# Introduction to Many-body Theory II

Part II : Feynman diagrams and the Green's function

- Why Green's functions?
  operator orderings and Wick's theorem
- Feynman diagrams and the self-energy
- The physical interpretation of the Green's function
- Spectral function and photo-emission

# Operator correlators

We have seen that the expansion of an expectation value leads to products of the form, so-called operator correlators

$$\mathcal{T}_\gamma \left\{ \hat{H}(z_1) \dots \hat{H}(z_n)\, \hat{O}(z) \right\}$$

We want to find an efficient way to evaluation such operator correlators.
Let us look at one of the simplest

$$\mathcal{T}_\gamma \left\{ \hat{O}_1(z_1) \hat{O}_2(z_2) \right\} = \theta(z_1, z_2)\, \hat{O}_1(z_1) \hat{O}_2(z_2) + \theta(z_2, z_1)\, \hat{O}_2(z_2) \hat{O}_1(z_1)$$

$$\theta(z_1, z_2) = \begin{cases} 1 & z_1 > z_2 \\ 0 & z_1 < z_2 \end{cases}$$

If we differentiate with respect to the contour times we can generate relations between various correlators

commutator

$$\frac{d}{dz_1}\mathcal{T}_\gamma\left\{\hat{O}_1(z_1)\hat{O}_2(z_2)\right\} = \delta(z_1,z_2)\left[\hat{O}_1(z_1),\hat{O}_2(z_2)\right] + \mathcal{T}_\gamma\left\{\frac{d}{dz_1}\hat{O}_1(z_1)\hat{O}_2(z_2)\right\}$$

where the contour delta function satisfies $\int_\gamma d\bar{z}\,\delta(z,\bar{z})\,A(\bar{z}) = A(z)$

For two fermionic field operators it is, however, more convenient to define

$$\mathcal{T}_\gamma\left\{\hat{O}_1(z_1)\hat{O}_2(z_2)\right\} = \theta(z_1,z_2)\,\hat{O}_1(z_1)\hat{O}_2(z_2) - \theta(z_2,z_1)\,\hat{O}_2(z_2)\hat{O}_1(z_1)$$

such that

anti-commutator

$$\frac{d}{dz_1}\mathcal{T}_\gamma\left\{\hat{O}_1(z_1)\hat{O}_2(z_2)\right\} = \delta(z_1,z_2)\left[\hat{O}_1(z_1),\hat{O}_2(z_2)\right]_+ + \mathcal{T}_\gamma\left\{\frac{d}{dz_1}\hat{O}_1(z_1)\hat{O}_2(z_2)\right\}$$

For example

$$\frac{d}{dz_1}\mathcal{T}_\gamma\left\{\hat{\psi}_H(\mathbf{x}_1,z_1)\hat{\psi}^\dagger_H(\mathbf{x}_2,z_2)\right\} = \delta(z_1,z_2)\delta(\mathbf{x}_1-\mathbf{x}_2) + \mathcal{T}_\gamma\left\{\frac{d}{dz_1}\hat{\psi}_H(\mathbf{x}_1,z_1)\hat{\psi}^\dagger_H(\mathbf{x}_2,z_2)\right\}$$

For a general string of fermionic operators we define

$$\mathcal{T}_\gamma \left\{ \hat{O}_1 \dots \hat{O}_n \right\} = (-1)^P \hat{O}_{P(1)} \dots \hat{O}_{P(n)} \quad z_{P(1)} > \dots > z_{P(n)}$$

where $\hat{O}_j = \hat{O}_j(z_j)$

We just put the operators in the correct order and add a plus/minus sign depending on whether the final permutation was even/odd

from this definition it follows that

$$\mathcal{T}_\gamma \left\{ \hat{O}_1 \dots \hat{O}_n \right\} = (-1)^P \mathcal{T}_\gamma \left\{ \hat{O}_{P(1)} \dots \hat{O}_{P(n)} \right\}$$

We further define that operators at equal time are kept in their relative order. For example

$$\mathcal{T}_\gamma \left\{ \psi(\mathbf{x}_1 z_1) \hat{\psi}^\dagger(\mathbf{x}_2 z_2) \hat{\psi}(\mathbf{x}_2 z_2) \right\} = -\mathcal{T}_\gamma \left\{ \hat{\psi}^\dagger(\mathbf{x}_2 z_2) \psi(\mathbf{x}_1 z_1) \hat{\psi}(\mathbf{x}_2 z_2) \right\}$$
$$= \mathcal{T}_\gamma \left\{ \hat{\psi}^\dagger(\mathbf{x}_2 z_2) \hat{\psi}(\mathbf{x}_2 z_2) \psi(\mathbf{x}_1 z_1) \right\} = \hat{\psi}^\dagger(\mathbf{x}_2 z_2) \hat{\psi}(\mathbf{x}_2 z_2) \psi(\mathbf{x}_1 z_1) \quad z_2 > z_1$$

It follows that operators containing an even number of equal time field operators (such as the Hamiltonian) commute under the time-ordered product, in agreement with our earlier definition

If we expand an expectation value in powers of one- or two-body interactions we obtain strings with an equal number of annihilation and creation operators. The most general such string has the form

$$\hat{G}_n(1\ldots,n;1'\ldots n') = (-i)^n \mathcal{T}_\gamma \left\{ \hat{\psi}(1)\ldots\hat{\psi}(n)\hat{\psi}^\dagger(n')\ldots\hat{\psi}^\dagger(1') \right\}$$

$$j = \mathbf{x}_j z_j$$

From the equation of motion of the field operator

$$[i\partial_t - h(\mathbf{x}t)]\,\hat{\psi}_H(\mathbf{x},t) = \int d\mathbf{y}\, w(\mathbf{x},\mathbf{y})\,\hat{n}_H(\mathbf{y}t)\hat{\psi}_H(\mathbf{x}t)$$

we can derive equations of motion for the operators $\hat{G}_n$

We find

$$i\frac{d}{dz_k}\hat{G}_n(1\dots n;1'\dots n') = (-i)\mathcal{T}_\gamma\left\{\hat{\psi}_H(1)\dots\left(i\frac{d}{dz_k}\hat{\psi}_H(k)\right)\dots\hat{\psi}_H(n)\hat{\psi}^\dagger_H(n')\dots\hat{\psi}^\dagger_H(1')\right\}$$
$$+\sum_{j=1}^{n}(-1)^{k+j}\delta(k,j')\,\hat{G}_{n-1}(1\dots\overset{\sqcap}{j}\dots n;1'\dots\overset{\sqcap}{k'}\dots n')$$

Which can be rewritten as

$$\left[i\frac{d}{dz_k}-h(k)\right]\hat{G}_n(1\dots n;1'\dots n') = -i\int d\bar{1}w(k,\bar{1})\,\hat{G}_{n+1}(1\dots n,\bar{1};1'\dots n',\bar{1}^+)$$
$$+\sum_{j=1}^{n}(-1)^{k+j}\delta(k,j')\,\hat{G}_{n-1}(1\dots\overset{\sqcap}{j}\dots n;1'\dots\overset{\sqcap}{k'}\dots n')$$

We therefore obtain a set of hierarchy equations for the correlators $\hat{G}_n$

The first equation in this hierarchy is

$$\left[i\frac{d}{dz_1} - h(1)\right] \hat{G}_1(1;1') = \delta(1,1') - i\int d\bar{1}\, w(1,\bar{1})\, \hat{G}_2(1,\bar{1};1',\bar{1}^+)$$

An example of an equation higher in the hierarchy is

$$\left[i\frac{d}{dz_2} - h(2)\right] \hat{G}_2(1,2;1',2') = -\,\delta(2,1')\, \hat{G}_1(1;2') + \delta(2,2')\, \hat{G}_1(2;2') - i\int d\bar{1}\, w(2,\bar{1})\, \hat{G}_3(1,2,\bar{1};1',2',\bar{1}^+)$$

In a next step we will convert these operator equations into differential equations

# Many-particle Green's function

The n-particle Green's function is defined as

$$G_n(1\dots n;1'\dots n') = \frac{\mathrm{Tr}\ \left[e^{-\beta\hat{H}^M}\hat{G}_n(1\dots n;1'\dots n')\right]}{\mathrm{Tr}\ \left[e^{-\beta\hat{H}^M}\right]}$$

or equivalently

$$G_n(1\dots n;1'\dots n') = (-i)^n \frac{\mathrm{Tr}\ \left[\mathcal{T}_\gamma\left\{e^{-i\int_\gamma d\bar{z}\hat{H}(\bar{z})}\hat{\psi}(1)\dots\hat{\psi}(n)\hat{\psi}^\dagger(n')\dots\hat{\psi}^\dagger(1')\right\}\right]}{\mathrm{Tr}\ \left[\mathcal{T}_\gamma\left\{e^{-i\int_\gamma d\bar{z}\hat{H}(\bar{z})}\right\}\right]}$$

The n-particle Green's function satisfies the same set of differential equations as the correlators $\hat{G}_n$

## Martin-Schwinger hierarchy

$$\left[i\frac{d}{dz_k} - h(k)\right] G_n(1\dots n; 1'\dots n') = -i\int d\bar{1} w(k,\bar{1})\, G_{n+1}(1\dots n,\bar{1}; 1'\dots n',\bar{1}^+)$$
$$+\sum_{j=1}^{n}(-1)^{k+j}\delta(k,j')\, G_{n-1}(1\dots \overset{\sqcap}{j}\dots n; 1'\dots \overset{\sqcap}{k'}\dots n')$$

(plus a set of similar equations with respect to the primed coordinates)

The hierarchy equations need to be solved with the boundary conditions

$$G_k(\dots, t_0, \dots) = -G_k(\dots, t_0 - i\beta, \dots)$$

which are known as the Kubo-Martin-Schwinger (KMS) boundary conditions (which can be derived from the definition of the Green's functions)

From the n-particle Green's function we can calculate any n-body observable

For example, if $\hat{O}(t)$ is a 1-body operator :

$$\hat{O}(t) = \int d\mathbf{x}\, \hat{\psi}^\dagger(\mathbf{x}) o(\mathbf{x}, t) \hat{\psi}(\mathbf{x})$$

then

$$\langle \hat{O}(t) \rangle = -i \int d\mathbf{x}\, o(\mathbf{x}, t)\, G(\mathbf{x}z, \mathbf{x}'z^+)|_{\mathbf{x}=\mathbf{x}', z=t}$$

The calculation of n-body observables is therefore possible once we know how to solve the Martin-Schwinger hierarchy equations. How to do this?

Further insight in the hierarchy is obtained by considering a non-interacting system which has the n-particle Green's function

$$g_n(1 \ldots n, 1' \ldots n') = \frac{1}{i^n} \frac{\mathrm{Tr}\ \mathcal{T} \left\{ e^{-i \int_\gamma dz\, \hat{H}_0(z)} \hat{\psi}(1) \ldots \hat{\psi}(n) \hat{\psi}^\dagger(n') \ldots \hat{\psi}^\dagger(1') \right\}}{\mathrm{Tr}\ \mathcal{T} \left\{ e^{-i \int_\gamma dz\, \hat{H}_0(z)} \right\}}$$

The Martin-Schwinger hierarchy becomes

$$\left[i\frac{d}{dz_k} - h(k)\right] g_n(1\ldots n;1'\ldots n') = \sum_{j=1}^{n}(-1)^{k+j}\delta(k,j')\, g_{n-1}(1\ldots \overset{\sqcap}{j}\ldots n;1'\ldots \overset{\sqcap}{k'}\ldots n')$$

The solution to this equation is

$$g_n(1\ldots n,1'\ldots n') = \begin{vmatrix} g(1,1') & \ldots & g(1,n') \\ \vdots & & \vdots \\ g(n,1') & \ldots & g(n,n') \end{vmatrix}$$

where we denote $g(1,1') = g_1(1,1')$

This is known as Wick's theorem

The proof of this identity is easy: Apply the operators

$$i\,\partial_{z_j} - h(\mathbf{x}_j, z_j) \qquad\qquad h(\mathbf{x}, z) = -\frac{1}{2}\nabla^2 + v(\mathbf{x}, z)$$

on both sides of the equation and check that we recover the Martin-Schwinger equations with the correct boundary conditions

To use Wick's theorem we need to solve

$$(i\,\partial_{z_j} - h(j))g(j, j') = \delta(j, j') \qquad\qquad (-i\,\partial_{z'_j} - h(j'))g(j, j') = \delta(j, j')$$

with the KMS boundary conditions. This is an easy problem in practice.

# Many-particle Green's function: Take home message

- The main motivation for defining the n-particle Green's function is that it for this object we can derive a set of coupled hierarchy equations, known as the Martin-Schwinger hierarchy, which forms a the basis for a systematic perturbation theory

- From the n-particle Green's function we can calculate n-body observables

- From the Martin-Schwinger hierarchy for a non-interacting system it is easy to derive an explicit expression for the n-particle Green's function in terms of the one-particle Green's function.
This expression is known as Wick's theorem and forms the basis of many-body perturbation theory

# Perturbation expansion

Wick's theorem allows for an expansion of the n-particle Green's function in powers of the non-interacting one-particle Green's function.

Let us illustrate this procedure for the one-particle Green's function given by

$$G(1,1') = \frac{1}{i}\frac{\mathrm{Tr}\ \mathcal{T}\left\{e^{-i\int_\gamma dz\,\hat{H}(z)}\hat{\psi}(1)\hat{\psi}^\dagger(1')\right\}}{\mathrm{Tr}\ \mathcal{T}\left\{e^{-i\int_\gamma dz\,\hat{H}(z)}\right\}}$$

We can expand this expression in powers of the two-body interaction

For the numerator we have

$$\mathrm{Tr}\ \mathcal{T}\left\{e^{-i\int_\gamma dz\,(\hat{H}_0(z)+\hat{W}(z))}\hat{\psi}(\mathbf{x}z)\hat{\psi}^\dagger(\mathbf{x}'z')\right\}$$

$$=\sum_{n=0}^{\infty}\frac{(-i)^n}{n!}\int_\gamma dz_1\ldots dz_n\,\mathrm{Tr}\ \mathcal{T}\left\{e^{-i\int_\gamma dz\,\hat{H}_0(z)}\hat{\psi}(\mathbf{x}z)\hat{\psi}^\dagger(\mathbf{x}'z')\hat{W}(z_1)\ldots\hat{W}(z_n)\right\}$$

The integrand has the form

$$\mathrm{Tr}\ \mathcal{T}\left\{e^{-\beta\hat{H}^M}\hat{\psi}_{H_0}(\mathbf{x}z)\hat{\psi}^\dagger_{H_0}(\mathbf{x}'z')\hat{W}_{H_0}(z_1)\ldots\hat{W}_{H_0}(z_n)\right\}=$$

$$\left(\prod_{j=1}^{n}\frac{1}{2}\int d\mathbf{x}_j d\mathbf{x}'_j w(\mathbf{x}_j,\mathbf{x}'_j)\right)\mathrm{Tr}\ \mathcal{T}\left\{e^{-\beta\hat{H}^M}\hat{\psi}_{H_0}(\mathbf{x}z)\hat{\psi}^\dagger_{H_0}(\mathbf{x}'z')\prod_{k=1}^{n}\hat{\psi}^\dagger_{H_0}(\mathbf{x}_k z_k)\hat{\psi}^\dagger_{H_0}(\mathbf{x}'_k z_k)\hat{\psi}_{H_0}(\mathbf{x}'_k z_k)\hat{\psi}_{H_0}(\mathbf{x}_k z_k)\right\}$$

This can be rewritten as a non-interacting (2n+1)-particle Green's function

This gives the following expansion for the one-particle Green's function

$$G(a,b) = \frac{\sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{i}{2}\right)^k \int w(1,1') \dots w(k,k')\, g_{2k+1}(a,1,1',\dots;b,1^+,1'^+,\dots)}{\sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{i}{2}\right)^k \int w(1,1') \dots w(k,k')\, g_{2k}(1,1',\dots;1^+,1'^+,\dots)}$$

$$w(1,1') = w(\mathbf{x}_1,\mathbf{x}_2)\delta(z_1,z_1')$$

Using Wick's theorem we can now replace the non-interacting n-particle Green's functions by determinants

This gives the perturbation expansion for the Green's function :

$$G(a,b) = \frac{\sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{i}{2}\right)^k \int w(1,1') \dots w(k,k') \begin{vmatrix} g(a,b) & g(a,1^+) & \dots & g(a,k'^+) \\ g(1,b) & g(1,1^+) & \dots & g(1,k'^+) \\ \vdots & \vdots & & \vdots \\ g(k',b) & g(k',1^+) & \dots & g(k',k'^+) \end{vmatrix}}{\sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{i}{2}\right)^k \int w(1,1') \dots w(k,k') \begin{vmatrix} g(1,1^+) & g(1,1'^+) & \dots & g(1,k'^+) \\ g(1',1^+) & g(1',1'^+) & \dots & g(1',k'^+) \\ \vdots & \vdots & & \vdots \\ g(k',1^+) & g(k',1'^+) & \dots & g(k',k'^+) \end{vmatrix}}$$

It is now only a technical matter to evaluate these terms

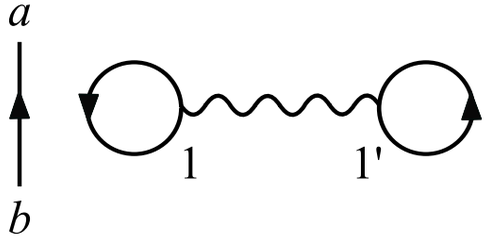
This leads to Feynman diagrams. Let us give an example an expand the numerator N(a,b) to first order

Expanding the 3x3 determinant along the first column we find

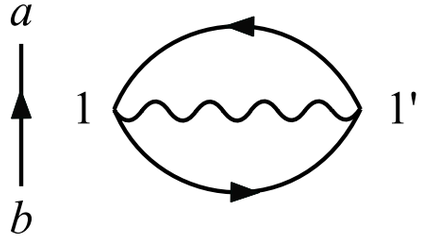
$$N^{(1)}(a;b) = \frac{i}{2} g(a;b) \int d1 d1' w(1,1') \begin{vmatrix} g(1;1^+) & g(1;1'^+) \\ g(1';1^+) & g(1';1'^+) \end{vmatrix}$$

$$\pm \frac{i}{2} \int d1 d1' w(1,1') g(1;b) \begin{vmatrix} g(a;1^+) & g(a;1'^+) \\ g(1';1^+) & g(1';1'^+) \end{vmatrix}$$

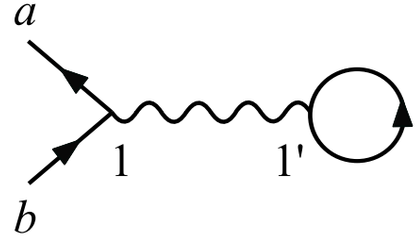
$$+ \frac{i}{2} \int d1 d1' w(1,1') g(1';b) \begin{vmatrix} g(a;1^+) & g(a;1'^+) \\ g(1;1^+) & g(1;1'^+) \end{vmatrix}$$



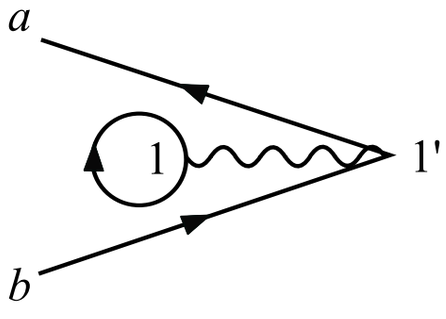

(*b*,1,1')



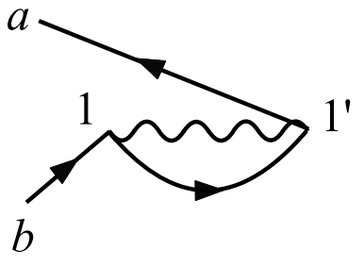

(*b*,1',1)



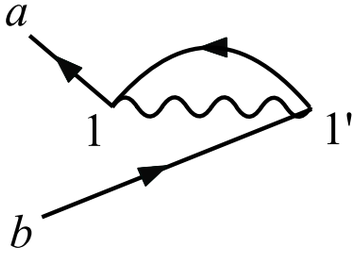

(1,*b*,1')




(1',1,*b*)




(1',*b*,1)

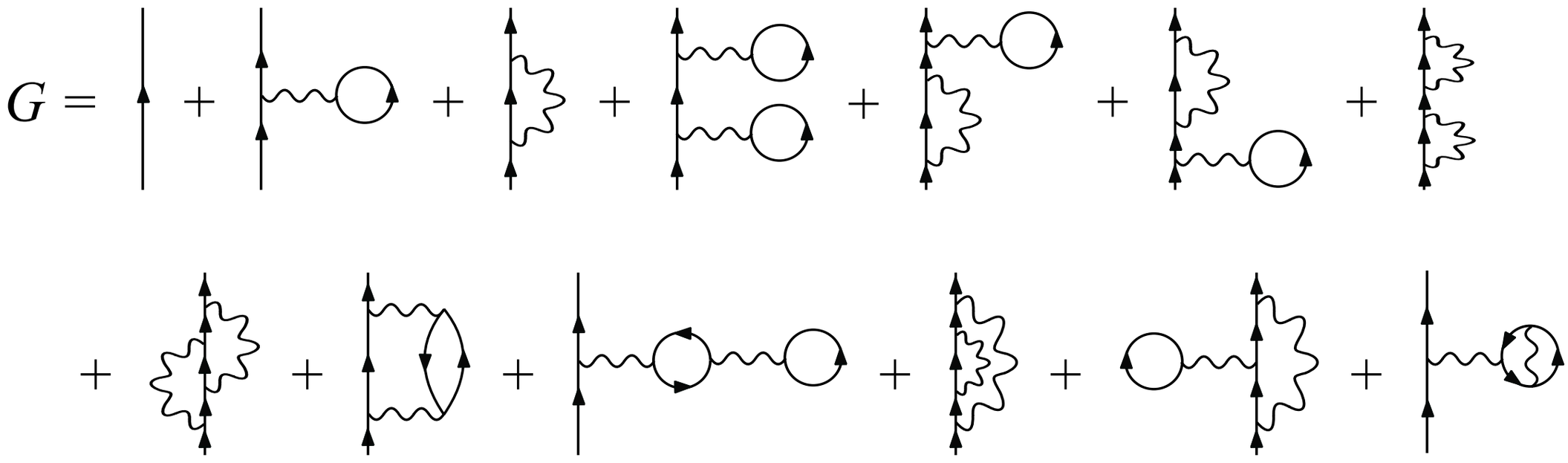



(1,1',*b*)

It is not difficult to prove that the disconnected diagrams from the numerator are cancelled by those of the denominator and we can further simplify to

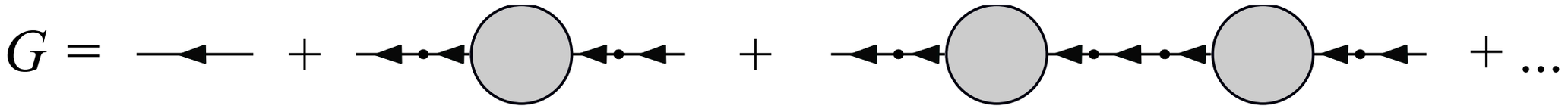
$$G(a,b) = \sum_{k=0}^{\infty} i^k \int w(1,1') \dots w(k,k') \left| \begin{array}{cccc} g(a,b) & g(a,1^+) & \dots & g(a,k'^+) \\ g(1,b) & g(1,1^+) & \dots & g(1,k'^+) \\ \vdots & \vdots & & \vdots \\ g(k',b) & g(k',1^+) & \dots & g(k',k'^+) \end{array} \right|_{CTI}$$

where in the expansion of the determinant we retain only the connected (C) and topologically inequivalent (TI) terms

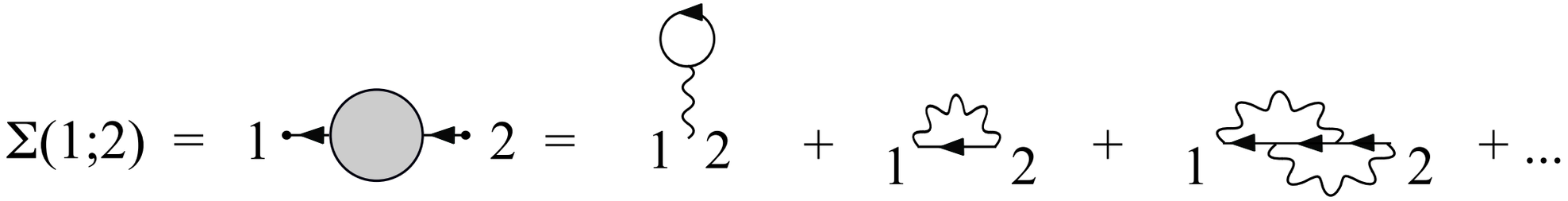


# Self energy

The expansion of G has the structure



where the self-energy is defined as the sum over irreducible diagrams
(i.e. can not be cut in two by cutting one g-line)

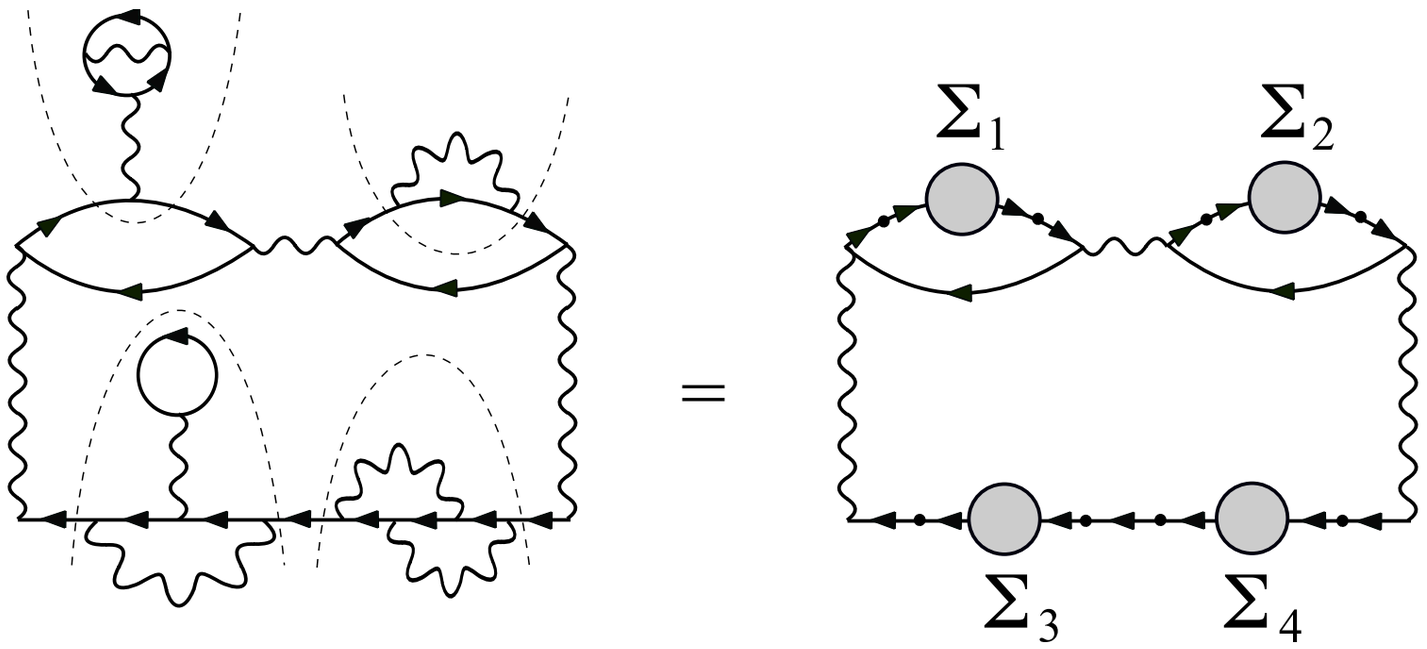


The Green's function thus satisfies the equation

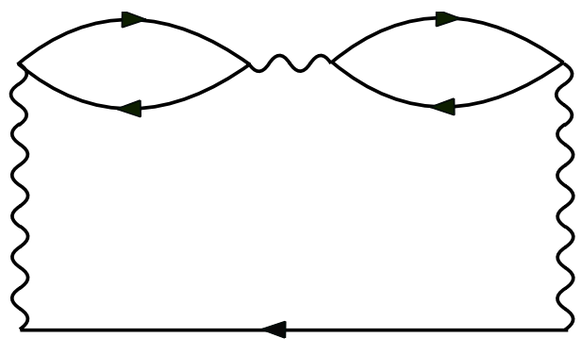
$$G(1,2) = g(1,2) + \int_\gamma d3d4\, g(1,3)\, \Sigma[g](3,4)\, G(4,2)$$

# Skeletons

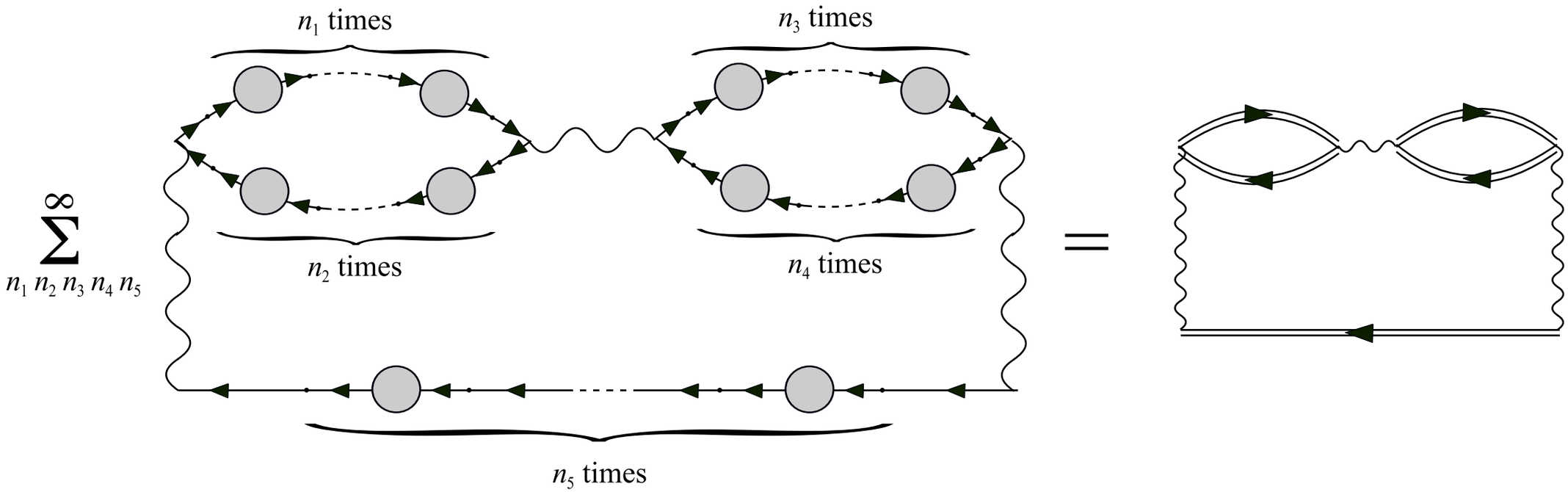
A skeleton diagram is a diagram without self-energy insertions, for example



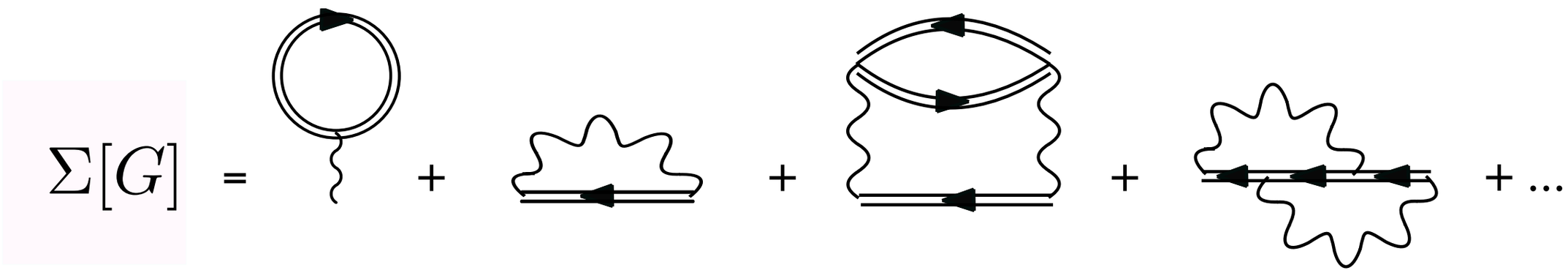

The corresponding skeleton is therefore



By replacing ‘g’ by ‘G’ in the skeleton we sum over all self-energy insertions




It follows that




where we sum over all dressed irreducible skeletons in terms of G

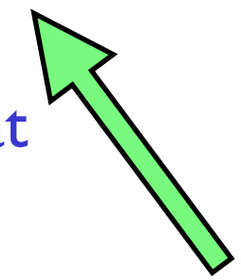
We therefore find the Dyson equation

$$G(1,2) = g(1,2) + \int_\gamma d3d4\, g(1,3)\, \Sigma[G](3,4)\, G(4,2)$$

or, if we use the equation of motion for g : $(i\,\partial_{z_1} - h(1))g(1,2) = \delta(1,2)$

$$(i\partial_{z_1} - h(1))G(1,1') = \delta(1,1') + \int_\gamma d2\, \Sigma[G](1,2)\, G(2,1')$$

This is a self-consistent equation of motion for the Green's function that needs to be solved with the boundary conditions



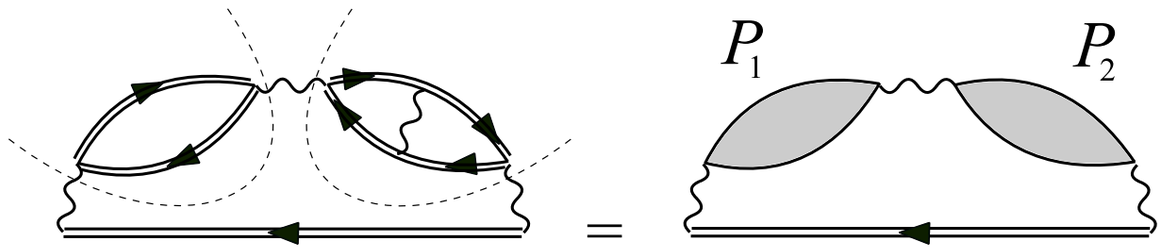
Kadanoff-Baym equations

$$G(\mathbf{x}_1 t_0 - i\beta, 2) = -G(\mathbf{x}_1 t_0, 2)$$

$$G(1, \mathbf{x}_2 t_0) = -G(1, \mathbf{x}_2 t_0 - i\beta)$$

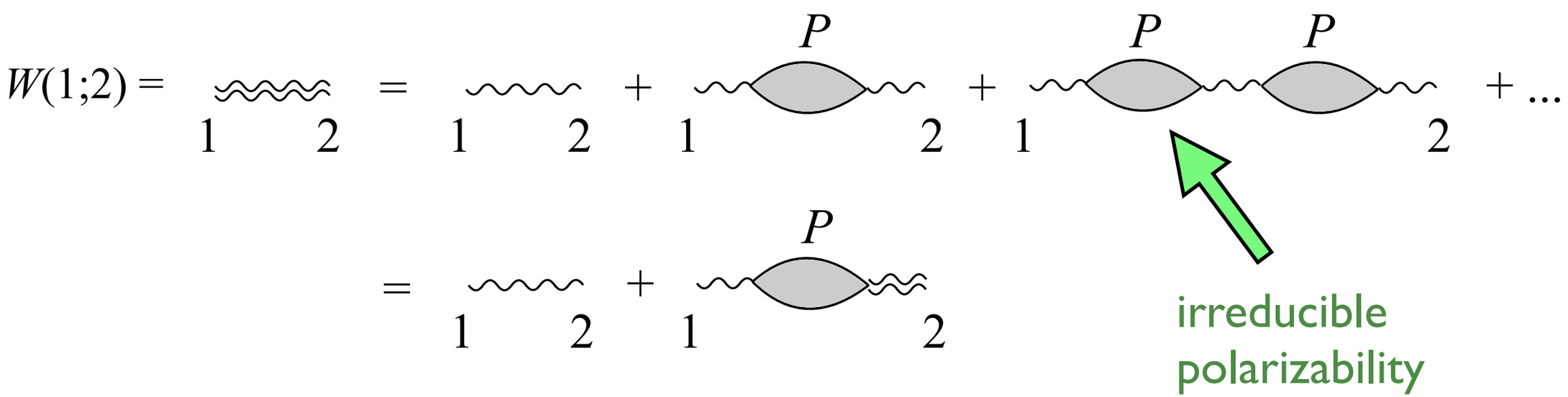
# W-skeletons

We can further renormalize the interaction lines, by removing all interaction line insertions. For example





We can then define the screened interaction W by



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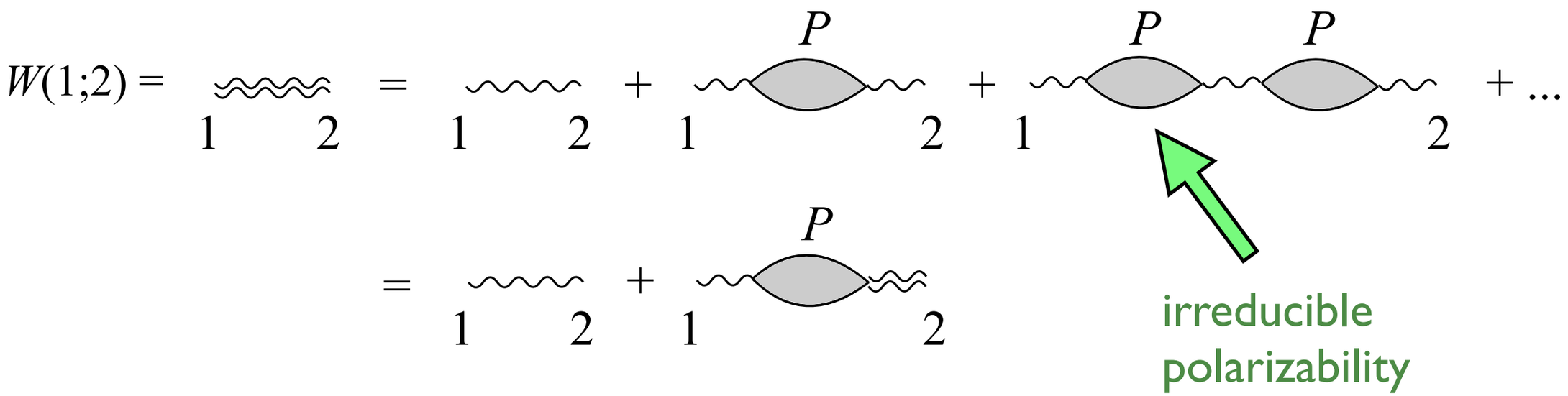
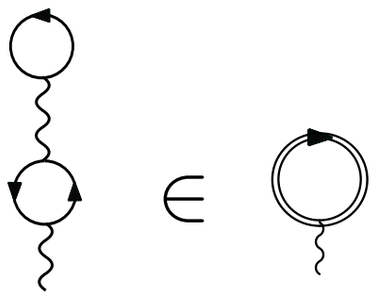



In formula

$$W(1,2) = w(1,2) + \int d3d4\, w(1,3)\, P(3,4)\, W(4,2)$$

We can then in W-skeletonic diagrams replace w by W with the exception of the Hartree diagram. We have

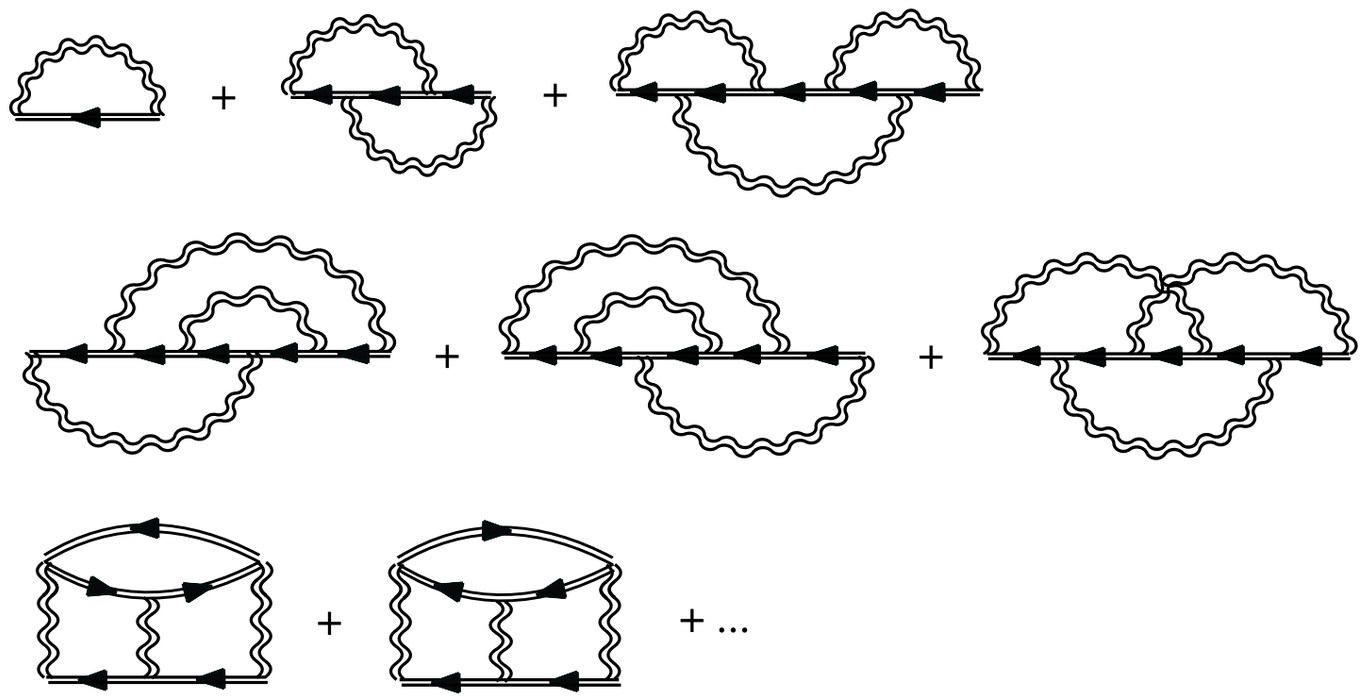


$$\Sigma = \Sigma_{ss}[G,W] = \Sigma_H[G,w] + \Sigma_{ss,\mathrm{xc}}[G,W]$$

double skeletonic

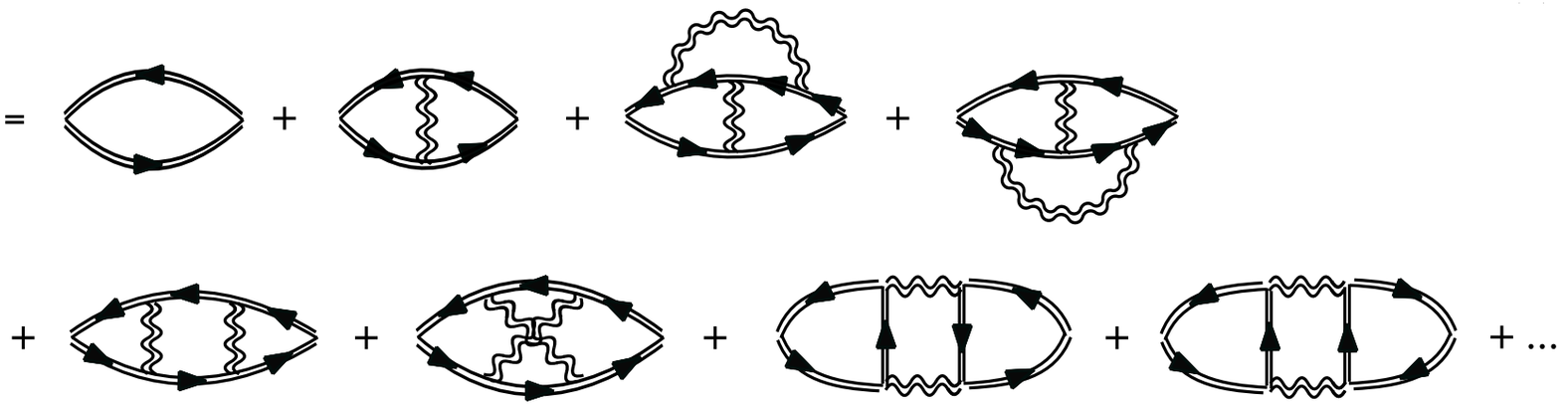
# This gives the double-skeletonic expansion for the self-energy

$\Sigma_{ss,\mathrm{xc}}[G,W]$ =



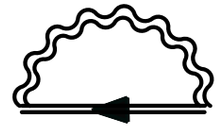
# and the polarizability

$P_{ss}[G,W]$ =

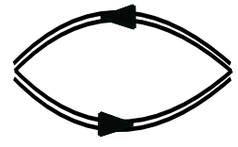


## The lowest order in W gives the GW approximation

$$\Sigma_{ss,\mathrm{xc}}(1,2) = -i\,G(1,2)W(1,2)$$



$$P(1,2) = -i\,G(1,2)G(2,1)$$



$$W(1,2) = w(1,2) + \int d3d4\, w(1,3)\, P(3,4)\, W(4,2)$$

$$G(1,2) = g(1,2) + \int_\gamma d3d4\, g(1,3)(\Sigma_H[G,w](3,4) + \Sigma_{ss,\mathrm{xc}}[G,W](3,4))\, W(4,2)$$

These form a self-consistent set of equations for G and W

# Diagrammatic expansion: Take home message

- Wick's theorem allows for a straightforward expansion of the Green's function in powers of the interaction

- The number of diagrammatic terms can be drastically reduced by introduction of the self-energy.

- The self-energy can be expanded in powers of the dressed Green's function and the screened interaction W by the introduction of skeletonic diagrams. This leads to self-consistent equations in terms of G and W.

- The lowest order in this expansion is the famous GW approximation

# Contours and formalisms

Let us now briefly clarify some issues that may confuse you in practice, namely the different flavours of many-body theory.

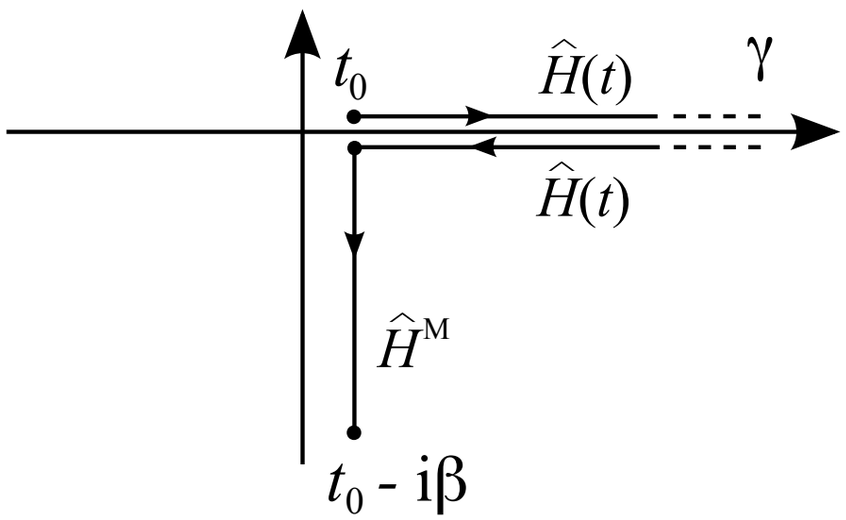
With different assumptions we can modify the contour

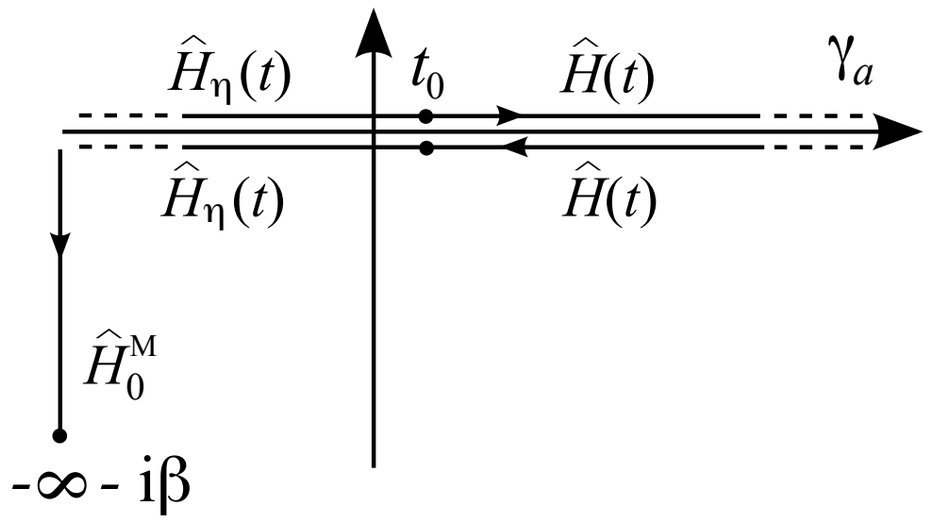
Adiabatic assumption

$$\hat{H}(t_\pm) = \begin{cases} \hat{H}_\eta(t) = \hat{H}_0 + e^{-\eta|t-t_0|}\hat{H}_{\rm int} & \text{for } t < t_0 \\ \hat{H}(t) = \hat{H}_0(t) + \hat{H}_{\rm int} & \text{for } t > t_0 \end{cases}$$

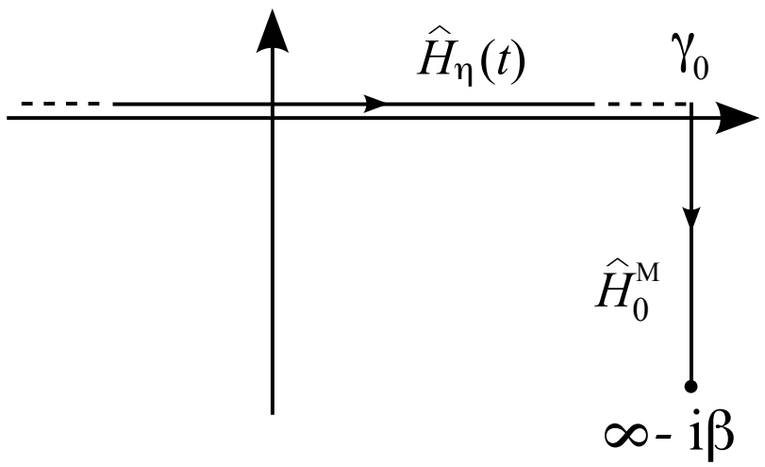
$$\hat{H}(z \in \gamma^{\rm M}) = \hat{H}_0^{\rm M} = \hat{H}_0 - \mu\hat{N},$$

$$\hat{\rho} = \frac{e^{-\beta\hat{H}^{\rm M}}}{Z} = \hat{U}_\eta(t_0, -\infty)\,\frac{e^{-\beta\hat{H}_0^{\rm M}}}{Z_0}\,\hat{U}_\eta(-\infty, t_0)$$



$$\hat{\rho}_0 = \hat{U}_\eta(-\infty, \infty)\, \hat{\rho}_0\, \hat{U}_\eta(\infty, -\infty)$$




## Zero-temperature assumption

When expanding in powers of the interaction only the terms on the real axis remain. This leads to 3 variants

1) Full formalism with the Matsubara approach
   (equilibrium finite temperature) as an initial case

2) Keldysh formalism (adiabatic assumption)

3) Zero-temperature standard time-ordered formalism
   (zero-temperature assumption)

In all the 3 formulations all diagrammatical expressions is identical.
The only thing that changes is the way the final integrals in the Feynman diagrams are done.

If we denote $\langle \hat{A} \rangle = \mathrm{Tr}\ \hat{\rho}\hat{A}$ then the Green's function has the structure

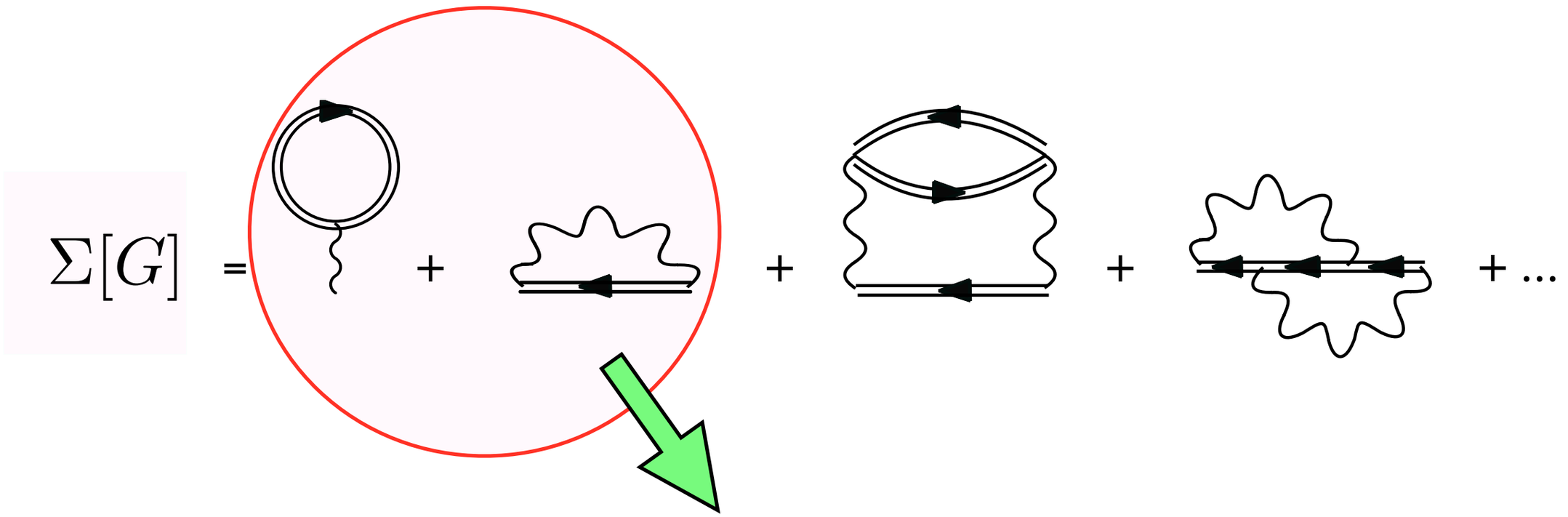
$$G(1,2) = -i\langle \mathcal{T}\left\{\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\right\}\rangle = \theta(z_1,z_2)\,G^{>}(1,2) + \theta(z_1,z_2)\,G^{<}(1,2)$$

Only information on the contour is in the Heaviside functions

Real-time functions

$$G^{>}(1,2) = -i\langle \hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\rangle \quad \text{Propagation of a "particle" (added electron)}$$

$$G^{<}(1,2) = i\langle \hat{\psi}_H^\dagger(2)\hat{\psi}_H(1)\rangle \quad \text{Propagation of a "hole" (removed electron)}$$




$$\Sigma^{\rm HF}(1,2) \sim \delta(z_1, z_2)$$

Hartree-Fock type diagrams are instantaneous since the Coulomb interaction is

The self-energy has the structure

$$\Sigma(1,2) = \Sigma^{\rm HF}(1,2) + \theta(z_1, z_2)\,\Sigma^{>}(1,2) + \theta(z_2, z_1)\,\Sigma^{<}(1,2)$$

A general contour function has the structure

$$k(z, z') = k^{\delta}(t)\,\delta(z, z') + \theta(z, z')\,k^{>}(t, t') + \theta(z', z)\,k^{>}(t, t')$$

One often needs to do integrals of the form

$$c(z,z') = \int_\gamma dz''\, a(z,z'')\, b(z'',z')$$

There are simple rules to convert these into real time functions.
For example, on the original contour:

$$c^< = a^< \cdot b^A + a^R \cdot b^< + a^\rceil \star b^\lceil$$

where

$$f \cdot g = \int_{t_0}^{\infty} f(t)g(t) \qquad\qquad f \star g = \int_0^\beta d\tau\, f(\tau)g(\tau)$$

and

$$c^R(t,t') = c^\delta(t)\delta(t-t') + \theta(t-t')[c^>(t,t') - c^<(t,t')] \qquad c^\lceil(\tau,t) = c(t_0 - i\tau, t)$$
$$c^A(t,t') = c^\delta(t)\delta(t-t') - \theta(t'-t)[c^>(t,t') - c^<(t,t')] \qquad c^\rceil(t,\tau) = c(t, t_0 - i\tau)$$

In this lecture I will not elaborate further on these so-called Langreth rules

# Different contours: Take home message

- The original contour can be deformed at the expense of additional approximations

- The adiabatic assumption leads to the standard Keldysh formalism without a vertical track

- The zero-temperature assumption leads to the standard time-ordered formalism restricted to equilibrium zero-temperature systems

- All equations of the three formalism are identical.
  Only the translation of the final contour integrals to real-time functions is different but in all cases straightforward.

# Green's function: Physical interpretation

We remove a particle from state j at time t. After this the system is left in a superposition of eigenstates of the ionized system

$$|\tilde{\Psi}_j(t)\rangle = \hat{U}(T,t)\,\hat{a}_j\,\hat{U}(t,t_0)|\Psi_0\rangle = e^{-i\hat{H}(T-t)}\sum_s |N-1,s\rangle\langle N-1,s|\hat{a}_j\,e^{-i\hat{H}(t-t_0)}|\Psi_0\rangle$$

$$= \sum_s e^{-iE_{N-1,s}(T-t)}e^{-iE_0(t-t_0)}c_{s,j}\,|N-1,s\rangle$$

where

$$c_{s,j} = \langle N-1,s|\hat{a}_j|\Psi_0\rangle$$

The probability to find the system in (N-1)-particle state after removal of the particle is then

$$P_{s,j} \propto |c_{s,j}|^2 = |\langle N-1,s|\hat{a}_j|\Psi_0\rangle|^2$$

The diagonal lesser Green's function has the form

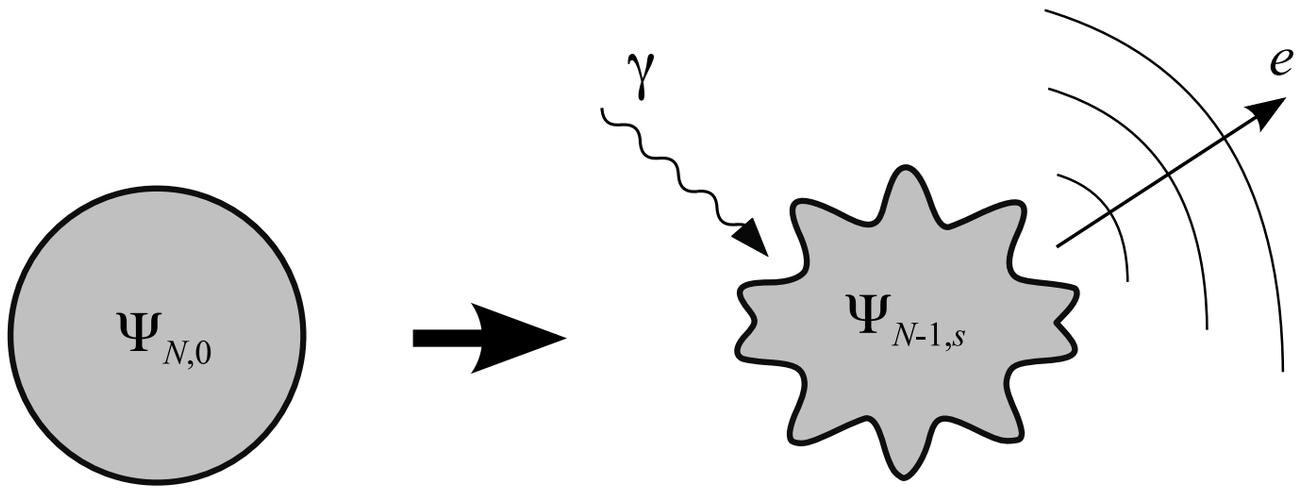
$$-i\,G^{<}_{jj}(t,t') = \langle\Psi_0|\hat{a}^{\dagger}_{j,H}(t')\hat{a}_{j,H}(t)|\Psi_0\rangle = \langle\tilde{\Psi}_j(t')|\tilde{\Psi}_j(t)\rangle = \sum_s |c_{s,j}|^2\, e^{-i(E_0-E_{N-1,s})(t-t')}$$

It will be convenient to write this in frequency space

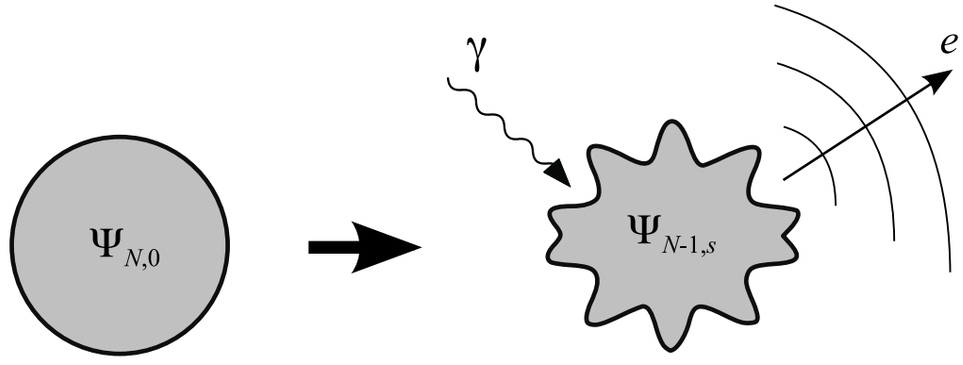
$$G^{<}_{jj}(t-t') = \int \frac{d\omega}{2\pi}\, G_{jj}(\omega)\, e^{-i\omega(t-t')}$$

$$-i\,G^{<}_{jj}(\omega) = 2\pi \sum_s |c_{s,j}|^2\, \delta(\omega - (E_0 - E_{N-1,s}))$$

Let us now see how this relates to a photo-current in a photo-emission experiment



## Electron-light interaction




$$\hat{H}_{l-e}(t) = \sum_{ij} (h_{ij}\, e^{i\omega_0 t} + h^*_{ij}\, e^{-i\omega_0 t})\, \hat{a}^\dagger_i \hat{a}_j$$

photon energy

## Fermi's Golden Rule

$$P_{0\to m} = 2\pi |\langle \Psi_{N,m}| \sum_{ij} h^*_{ij}\, \hat{a}^\dagger_i \hat{a}_j |\Psi_{N,0}\rangle|^2\, \delta(\omega_0 - (E_{N,m} - E_{N,0}))$$

Final states (sudden approximation) : $\quad |\Psi_{N,m}\rangle = \hat{a}^\dagger_\epsilon\, |\Psi_{N-1,s}\rangle$

$$P_s(\epsilon) = 2\pi |\langle \Psi_{N-1,s}| \sum_{j} h^*_{\epsilon j}\, \hat{a}_j |\Psi_{N,0}\rangle|^2\, \delta(\omega_0 - \epsilon - (E_{N-1,s} - E_{N,0}))$$

kinetic energy
photo-electron

The photo-current is then given by

$$I_{\rm ph}(\epsilon) \propto \sum_s P_s(\epsilon) = -i \sum_{j,j'} h^*_{\epsilon j} h_{\epsilon j'}\, G^<_{jj'}(\epsilon - \omega_0)$$

Similarly in an inverse photo-emission experiment the light intensity is given by i $G^>$

These two quantities are often combined in a single function known as the spectral function

$$A_{ij}(\omega) = i\left[G^>_{ij}(\omega) - G^<_{ij}(\omega)\right] = -2\,\mathrm{Im}\, G^R_{ij}(\omega)$$

$$A_{ii}(\omega) \geq 0$$

This equality follows from short manipulations which are omitted here

# Physical interpretation: Take home message

- The hole and particle Green's functions relate directly to the spectra measured in photo-emission and inverse photo-emission experiments

- These spectra contain information on band structure and probabilities for various inelastic events

- The renormalisation and broadening of the main single-particle peak due to interactions in metallic systems leads to a quasi-particle picture which forms the basis of Landau's theory of quantum liquids.