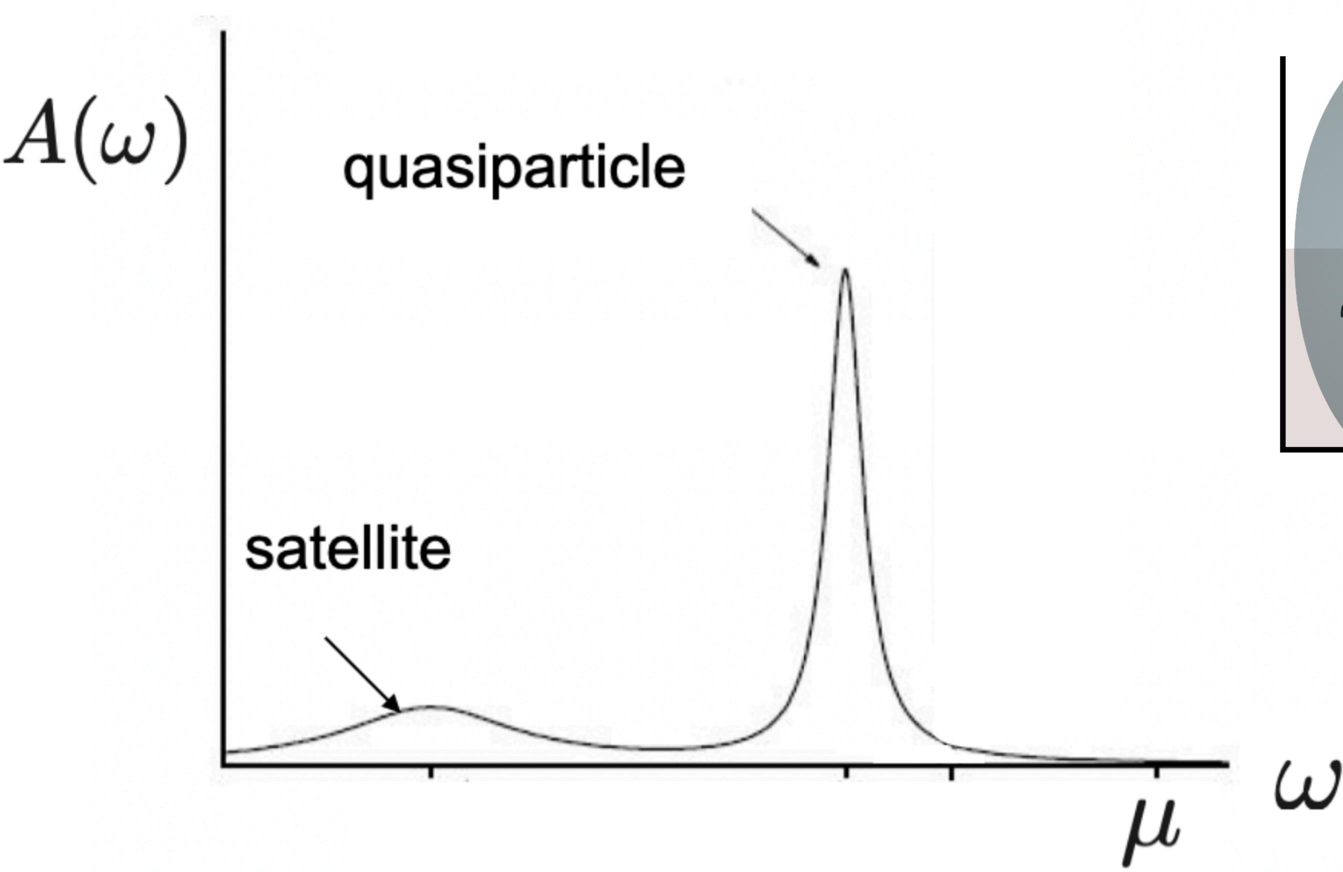
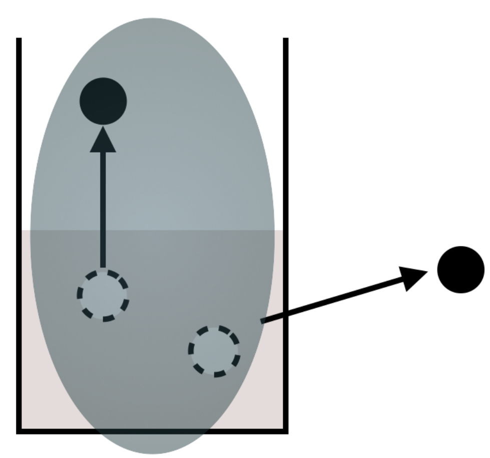
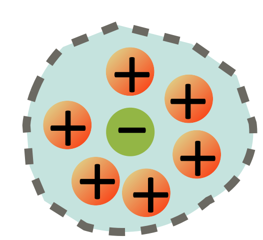
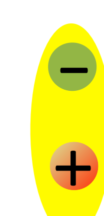






quasiparticles

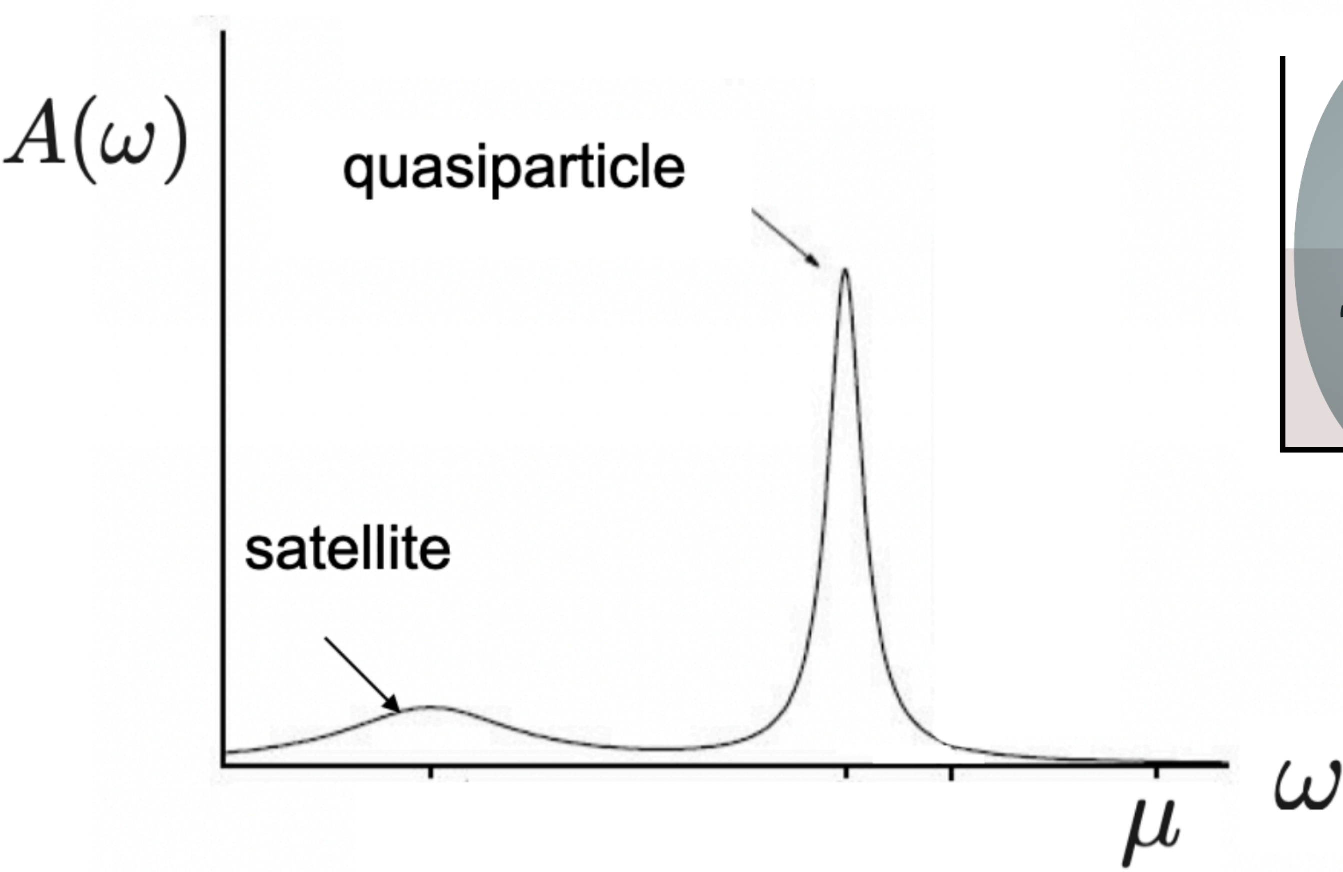
satellites (e.g., neutral excitations )

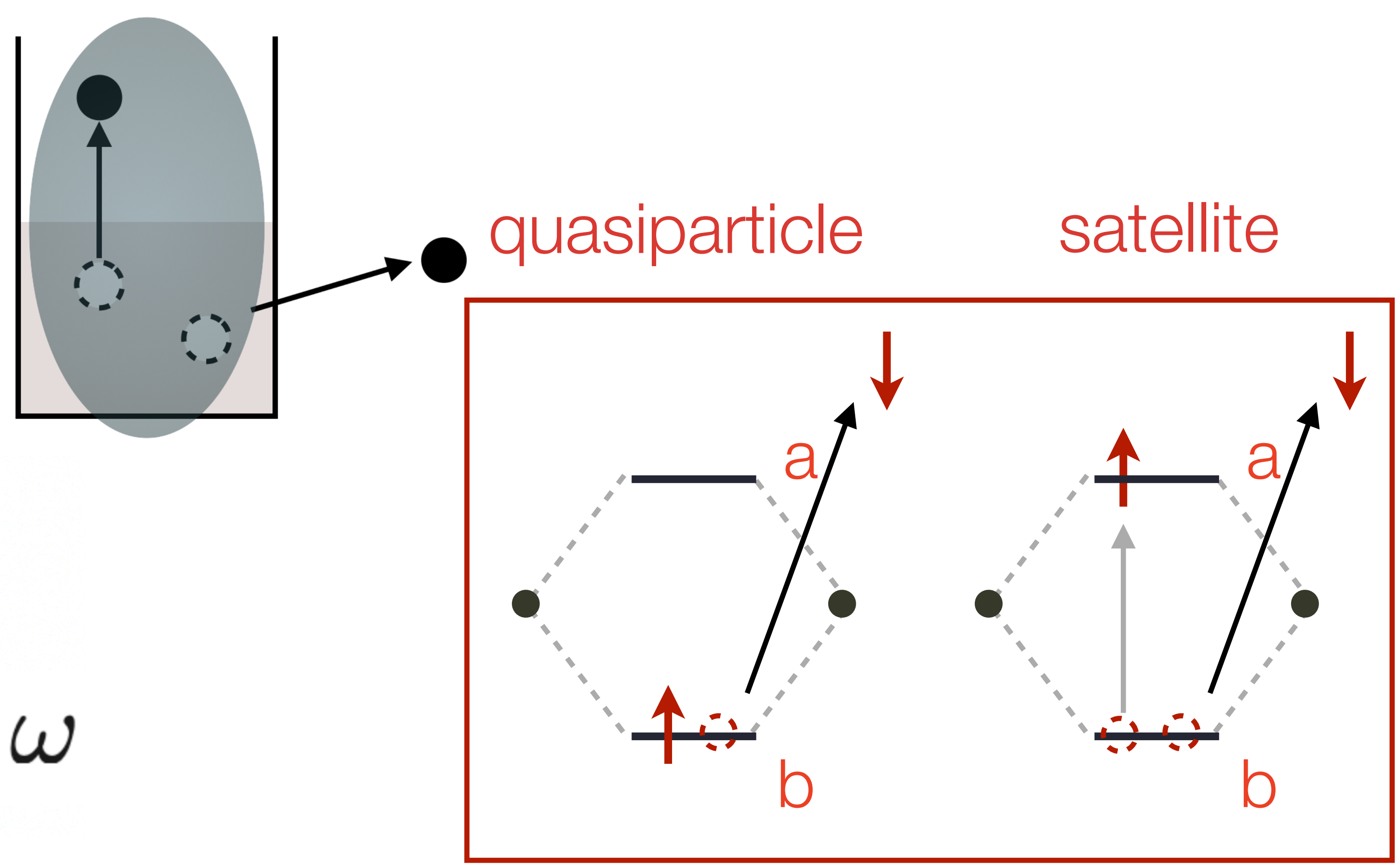
1-body Green's function

- **Spectral function**

$$A(\mathbf{x},\mathbf{x}';\omega) = -\frac{1}{2\pi i}[G^R(\mathbf{x},\mathbf{x}';\omega) - G^A(\mathbf{x},\mathbf{x}';\omega)] = \frac{1}{\pi}\mathrm{sgn}(\mu-\omega)\Im G(\mathbf{x},\mathbf{x}';\omega)$$

$$= \sum_m B_m^A(\mathbf{x},\mathbf{x}')\delta(\omega - (E_m^{N+1} - E_0^N)) + \sum_n B_n^R(\mathbf{x},\mathbf{x}')\delta(\omega - (E_n^{N-1} - E_0^N))$$





1-body Green's function

- **Spectral function**

$$A(\mathbf{x},\mathbf{x}';\omega) = -\frac{1}{2\pi i}[G^R(\mathbf{x},\mathbf{x}';\omega) - G^A(\mathbf{x},\mathbf{x}';\omega)] = \frac{1}{\pi}\mathrm{sgn}(\mu-\omega)\Im G(\mathbf{x},\mathbf{x}';\omega)$$

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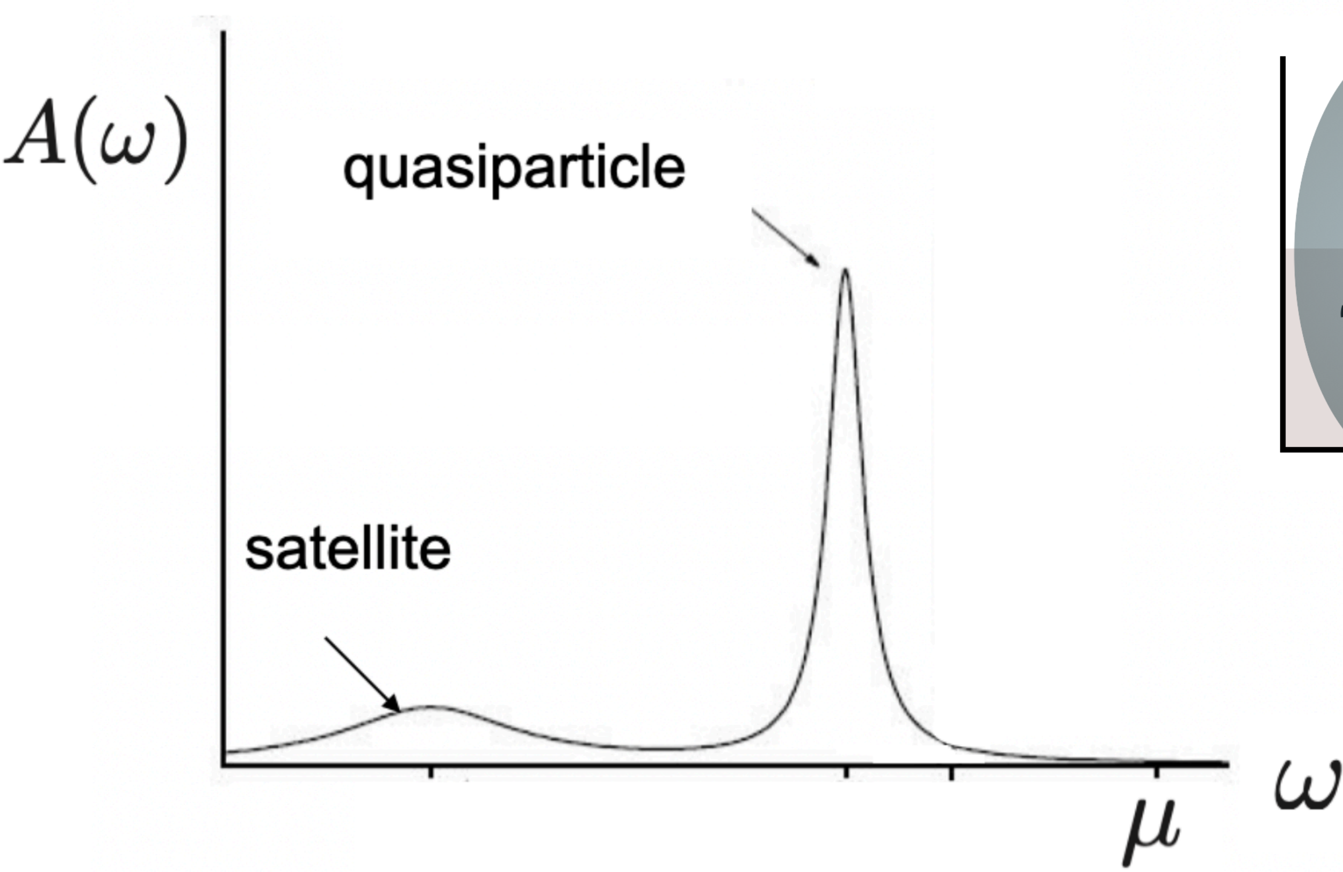

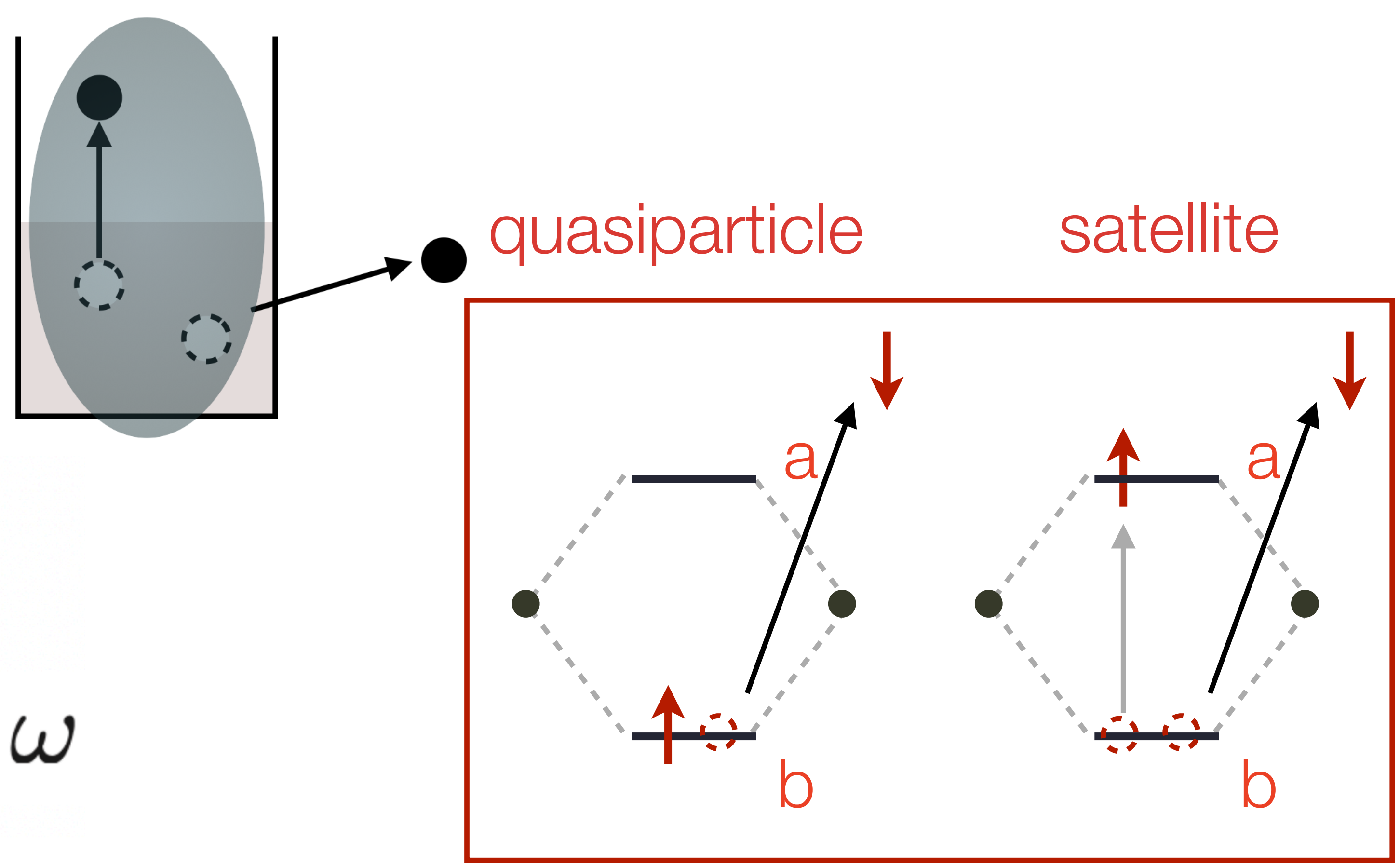

1-body Green's function

Physical content of 1-GF

- the one-particle excitation spectrum of the system

- the ground-state expectation value of any one-body operator, e.g., the density ρ or the density matrix γ

$$\rho(\mathbf{x}) = -iG(\mathbf{x},\mathbf{x};t-t^+) \qquad \gamma(\mathbf{x},\mathbf{x}') = -iG(\mathbf{x},\mathbf{x}';t-t^+)$$

- the ground state total energy

$$E = -\frac{i}{2}\int dx_1 \lim_{t_1'\to t_1^+}\lim_{x_1'\to x_1}\left[i\frac{\partial}{\partial t_1} + h(x_1)\right]G(1,1')$$

1-body Green's function

- **How do we get G ?**

$$G(1,1') = -i\langle\Psi_0|\hat{T}[\hat{\psi}_H(1)\hat{\psi}^\dagger_H(1')]|\Psi_0\rangle$$

1-body Green's function

- **Equation of motion of G:** $\dfrac{\partial G(1,2)}{\partial t_1}$

1-body Green's function

- **Equation of motion of G:** $\dfrac{\partial G(1,2)}{\partial t_1}$

EoM operators $$\mathrm{i}\frac{\partial \hat{\psi}_H(1)}{\partial t_1} = [\hat{\psi}_H(1), \hat{H}]$$

commutators

$$[\hat{\psi}(\mathbf{x}), \hat{H}] = h(\mathbf{x})\hat{\psi}(\mathbf{x}) + \int d\mathbf{y} v_c(\mathbf{x},\mathbf{y})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x})$$

$$[\hat{\psi}^\dagger(\mathbf{x}), \hat{H}] = -h(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x}) - \int d\mathbf{y} v_c(\mathbf{x},\mathbf{y})\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y})$$

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$$\mathrm{i}\frac{\partial G(1,1')}{\partial t_1} = \delta(1-1') + h(1)G(1,1')$$

$$-i\int d2 v_c(1^+,2)\langle\Psi_0|T[\hat{\psi}_H^\dagger(2)\hat{\psi}_H(2)\hat{\psi}_H(1)\hat{\psi}_H^\dagger(1')]\,|\Psi_0\rangle$$

1-body Green's function

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commutators

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$$v_c(1^+,2) = v_c(\mathbf{r}_1,\mathbf{r}_2)\delta(t_1^+ - t_2)$$

1-body Green's function

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1-body Green's function

- **Equation of motion of G:** $\dfrac{\partial G(1,2)}{\partial t_1}$

2-body GF

$$\langle \Psi_0 | \hat{T}[\hat{\psi}_H^\dagger(2^+)\hat{\psi}_H(2)\hat{\psi}_H(1)\hat{\psi}_H^\dagger(1')]\ |\Psi_0\rangle = -\langle \Psi_0 | \hat{T}[\hat{\psi}_H(1)\hat{\psi}_H(2)\hat{\psi}_H^\dagger(2^+)\hat{\psi}_H^\dagger(1')]\ |\Psi_0\rangle$$

$$= G^{(2)}(1,2;1',2^+)$$

1-body Green's function

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$$\left[\mathrm{i}\frac{\partial}{\partial t_1} - h(1)\right] G(1,1') + \mathrm{i}\int d2 v_c(1,2^+) G^{(2)}(1,2;1',2^+) = \delta(1-1')$$

1-body Green's function

- Equation of motion of G: $\dfrac{\partial G(1,2)}{\partial t_1}$

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How do we get rid of $G^{(2)}$?

1-body Green's function

- Equation of motion of G: $\frac{\partial G(1,2)}{\partial t_1}$

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How do we get rid of $G^{(2)}$?

Equation of motion of $G^{(2)}$

1-body Green's function

- **Martin-Schwinger hierarchy**

$$G^{(1)} \leftarrow G^{(2)}$$

$$G^{(2)} \leftarrow G^{(3)}$$

$$\dots$$

$$\left[\mathrm{i}\frac{d}{dt_k} - h(k)\right] G^{(n)}(1,\dots,n;1',\dots,n') = \sum_j (-1)^{k+j}\delta(k,j')G^{(n-1)}(1,\dots,\tilde{j},\dots,n;1',\dots,\tilde{k}',\dots,n')$$

$$-\mathrm{i}\int d\bar{1} v_c(k,\bar{1})G^{(n+1)}(1,\dots,n,\bar{1};1',\dots,n',\bar{1}^+)$$

1-body Green's function

- Martin-Schwinger hierarchy

$$G^{(1)} \leftarrow G^{(2)}$$

$$G^{(2)} \leftarrow G^{(3)}$$

...

$$\left[\mathrm{i}\frac{d}{dt_k} - h(k)\right] G^{(n)}(1,...,n;1',...,n') = \sum_j (-1)^{k+j}\delta(k,j')G^{(n-1)}(1,...,\tilde{j},...,n;1',...,\tilde{k}',...,n')$$

$$-\mathrm{i}\int d\bar{1} v_c(k,\bar{1})G^{(n+1)}(1,...,n,\bar{1};1',...,n',\bar{1}^+)$$

How to truncate this hierarchy?

1-body Green's function

Self-energy and Dyson equation

self-energy $$\Sigma(1,1') = -\mathrm{i}v_c(1,2^+)G^{(2)}(1,2;2',2^+)G^{-1}(2',1')$$

$$\left[i\frac{\partial}{\partial t_1} - h(1)\right]G(1,1') - \int d2\Sigma(1,2)G(2,1') = \delta(1-1')$$

1-body Green's function

Self-energy and Dyson equation

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noninteracting G $$\left[\mathrm{i}\frac{\partial}{\partial t_1} - h(1)\right]G_0(1,1') = \delta(1-1')$$

Dyson eq. $$G(1,1') = G_0(1,1') + G_0(1,2)\Sigma(2,2')G(2',1')$$

1-body Green's function

Self-energy and Dyson equation

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Dyson eq. $$G(1,1') = G_0(1,1') + G_0(1,2)\Sigma(2,2')G(2',1')$$

1-body Green's function

- **Why a Dyson equation?**

$$G(\omega) = [1 - G_0(\omega)\Sigma(\omega)]^{-1} G_0(\omega)$$
$$= G_0(\omega) + G_0(\omega)\Sigma(\omega)G_0(\omega) + G_0(\omega)\Sigma(\omega)G_0(\omega)\Sigma(\omega)G_0(\omega) + \ldots$$

Even approximating Σ to low order in the interaction, solving the Dyson equation creates contributions to all orders

1-body Green's function

- **Self-energy and Dyson equation**

self-energy
$$\Sigma(1,1') = -\mathrm{i}v_c(1,2^+)G^{(2)}(1,2;2',2^+)G^{-1}(2',1')$$

$$\left[i\frac{\partial}{\partial t_1} - h(1)\right]G(1,1') - \int d2\Sigma(1,2)G(2,1') = \delta(1-1')$$

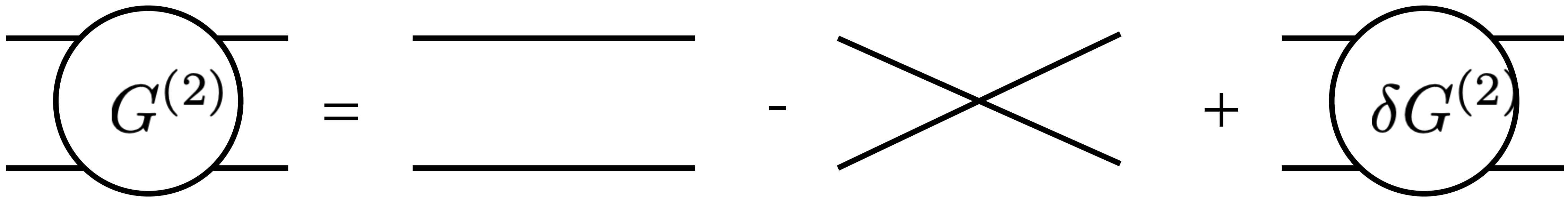
noninteracting G
$$\left[\mathrm{i}\frac{\partial}{\partial t_1} - h(1)\right]G_0(1,1') = \delta(1-1')$$

Dyson eq.
$$G(1,1') = G_0(1,1') + G_0(1,2)\Sigma(2,2')G(2',1')$$

1-body Green's function

- **Hartree-Fock approximation**

$$G^{(2)}(1,2;1',2') = G(1,1')G(2,2') - G(1,2')G(2,1') + \delta G^{(2)}(1,2;1',2')$$



1-body Green's function

- **Hartree-Fock approximation**

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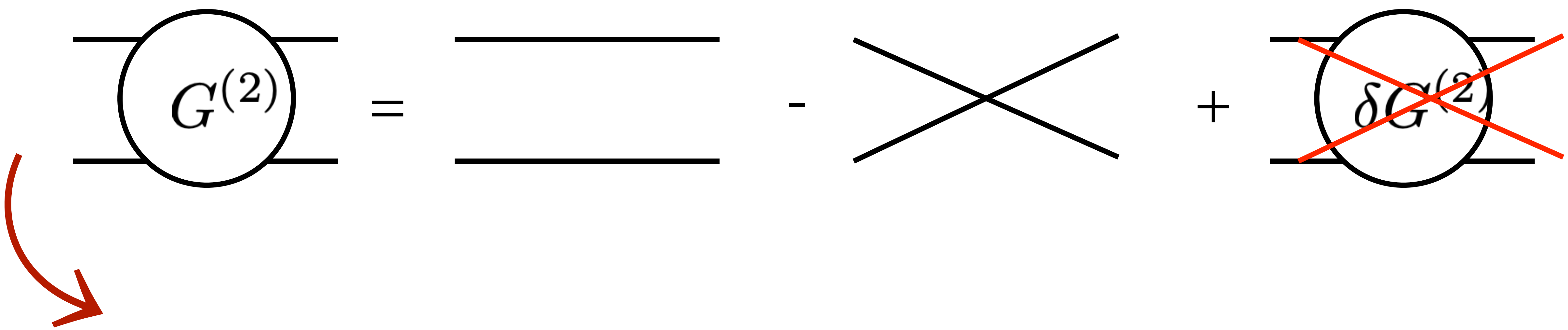


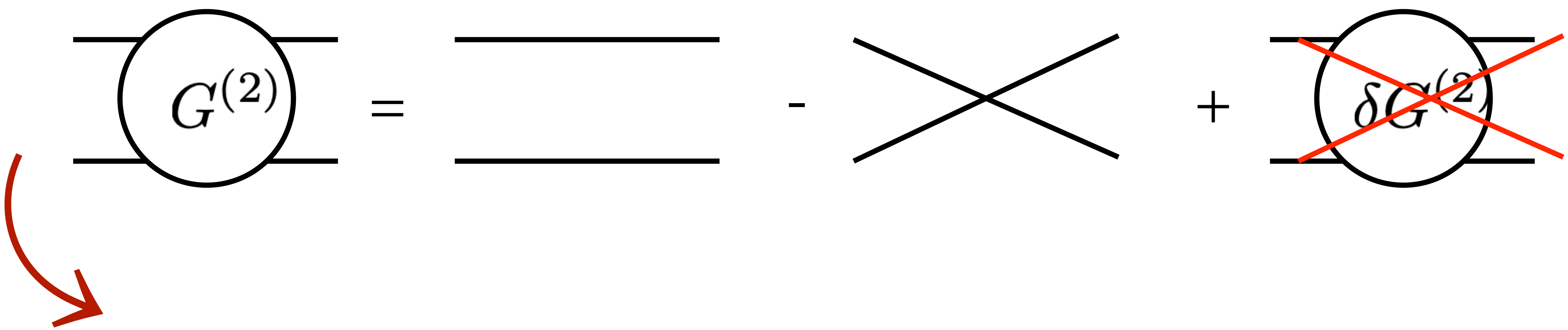
$$\Sigma^{\mathrm{HF}}(1,1') = -iv_c(1,2^+)[G(1,2')G(2,2^+) - G(1,2^+)G(2,2')]G^{-1}(2',1')$$

$$= -iv_c(1,2)G(2,2^+)\delta(1,1') + iv_c(1,1')G(1,1'^+)$$

1-body Green's function

- **Hartree-Fock approximation**

$$G^{(2)}(1,2;1',2') = G(1,1')G(2,2') - G(1,2')G(2,1') + \delta G^{(2)}(1,2;1',2')$$



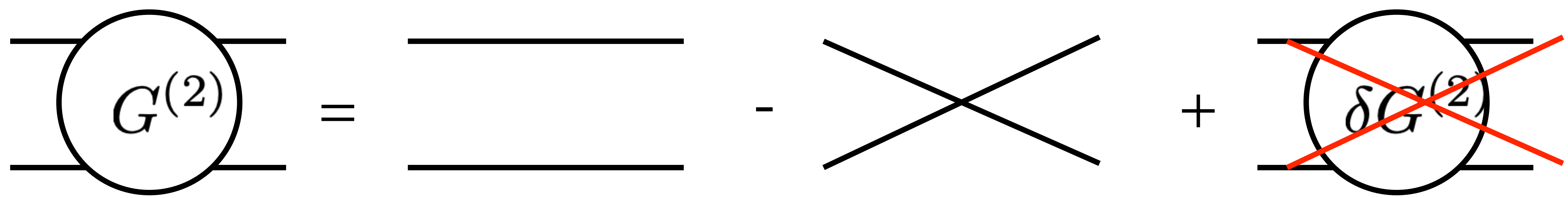
$$\Sigma^{\text{HF}}(1,1') = -iv_c(1,2^+)[G(1,2')G(2,2^+) - G(1,2^+)G(2,2')]G^{-1}(2',1')$$

$$= \underbrace{-iv_c(1,2)G(2,2^+)\delta(1,1')}_{v_H(1)\delta(1,1')} + \underbrace{iv_c(1,1')G(1,1'^+)}_{\Sigma_x(1,1')}$$

1-body Green's function

Hartree-Fock approximation

$$G^{(2)}(1,2;1',2') = G(1,1')G(2,2') - G(1,2')G(2,1') + \delta G^{(2)}(1,2;1',2')$$



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$$= \underbrace{-iv_c(1,2)G(2,2^+)\delta(1,1')}_{v_H(1)\delta(1,1')} + \underbrace{iv_c(1,1')G(1,1'^+)}_{\Sigma_x(1,1')}$$

How to go beyond HF?

1-body Green's function

- **Schwinger relation**

$$\frac{\delta G(1,1';[V_{ext}])}{\delta V_{ext}(2',2)} = -G^{(2)}(1,2;1',2^+;[V_{ext}]) + G(1,1';[V_{ext}])G(2,2^+;[V_{ext}])$$

1-body Green's function

- Schwinger relation

$$\frac{\delta G(1,1';[V_{ext}])}{\delta V_{ext}(2',2)} = -G^{(2)}(1,2;1',2^+;[V_{ext}]) + G(1,1';[V_{ext}])G(2,2^+;[V_{ext}])$$

$$\Sigma(1,1') = v_H(1)\delta(1-1') + \mathrm{i}v_c(1,2)\left.\frac{\delta G(1,2';[V_{ext}])}{\delta V_{ext}(2)}\right|_{V_{ext}=0} G^{-1}(2',1')$$

1-body Green's function

- **Schwinger relation**

$$\frac{\delta G(1,1';[V_{ext}])}{\delta V_{ext}(2',2)} = -G^{(2)}(1,2;1',2^+;[V_{ext}]) + G(1,1';[V_{ext}])G(2,2^+;[V_{ext}])$$

$$\Sigma(1,1') = v_H(1)\delta(1-1') + iv_c(1,2)\left.\frac{\delta G(1,2';[V_{ext}])}{\delta V_{ext}(2)}\right|_{V_{ext}=0} G^{-1}(2',1')$$

And now?

1-body Green's function

- Schwinger relation

$$\frac{\delta G(1,1';[V_{ext}])}{\delta V_{ext}(2',2)} = -G^{(2)}(1,2;1',2^+;[V_{ext}]) + G(1,1';[V_{ext}])G(2,2^+;[V_{ext}])$$

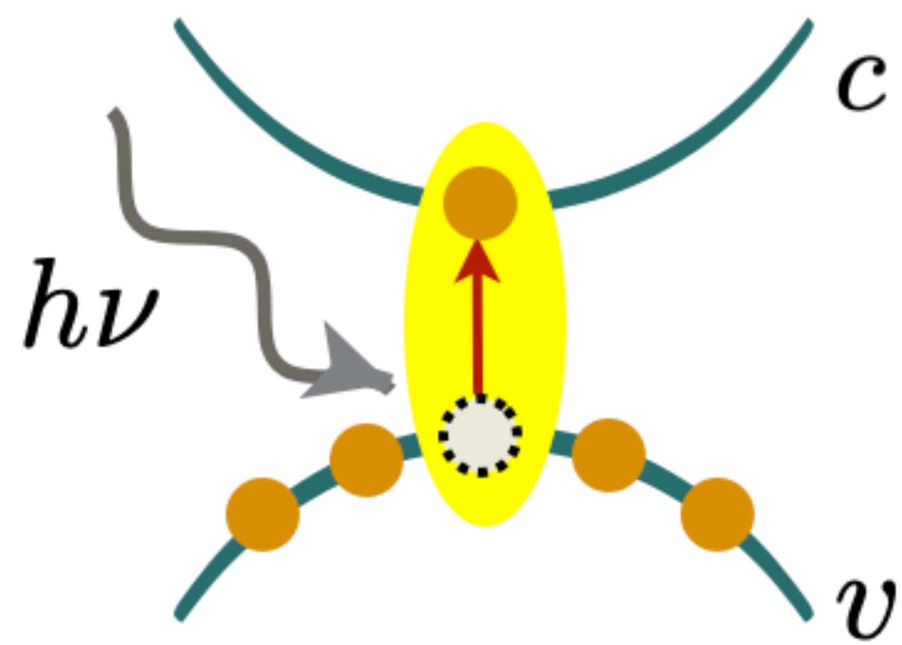
$$\Sigma(1,1') = v_H(1)\delta(1-1') + iv_c(1,2)\left.\frac{\delta G(1,2';[V_{ext}])}{\delta V_{ext}(2)}\right|_{V_{ext}=0} G^{-1}(2',1')$$

And now?

See next week!

2-body Green's function

- **Neutral excitations/Absorption spectrum**



The excited electron and the hole left behind interact

A two-particle correlation function is needed ($G^{(2)}$)

2-body Green's function

2-body Green's function

$$G^{(2)}(1,2,1',2') = (-i)^2 \langle N|\hat{T}[\hat{\psi}_H(1)\hat{\psi}_H(2)\hat{\psi}^\dagger_H(2')\hat{\psi}^\dagger_H(1')]|N\rangle$$

particle-particle

electron-hole

2-body Green's function

2-body Green's function

$$G^{(2)}(1,2,1',2') = (-i)^2 \langle N|\hat{T}[\hat{\psi}_H(1)\hat{\psi}_H(2)\hat{\psi}^\dagger_H(2')\hat{\psi}^\dagger_H(1')]|N\rangle$$

particle-particle

electron-hole

$t_1, t_{1'} > t_2, t_{2'}$ →

$$G^{(2),I}(1,2;1',2') = -\langle N|\hat{T}[\hat{\psi}(1)\hat{\psi}^\dagger(1')]\hat{T}[\hat{\psi}(2)\hat{\psi}^\dagger(2')]|N\rangle$$

$t_2, t_{2'} > t_1, t_{1'}$

$$= -\sum_{i=0}^{\infty}\langle N|\hat{T}[\hat{\psi}(1)\hat{\psi}^\dagger(1')]|N,i\rangle\langle N,i|\hat{T}[\hat{\psi}(2)\hat{\psi}^\dagger(2')]|N\rangle$$

$t_1, t_{2'} > t_2, t_{1'}$

$$= -\sum_{i=0}^{\infty}\chi_i(1,1')\tilde{\chi}_i(2,2')$$

$t_2, t_{1'} > t_1, t_{2'}$

$$= -\sum_{i=0}^{\infty}e^{i(E_0-E_i)\tau}\chi_i(x_1,x_{1'},\tau_1)\tilde{\chi}_i(x_2,x_{2'},\tau_2)$$

2-body Green's function

2-body Green's function

$$G^{(2)}(1,2,1',2') = (-i)^2 \langle N|\hat{T}[\hat{\psi}_H(1)\hat{\psi}_H(2)\hat{\psi}^\dagger_H(2')\hat{\psi}^\dagger_H(1')]|N\rangle$$

particle-particle

electron-hole

$$G^{(2),eh}(1,2,1',2') = G^{(2),I}(1,2,1',2')\Theta(\tau - |\tau_1|/2 - |\tau_2|/2)$$

$$+G^{(2),II}(1,2,1',2')\Theta(-\tau - |\tau_1|/2 - |\tau_2|/2)$$

$$+G^{(2),III}(1,2,1',2')\Theta(-(\tau_1-\tau_2)/2 - |-\tau+\tau_1/2+\tau_2/2|/2 - |\tau+\tau_1/2+\tau_2/2|)$$

$$+G^{(2),IV}(1,2,1',2')\Theta((\tau_1-\tau_2)/2 - |-\tau+\tau_1/2+\tau_2/2|/2 - |\tau+\tau_1/2+\tau_2/2|)$$

2-body Green's function

2-body Green's function

$$G^{(2)}(1,2,1',2') = (-i)^2 \langle N|\hat{T}[\hat{\psi}_H(1)\hat{\psi}_H(2)\hat{\psi}^\dagger_H(2')\hat{\psi}^\dagger_H(1')]|N\rangle$$

particle-particle

electron-hole

$$G^{(2),eh}(\tau_1,\tau_2,\omega) = \frac{1}{i}\lim_{\eta\to 0^+}\sum_{\omega_i}\frac{X_i(x_1,x_{1'},\tau_1)\tilde{X}_i(x_2,x_{2'},\tau_2)\text{sign}(\omega_i)}{\omega-\omega_i+i\eta\,\text{sign}(\omega_i)}$$

$$\omega_i = E_i - E_0$$

$$\times\exp\left\{\frac{i}{2}\text{sign}(\omega_i)[\omega-\omega_i][|\tau_1|+|\tau_2|]\right\}$$

$$+\text{contributions non singular at}\ \omega_i$$

2-body Green's function

- **2-body Green's function**

$$G^{(2)}(1,2,1',2') = (-i)^2 \langle N|\hat{T}[\hat{\psi}_H(1)\hat{\psi}_H(2)\hat{\psi}^\dagger_H(2')\hat{\psi}^\dagger_H(1')]|N\rangle$$

2-body Green's function

- **2-body Green's function**

$$G^{(2)}(1,2,1',2') = (-i)^2 \langle N | \hat{T}[\hat{\psi}_H(1)\hat{\psi}_H(2)\hat{\psi}^\dagger_H(2')\hat{\psi}^\dagger_H(1')] | N \rangle$$

How to get a Dyson equation for $G^{(2)}$?

2-body Green's function

- **2-body Green's function**

$$G^{(2)}(1,2,1',2') = (-i)^2 \langle N|\hat{T}[\hat{\psi}_H(1)\hat{\psi}_H(2)\hat{\psi}^\dagger_H(2')\hat{\psi}^\dagger_H(1')]|N\rangle$$

How to get a Dyson equation for $G^{(2)}$?

See next week!

2-body Green's function

- **2-body Green's function**

$$G^{(2)}(1,2,1',2') = (-i)^2 \langle N|\hat{T}[\hat{\psi}_H(1)\hat{\psi}_H(2)\hat{\psi}^\dagger_H(2')\hat{\psi}^\dagger_H(1')]|N\rangle$$

How to get a Dyson equation for $G^{(2)}$?

See next week!

Spoiler: use Schwinger relation

$$\frac{\delta G(1,1';[V_{ext}])}{\delta V_{ext}(2',2)} = -G^{(2)}(1,2;1',2^+;[V_{ext}]) + G(1,1';[V_{ext}])G(2,2^+;[V_{ext}])$$

n-body Green's function

Dyson equation

$$\left[\mathrm{i}\frac{d}{dt_k} - h(k)\right] G^{(n)}(1,...,n;1',...,n') = \sum_j (-1)^{k+j}\delta(k,j')G^{(n-1)}(1,...,\tilde{j},...,n;1',...,\tilde{k}',...,n')$$

$$-\mathrm{i}\int d\bar{1}v_c(k,\bar{1})G^{(n+1)}(1,...,n,\bar{1};1',...,n',\bar{1}^+)$$

$$G^{(n)}(\omega) = G_0^{(n)}(\omega) + G_0^{(n)}(\omega)\Sigma_n(\omega)G^{(n)}(\omega)$$

One can recast the EoM of the n-GF in a Dyson equation at the price of a very complicated self-energy…or

n-body Green's function

n-body self-energy

$$\Sigma_n(\omega) = G_0^{(n),-1} - G^{(n),-1}$$

$G_0^{(n)}$ defines the space in which the Dyson equation has to be solved

Express Σ_n in terms of Σ_2

n-body Green's function

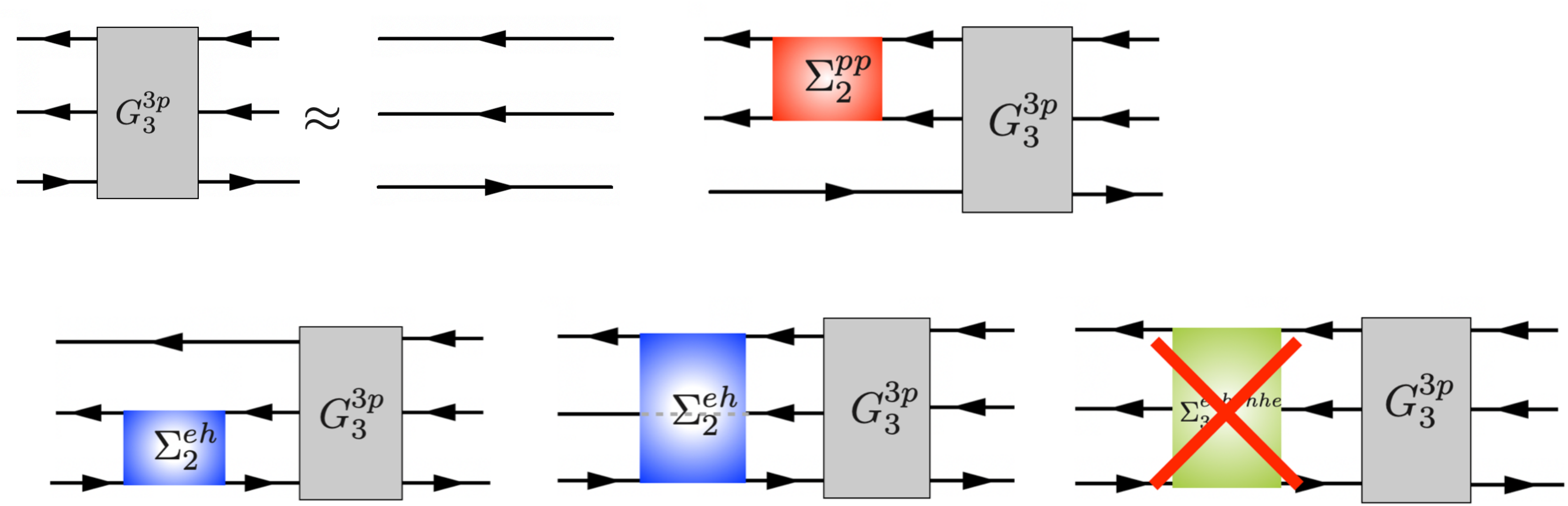
Example: the 3-GF

$$G_3(\omega) = G_{03}(\omega) + G_{03}(\omega)\Sigma_3(\omega)G_3(\omega)$$

$$G_{03}(\omega) = \begin{pmatrix} G_{01}(\omega) & 0 \\ 0 & G_{03}^{3p}(\omega) \end{pmatrix}$$

$$G_{01,(im)}(\omega) = \frac{\delta_{im}}{\omega - \epsilon_i + i\eta \mathrm{sign}(\epsilon_i - \mu)}$$

$$G^{3\mathrm{p}}_{03,(i>jl;m>ok)}(\omega) = \frac{\delta_{im}\delta_{jo}\delta_{lk}(f_i - f_l)(f_j - f_l)}{\omega - \epsilon_i^0 - (\epsilon_j^0 - \epsilon_l^0) + i\eta \mathrm{sign}(\epsilon_i^0 - \mu)}$$



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