Introduction to Many-body Theory

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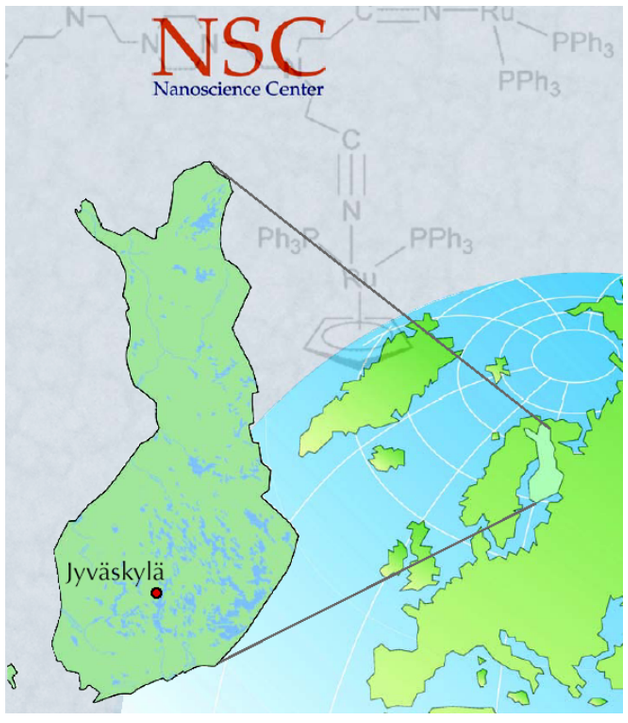

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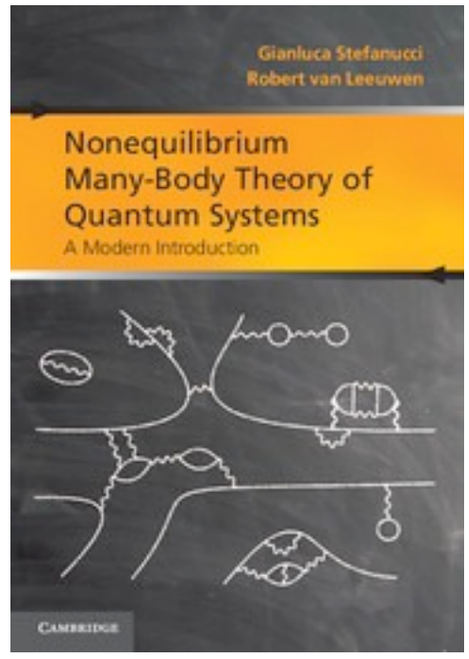
Overview



Part I : Basics

- Time-dependent Schrödinger equation
- Second quantization
- Time-evolution
- The contour idea

Part II : Feynman diagrams and the Green's function

- Why Green's functions?
- Feynman diagrams and the self-energy
- The physical meaning of the Green's function
- Spectral function and photo-emission

Part III: Linear response and examples

- The 2-particle Green's function and optical spectra (Bethe-Salpeter)
- Hedin's equations
- Linear response
- Examples: Time-dependent screening in an electron gas

Introduction to Many-body Theory I

Part I : Basics

- Time-dependent Schrödinger equation
- Second quantization
- Time-evolution
- The contour idea

Basic quantum mechanics

To describe time-dependent phenomena in nature we have to calculate the time evolution of the relevant quantum states. These states are usually given in a basis representation

$$|\Psi\rangle = \sum_n \Psi_n |n\rangle \quad \Rightarrow \quad \langle m|\Psi\rangle = \Psi_m$$

$$\langle m|n\rangle = \delta_{mn}$$

We can therefore write

$$|\Psi\rangle = \sum_n |n\rangle\langle n|\Psi\rangle \quad \Rightarrow \quad \sum_n |n\rangle\langle n| = 1$$

Resolution of the identity

The time-evolution of a quantum state is given by the Schrödinger equation

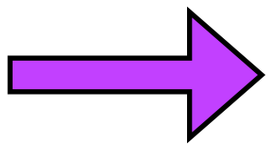
$$i\partial_t|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle \qquad\qquad |\Psi(t_0)\rangle = |\Psi_0\rangle$$

To solve this equation we need to know the representation of the Hamiltonian in a given basis. If we define

$$H_{nm}(t) = \langle n|\hat{H}(t)|m\rangle \qquad\qquad c_n(t) = \langle n|\Psi(t)\rangle$$

Then we can write

$$i\partial_t\langle n|\Psi(t)\rangle = \langle n|\hat{H}(t)|\Psi(t)\rangle = \sum_m \langle n|\hat{H}(t)|m\rangle\langle m|\Psi(t)\rangle = \sum_m H_{nm}(t)\langle m|\Psi(t)\rangle$$



$$i\partial_t \mathbf{c}(t) = \mathbf{H}(t)\,\mathbf{c}(t)$$

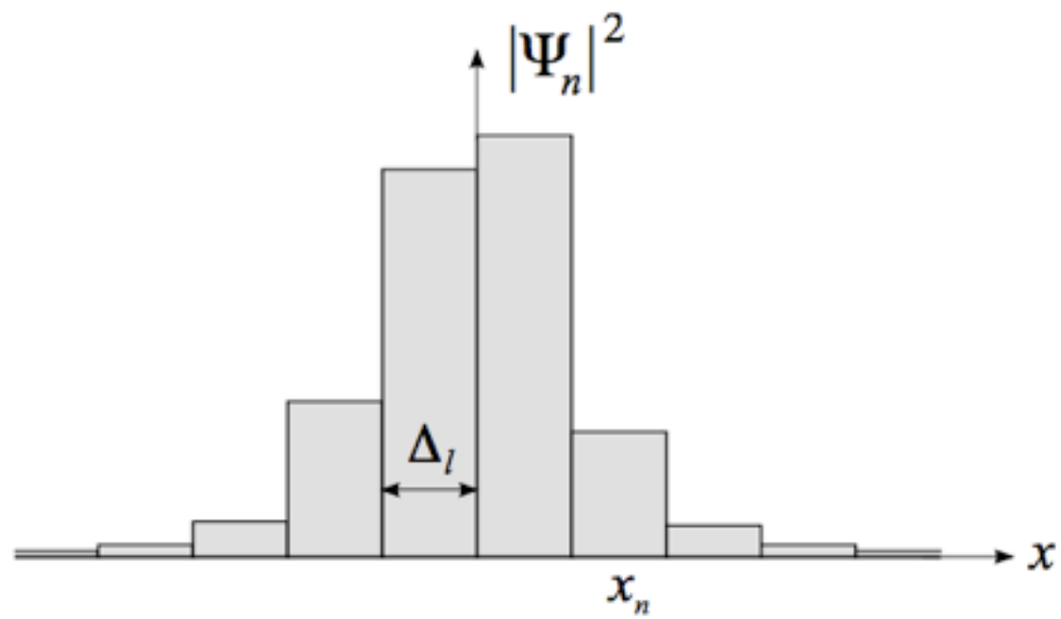
Position basis

We measure a particle to be in interval Δ_n
Its corresponding state is denoted by

$$|x_n\rangle$$

These states have the property

$$\langle x_n|x_m\rangle = \delta_{nm}$$



and form a complete set

$$|\Psi\rangle = \sum_n |x_n\rangle\langle x_n|\Psi\rangle$$

If the system is in state $|\Psi\rangle$ then the probability to measure state $|x_n\rangle$ is

$$P_n = |\langle x_n|\Psi\rangle|^2 = |\Psi(x_n)|^2$$

For one particle in position basis we can, for example, define the Hamiltonian

$$\langle \mathbf{x}|\hat{h}|\mathbf{x}'\rangle = (-\frac{1}{2}\nabla^2 + v(\mathbf{x},t))\langle \mathbf{x}|\mathbf{x}'\rangle$$

The Schrödinger equation

$$\hat{h}|\psi(t)\rangle = i\partial_t|\psi(t)\rangle \qquad\qquad \psi(\mathbf{x},t) = \langle \mathbf{x}|\psi(t)\rangle$$

in the position representation then has the form

$$\begin{aligned} i\partial_t\psi(\mathbf{x},t) &= \langle \mathbf{x}|\hat{h}|\psi(t)\rangle = \int d\mathbf{x}'\, \langle \mathbf{x}|\hat{h}|\mathbf{x}'\rangle\langle \mathbf{x}'|\psi(t)\rangle \\ &= \int d\mathbf{x}' \left(-\frac{1}{2}\nabla^2 + v(\mathbf{x},t)\right) \langle \mathbf{x}|\mathbf{x}'\rangle\langle \mathbf{x}'|\psi(t)\rangle \\ &= \left(-\frac{1}{2}\nabla^2 + v(\mathbf{x},t)\right) \psi(\mathbf{x},t) \end{aligned}$$

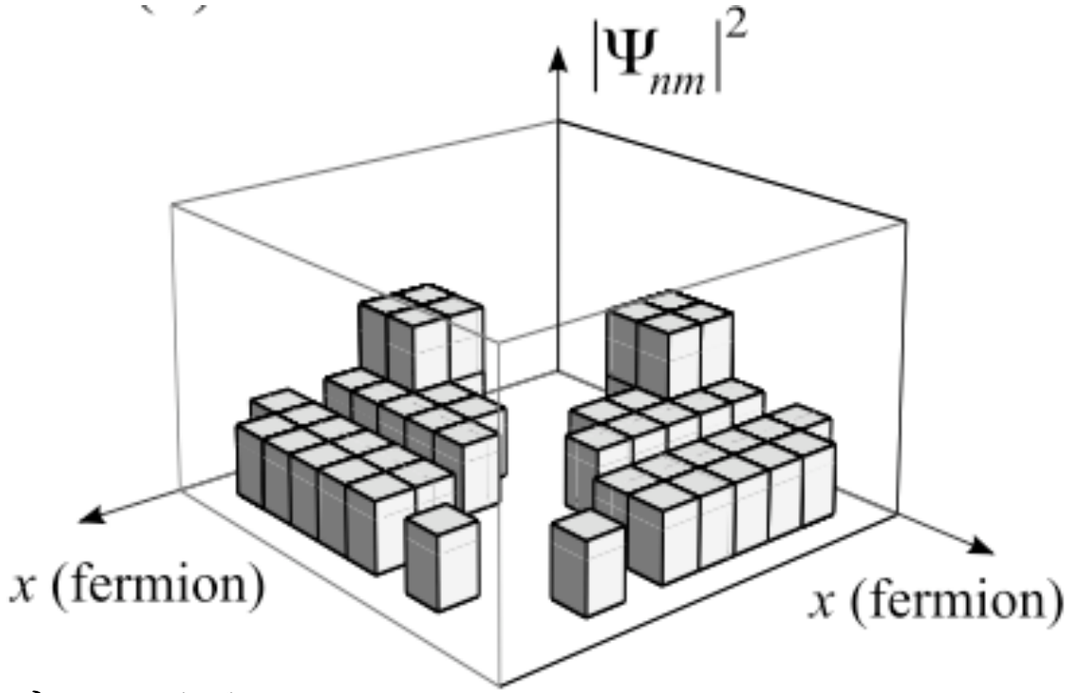
Two particles

If we simultaneously measure a particle in intervals Δ_n and Δ_m the state is

$$|x_n\, x_m\rangle$$

The particles are indistinguishable

$$|x_n\, x_m\rangle = \lambda |x_m\, x_n\rangle = \lambda^2 |x_n\, x_m\rangle \rightarrow \lambda = \pm 1$$



The states are normalized

$$\langle x_n x_m | x_{n'} x_{m'} \rangle = \delta_{nn'}\delta_{mm'} \pm \delta_{nm'}\delta_{mn'} = \left| \begin{array}{cc} \delta_{nn'} & \delta_{nm'} \\ \delta_{mn'} & \delta_{mm'} \end{array} \right|_{\pm}$$

Let us consider fermions. Only the states with n > m are linearly independent and we have

$$|\Psi\rangle = \sum_{n>m} |x_n\, x_m\rangle\langle x_n\, x_m|\Psi\rangle$$

$$P_{nm} = |\langle x_n\, x_m|\Psi\rangle|^2 = |\Psi(x_n, x_m)|^2$$

Second quantization

For N fermions we have (with P a permutation)

$$|\mathbf{x}_1 \dots \mathbf{x}_N\rangle = (-1)^P \, |\mathbf{x}_{P(1)} \dots \mathbf{x}_{P(N)}\rangle \qquad \mathbf{x} = \mathbf{r}, \sigma$$

$$\langle \mathbf{x}_1 \dots \mathbf{x}_N | \mathbf{y}_1 \dots \mathbf{y}_N \rangle = \sum_P (-1)^P \prod_{j=1}^{N} \delta(\mathbf{x}_j - \mathbf{y}_{P(j)})$$

Determinant

There is a unique operator $\hat{\psi}^\dagger(\mathbf{x})$ that generates the position basis. It is defined by

$$\begin{aligned} |\mathbf{x}_1\rangle &= \hat{\psi}^\dagger(\mathbf{x}_1)|0\rangle \\ |\mathbf{x}_1\, \mathbf{x}_2\rangle &= \hat{\psi}^\dagger(\mathbf{x}_2)|\mathbf{x}_1\rangle = \hat{\psi}^\dagger(\mathbf{x}_2)\hat{\psi}^\dagger(\mathbf{x}_1)|0\rangle \\ |\mathbf{x}_1 \dots \mathbf{x}_N\rangle &= \hat{\psi}^\dagger(\mathbf{x}_N)|\mathbf{x}_1 \dots \mathbf{x}_{N-1}\rangle = \hat{\psi}^\dagger(\mathbf{x}_N) \dots \hat{\psi}^\dagger(\mathbf{x}_1)|0\rangle \end{aligned}$$

$\hat{\psi}^\dagger(\mathbf{x})$ is called creation operator

It follows : $$\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y}) = -\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}^\dagger(\mathbf{x})$$

Remember that the adjoint of an operator $\hat{O}$ is defined by

$$\langle\Phi|\hat{O}^\dagger|\chi\rangle = \langle\chi|\hat{O}|\Phi\rangle^*$$

The adjoint $\hat{\psi}(\mathbf{x})$ of the creation operator therefore satisfies

$$\langle\mathbf{x}_1\ldots\mathbf{x}_{N-1}|\hat{\psi}(\mathbf{x}_N)|\mathbf{y}_1\ldots\mathbf{y}_N\rangle^* = \langle\mathbf{y}_1\ldots\mathbf{y}_N|\hat{\psi}^\dagger(\mathbf{x}_N)|\mathbf{x}_1\ldots\mathbf{x}_{N-1}\rangle$$
$$= \langle\mathbf{y}_1\ldots\mathbf{y}_N|\mathbf{x}_1\ldots\mathbf{x}_N\rangle = \sum_P(-1)^P\prod_{j=1}^N\delta(\mathbf{y}_j-\mathbf{x}_{P(j)})$$

and hence (by expanding the determinant along column N) we have

$$\hat{\psi}(\mathbf{x})|\mathbf{y}_1\ldots\mathbf{y}_N\rangle = \sum_{k=1}^N(-1)^{N-k}\,\delta(\mathbf{x}-\mathbf{y}_k)\,|\mathbf{y}_1\ldots\mathbf{y}_{k-1}\mathbf{y}_{k+1}\ldots\mathbf{y}_N\rangle$$

For example:

$$
\begin{aligned}
\hat{\psi}(\mathbf{x})|0\rangle &= 0 \\
\hat{\psi}(\mathbf{x})|\mathbf{y}_1\rangle &= \delta(\mathbf{x}-\mathbf{y}_1)|0\rangle \\
\hat{\psi}(\mathbf{x})|\mathbf{y}_1\,\mathbf{y}_2\rangle &= \delta(\mathbf{x}-\mathbf{y}_2)|\mathbf{y}_1\rangle - \delta(\mathbf{x}-\mathbf{y}_1)|\mathbf{y}_2\rangle \\
\hat{\psi}(\mathbf{x})|\mathbf{y}_1\,\mathbf{y}_2\,\mathbf{y}_3\rangle &= \delta(\mathbf{x}-\mathbf{y}_3)|\mathbf{y}_1\,\mathbf{y}_2\rangle - \delta(\mathbf{x}-\mathbf{y}_2)|\mathbf{y}_1\,\mathbf{y}_3\rangle + \delta(\mathbf{x}-\mathbf{y}_1)|\mathbf{y}_2\,\mathbf{y}_3\rangle
\end{aligned}
$$

The operator $\hat{\psi}(\mathbf{x})$ is called annihilation operator

It follows (with anti-commutator $[A,B]_+ = AB + BA$):

$$
\begin{aligned}
\left[\hat{\psi}(\mathbf{x}),\hat{\psi}(\mathbf{y})\right]_+ &= \left[\hat{\psi}^\dagger(\mathbf{x}),\hat{\psi}^\dagger(\mathbf{y})\right]_+ = 0 \\
\left[\hat{\psi}(\mathbf{x}),\hat{\psi}^\dagger(\mathbf{y})\right]_+ &= \delta(\mathbf{x}-\mathbf{y})
\end{aligned}
$$

The density operator is defined by

$$\hat{n}(\mathbf{x}) = \hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})$$

and has the property

$$\hat{n}(\mathbf{x})|\mathbf{x}_1 \ldots \mathbf{x}_N\rangle = \sum_{j=1}^{N} \delta(\mathbf{x} - \mathbf{x}_j)\,|\mathbf{x}_1 \ldots \mathbf{x}_N\rangle$$

For example:

$$\begin{aligned}
\hat{\psi}^\dagger(\mathbf{x})\,\hat{\psi}(\mathbf{x})|\mathbf{y}_1\mathbf{y}_2\rangle &= \hat{\psi}^\dagger(\mathbf{x})\ (\delta(\mathbf{x}-\mathbf{y}_2)|\mathbf{y}_1\rangle - \delta(\mathbf{x}-\mathbf{y}_1)|\mathbf{y}_2\rangle) \\
&= \delta(\mathbf{x}-\mathbf{y}_2)|\mathbf{y}_1\mathbf{x}\rangle - \delta(\mathbf{x}-\mathbf{y}_1)|\mathbf{y}_2\mathbf{x}\rangle \\
&= (\delta(\mathbf{x}-\mathbf{y}_1) + \delta(\mathbf{x}-\mathbf{y}_2))|\mathbf{y}_1\mathbf{y}_2\rangle
\end{aligned}$$

The expectation value $n(\mathbf{x}) = \langle\Psi|\hat{n}(\mathbf{x})|\Psi\rangle$

is the particle density of the system in state $|\Psi\rangle$

For N particles we define the Hamiltonian by

$$\langle \mathbf{x}_1 \dots \mathbf{x}_N | \hat{H} | \mathbf{x}'_1 \dots \mathbf{x}'_N \rangle$$

$$= \left(\sum_j^N -\frac{1}{2}\nabla_j^2 + v(\mathbf{x}_j, t) + \frac{1}{2}\sum_{i \neq j}^N w(\mathbf{x}_i, \mathbf{x}_j) \right) \langle \mathbf{x}_1 \dots \mathbf{x}_N | \mathbf{x}'_1 \dots \mathbf{x}'_N \rangle$$

or equivalently, for any state $|\Psi\rangle$

Many-body wave function

$$\langle \mathbf{x}_1 \dots \mathbf{x}_N | \hat{H} | \Psi \rangle$$

$$= \left(\sum_j^N -\frac{1}{2}\nabla_j^2 + v(\mathbf{x}_j, t) + \frac{1}{2}\sum_{i \neq j}^N w(\mathbf{x}_i, \mathbf{x}_j) \right) \langle \mathbf{x}_1 \dots \mathbf{x}_N | \Psi \rangle$$

Since the one- and two-body potentials are diagonal in the position representation it is easy to express them in second quantization

For the 2-particle interaction we have

$$\hat{W}|\mathbf{x}_1 \ldots \mathbf{x}_N\rangle = \frac{1}{2}\sum_{i\neq j}^{N} w(\mathbf{x}_i, \mathbf{x}_j)|\mathbf{x}_1 \ldots \mathbf{x}_N\rangle$$

Since the density operator has the property

$$\hat{n}(\mathbf{x})|\mathbf{x}_1 \ldots \mathbf{x}_N\rangle = \sum_{j=1}^{N} \delta(\mathbf{x}-\mathbf{x}_j)\,|\mathbf{x}_1 \ldots \mathbf{x}_N\rangle$$

it follows that

$$\begin{aligned}
\hat{W} &= \frac{1}{2}\int d\mathbf{x}d\mathbf{y}\, w(\mathbf{x},\mathbf{y})\hat{n}(\mathbf{x})\hat{n}(\mathbf{y}) - \frac{1}{2}\int d\mathbf{x}\, w(\mathbf{x},\mathbf{x})\hat{n}(\mathbf{x}) \\
&= \frac{1}{2}\int d\mathbf{x}d\mathbf{y}\, w(\mathbf{x},\mathbf{y})\left(\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y}) - \delta(\mathbf{x}-\mathbf{y})\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}(\mathbf{x})\right) \\
&= \frac{1}{2}\int d\mathbf{x}d\mathbf{y}\, w(\mathbf{x},\mathbf{y})\,\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x})
\end{aligned}$$

$$\hat{W} = \frac{1}{2}\int d\mathbf{x}d\mathbf{y}\, w(\mathbf{x},\mathbf{y})\,\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x})$$

Similarly for the one-body potential

$$\hat{V}(t)|\mathbf{x}_1 \dots \mathbf{x}_N\rangle = \sum_j^N v(\mathbf{x}_j, t)|\mathbf{x}_1 \dots \mathbf{x}_N\rangle = \int d\mathbf{x}\, \hat{n}(\mathbf{x}) v(\mathbf{x}, t)|\mathbf{x}_1 \dots \mathbf{x}_N\rangle$$

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

The kinetic energy operator is only slightly more difficult. Let's illustrate it for 3 particles. Remember that

$$\hat{\psi}(\mathbf{x})|\mathbf{y}_1\, \mathbf{y}_2\, \mathbf{y}_3\rangle \quad = \quad \delta(\mathbf{x} - \mathbf{y}_3)|\mathbf{y}_1\, \mathbf{y}_2\rangle - \delta(\mathbf{x} - \mathbf{y}_2)|\mathbf{y}_1\, \mathbf{y}_3\rangle + \delta(\mathbf{x} - \mathbf{y}_1)|\mathbf{y}_2\, \mathbf{y}_3\rangle$$

$$\hat{\psi}^\dagger(\mathbf{x})\nabla^2\hat{\psi}(\mathbf{x})\, |\mathbf{y}_1\mathbf{y}_2\mathbf{y}_3\rangle$$

$$= \nabla^2\delta(\mathbf{x} - \mathbf{y}_3)|\mathbf{y}_1\, \mathbf{y}_2\, \mathbf{x}\rangle + \nabla^2\delta(\mathbf{x} - \mathbf{y}_2)|\mathbf{y}_1\mathbf{x}\, \mathbf{y}_3\rangle + \nabla^2\delta(\mathbf{x} - \mathbf{y}_1)|\mathbf{x}\, \mathbf{y}_2\, \mathbf{y}_3\rangle$$

If we therefore define

$$\hat{T} = -\frac{1}{2}\int d\mathbf{x}\,\hat{\psi}^\dagger(\mathbf{x})\nabla^2\hat{\psi}(\mathbf{x})$$

then since T is Hermitian

$$\langle \mathbf{y}_1\mathbf{y}_2\mathbf{y}_3|\hat{T}|\mathbf{x}_1\mathbf{x}_2\mathbf{x}_3\rangle = \langle \mathbf{x}_1\mathbf{x}_2\mathbf{x}_3|\hat{T}|\mathbf{y}_1\mathbf{y}_2\mathbf{y}_3\rangle^*$$

$$= -\frac{1}{2}\left(\nabla^2_{\mathbf{y}_1} + \nabla^2_{\mathbf{y}_2} + \nabla^2_{\mathbf{y}_3}\right)\langle \mathbf{x}_1\mathbf{x}_2\mathbf{x}_3|\mathbf{y}_1\mathbf{y}_2\mathbf{y}_3\rangle^*$$

$$= -\frac{1}{2}\left(\nabla^2_{\mathbf{y}_1} + \nabla^2_{\mathbf{y}_2} + \nabla^2_{\mathbf{y}_3}\right)\langle \mathbf{y}_1\mathbf{y}_2\mathbf{y}_3|\mathbf{x}_1\mathbf{x}_2\mathbf{x}_3\rangle$$

yielding exactly the matrix element of the kinetic energy operator. Hence

$$\hat{H}(t) = \int d\mathbf{x}\,\hat{\psi}^\dagger(\mathbf{x})\left(-\frac{1}{2}\nabla^2 + v(\mathbf{x},t)\right)\hat{\psi}(\mathbf{x})$$

$$+\frac{1}{2}\int d\mathbf{x}d\mathbf{y}\,w(\mathbf{x},\mathbf{y})\,\hat{\psi}^\dagger(\mathbf{x})\hat{\psi}^\dagger(\mathbf{y})\hat{\psi}(\mathbf{y})\hat{\psi}(\mathbf{x})$$

We can also rewrite everything in a general basis. If we define

$$\langle \mathbf{x}|n\rangle = \varphi_n(\mathbf{x})$$

then φ_n is an orthonormal set of orbitals

$$\delta_{nm} = \langle n|m\rangle = \int d\mathbf{x}\, \langle n|\mathbf{x}\rangle\langle \mathbf{x}|m\rangle = \int d\mathbf{x}\, \varphi_n^*(\mathbf{x})\varphi_m(\mathbf{x})$$

If we define

$$\hat{a}_n = \int d\mathbf{x}\, \varphi_n^*(\mathbf{x})\hat{\psi}(\mathbf{x}) \qquad \hat{a}_n^\dagger = \int d\mathbf{x}\, \varphi_n(\mathbf{x})\hat{\psi}^\dagger(\mathbf{x})$$

then

$$[\hat{a}_n, \hat{a}_m^\dagger]_+ = \delta_{nm} \qquad [\hat{a}_n, \hat{a}_m]_+ = [\hat{a}_n^\dagger, \hat{a}_m^\dagger]_+ = 0$$

$$a_n^\dagger|0\rangle = \int d\mathbf{x}\, \varphi_n(\mathbf{x}) \underbrace{\hat{\psi}^\dagger(\mathbf{x})|0\rangle}_{|\mathbf{x}\rangle} = \int d\mathbf{x}|\mathbf{x}\rangle\langle \mathbf{x}|n\rangle = |n\rangle$$

In general we can generate N-particle states

$$|n_1 \dots n_N\rangle = \hat{a}^\dagger_{n_N} \dots \hat{a}^\dagger_{n_1} |0\rangle$$

We can relate them to position basis states as follows

$$|n_1 \dots n_N\rangle = \int d\mathbf{x}_1 \dots d\mathbf{x}_N \, \varphi_{n_1}(\mathbf{x}_1) \dots \varphi_{n_N}(\mathbf{x}_N) \, \hat{\psi}^\dagger(\mathbf{x}_N) \dots \hat{\psi}^\dagger(\mathbf{x}_1) |0\rangle$$

$$= \int d\mathbf{x}_1 \dots d\mathbf{x}_N \, \varphi_{n_1}(\mathbf{x}_1) \dots \varphi_{n_N}(\mathbf{x}_N) |\mathbf{x}_1 \dots \mathbf{x}_N\rangle$$

and find that their overlaps are given by Slater determinants

$$\langle \mathbf{x}_1 \dots \mathbf{x}_N | n_1 \dots n_N \rangle = \sum_P (-1)^P \varphi_{n_1}(\mathbf{x}_{P(1)}) \dots \varphi_{n_N}(\mathbf{x}_{P(N)}) = \begin{vmatrix} \varphi_{n_1}(\mathbf{x}_1) & \dots & \varphi_{n_N}(\mathbf{x}_1) \\ \vdots & & \vdots \\ \varphi_{n_1}(\mathbf{x}_N) & \dots & \varphi_{n_N}(\mathbf{x}_N) \end{vmatrix}$$

The creation and annihilation operators therefore add and remove orbitals from Slater determinants

The Hamiltonian in a general one-particle basis then attains the form

$$\hat{H}(t) = \sum_{ij} h_{ij}(t)\, \hat{a}_i^\dagger\, \hat{a}_j + \frac{1}{2} \sum_{ijkl} v_{ijkl}\, \hat{a}_i^\dagger\, \hat{a}_j^\dagger\, \hat{a}_k\, \hat{a}_l$$

where

$$h_{ij}(t) = \int d\mathbf{x}\, \varphi_i^*(\mathbf{x}) h(\mathbf{x}, t) \varphi_j(\mathbf{x})$$

$$v_{ijkl} = \int d\mathbf{x} d\mathbf{y}\, w(\mathbf{x}, \mathbf{y})\, \varphi_i^*(\mathbf{x}) \varphi_j^*(\mathbf{y}) \varphi_k(\mathbf{y}) \varphi_l(\mathbf{x})$$

The convenient basis states in practice depend on the problem.
Commonly used ones are, for example, Kohn-Sham or Hartree-Fock orbitals

Second quantization: Take home message

- Second quantization is nothing but a convenient way to generate a many-particle basis that automatically has the correct (anti)symmetry.

  Basis states are created by (anti)-commuting operators with simple (anti)-commutation relations

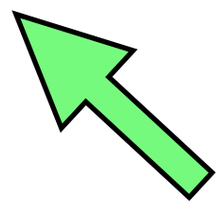
- As we will see, second quantization is very convenient in many-body theory as it allows for simple manipulation of perturbative terms without the need to deal with (anti)-symmetrized orbital products

- The derivation of the Hamiltonian in second quantization is easy in position basis as the Hamiltonian is almost diagonal in this basis

Expectation values

A general expectation value is of the form

$$\langle \hat{O}(t) \rangle = \langle \Psi(t) | \hat{O}(t) | \Psi(t) \rangle = \langle \Psi_0 | \hat{U}(t_0, t)\, \hat{O}(t)\, \hat{U}(t, t_0) | \Psi_0 \rangle = \langle \Psi_0 | \hat{O}_H(t) | \Psi_0 \rangle$$



initial state

where we defined the evolution operator as

$$|\Psi(t)\rangle = \hat{U}(t, t') |\Psi(t')\rangle$$

and the operator Ô(t) in the Heisenberg picture as

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

The Heisenberg operator satisfies an equation of motion

It follows from the Schrödinger equation that

$$i\partial_t \hat{U}(t,t') = \hat{H}(t)\hat{U}(t,t')$$

and therefore that the Heisenberg operator satisfies the equation of motion

$$\partial_t \hat{O}_H(t) = -i\left[\hat{O}_H(t), \hat{H}_H(t)\right] + \left(\partial_t \hat{O}(t)\right)_H$$

For example, you can check that the field operator satisfies

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

Let us now derive a more explicit expression for the evolution operator

We start again from the Schrödinger equation $i\partial_t|\Psi(t)\rangle = \hat{H}(t)|\Psi(t)\rangle$

If we divide [t_0 , T] into small intervals Δ then

$$|\Psi(T)\rangle \approx e^{-i\hat{H}(t_n)\Delta}\dots e^{-i\hat{H}(t_0)\Delta}|\Psi(t_0)\rangle = \mathcal{T}\left\{e^{-i\hat{H}(t_n)\Delta}\dots e^{-i\hat{H}(t_0)\Delta}\right\}|\Psi(t_0)\rangle$$

$$= \mathcal{T}\left\{e^{-i\sum_j^n \hat{H}(t_j)\Delta}\right\}|\Psi(t_0)\rangle$$

where $\mathcal{T}$ denotes time-ordering that orders the latest operator most left.
We used that operators commute under time-ordering

$$\mathcal{T}\left\{\hat{A}(t_1)\hat{B}(t_2)\right\} = \mathcal{T}\left\{\hat{B}(t_2)\hat{A}(t_1)\right\}$$

and hence, in particular

$$\mathcal{T}\left\{e^{\hat{A}(t_1)}e^{\hat{B}(t_2)}\right\} = \mathcal{T}\left\{e^{\hat{A}(t_1)+\hat{B}(t_2)}\right\}$$

In the limit Δ => 0 then

$$|\Psi(T)\rangle = \mathcal{T}\left\{e^{-i\int_{t_0}^{T} dt\, \hat{H}(t)}\right\}|\Psi(t_0)\rangle = \hat{U}(T,t_0)|\Psi(t_0)\rangle$$

Time-evolution operator

By as similar procedure we have

$$U(t_0,T) = e^{i\hat{H}(t_1)\Delta}e^{i\hat{H}(t_2)\Delta}\ldots e^{i\hat{H}(t_n)\Delta} = \bar{\mathcal{T}}\left\{e^{i\sum_j^n \hat{H}(t_j)\Delta}\right\}$$

$$U(t_0,T) = \bar{\mathcal{T}}\left\{e^{i\int_{t_0}^{T}\hat{H}(t)dt}\right\}$$

where $\bar{\mathcal{T}}$ denotes anti-time-ordering that orders the latest operator most right.

The evolution operator can then be written as

$$\hat{U}(t_1,t_2) = \begin{cases} \mathcal{T} e^{-i\int_{t_1}^{t_2} dt\, \hat{H}(t)dt} & t_1 < t_2 \\ \bar{\mathcal{T}} e^{+i\int_{t_2}^{t_1} dt\, \hat{H}(t)dt} & t_2 < t_1 \end{cases}$$

and the expectation value

$$\langle \hat{O}(t) \rangle = \langle \Psi_0 | \hat{U}(t_0,t) \hat{O}(t) \hat{U}(t,t_0) | \Psi_0 \rangle$$

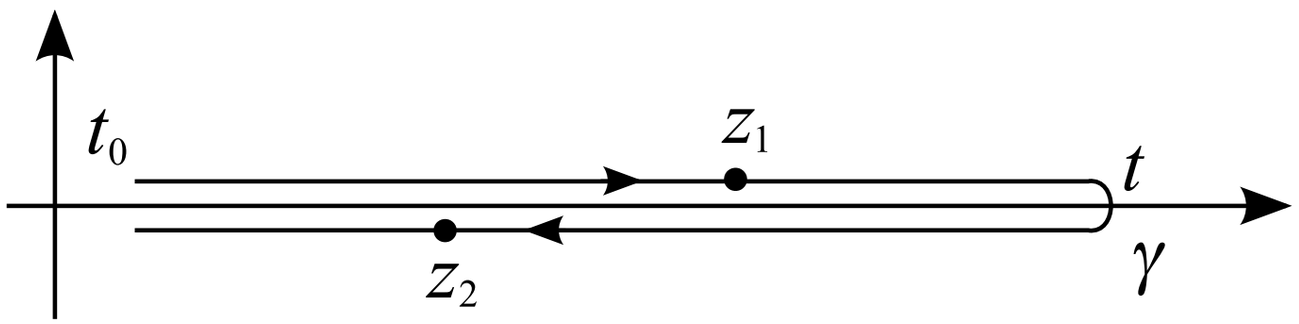
can therefore be written as

$$\langle \hat{O}(t) \rangle = \langle \Psi_0 | \bar{\mathcal{T}} e^{i\int_{t_0}^{t} dt\, \hat{H}(t)dt}\, \hat{O}(t)\, \mathcal{T} e^{-i\int_{t_0}^{t} dt\, \hat{H}(t)dt} | \Psi_0 \rangle$$

If we expand in powers of the Hamiltonian then a typical term is

$$\bar{\mathcal{T}} \left\{ \hat{H}(t_1) \dots \hat{H}(t_n) \right\} \hat{O}(t)\, \mathcal{T} \left\{ \hat{H}(t'_1) \dots \hat{H}(t'_n) \right\}$$

early ⟵ late late ⟵ early



$$\gamma \equiv \underbrace{(t_0, t)}_{\gamma_-} \oplus \underbrace{(t, t_0)}_{\gamma_+}$$

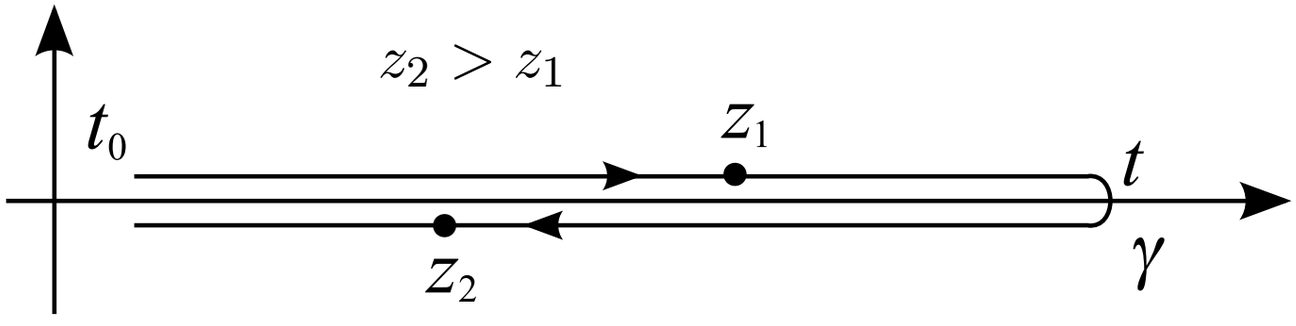
We define a contour γ consisting of two copies of the interval [t_0 , t] .A generic element z of γ can lie on the forward branch γ_- or the backward branch γ_+

Notation

$$z = t'_- \quad \text{when} \quad z \in \gamma_- \quad \text{and its real value is} \quad t'$$
$$z = t'_+ \quad \text{when} \quad z \in \gamma_+ \quad \text{and its real value is} \quad t'$$

We can define operators on the contour

$$\hat{O}(z') = \begin{cases} \hat{O}_-(t') & z' = t'_- \\ \hat{O}_+(t') & z' = t'_+ \end{cases}$$



$$\mathcal{T}_\gamma \left\{ \hat{A}_{P(1)}(z_{P(1)}) \dots \hat{A}_{P(1)}(z_{P(1)}) \right\} = \hat{A}_1(z_1) \dots \hat{A}_n(z_n) \quad z_1 > \dots > z_n$$

With this definition we can write

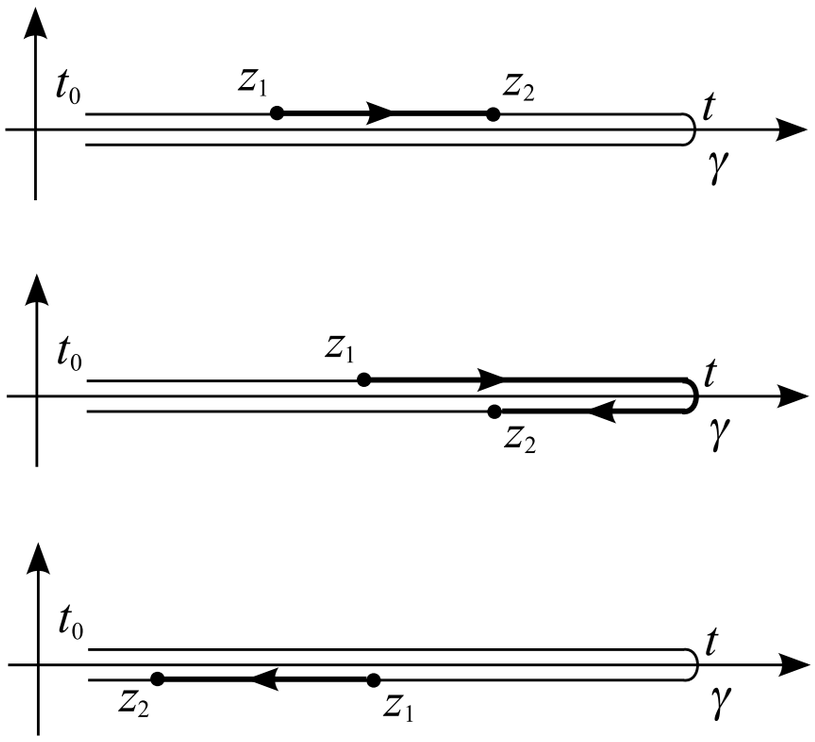
$$\bar{\mathcal{T}} \left\{ \hat{H}(t_1) \dots \hat{H}(t_n) \right\} \hat{O}(t) \mathcal{T} \left\{ \hat{H}(t'_1) \dots \hat{H}(t'_n) \right\}$$

$$= \mathcal{T}_\gamma \left\{ \hat{H}(t_{1+}) \dots \hat{H}(t_{n+}) \hat{O}(t) \hat{H}(t'_{1-}) \dots \hat{H}(t'_{n-}) \right\}$$

where

$$\hat{H}(z = t'_\pm) = \hat{H}(t')$$

With this trick we can write the expectation value in a compact way



$$\int_{z_1}^{z_2} d\bar{z}\,\hat{A}(\bar{z}) = \begin{cases} \int_{t_1}^{t_2} d\bar{t}\,\hat{A}_-(\bar{t}) & \text{if } z_1 = t_{1-} \text{ and } z_2 = t_{2-} \\ \int_{t_1}^{t} d\bar{t}\,\hat{A}_-(\bar{t}) + \int_{t}^{t_2} d\bar{t}\,\hat{A}_+(\bar{t}) & \text{if } z_1 = t_{1-} \text{ and } z_2 = t_{2+} \\ \int_{t_1}^{t_2} d\bar{t}\,\hat{A}_+(\bar{t}) & \text{if } z_1 = t_{1+} \text{ and } z_2 = t_{2+} \end{cases}$$

The expectation value can then be written as

$$\langle \hat{O}(t) \rangle = \langle \Psi_0 | \mathcal{T}_\gamma \left\{ e^{-i\int_{\gamma_+} \hat{H}(\bar{z})d\bar{z}}\, \hat{O}(t_\pm)\, e^{-i\int_{\gamma_-} \hat{H}(\bar{z})d\bar{z}} \right\} |\Psi_0\rangle$$

and since the operators commute under the time-ordering

$$\langle \hat{O}(t) \rangle = \langle \Psi_0 | \mathcal{T}_\gamma \left\{ e^{-i\int_{\gamma} \hat{H}(\bar{z})d\bar{z}}\, \hat{O}(t_\pm) \right\} |\Psi_0\rangle$$

It will be useful to extend the concept of expectation value to ensembles

$$\langle \hat{O}_H(t) \rangle = \sum_n w_n \langle \Psi_n | \hat{O}_H(t) | \Psi_n \rangle = \mathrm{Tr} \left\{ \hat{\rho}\, \hat{O}_H(t) \right\}$$

$$\hat{\rho} = \sum_n w_n |\Psi_n\rangle\langle\Psi_n| \qquad \sum_n w_n = 1 \qquad w_m \geq 0$$

where we defined $\mathrm{Tr}\ \hat{A} = \sum_m \langle \Phi_m | \hat{A} | \Phi_m \rangle$ with $|\Phi_m\rangle$ any complete orthonormal set

An important special case is

$$w_n = \frac{e^{-\beta E_n}}{\sum_m e^{-\beta E_m}} \qquad \hat{H}^M |\Psi_n\rangle = E_n |\Psi_n\rangle \qquad \hat{H}^M = \hat{H}(t_0) - \mu \hat{N}$$

$$\hat{\rho} = \sum_n w_n |\Psi_n\rangle\langle\Psi_n| = \frac{e^{-\beta \hat{H}^M}}{\mathrm{Tr} \left\{ e^{-\beta \hat{H}^M} \right\}}$$

This corresponds to an initial system at inverse temperature β and chemical potential μ

$$e^{-\beta \hat{H}^M} = e^{-i[(t_0 - i\beta) - t_0]\hat{H}^M} = \hat{U}(t_0 - i\beta, t_0)$$

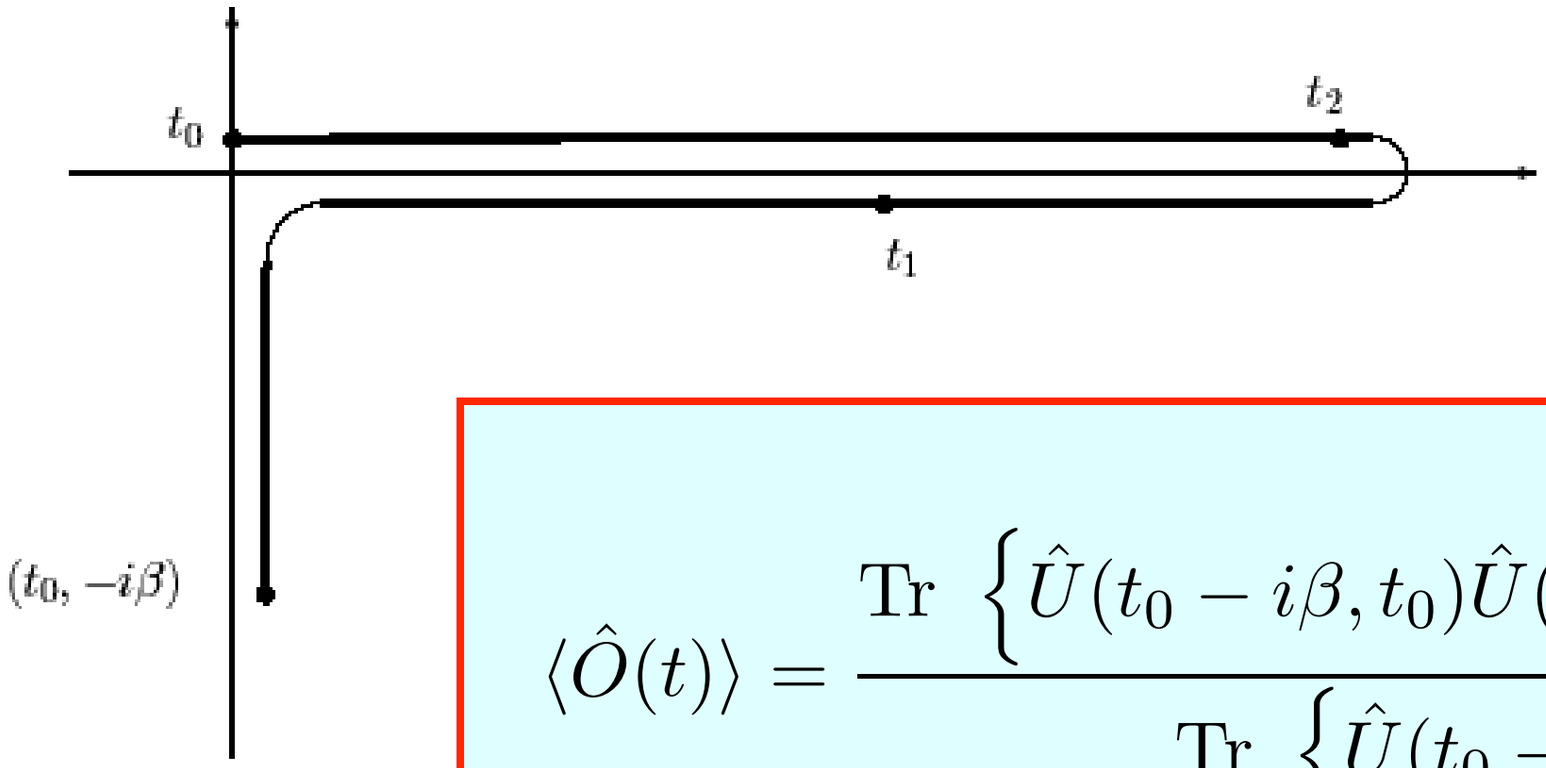
If we therefore define

$$\hat{H}(z) = \begin{cases} \hat{H}(t) & z \in [t_0, \infty[\\ \hat{H}^M & z \in [t_0, t_0 - i\beta] \end{cases}$$

then we can write

$$\langle \hat{O}(t) \rangle = \frac{\mathrm{Tr}\ \left\{ \hat{U}(t_0 - i\beta, t_0)\hat{U}(t_0, t)\hat{O}(t)\hat{U}(t, t_0) \right\}}{\mathrm{Tr}\ \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}}$$

(L.V.Keldysh, Sov.Phys.JETP20, 1018 (1965),
Konstantinov, Perel', JETP12,142 (1961))



$$\langle \hat{O}(t) \rangle = \frac{\mathrm{Tr}\ \left\{ \hat{U}(t_0 - i\beta, t_0) \hat{U}(t_0, t) \hat{O}(t) \hat{U}(t, t_0) \right\}}{\mathrm{Tr}\ \left\{ \hat{U}(t_0 - i\beta, t_0) \right\}}$$

$$\langle \hat{O}(t) \rangle = \frac{\mathrm{Tr}\ \mathcal{T} \left\{ e^{-i \int_\gamma dz\, \hat{H}(z)} \hat{O}(t) \right\}}{\mathrm{Tr}\ \mathcal{T} \left\{ e^{-i \int_\gamma dz\, \hat{H}(z)} \right\}}$$

Time ordering is now defined along the extended contour

Time-ordering: Take home message

- Time-ordering is a direct consequence of the structure of time-dependent Schrödinger equation.

- Expectation values consist of a time-ordered evolution operator for the ket state and an anti-time-ordering for the bra state

- The expectation of any operator value can be rewritten in terms of a single time-ordered exponential by introducing contour ordering

- In case of systems prepared in an initial ensemble the expectation value can be rewritten as a time-ordering on a contour with an additional vertical track

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

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

The solution to this equation is

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

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

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

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

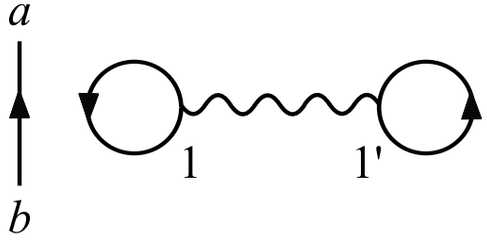
This leads to Feynman diagrams. Let us give an example an expand the numerator N(a,b) to first order

Expanding the 3x3 determinant along the first column we find

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

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

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



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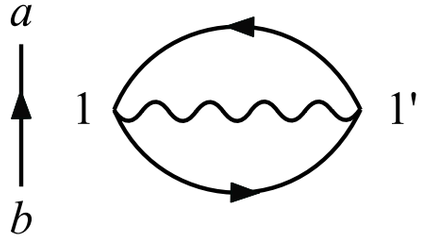

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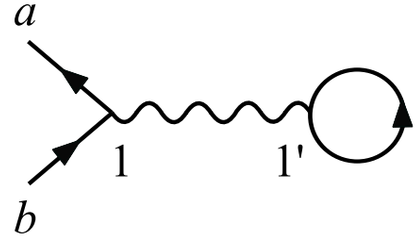

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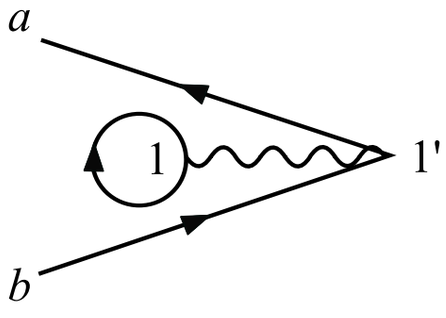
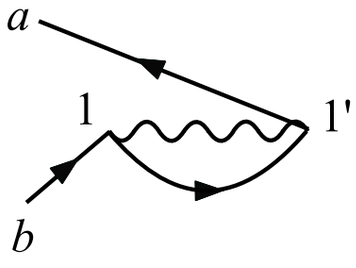
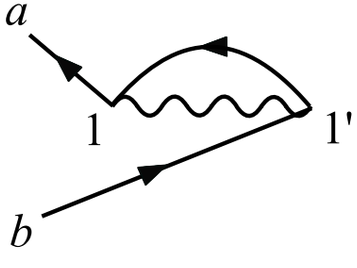


(1',1,*b*)



(1',*b*,1)

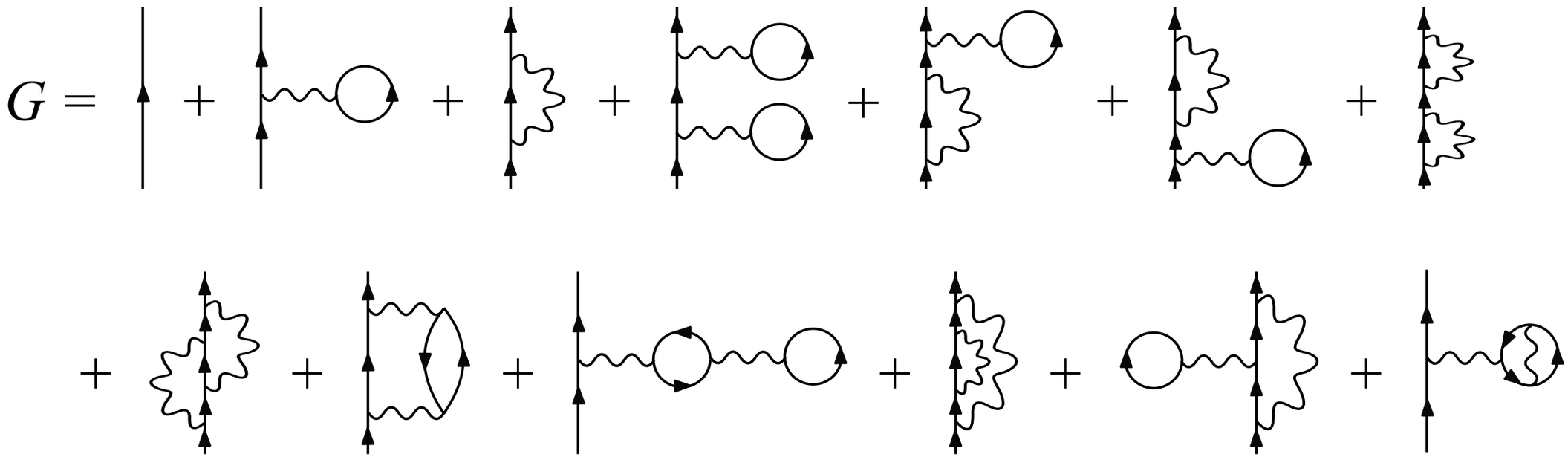


(1,1',*b*)

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

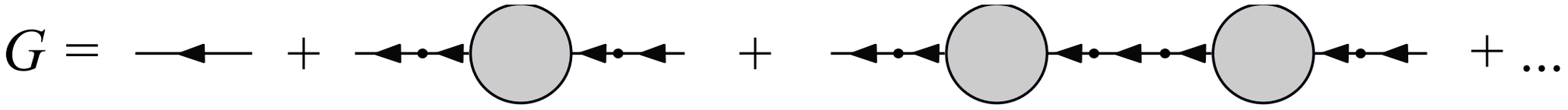
$$G(a,b) = \sum_{k=0}^{\infty} i^k \int w(1,1') \dots w(k,k') \left| \begin{array}{cccc} g(a,b) & g(a,1^+) & \dots & g(a,k'^+) \\ g(1,b) & g(1,1^+) & \dots & g(1,k'^+) \\ \vdots & \vdots & & \vdots \\ g(k',b) & g(k',1^+) & \dots & g(k',k'^+) \end{array} \right|_{CTI}$$

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

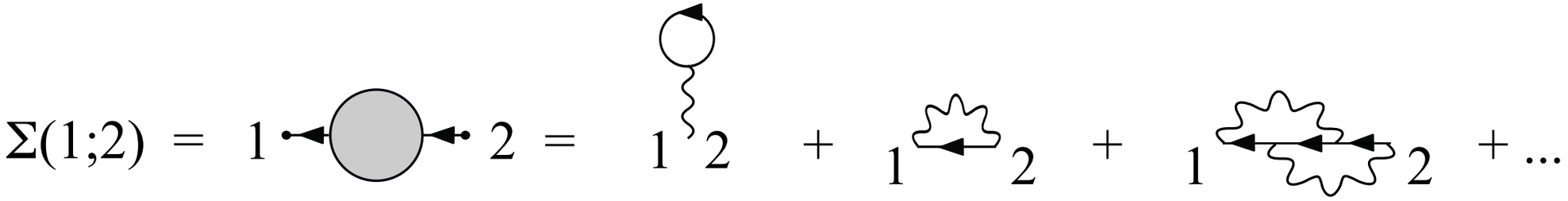


Self energy

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)

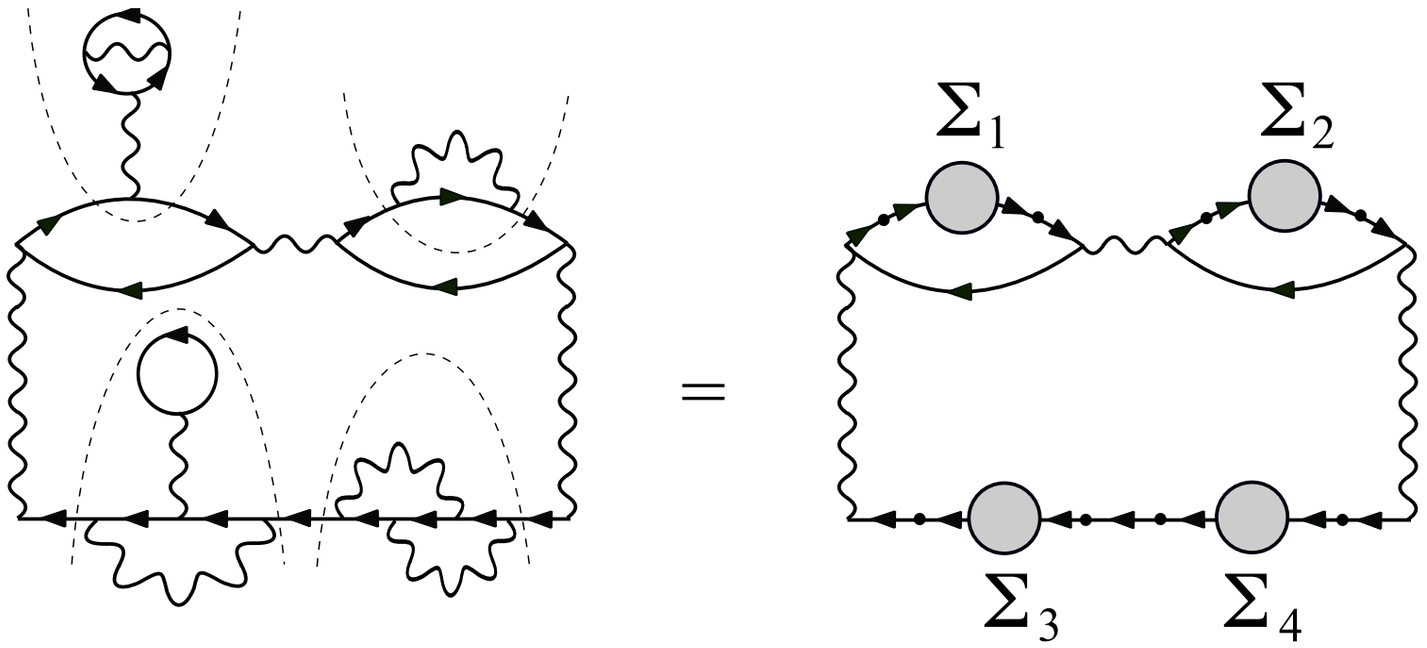


The Green's function thus satisfies the equation

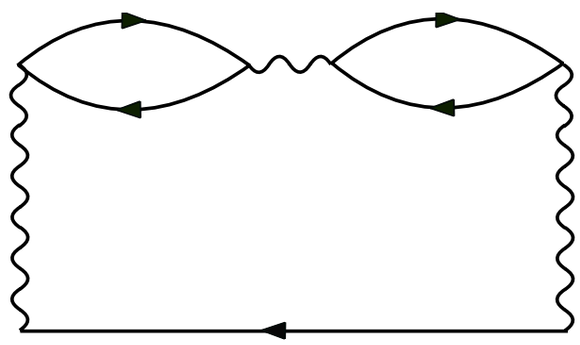
$$G(1,2) = g(1,2) + \int_\gamma d3d4\, g(1,3)\, \Sigma[g](3,4)\, G(4,2)$$

Skeletons

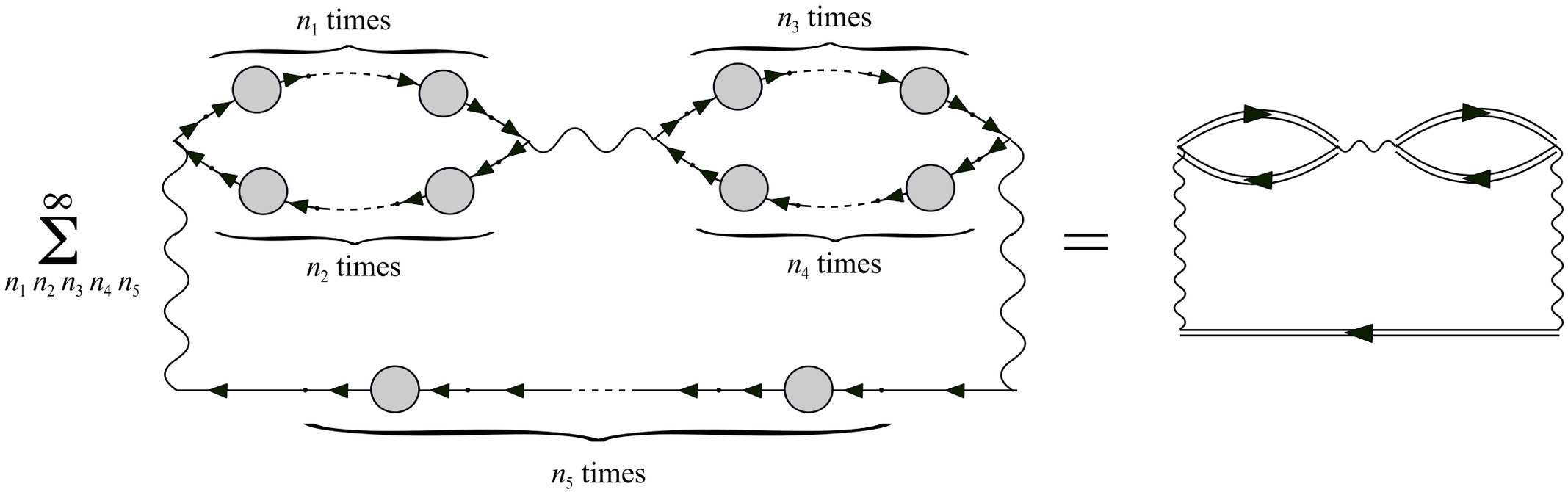
A skeleton diagram is a diagram without self-energy insertions, for example



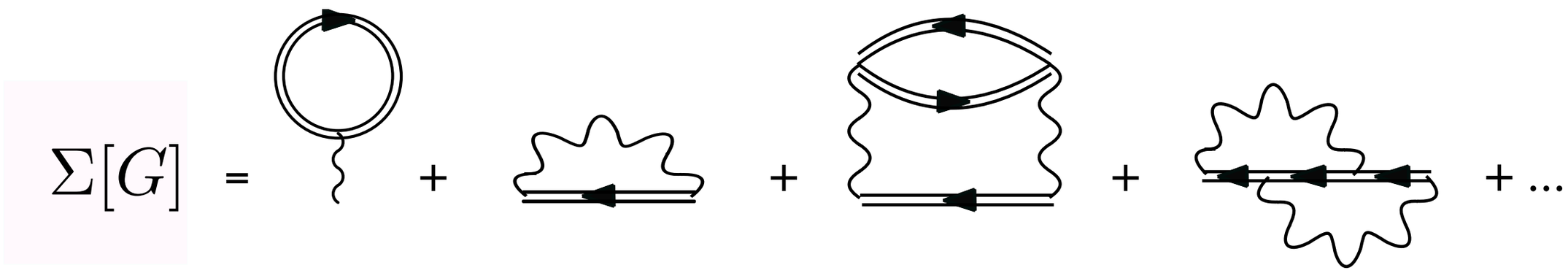
The corresponding skeleton is therefore



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

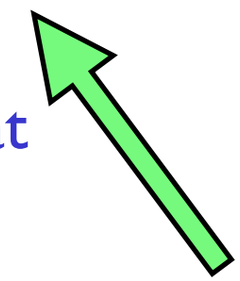
We therefore find the Dyson equation

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

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



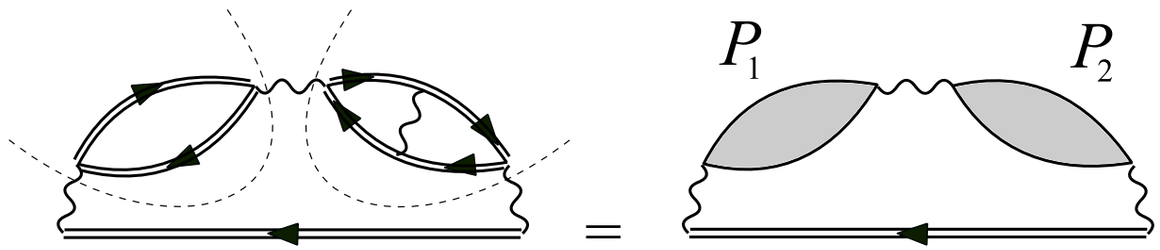
Kadanoff-Baym equations

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

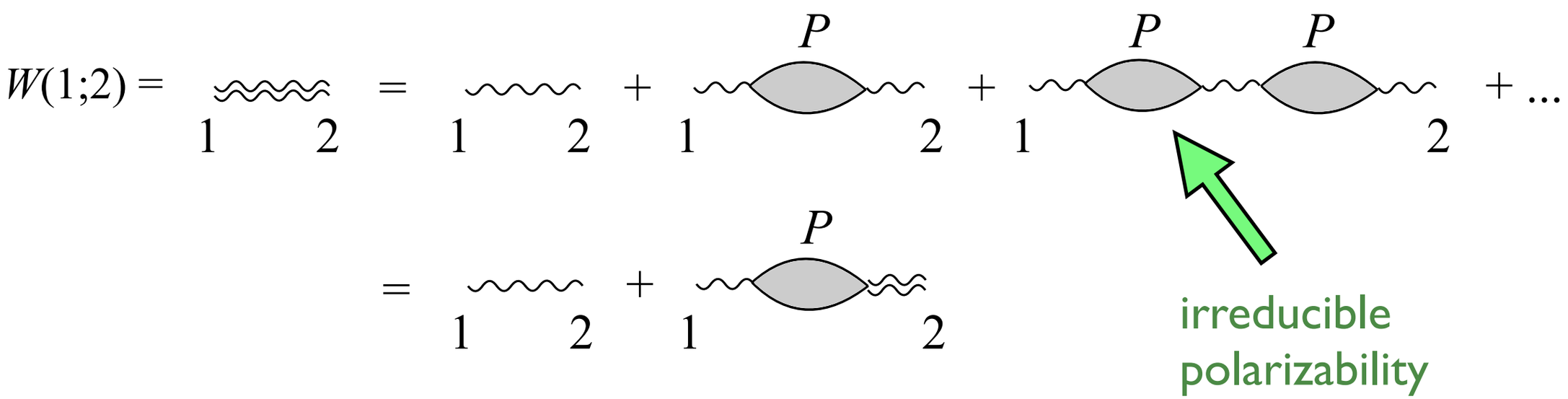
$$G(1, \mathbf{x}_2 t_0) = -G(1, \mathbf{x}_2 t_0 - i\beta)$$

W-skeletons

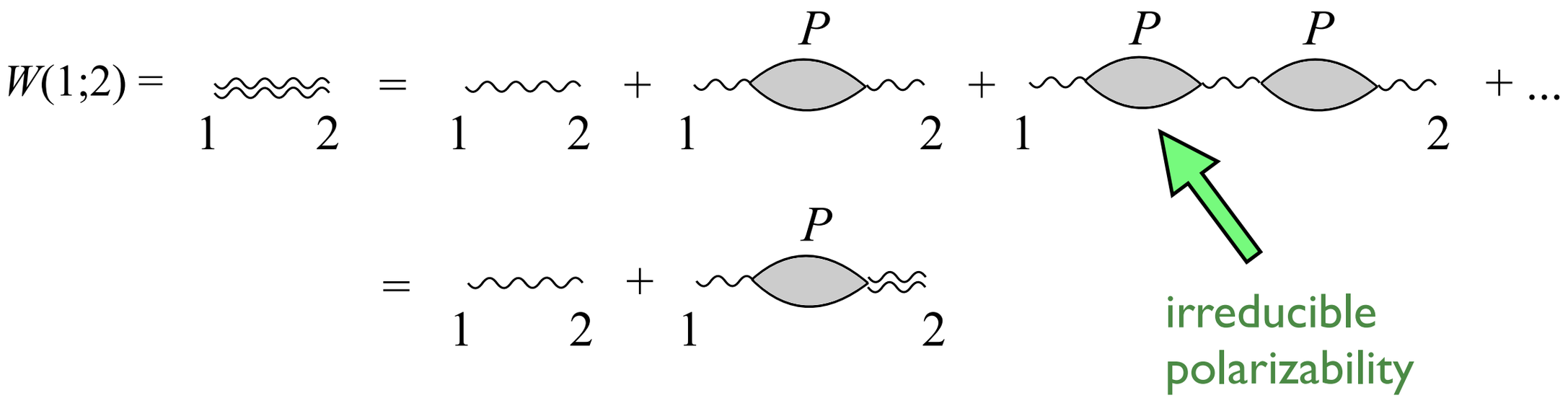
We can further renormalize the interaction lines, by removing all interaction line insertions. For example



We can then define the screened interaction W by



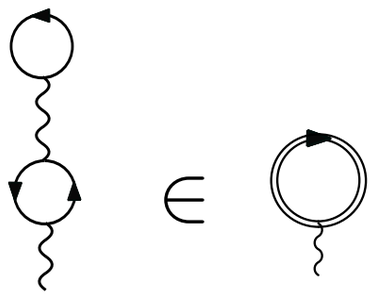
We can then define the screened interaction W by



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

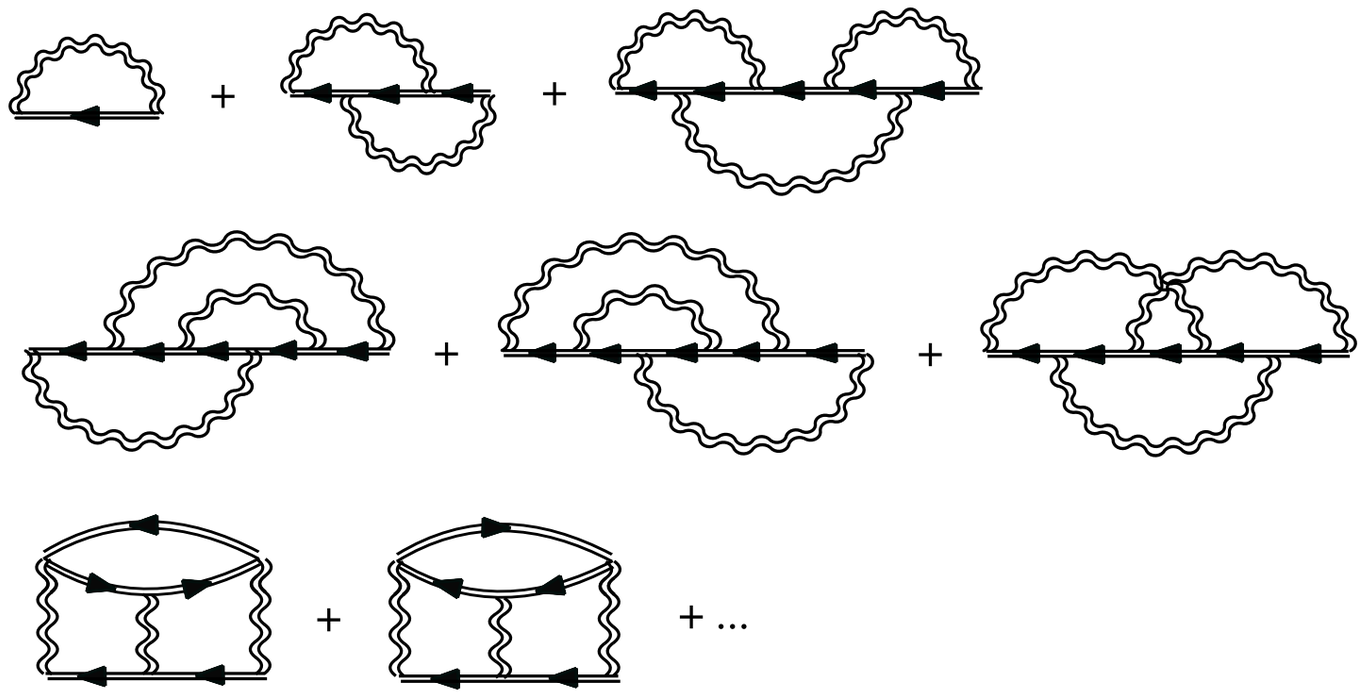


$$\Sigma = \Sigma_{ss}[G,W] = \Sigma_H[G,w] + \Sigma_{ss,\mathrm{xc}}[G,W]$$

double skeletonic

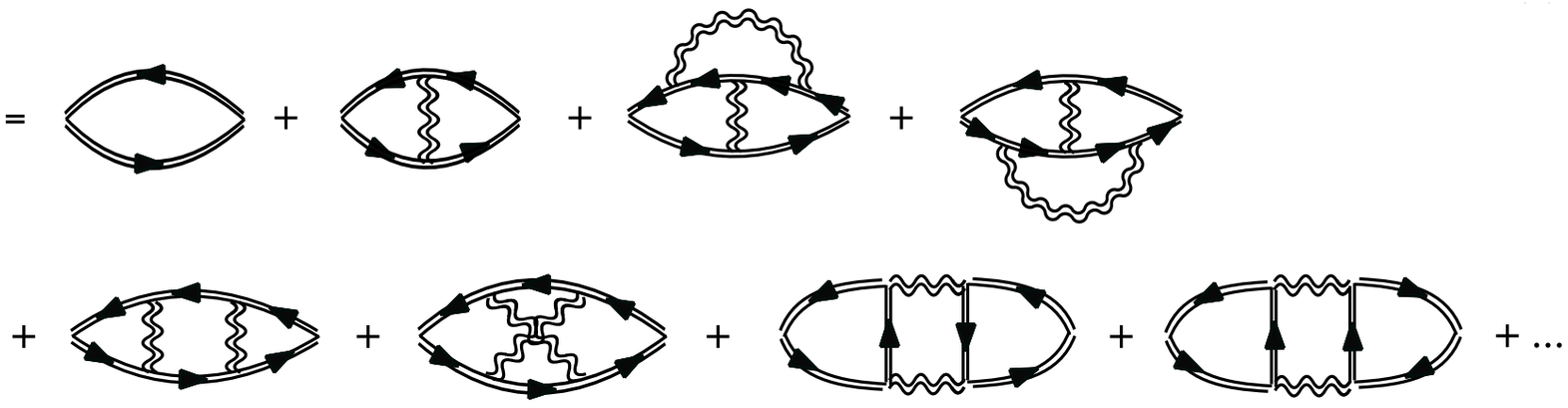
This gives the double-skeletonic expansion for the self-energy

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



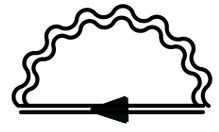
and the polarizability

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

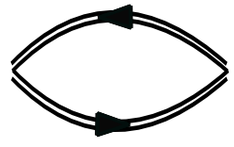


The lowest order in W gives the GW approximation

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



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



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

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

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 (see lectures Matteo Gatti)

Contours and formalisms

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

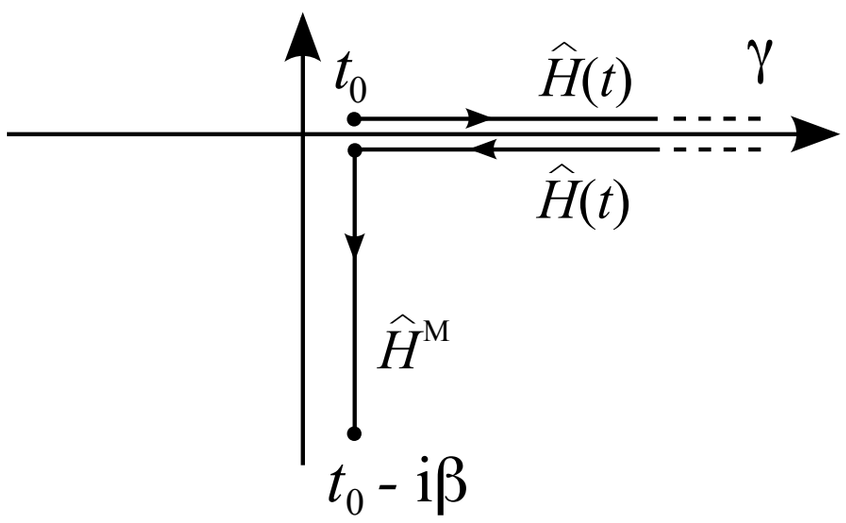
With different assumptions we can modify the contour

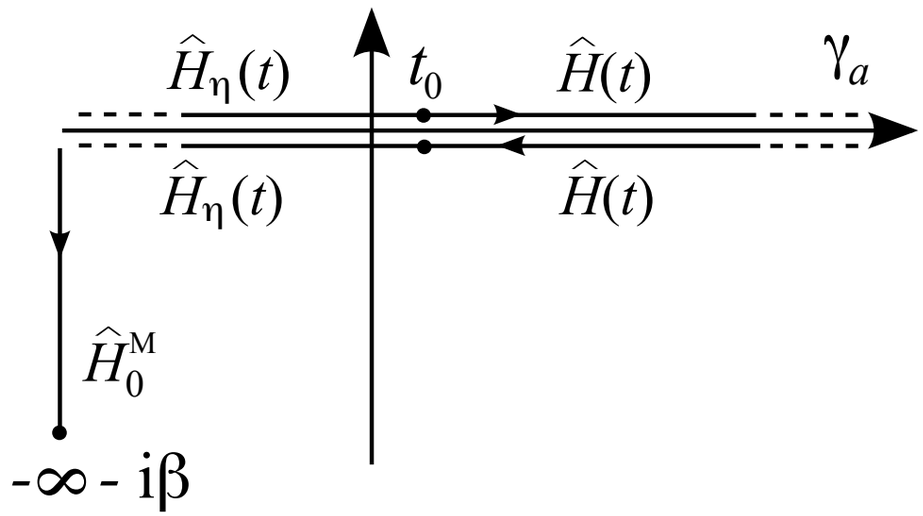
Adiabatic assumption

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

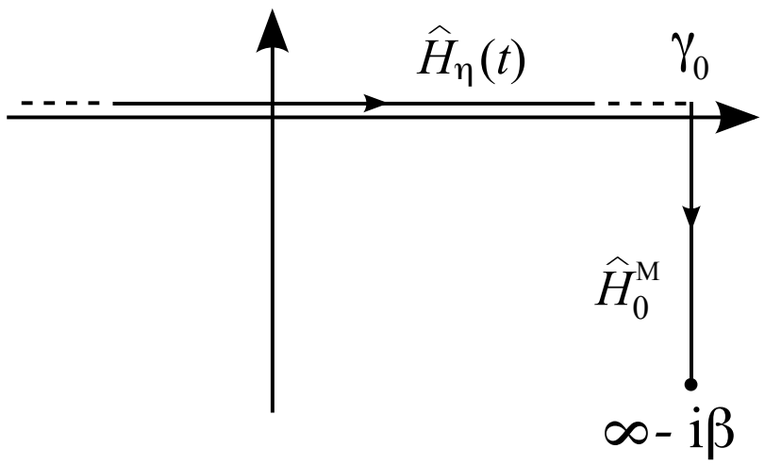
$$\hat{H}(z \in \gamma^{\rm M}) = \hat{H}_0^{\rm M} = \hat{H}_0 - \mu\hat{N},$$

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





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



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

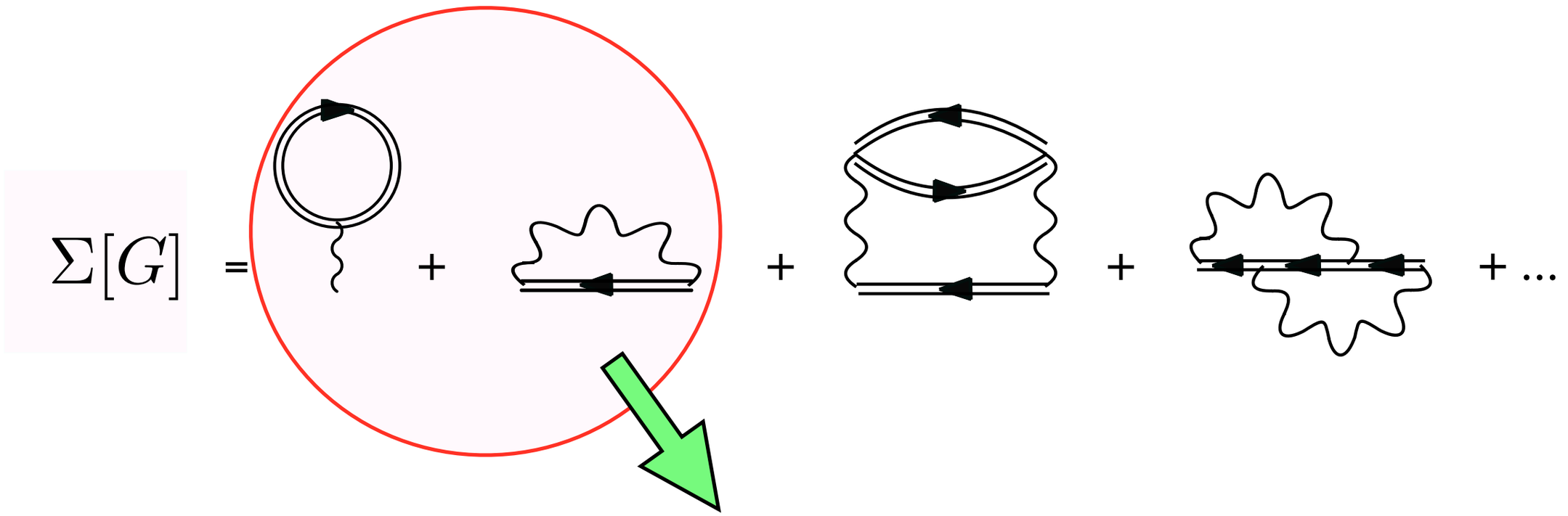
$$G(1,2) = -i\langle \mathcal{T}\left\{\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)\right\}\rangle = \theta(z_1,z_2)\,G^{>}(1,2) + \theta(z_1,z_2)\,G^{<}(1,2)$$

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

$$c^R(t,t') = c^\delta(t)\delta(t-t') + \theta(t-t')[c^>(t,t') - c^<(t,t')]$$
$$c^A(t,t') = c^\delta(t)\delta(t-t') - \theta(t'-t)[c^>(t,t') - c^<(t,t')]$$

$$c^\lceil(\tau,t) = c(t_0 - i\tau, t)$$
$$c^\rceil(t,\tau) = c(t, t_0 - i\tau)$$

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

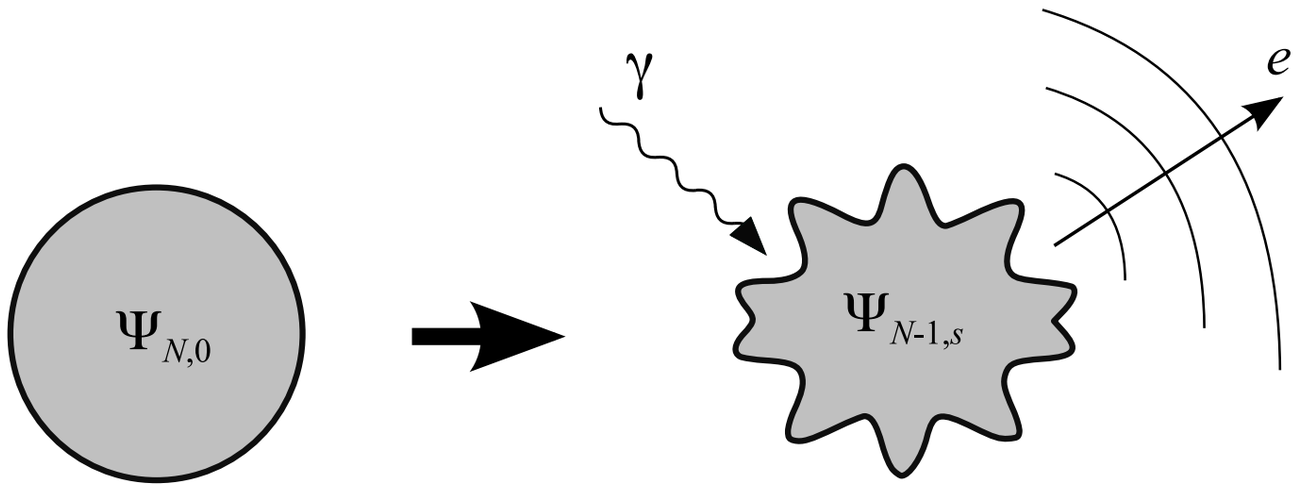
$$-i\,G^{<}_{jj}(t,t') = \langle\Psi_0|\hat{a}^{\dagger}_{j,H}(t')\hat{a}_{j,H}(t)|\Psi_0\rangle = \langle\tilde{\Psi}_j(t')|\tilde{\Psi}_j(t)\rangle = \sum_s |c_{s,j}|^2\, e^{-i(E_0-E_{N-1,s})(t-t')}$$

It will be convenient to write this in frequency space

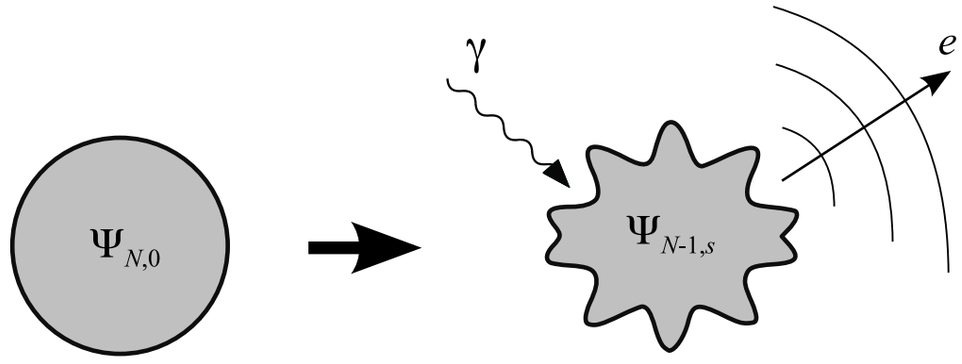
$$G^{<}_{jj}(t-t') = \int \frac{d\omega}{2\pi}\, G_{jj}(\omega)\, e^{-i\omega(t-t')}$$

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

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 (See Simo Huotari's lectures)

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

- The renormalization 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.

Introduction to Many-body Theory III

Part III: Linear response and examples

- The 2-particle Green's function and optical spectra
- Hedin's equations
- Linear response
- Examples: Time-dependent screening in an electron gas

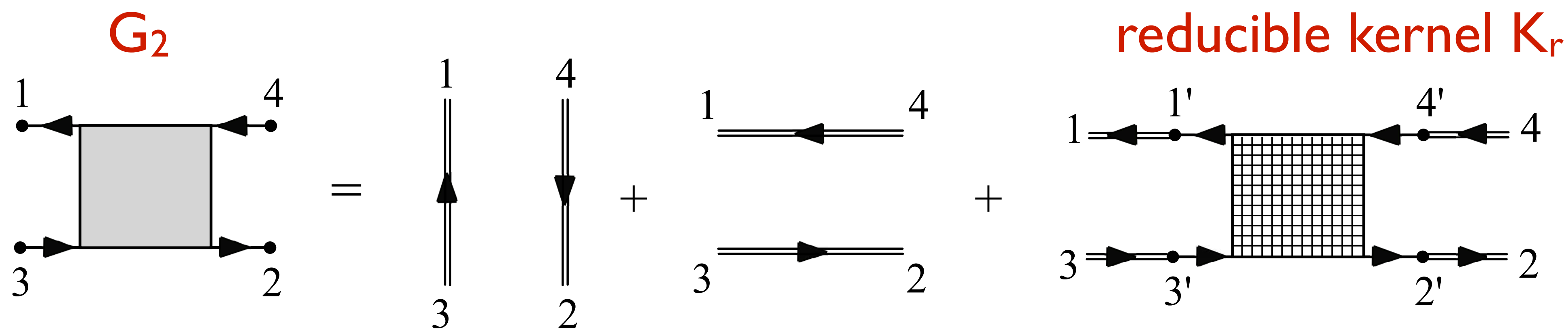
The 2-particle Green's function

See also lectures by Ilya Tokatly

We can further expand the two-particle Green's function using Wick's theorem

$$G_2(a,b;c,d) = \frac{\sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{\mathrm{i}}{2}\right)^k \int v(1;1') \dots v(k;k') \begin{vmatrix} G_0(a;c) & G_0(a;d) & \dots & G_0(a;k'^+) \\ G_0(b;c) & G_0(b;d) & \dots & G_0(b;k'^+) \\ \vdots & \vdots & \ddots & \vdots \\ G_0(k';c) & G_0(k';d) & \dots & G_0(k';k'^+) \end{vmatrix}_{\pm}}{\sum_{k=0}^{\infty} \frac{1}{k!} \left(\frac{\mathrm{i}}{2}\right)^k \int v(1;1') \dots v(k;k') \begin{vmatrix} G_0(1;1^+) & G_0(1;1'^+) & \dots & G_0(1;k'^+) \\ G_0(1';1^+) & G_0(1';1'^+) & \dots & G_0(1';k'^+) \\ \vdots & \vdots & \ddots & \vdots \\ G_0(k';1^+) & G_0(k';1'^+) & \dots & G_0(k';k'^+) \end{vmatrix}_{\pm}}$$

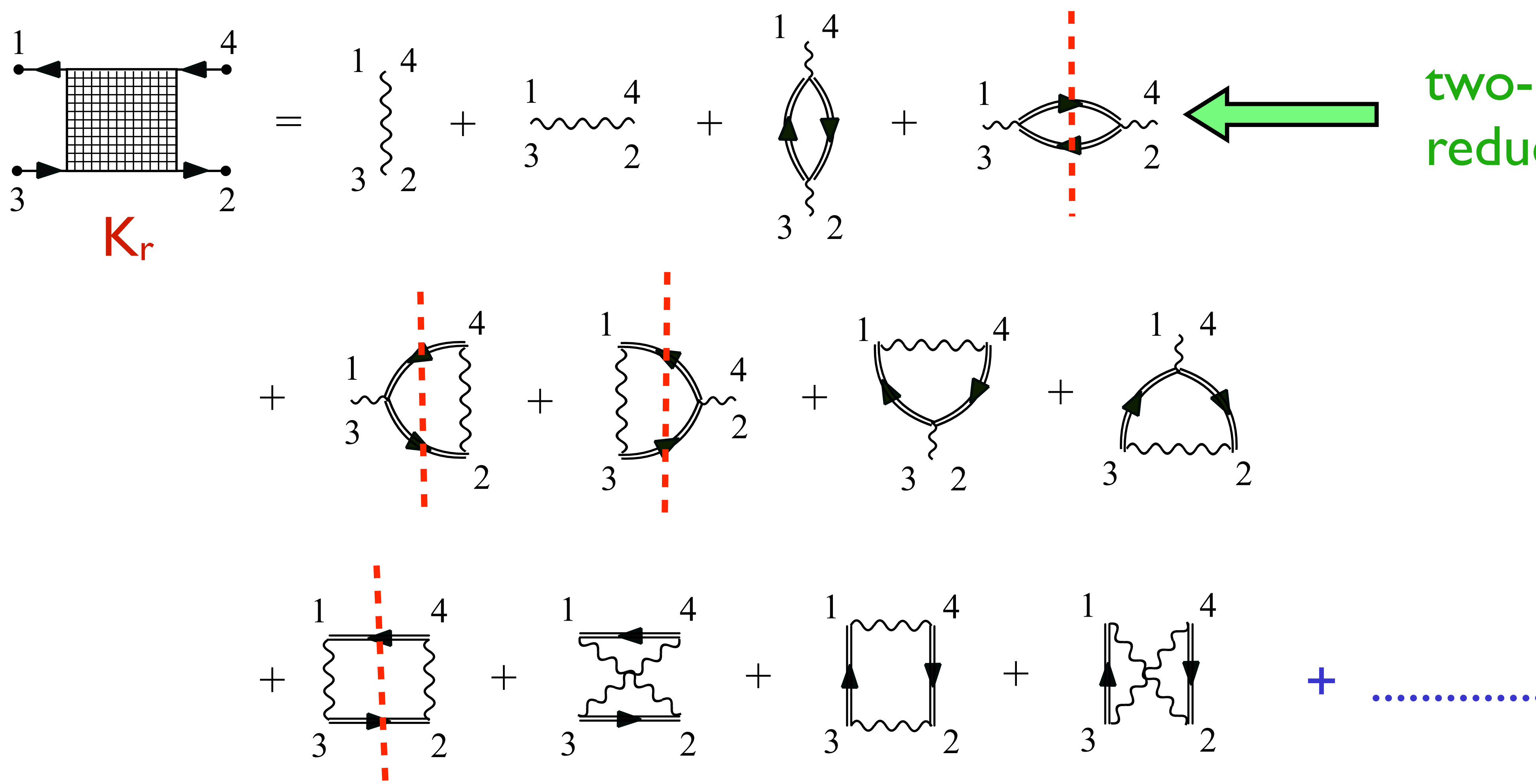
Again only connected diagrams contribute. In the same way as before non-connected diagrams cancel and we can expand in G-skeletons by removing self-energy insertions



$$G_2(1,2;3,4) = G(1;3)G(2;4) \pm G(1;4)G(2;3)$$

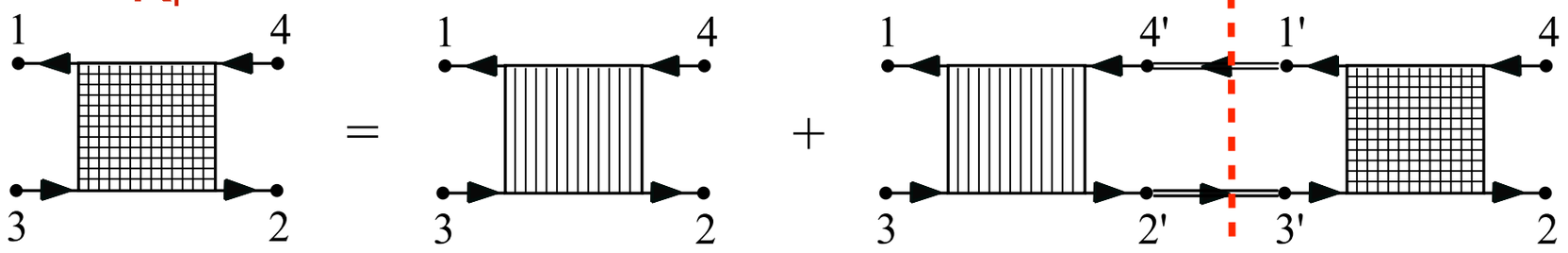
noninteracting form

$$+ \int G(1;1')G(3';3)K_r(1',2';3',4')G(4';4)G(2;2')$$



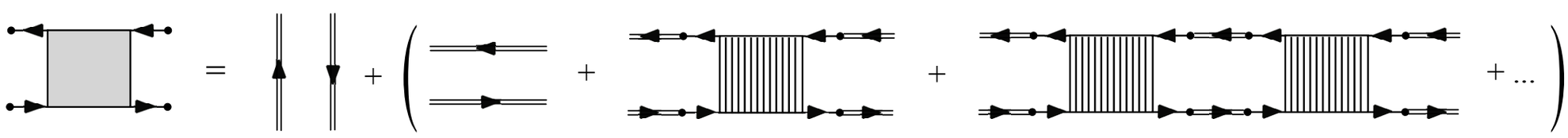
two-particle reducible

K_r irreducible kernel K

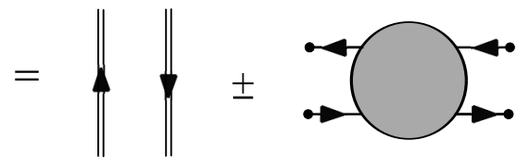


$$K_r(1,2;3,4) = K(1,2;3,4) \pm \int K(1,2';3,4')G(4';1')G(3';2')K_r(1',2;3',4)$$

K K K

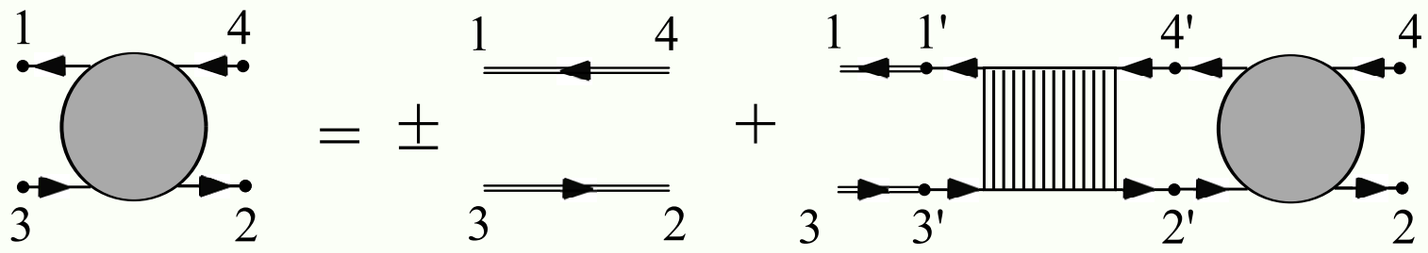


G_2 L



$$L(1,2;3,4) \equiv \pm\big[G_2(1,2;3,4) - G(1;3)G(2;4)\big]$$

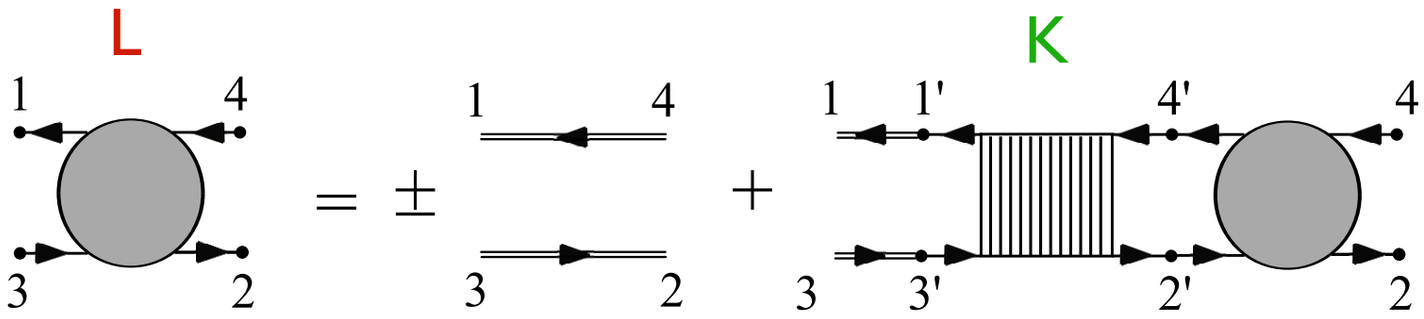
L K



Bethe-Salpeter equation

$$L(1,2;3,4) = G(1;4)G(2;3) \pm \int G(1;1')G(3';3)K(1',2';3',4')L(4',2;2',4)$$

To find the 2-particle Green's function we have to solve the Bethe-Salpeter equation



Bethe-Salpeter equation

$$L(1,2;3,4) = G(1;4)G(2;3) \pm \int G(1;1')G(3';3)K(1',2';3',4')L(4',2;2',4)$$

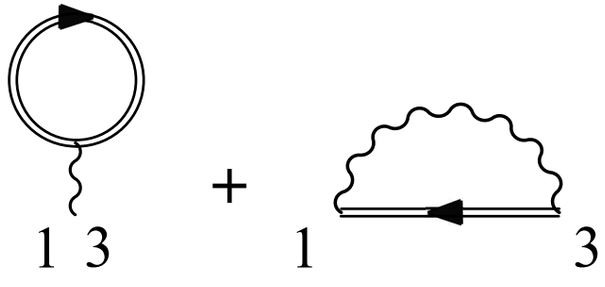
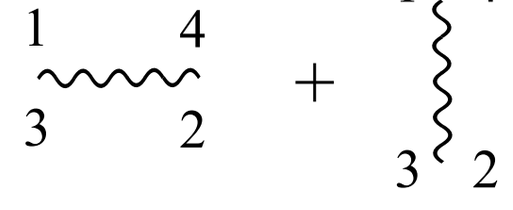
If we expand the self-energy in G-skeletonic diagrams then the following important relation is valid

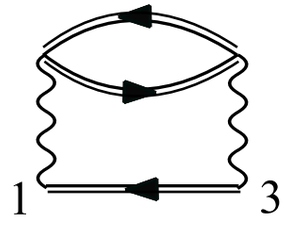
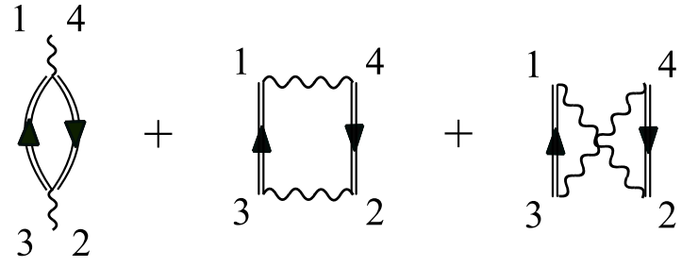
$$K(1,2;3,4) = \pm \frac{\delta \Sigma(1;3)}{\delta G(4;2)}$$

It is not hard to prove this diagrammatically

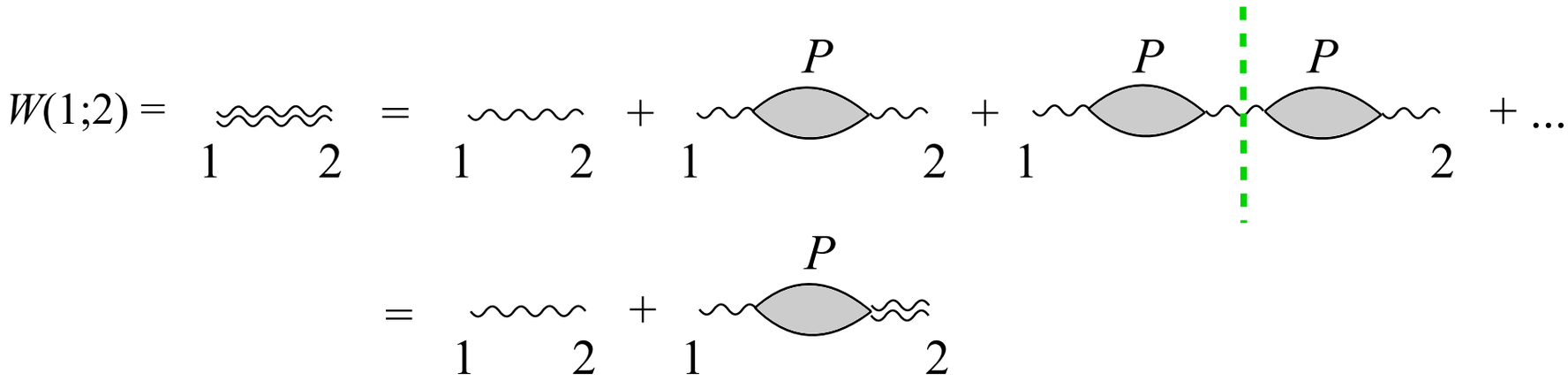
Let us give some examples

K

$$\Sigma_{\rm HF}(1;3) =$$  $$\pm\frac{\delta\Sigma_{\rm HF}(1;3)}{\delta G(4;2)} =$$ 

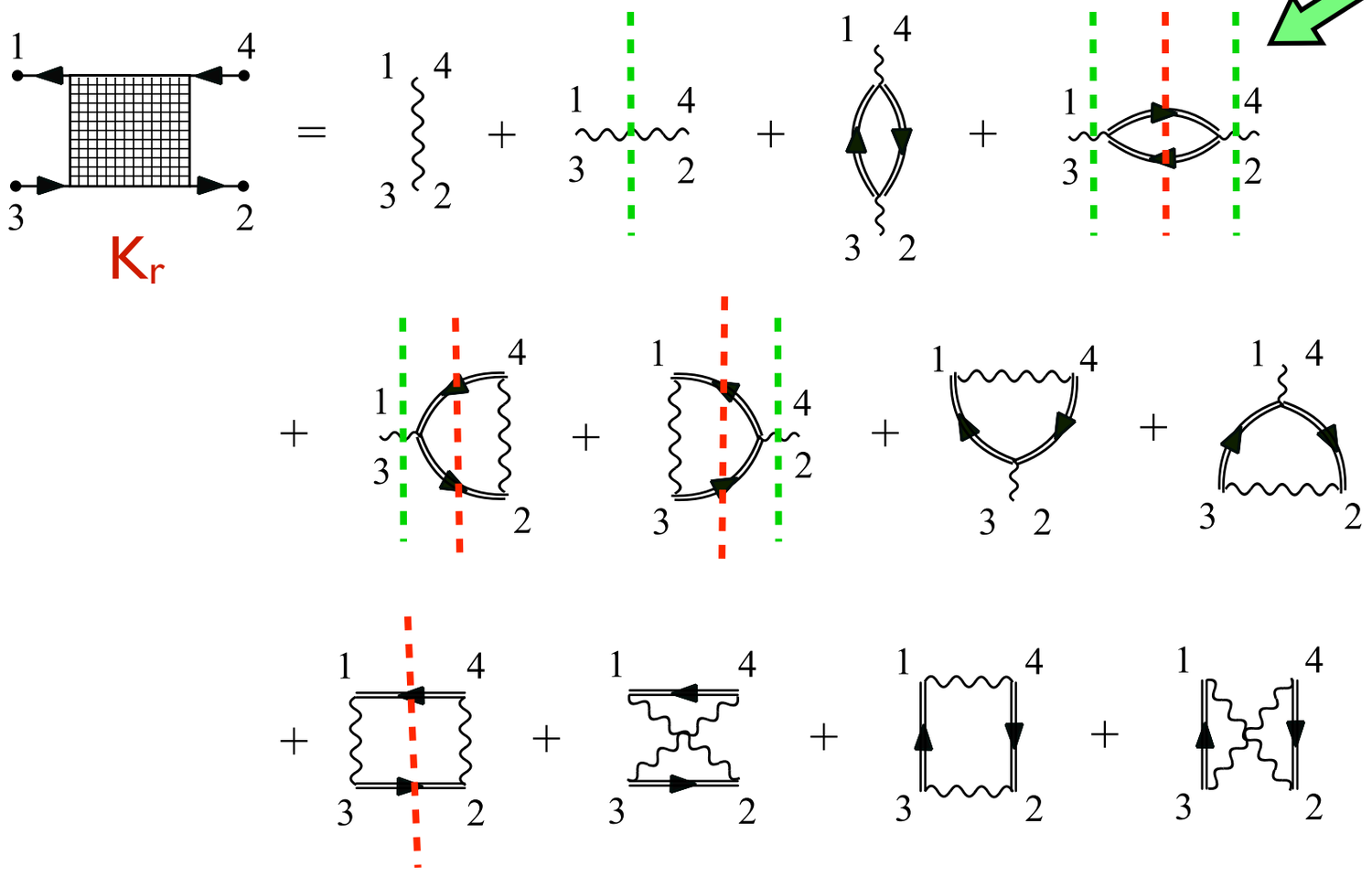
$$\Sigma_{\rm 2B,bubble}(1;3) =$$  $$\pm\frac{\delta\Sigma_{\rm 2B,bubble}(1;3)}{\delta G(4;2)} =$$ 

What about the W-skeletons? Remember that



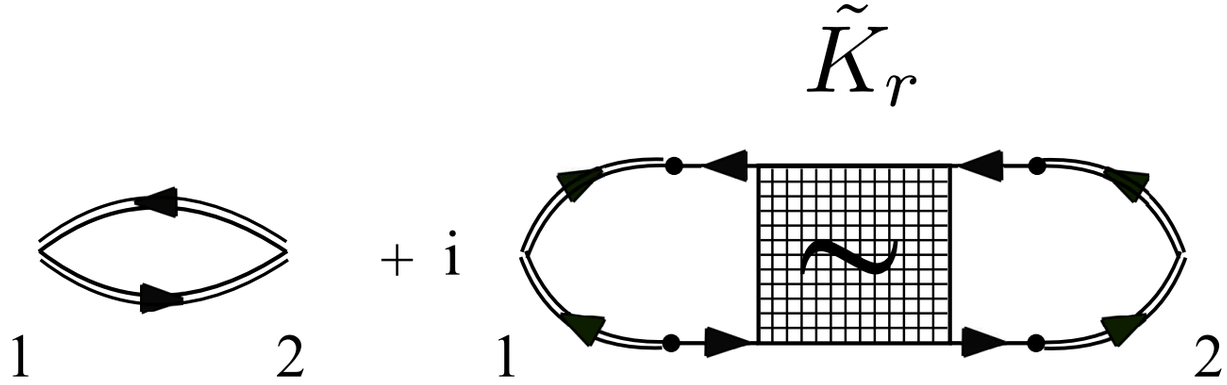
Let us look at the reducible kernel again

interaction line reducible

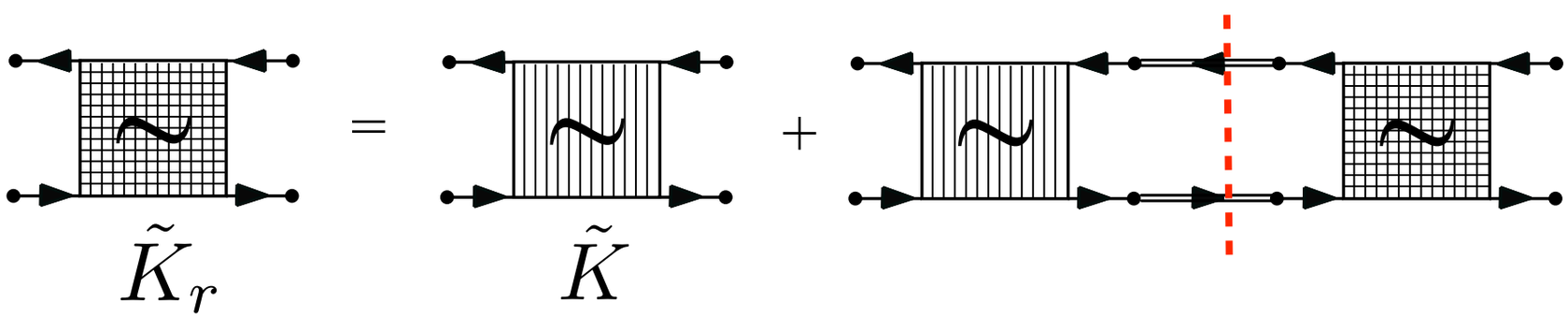


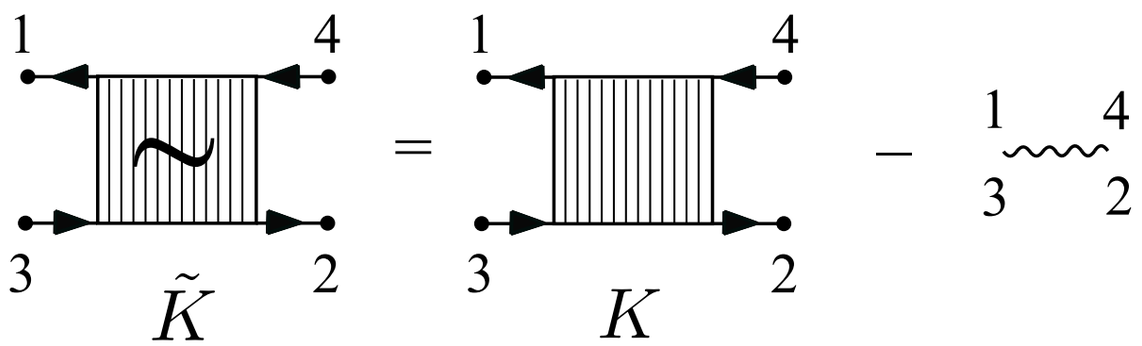
If we remove from K_r all interaction line reducible we obtain a new kernel $\tilde{K}_r$

$$P(1;2) =$$



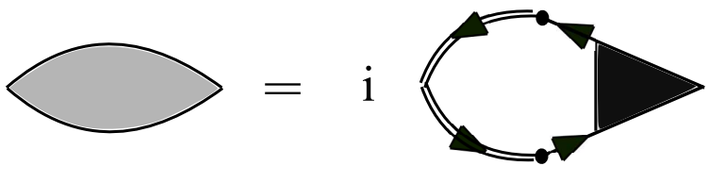
The reducible kernel can again be expanded in a G-line irreducible one





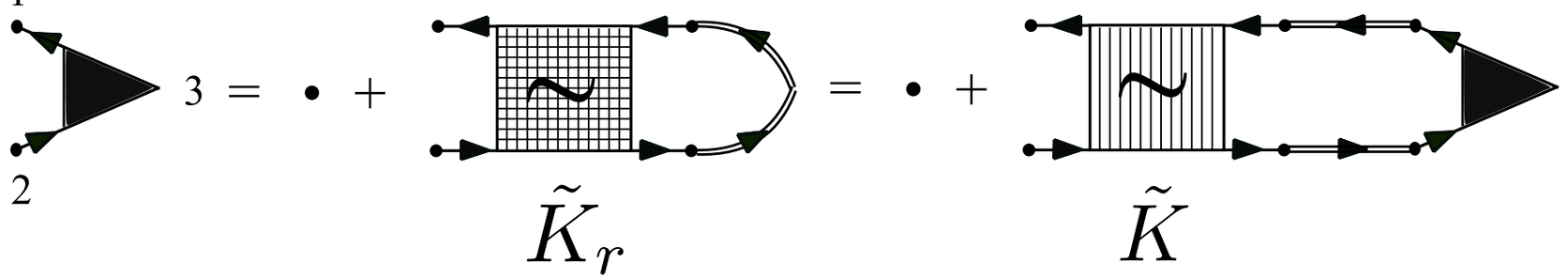
$$\tilde{K}(1,2;3,4) = K(1,2;3,4) - \mathrm{i}\,\delta(1;3)\delta(2;4)v(1;2)$$

The polarizability can then be expressed as



$$P(1,2) = -i \int d4\, G(1,3)\, G(4,1)\, \Gamma(3,4;2)$$

where we defined the vertex function as



$$\Gamma(1,2;3) = \delta(1,2^+)\delta(3,2) - \int d(4567)\, \tilde{K}(1,5;2,4)\, G(4,6)\, G(7,5)\, \Gamma(6,7;3)$$

For the kernel $\tilde{K}$ the following relation is valid

$$\tilde{K}(1,2;3,4) = -\frac{\delta\Sigma_{\rm xc}(1,3)}{\delta G(4,2)}$$

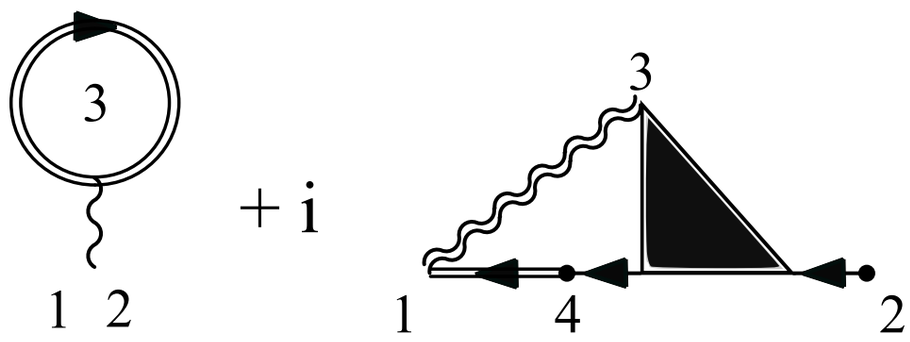
as follows from a diagrammatic proof

The equation for the vertex therefore becomes

$$\Gamma(1,2;3) = \delta(1;2^+)\delta(3;2) + \int d4d5d6d7\, \frac{\delta\Sigma_{\rm xc}(1;2)}{\delta G(4;5)}\, G(4;6)G(7;5)\Gamma(6,7;3)$$

If we can further express the vertex in terms of the vertex we have a closed set of functional differential equations

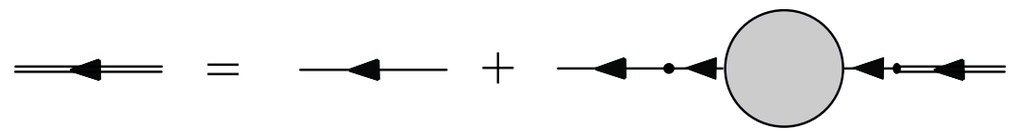
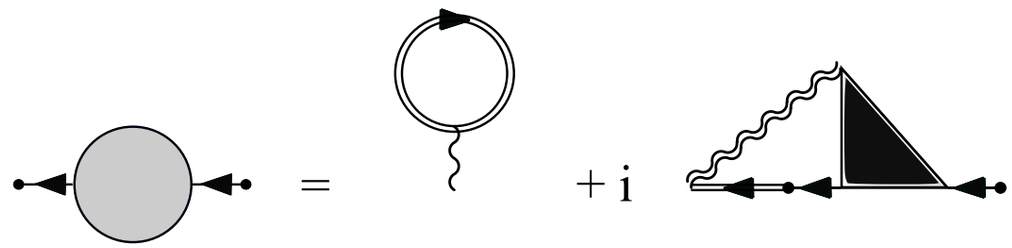
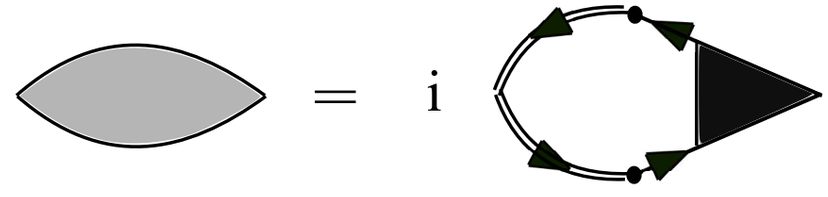
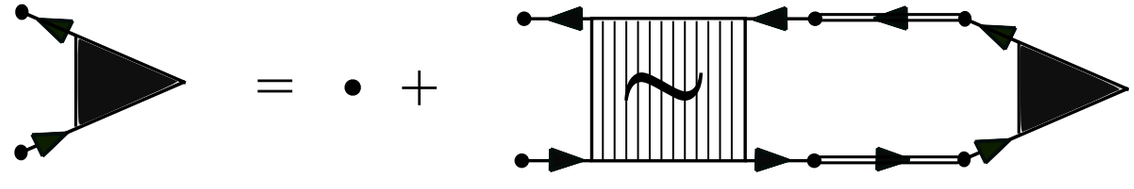
By a diagrammatic derivation we can also show that the self-energy can be expressed in terms of the vertex

$\Sigma(1;2) =$ 

$$\Sigma(1;2) = \pm \mathrm{i}\,\delta(1;2)\int d3\, v(1;3)G(3;3^{+}) + \mathrm{i}\int d3d4\, W(1;3)G(1;4)\Gamma(4,2;3)$$

Let us collect all the equations that we derived

Hedin's equations

$G = G_0 + G_0 \Sigma G$	
$\Sigma = \Sigma_{\mathrm{H}} + \mathrm{i} G W \Gamma$	
$P = \pm \mathrm{i} G G \Gamma$	
$W = v + vPW$	
$\Gamma = \delta + \frac{\delta \Sigma_{\mathrm{xc}}}{\delta G} G G \Gamma$	

2-particle Green's function and Hedin's equations: Take home message

- For the 2-particle Green's function we can derive an equation with a reducible kernel, known as the Bethe-Salpeter equation.

- The reducible kernel is the functional derivative of the self-energy with respect to the Green's function.

- From the diagrammatic rules we can derive a set of functional differential equations relating the vertex, the Dyson and the Bethe-Salpeter equation. These equations are known as the Hedin equations.

- The Hedin equations can be iterated in various ways to generate different perturbation series.
  It is not known whether all skeleton diagrams are generated once by such a procedure.

Linear response functions

$$\langle \hat{n}(\mathbf{x},t)\rangle = \frac{\mathrm{Tr}\ \mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\,\hat{H}(\bar{z})}\hat{n}(\mathbf{x},t)\right\}}{\mathrm{Tr}\ \mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\,\hat{H}(\bar{z})}\right\}}$$

If we make the variation $\hat{H}(z) \to \hat{H}(z) + \delta\hat{V}(z)$ $\qquad \delta\hat{V}(z) = \int d\mathbf{x}\,\hat{n}(\mathbf{x})\,\delta v(\mathbf{x}z)$

then

$$\delta\langle \hat{n}(\mathbf{x},t)\rangle = -i\int_\gamma dz_1 \frac{\mathrm{Tr}\ \mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\,\hat{H}(\bar{z})}\hat{n}(\mathbf{x},t)\delta\hat{V}(z_1)\right\}}{\mathrm{Tr}\ \mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\,\hat{H}(\bar{z})}\right\}} + i\langle \hat{n}(\mathbf{x},t)\rangle \int_\gamma dz_1 \frac{\mathrm{Tr}\ \mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\,\hat{H}(\bar{z})}\delta\hat{V}(z_1)\right\}}{\mathrm{Tr}\ \mathcal{T}\left\{e^{-i\int_\gamma d\bar{z}\,\hat{H}(\bar{z})}\right\}}$$

which can be rewritten as

$$\delta n(1) = \int d2\,\chi(1,2)\,\delta v(2)$$

$$\chi(1,2) = -i\left[\,\langle \mathcal{T}\{\hat{n}_H(1)\hat{n}_H(2)\}\rangle - n(1)n(2)\,\right]$$

There is a close relation between the density response function and the Bethe-Salpeter equation. We have

$$
\begin{aligned}
L(1,2;1',2') &= -\left[G_2(1,2;1',2') - G(1,1')G(2,2')\right] \\
&= \langle \mathcal{T}\left\{\hat{\psi}_H(1)\hat{\psi}_H(2)\hat{\psi}^\dagger_H(2')\hat{\psi}^\dagger_H(1')\right\}\rangle - \langle \mathcal{T}\left\{\hat{\psi}_H(1)\hat{\psi}^\dagger_H(1')\right\}\rangle\langle \mathcal{T}\left\{\hat{\psi}_H(2)\hat{\psi}^\dagger_H(2')\right\}\rangle
\end{aligned}
$$

and therefore

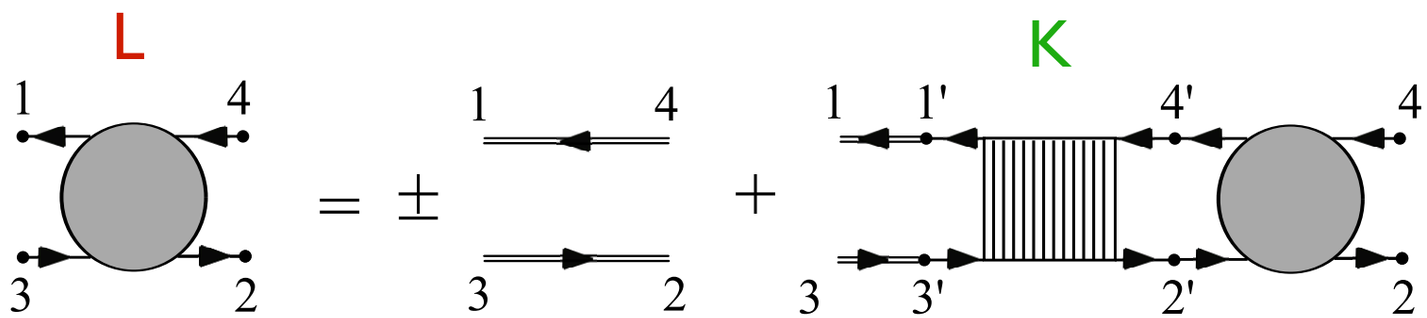
$$
\chi(1,2) = -i\left[\langle \mathcal{T}\left\{\hat{n}_H(1)\hat{n}_H(2)\right\}\rangle - n(1)n(2)\right] = -i\,L(1,2;1^+,2^+)
$$

In combination with the Bethe-Salpeter equation we can then further derive that

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

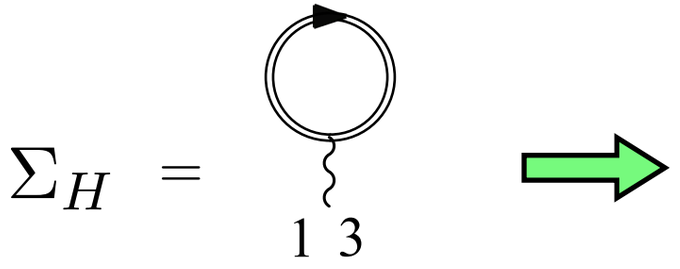
A diagrammatic expansion of the polarizability therefore directly gives an approximation for the density response function

Random Phase Approximation and plasmons

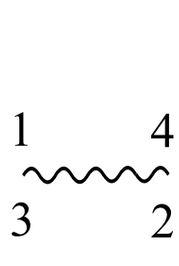


Bethe-Salpeter equation

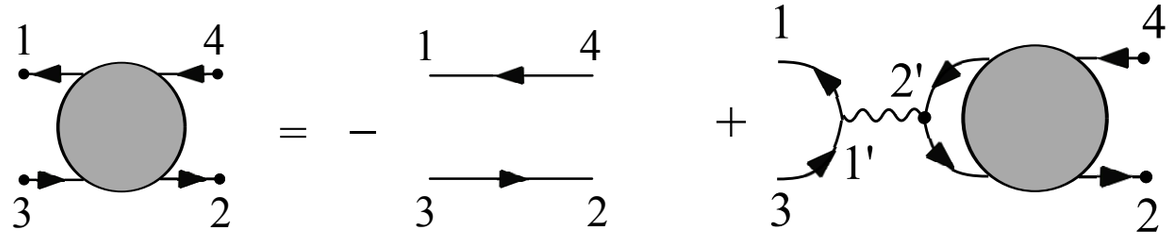
If we calculate the Bethe-Salpeter from the Hartree self-energy



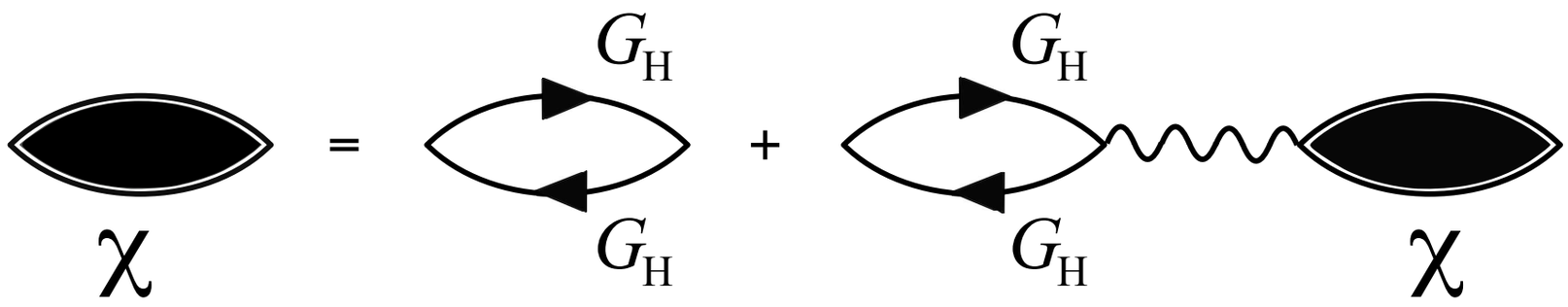
$$K_H(1,2;3,4) = -\frac{\delta\Sigma_H(1,3)}{\delta G(4,2)} =$$



then the Bethe-Salpeter equation becomes



From $\chi(1,2) = -i\,L(1,2;1^+,2^+)$ it then follows



if we take the retarded component of this expression and Fourier transform then we find

$$\chi^{\rm R}(\mathbf{x}_1,\mathbf{x}_2;\omega) = \chi_0^{\rm R}(\mathbf{x}_1,\mathbf{x}_2;\omega) + \int d\mathbf{x}_3 d\mathbf{x}_4\, \chi_0^{\rm R}(\mathbf{x}_1,\mathbf{x}_3;\omega) v(\mathbf{x}_3,\mathbf{x}_4) \chi^{\rm R}(\mathbf{x}_4,\mathbf{x}_2;\omega)$$

This approximation for the density response function is also known as the Random Phase Approximation (RPA).

A better name is the Time-Dependent Hartree Approximation (it amounts to TDDFT with zero xc-kernel)

Let us now take the case of the homogeneous electron gas. Since the system is translational invariant we can write

$$\sum_{\sigma\sigma'} \chi^{\mathrm{R}}(\mathbf{x},\mathbf{x}';\omega) = \int \frac{d\mathbf{p}}{(2\pi)^3} e^{\mathrm{i}\mathbf{p}\cdot(\mathbf{r}-\mathbf{r}')} \chi^{\mathrm{R}}(\mathbf{p},\omega)$$

$$\chi^{\mathrm{R}}(\mathbf{q},\omega) = \frac{\chi_0^{\mathrm{R}}(\mathbf{q},\omega)}{1-\tilde{v}_{\mathbf{q}}\chi_0^{\mathrm{R}}(\mathbf{q},\omega)}, \qquad \tilde{v}_{\mathbf{q}} = \frac{4\pi}{q^2}$$

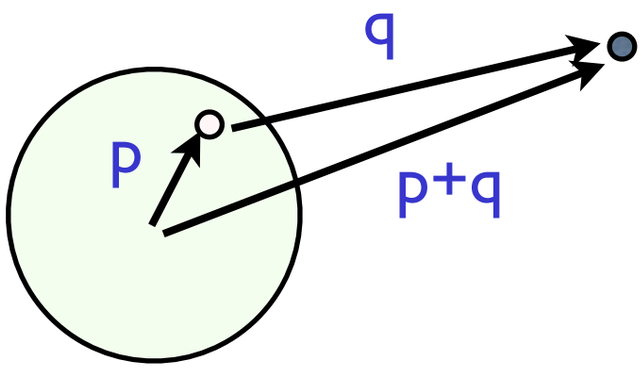
⇐ Fourier transform Coulomb potential

⇓

The RPA response function has poles at the poles of $\chi_0(\mathbf{q},\omega)$ and when

$$1 - \tilde{v}_{\mathbf{q}}\,\chi_0(\mathbf{q},\omega) = 0$$

The extra pole corresponding to this condition is known as the plasmon and corresponds to a collective mode of the electron gas



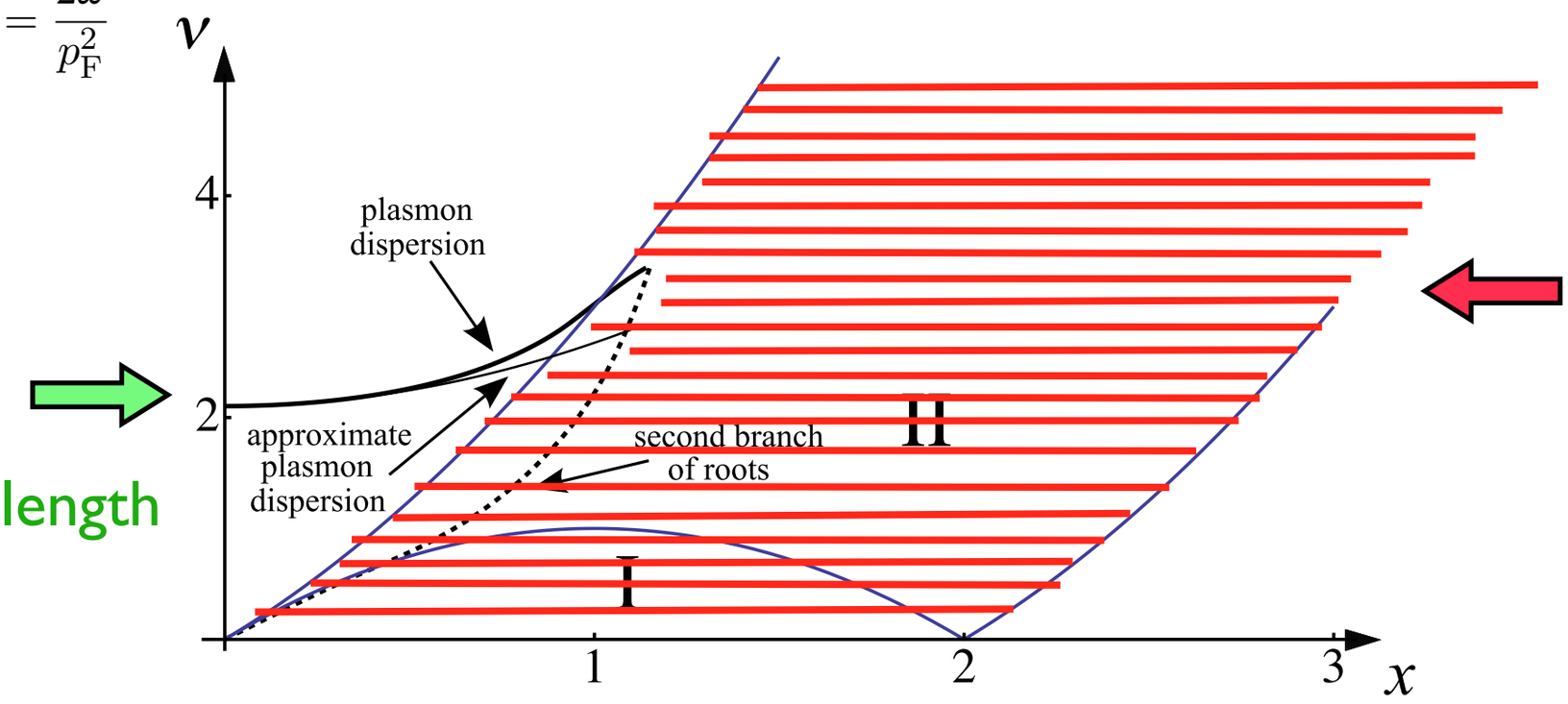
Fermi sphere
with radius p_F

$$\epsilon = \frac{(\mathbf{p}+\mathbf{q})^2}{2} - \frac{\mathbf{p}^2}{2} = \frac{\mathbf{q}^2}{2} + |\mathbf{p}||\mathbf{q}|\cos\theta$$

$$\frac{q^2}{2} - q\,p_{\rm F} \;\le \epsilon \le \frac{q^2}{2} + q\,p_{\rm F} \qquad\qquad q = |\mathbf{q}|$$

The particle-hole excitations lie between two parabolas in the q-ω plane

$$\nu = \frac{2\omega}{p_{\rm F}^2}$$



ω_p
plasma
frequency
Long wavelength
plasmon

particle-hole
continuum

$$x = \frac{q}{p_{\rm F}}$$

Sudden creation of a positive charge (such as in the creation of a core-hole)

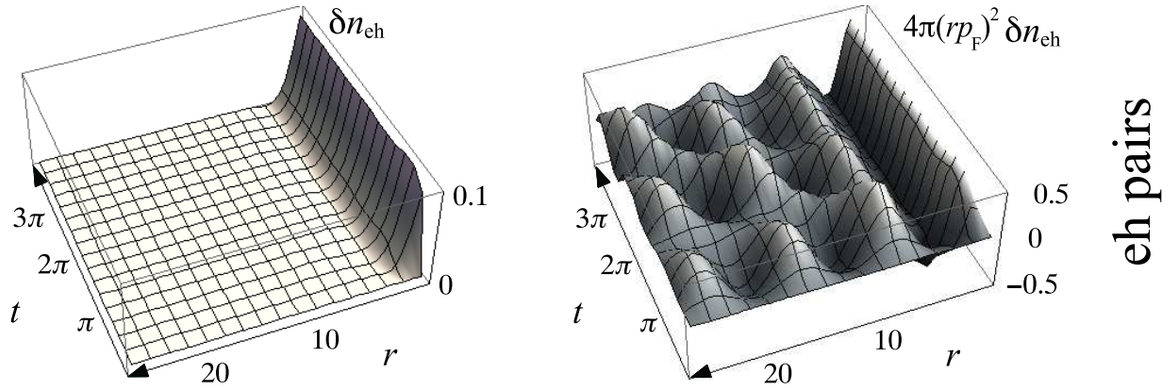
$$\delta V(\mathbf{x},t) = \theta(t)\frac{Q}{r} = \int \frac{d\mathbf{q}}{(2\pi)^3}\int \frac{d\omega}{2\pi} e^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}-\mathrm{i}\omega t}\,\delta V(\mathbf{q},\omega)$$

$$\delta V(\mathbf{q},\omega) = \frac{4\pi Q}{q^2}\frac{\mathrm{i}}{\omega+\mathrm{i}\eta} = \tilde{v}_{\mathbf{q}}\,Q\frac{\mathrm{i}}{\omega+\mathrm{i}\eta}.$$

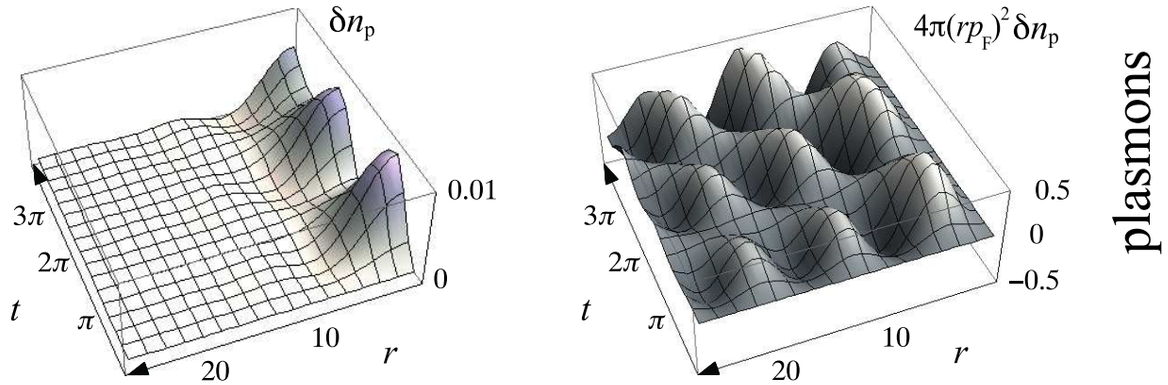
We can calculate the induced density change from the RPA response function. A few manipulations lead to

$$\delta n(\mathbf{r},t) = -\frac{16\pi Q}{(2\pi)^4}\frac{1}{r}\int_0^\infty dq\, q\,\sin qr \int_0^\infty \mathrm{Im}\chi^{\mathrm{RPA}}(q,\omega)\,\tilde{v}_{\mathbf{q}}\frac{1-\cos\omega t}{\omega}$$

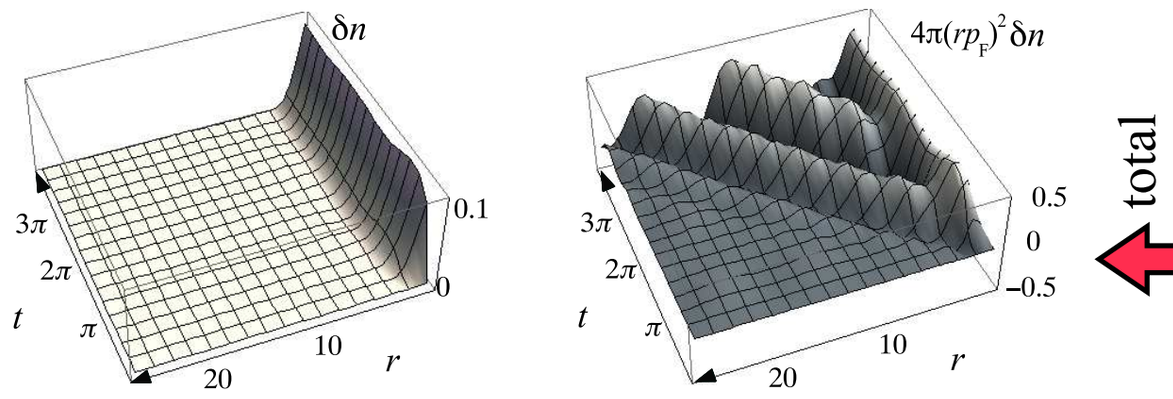
The integral can be split into a contribution from particle-hole excitations and a contribution from the plasmon



(a)



(b)



(c)

The positive charge is screened at a time-scale of the inverse plasmon frequency

Figure 15.7: This figure shows the 3D plot of the transient density in an electron gas with $r_s = 3$ induced by the sudden creation of a point-like positive charge $Q = 1$ in the origin at $t = 0$. The contribution due to the excitation of electron-hole pairs (a) and plasmons (b) is, for clarity, multiplied by $4\pi(rp_{\rm F})^2$ in the plots to the right. Panel (c) is simply the sum of the two contributions. Units: r is in units of $1/p_{\rm F}$, t is in units of $1/\omega_{\rm p}$ and all densities are in units of $p_{\rm F}^3$.

In the long time limit we have

$$\delta n_s(\mathbf{r}) \equiv \lim_{t\to\infty} \delta n(\mathbf{r},t) = -\frac{Q}{2\pi^2}\frac{1}{r}\int_0^\infty dq\, q \sin(qr)\tilde{v}_{\mathbf{q}}\,\chi^{\mathrm{R}}(\mathbf{q},0)$$

has spatial oscillations known as Friedel oscillations

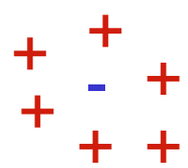
Suppose now that $Q = q = -1$ is the same a the electron charge. The total density change due to this test charge is

$$q\,\delta n_{\mathrm{tot}}(\mathbf{r}) = q[\delta(\mathbf{r}) + \delta n_s(\mathbf{r})]$$

The interaction energy between this charge and a generic electron is

$$e_{\mathrm{int}}(\mathbf{r}) = \int d\mathbf{r}' v(\mathbf{r},\mathbf{r}')\delta n_{\mathrm{tot}}(\mathbf{r}')$$

$$\begin{aligned} e_{\mathrm{int}}(\mathbf{r}) &= \int d\mathbf{r}' v(\mathbf{r},\mathbf{r}')\left[\delta(\mathbf{r}) + \int \frac{d\mathbf{q}}{(2\pi)^3}\, e^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}'}\,\tilde{v}_{\mathbf{q}}\,\chi^{\mathrm{R}}(\mathbf{q},0)\right] \\ &= \int \frac{d\mathbf{q}}{(2\pi)^3}\, e^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}}\left[\tilde{v}_{\mathbf{q}} + \tilde{v}_{\mathbf{q}}^2\chi^{\mathrm{R}}(\mathbf{q},0)\right] \\ &= \int \frac{d\mathbf{q}}{(2\pi)^3}\, e^{\mathrm{i}\mathbf{q}\cdot\mathbf{r}}\, W^{\mathrm{R}}(\mathbf{q},0) \xrightarrow[r\to\infty]{} \frac{e^{-r/\lambda_{\mathrm{TF}}}}{r} \end{aligned}$$



In the static limit W describes the interaction between a test charge and an electron

Linear response: Take home message

- We can derive a diagrammatic expansion for the linear response function from the diagrammatic rules for the 2-particle Green's function

- The linear response function gives direct information on neutral excitation spectra such as measured in optical absorption experiments

- The random phase approximation to the linear response function describes the phenomena of plasmon excitation in metallic systems

- The screening of a an added charge in the electron gas happens at a time-scale of the inverse plasmon frequency

Spectral properties of an electron gas : GW

We have seen that the spectral function describes the energy distribution of excitations upon addition or removal of an electron. We therefore expect so see both plasmon and particle-hole excitations when we do a photo-emission experiment on an electron gas (or electron gas like metals such a sodium)

Dyson equation

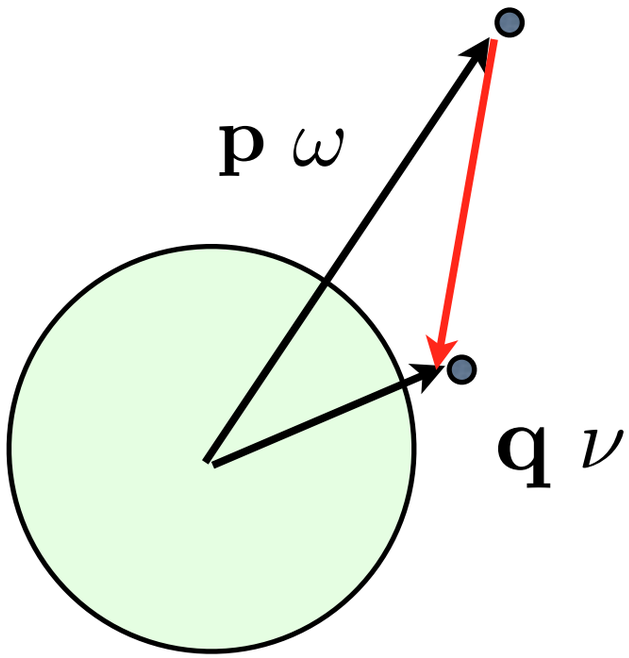
$$G^R(\mathbf{p},\omega) = g^R(\mathbf{p},\omega) + g^R(\mathbf{p},\omega)\Sigma^R(\mathbf{p},\omega)G^R(\mathbf{p},\omega)$$

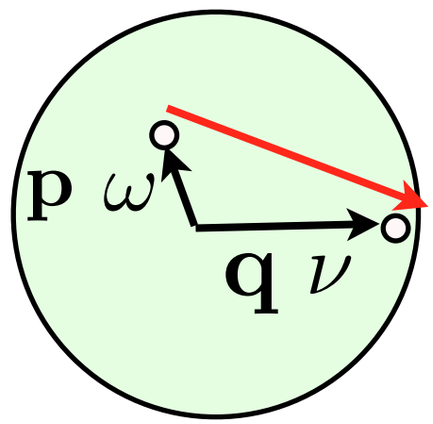
$$g^R(\mathbf{p},\omega) = \frac{1}{\omega - \epsilon_{\mathbf{p}} + i\eta} \qquad\qquad \epsilon_{\mathbf{p}} = \frac{|\mathbf{p}|^2}{2}$$

$$\Rightarrow \qquad G^R(\mathbf{p},\omega) = \frac{g^R(\mathbf{p},\omega)}{1 - g^R(\mathbf{p},\omega)\Sigma^R(\mathbf{p},\omega)} = \frac{1}{\omega - \epsilon_{\mathbf{p}} - \Sigma^R(\mathbf{p},\omega)}$$

Let us first discuss the scattering processes contained in the self-energy

Scattering processes : energy transfer to/from particle-hole excitations or plasmons





Loss of energy by a particle.
Scattering rate given by $i\,\Sigma^{>}(\mathbf{p},\omega)$

Only relevant when $p \geq p_{\rm F}$

A plasmon can be excited only when $\omega \geq \mu + \omega_p$

Absorption of energy by a hole.
Scattering rate given by $-i\,\Sigma^{<}(\mathbf{p},\omega)$

Only relevant when $p \leq p_{\rm F}$

A plasmon can be absorbed only when $\omega \leq \mu - \omega_p$

The greater and lesser self-energies describe scattering rates for added or removed particles with energy ω and momentum p

$$\omega > \mu \quad \Rightarrow \quad i\,\Sigma^{>}(\mathbf{p},\omega) \quad \text{non-zero and positive}$$

$$\omega < \mu \quad \Rightarrow \quad -i\,\Sigma^{>}(\mathbf{p},\omega) \quad \text{non-zero and positive}$$

The self-energy vanishes when $\omega \to \mu$ due to the fact an added particle can maximally lose energy $\omega - \mu$ as states below the Fermi energy are occupied

$$i(\Sigma^{>}(\mathbf{p},\omega) - \Sigma^{<}(\mathbf{p},\omega)) = -2\,\mathrm{Im}\,\Sigma^{R}(\mathbf{p},\omega) = \Gamma(\mathbf{p},\omega)$$

$$\lim_{\omega\to\mu} \mathrm{Im}\,\Sigma^{R}(\mathbf{p},\omega) = 0 \qquad\qquad \Sigma^{R}(\mathbf{p},\omega) = \Lambda(\mathbf{p},\omega) - \frac{i}{2}\Gamma(\mathbf{p},\omega)$$

We calculate the self-energy in the GW approximation using noninteracting Green's function we find

$$\Sigma^{\lessgtr}(p,\omega) = \frac{\mathrm{i}}{(2\pi)^3\,p}\int d\omega' \int_0^\infty dk\,k\,G^{\lessgtr}(k,\omega') \int_{|k-p|}^{k+p} dq\,q\,W^{\gtrless}(q,\omega'-\omega)$$

Absorption of plasmons
by hole states

Energy loss to plasmons
by particle states

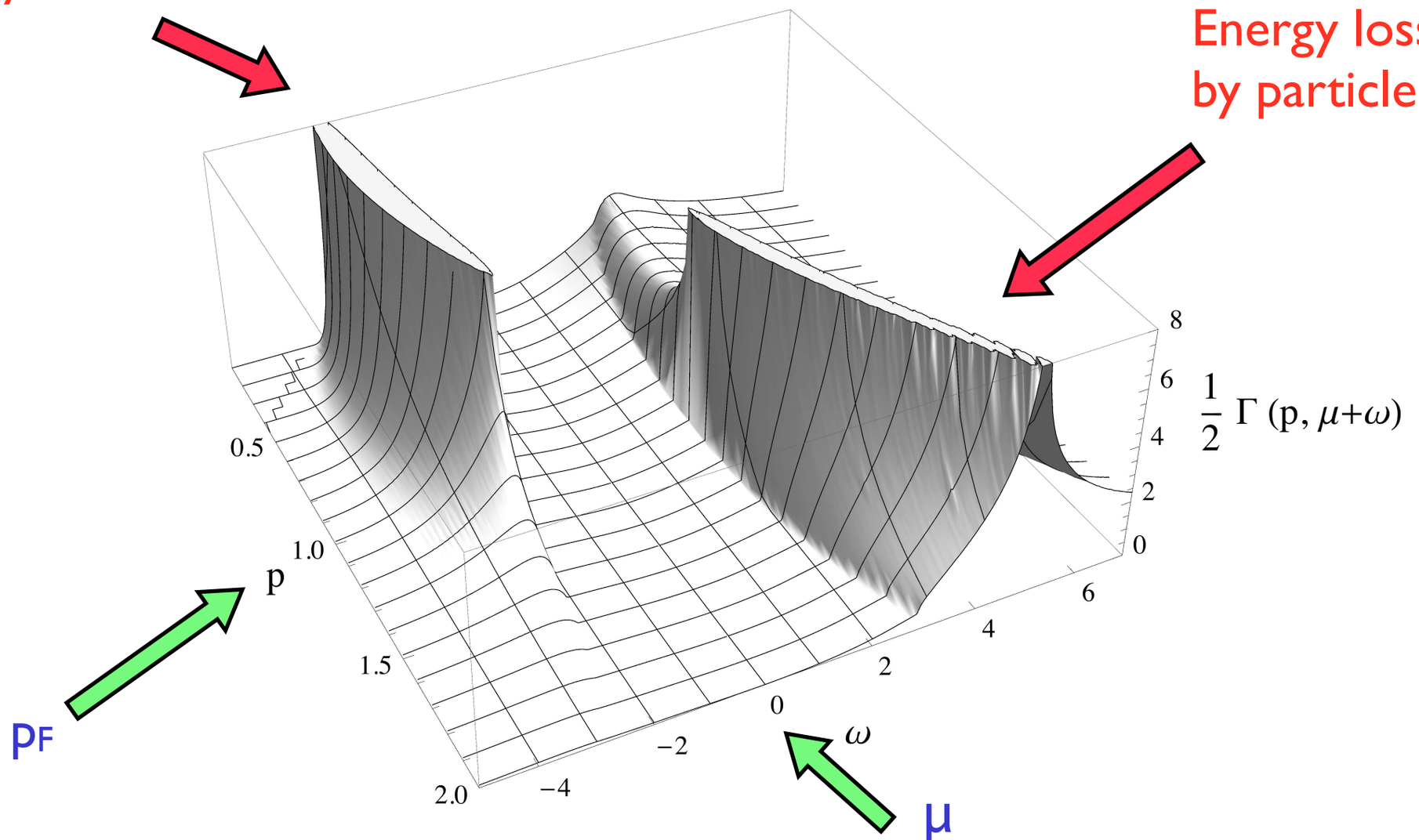


Figure 15.9: The imaginary part of the retarded self-energy $-\mathrm{Im}[\Sigma^{\mathrm{R}}(p,\omega+\mu)] = \Gamma(p,\omega+\mu)/2$ for an electron gas at $r_s = 4$ within the G_0W_0 approximation as a function of the momentum and energy. The momentum p is measured in units of p_{F} and the energy ω and the self-energy in units of $\epsilon_{p_{\mathrm{F}}} = p_{\mathrm{F}}^2/2$.

For the spectral function this implies the following $\Sigma^R(\mathbf{p},\omega) = \Lambda(\mathbf{p},\omega) - \frac{i}{2}\Gamma(\mathbf{p},\omega)$

$$A(\mathbf{p},\omega) = -2\,\mathrm{Im}\,G^R(\mathbf{p},\omega) = \frac{\Gamma(\mathbf{p},\omega)}{(\omega - \epsilon_{\mathbf{p}} - \Lambda(\mathbf{p},\omega))^2 + \left(\frac{\Gamma(\mathbf{p},\omega)}{2}\right)^2}$$

If $\Gamma(\mathbf{p},\omega)$ is small then the spectral function can only become large ($\sim 1/\Gamma$) when

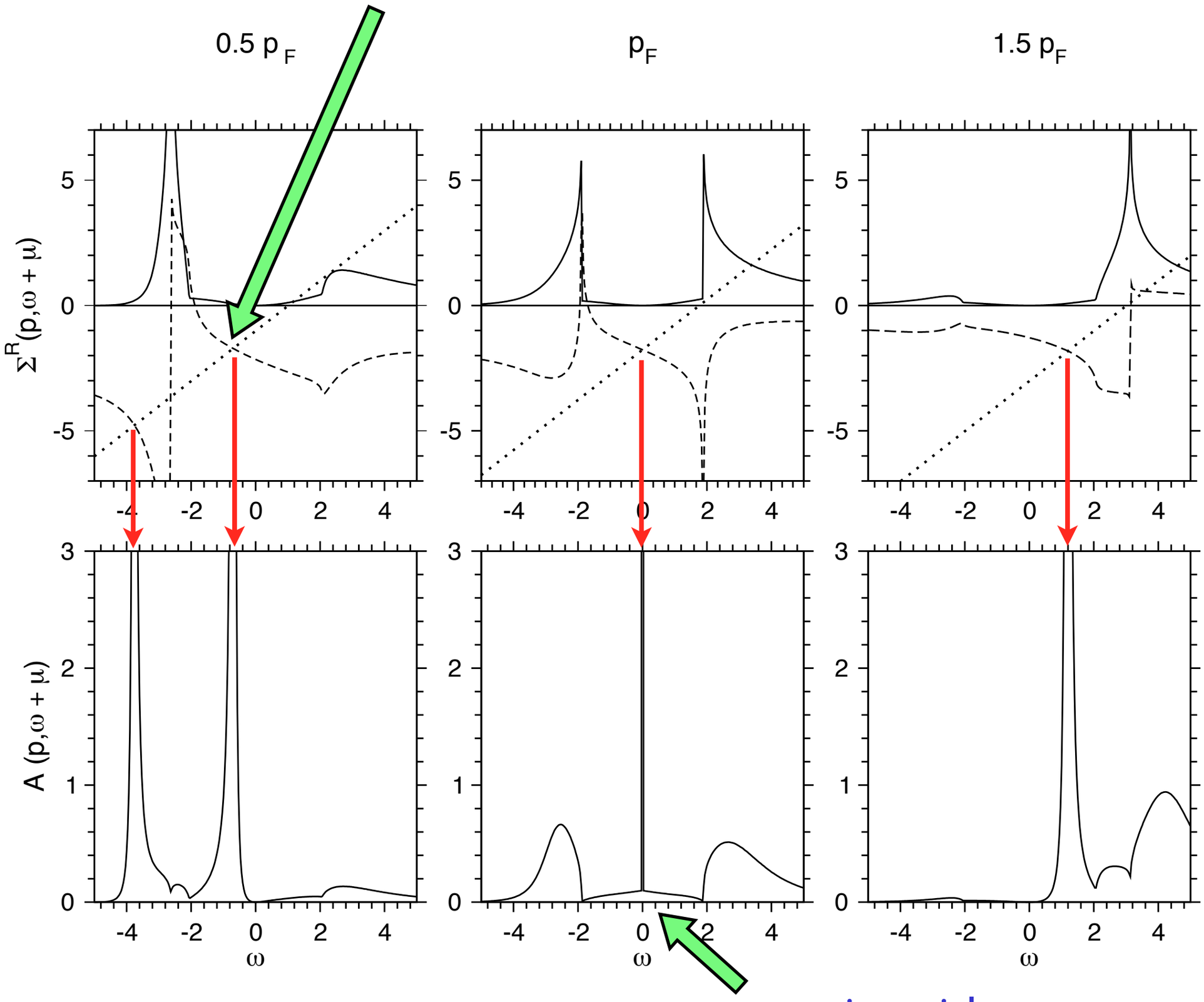
$$\omega - \epsilon_{\mathbf{p}} - \Lambda(\mathbf{p},\omega) = 0$$

The Luttinger-Ward theorem tells that this happens when $q = p_{\mathrm{F}}\ ,\ \omega = \mu$

$$\mu - \epsilon_{p_{\mathrm{F}}} - \Lambda(p_{\mathrm{F}},\mu) = 0$$

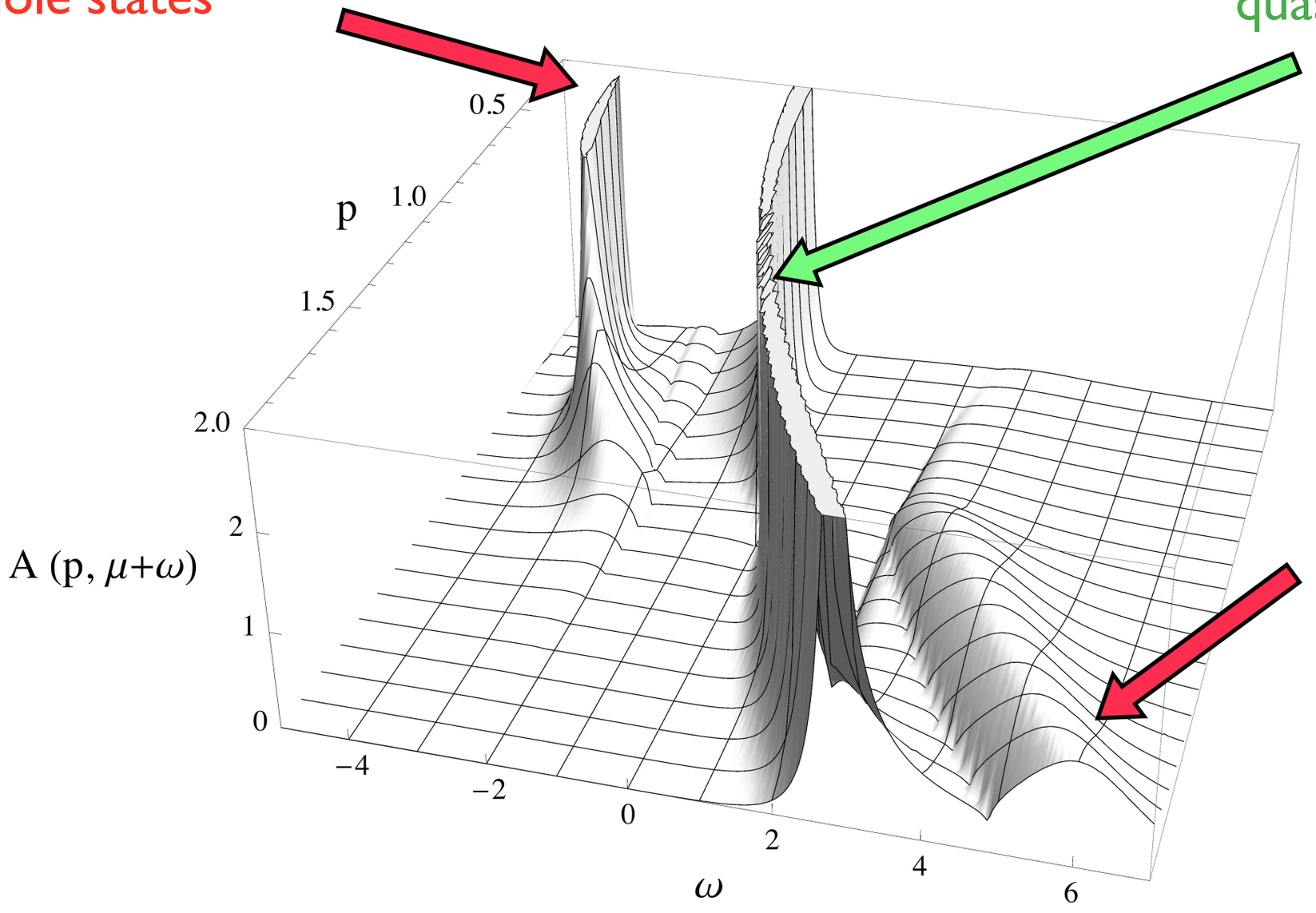
(not explained in these lectures, requires a derivation of the Luttinger-Ward functional, see G.Stefanucci, RvL, Nonequilibrium Many-Body Theory of Quantum Systems)

$$\omega - \epsilon_{\mathbf{p}} - \Lambda(\mathbf{p}, \omega) = 0$$



Absorption of plasmons
by hole states

quasi-particle state



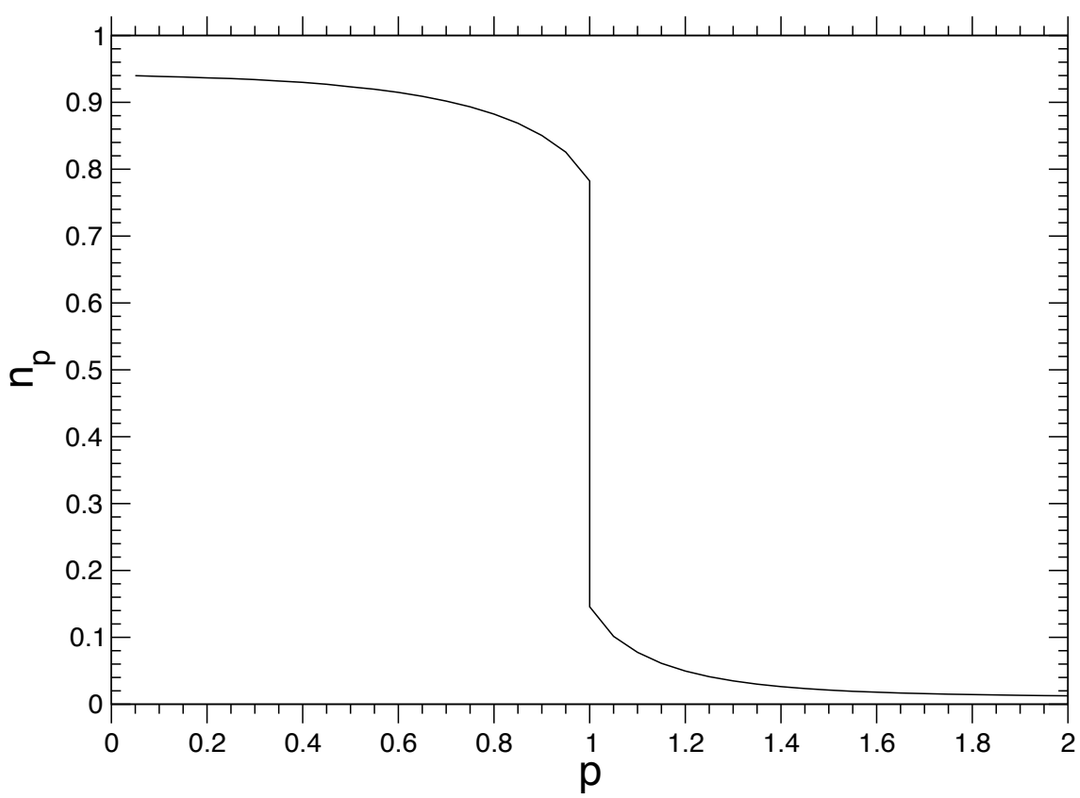
Energy loss
to plasmons
by particle
states

Figure 15.12: The spectral function $A(p, \mu+\omega)$ as a function of the momentum and energy for an electron gas at $r_s = 4$ within the G_0W_0 approximation. The momentum p is measured in units of p_{F} and the energy ω and the spectral function in units of $\epsilon_{p_{\mathrm{F}}} = p_{\mathrm{F}}^2/2$.

The momentum distribution in the electron gas is given by

$$n_p = \int_{-\infty}^{\mu} \frac{d\omega}{2\pi} A(p,\omega)$$

Due to the appearance of a delta peak in the spectral function at the Fermi momentum p_F the momentum distribution jumps discontinuously at the Fermi momentum. The jump is the strength of the quasi-particle peak.



Spectral properties of the electron gas: Take home message

- By addition or removal of an electron we create particle-hole and plasmon excitations

- The self-energy at the Fermi-surface vanishes due to phase-space restrictions. This has various consequences:

  1) The momentum distribution of the electron gas jumps discontinuously at the Fermi momentum

  2) Quasi-particles at the Fermi surface have an infinite life-time.

- The GW approximation gives extra plasmon structure in the spectral function due to plasmons

- Multiple-plasmons excitations (satellites) are beyond GW and require vertex corrections.

Things we did not talk about

- Feynman diagrams for the grand canonical potential and the action. Luttinger-Ward functionals, variational principles

- Connections to TDDFT and TD current DFT :
  - Diagrammatic expansion of xc-kernel
  - Sham-Schlüter equation and TDOEP

- General initial states

- Bethe-Salpeter and excitons, Lehmann representation

- Non-equilibrium phenomena and the Kadanoff-Baym equations (quantum transport)

- Conserving approximations and Ward identities

- Open quantum systems, T-matrix, superconductivity, phonons, Bose condensates,.....etc.