Introduction to Many-body Theory II

Part II : Feynman diagrams, the Green's function and TDDFT

- Why Green's functions?
  operator orderings and Wick's theorem
- Feynman diagrams and the self-energy
- Connections to TDDFT: Sham-Schlüter equation and linear response kernel

Operator correlators

We have seen that the expansion of an expectation value leads to products of the form of 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

If we differentiate a time-ordered product with respect to a time variable we find

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 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 therefore 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

$$\mathcal{T}_\gamma\left\{\psi(\mathbf{x}_1z_1)\hat{\psi}^\dagger(\mathbf{x}_2z_2)\hat{\psi}(\mathbf{x}_2z_2)\right\}=-\mathcal{T}_\gamma\left\{\hat{\psi}^\dagger(\mathbf{x}_2z_2)\psi(\mathbf{x}_1z_1)\hat{\psi}(\mathbf{x}_2z_2)\right\}$$

$$=\mathcal{T}_\gamma\left\{\hat{\psi}^\dagger(\mathbf{x}_2z_2)\hat{\psi}(\mathbf{x}_2z_2)\psi(\mathbf{x}_1z_1)\right\}=\hat{\psi}^\dagger(\mathbf{x}_2z_2)\hat{\psi}(\mathbf{x}_2z_2)\psi(\mathbf{x}_1z_1)\quad z_2>z_1$$

Pairs of fermionic operators behave like bosonic operators

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

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

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

The hierarchy equations need to be solved with the boundary conditions

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

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

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

For instance, the density is given by

$$n(\mathbf{x}, t) = -iG(\mathbf{x}t, \mathbf{x}t^+)$$

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 simplifies to

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

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

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 and expand the numerator N(a,b) to first order

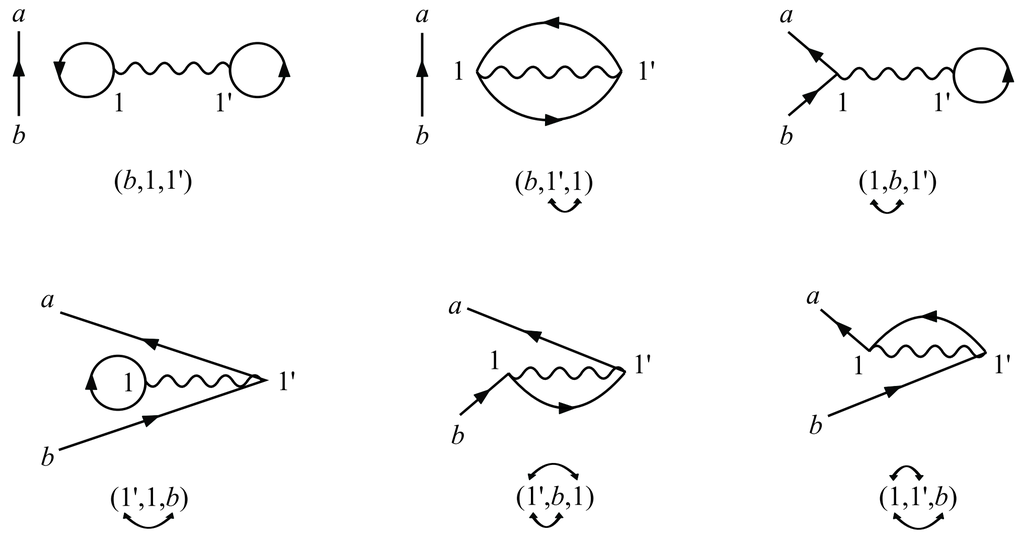
Expanding the 3x3 determinant in the numerator along the first column we find

$$N^{(1)}(a;b) = \frac{i}{2} g(a;b) \int d1d1' w(1,1') \begin{vmatrix} g(1;1^+) & g(1;1'^+) \\ g(1';1^+) & g(1';1'^+) \end{vmatrix}$$

$$\pm \frac{i}{2} \int d1d1' w(1,1') g(1;b) \begin{vmatrix} g(a;1^+) & g(a;1'^+) \\ g(1';1^+) & g(1';1'^+) \end{vmatrix}$$

$$+ \frac{i}{2} \int d1d1' w(1,1') g(1';b) \begin{vmatrix} g(a;1^+) & g(a;1'^+) \\ g(1;1^+) & g(1;1'^+) \end{vmatrix}$$

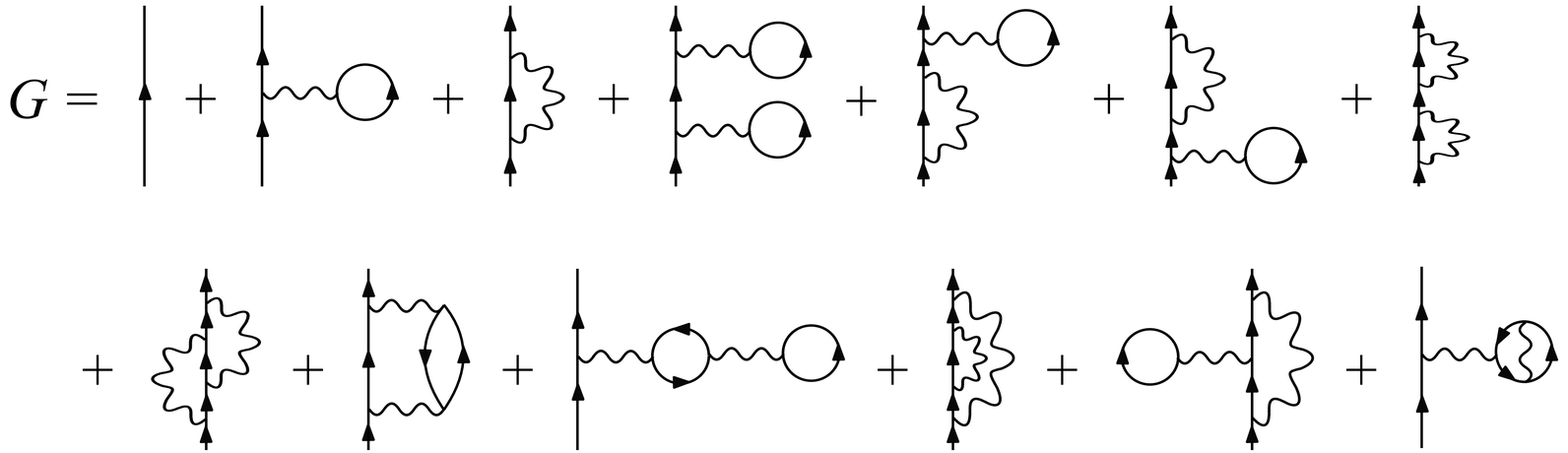
which is represented by the following six diagrams



By a combinatorial argument is follows that the disconnected diagrams from the numerator are cancelled by those of the denominator and we can further simplify to

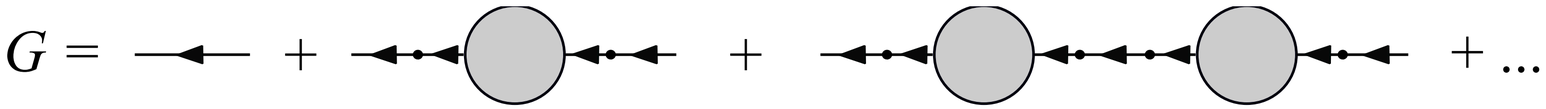
$$G(a,b) = \sum_{k=0}^{\infty} i^k \int w(1,1') \dots w(k,k') \begin{vmatrix} g(a,b) & g(a,1^+) & \dots & g(a,k'^+) \\ g(1,b) & g(1,1^+) & \dots & g(1,k'^+) \\ \vdots & \vdots & & \vdots \\ g(k',b) & g(k',1^+) & \dots & g(k',k'^+) \end{vmatrix}_{CTI}$$

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

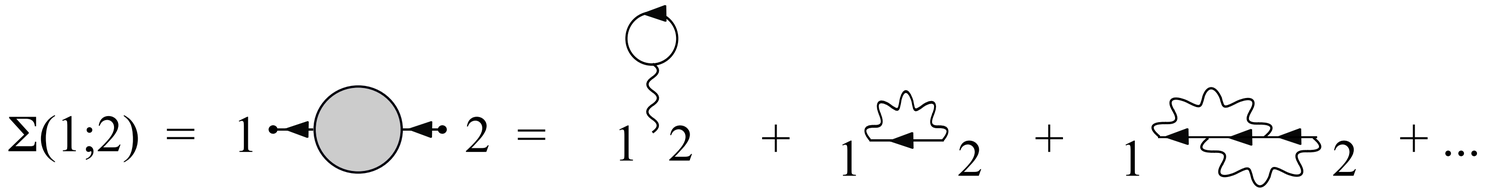


Self energy

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)



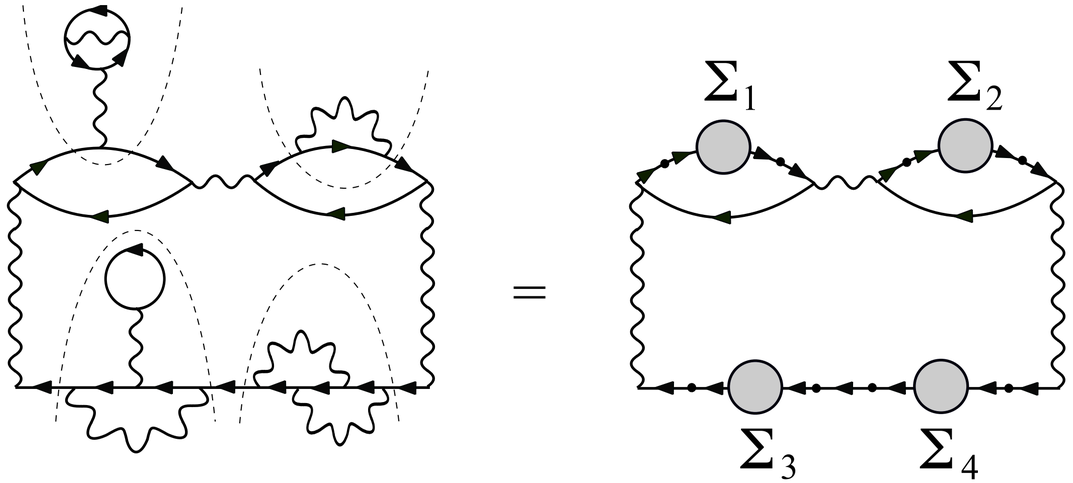
The Green's function thus satisfies the equation

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

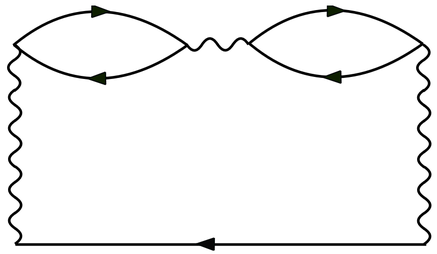
Dyson equation

Skeletons

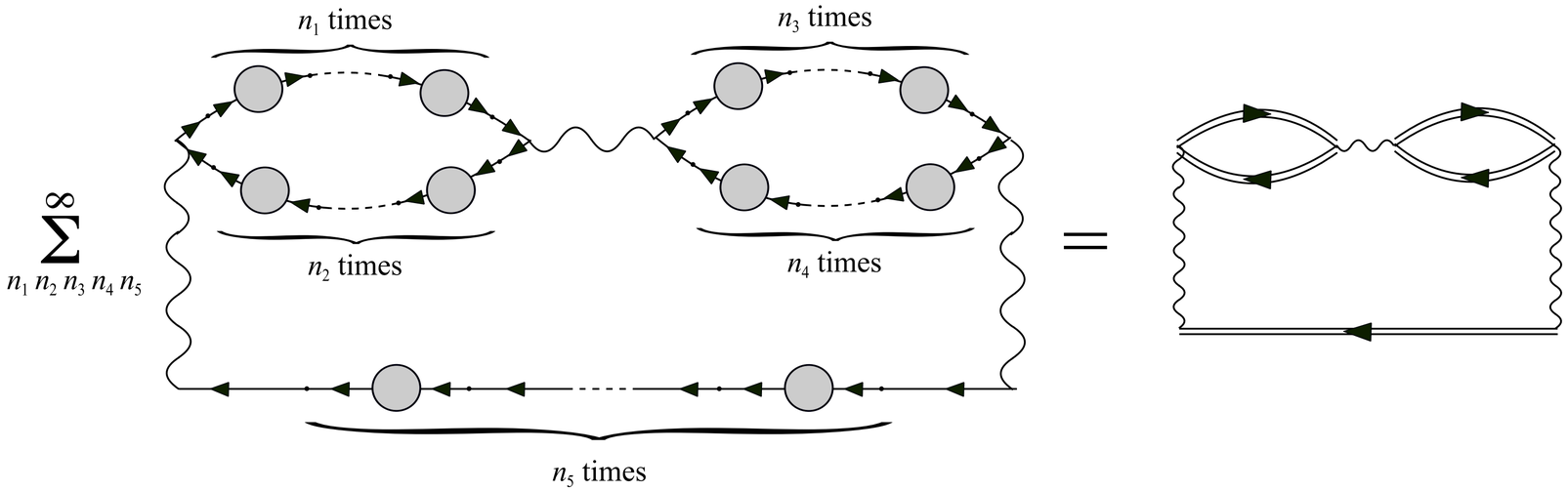
A skeleton diagram is a diagram without self-energy insertions, for example



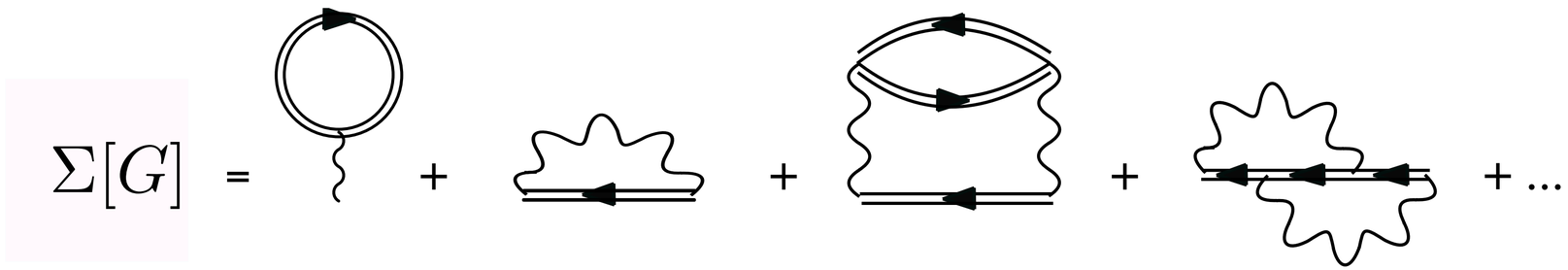
The corresponding skeleton is therefore



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

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

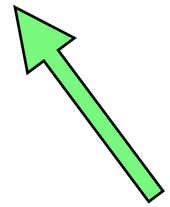
or, if we use the equation of motion for g : $(i\,\partial_{z_1} - h(1))g(1,2) = \delta(1,2)$

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

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

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

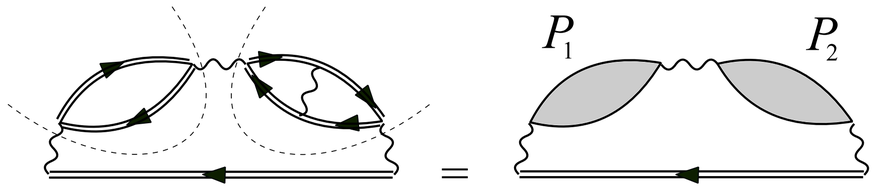
$$G(1, \mathbf{x}_2 t_0) = -G(1, \mathbf{x}_2 t_0 - i\beta)$$



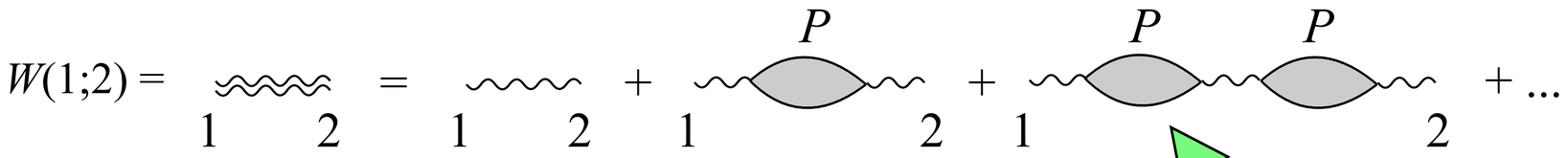
Kadanoff-Baym equations

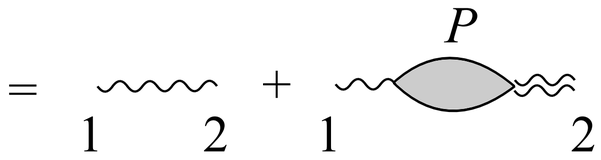
W-skeletons

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



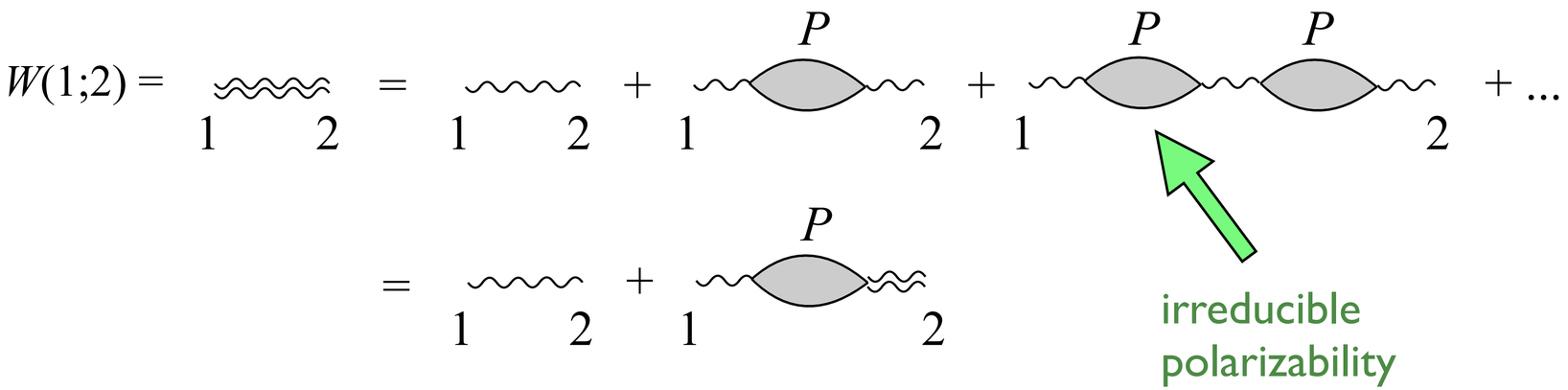
We can then define the screened interaction W by





irreducible polarizability

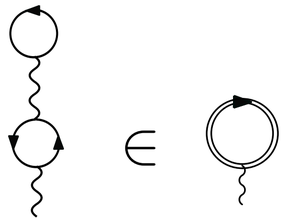
We can then define the screened interaction W by



In formula

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

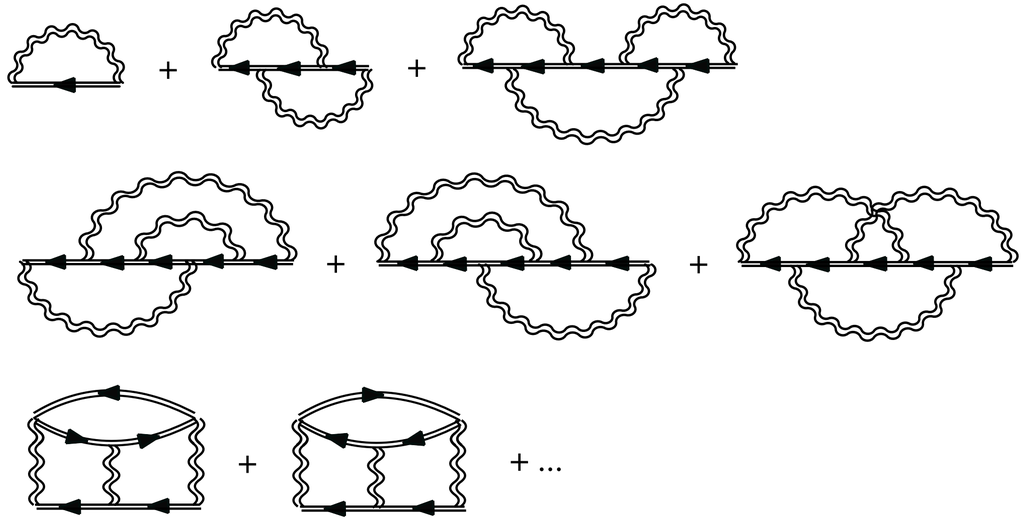
We can then in W-skeletonic diagrams replace w by W with the exception of the Hartree diagram. We have



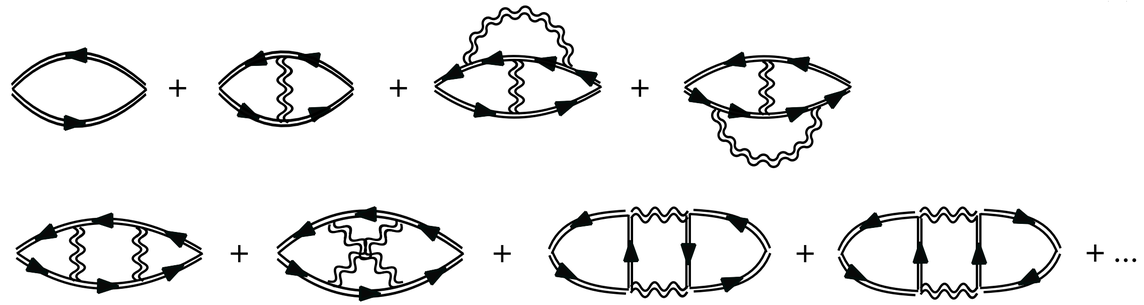
$$\Sigma = \Sigma_{ss}[G,W] = \Sigma_H[G,w] + \Sigma_{ss,\mathrm{xc}}[G,W]$$

double skeletonic

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

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

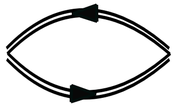
and the polarizability

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

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

Connection to TDDFT: Sham-Schlüter equation

Many-body theory can be used to derive an equation for the exchange-correlation potential of TDDFT for a given diagrammatic expansion

The Kohn-Sham system is a particular many-body system and therefore has a Green's function

$$\left(i\partial_t - [-\frac{1}{2}\nabla^2 + v(1) + v_{\mathrm{Hxc}}(1)]\right) G_s(1,2) = \delta(1,2)$$

Hartree + xc potential

Kohn-Sham Green's function

The interacting many-body system satisfies the equation

$$\left(i\partial_t - [-\frac{1}{2}\nabla^2 + v(1)]\right) G(1,2) = \delta(1,2) + \int d3\, \Sigma[G](1,3)G(3,2)$$

Many-body interactions in the self-energy

We now rewrite this equation

$$\left(i\partial_t - [-\frac{1}{2}\nabla^2 + v(1) + v_{\mathrm{Hxc}}(1)]\right) G(1,2) = \delta(1,2) + \int d3\,(\Sigma[G](1,3) - \delta(1,3)v_{\mathrm{Hxc}}(1))G(3,2)$$

and we see from the equation of motion of the Kohn-Sham Green's function that

$$G(1,2) = G_s(1,2) + \int d3d4\, G_s(1,3)(\Sigma[G](3,4) - \delta(3,4)v_{\mathrm{Hxc}}(3))G(4,2)$$

Since both the exact and the Kohn-Sham system have the same density we have

$$n(\mathbf{x},t) = -iG(\mathbf{x}t,\mathbf{x}t^+) = -iG_s(\mathbf{x}t,\mathbf{x}t^+)$$

and by taking an equal space-time limit we there obtain that

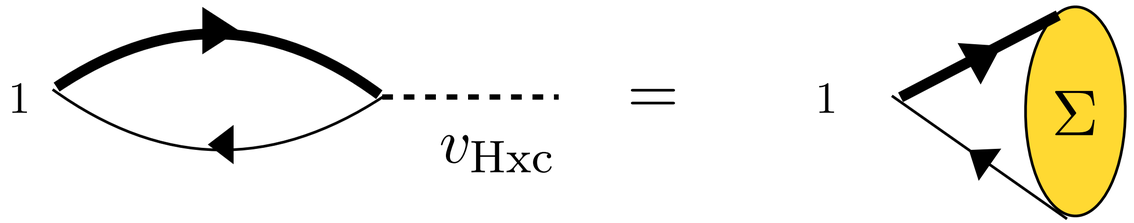
$$0 = \int d3d4\, G_s(1,3)(\Sigma[G](3,4) - \delta(3,4)v_{\mathrm{Hxc}}(3))G(4,1)$$

which we can rewrite as

$$\int d3\, G_s(1,3)G(3,1)v_{\rm Hxc}(3) = \int d3d4\, G_s(1,3)\Sigma[G](3,4)G(4,1)$$

Sham-Schlüter equation

It is an integral equation of the form $\int d3K(1,3)v_{\rm Hxc}(3) = Q(1)$ with diagrammatic representation



The equation can be used to derive approximate xc-potentials in TDDFT if we make the replacement $G \to G_s$

$$\int d3\, G_s(1,3)G_s(3,1)v_{\rm Hxc}(3) = \int d3d4\, G_s(1,3)\Sigma[G_s](3,4)G_s(4,1)$$

This is the so-called linearized Sham-Schlüter (LSS) equation

TDOEP equations

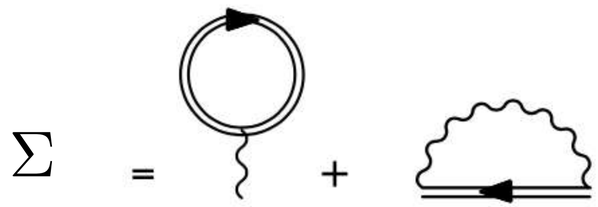
Solve the Kohn-Sham equations together with the LSS equation using the self-consistency loop

$$i\partial_t \varphi_i(1) = (-\frac{1}{2}\nabla_1^2 + v(1) + v_{\mathrm{Hxc}}(1))\varphi_i(1) \quad \rightarrow \quad G_s(1,2)$$

$$\int d3\, G_s(1,3)G_s(3,1)v_{\mathrm{Hxc}}(3) = \int d3d4\, G_s(1,3)\Sigma[G_s](3,4)G_s(4,1)$$

Induces memory effects in TDDFT

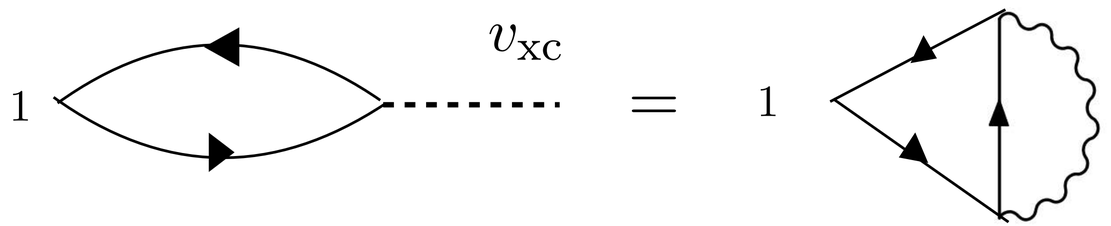
These are the so-called optimised effective potential (OEP) equations. In case the self-energy is given by the Hartree-Fock terms obtain the exchange-only TDOEP equations



v_H Hartree potential

In the case of x-only TDOEP we have the self-consistency loop

$$i\partial_t\varphi_i(1) = (-\frac{1}{2}\nabla_1^2 + v(1) + v_H(1) + v_{\rm xc}(1))\varphi_i(1) \quad \rightarrow \quad G_s(1,2)$$



The integral equation can also be written directly in terms of orbitals.

An excellent discussion of TDDFT and many of the issues is given in the textbook

Carsten Ullrich, "Time-dependent density-functional theory: Concepts and applications"

Many more intriguing features of time-dependent xc-potentials in the lectures of Neepa Maitra

The xc-kernel of linear response TDDFT

Let us first see what happens when we make a small change in the Kohn-Sham potential

$$\left(i\partial_t - [-\frac{1}{2}\nabla^2 + v_s(1)]\right) G_s(1,2) = \delta(1,2)$$

We get

$$\left(i\partial_t - [-\frac{1}{2}\nabla^2 + v_s(1) + \delta v_s(1)]\right) G'_s(1,2) = \delta(1,2)$$

$$\left(i\partial_t - [-\frac{1}{2}\nabla^2 + v_s(1)]\right) G'_s(1,2) = \delta(1,2) + \delta v_s(1) G'_s(1,2)$$

The solution of which is

$$G'_s(1,2) = G_s(1,2) + \int d3\, G_s(1,3)\delta v_s(3) G'_s(3,2)$$

$$= G_s(1,2) + \int d3\, G_s(1,3)\delta v_s(3) G_s(3,2) + \int d3d4\, G_s(1,3)\delta v_s(3) G_s(3,4)\delta v_s(4) G_s(4,2) + \ldots\ldots$$

From this expression we see that

$$\frac{\delta G_s(1,2)}{\delta v_s(3)} = G_s(1,3)G_s(3,2)$$

In particular we see that the Kohn-Sham density response function is given by

$$\chi_s(1,2) = \frac{\delta n(1)}{\delta v_s(2)} = -i\frac{\delta G_s(1,1^+)}{\delta v_s(2)} = -iG_s(1,2)G_s(2,1)$$

So we could rewrite the linearised Sham-Schlüter equation also as

$$\int d3\, \chi_s(1,2)v_{\mathrm{Hxc}}(3) = -i\int d3d4\, G_s(1,3)\Sigma[G_s](3,4)G_s(4,1)$$

or, if we subtract out the Hartree potential

$$\Sigma_{\mathrm{xc}}[G_s](1,2) = \Sigma[G_s](1,2) - \delta(1,2)v_H(1)$$

So we obtain

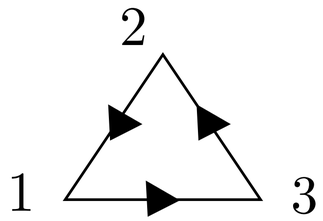
$$\int d3\,\chi_s(1,3)v_{\rm xc}(3) = -i\int d3d4\,G_s(1,3)\Sigma_{\rm xc}[G_s](3,4)G_s(4,1)$$

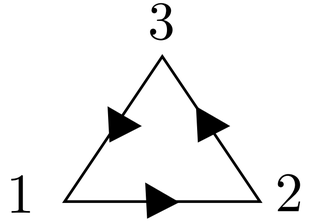
We can derive an equation for the xc-kernel if we take the functional derivative with respect to the Kohn-Sham potential. On the left hand side we obtain

$$\frac{\delta}{\delta v_s(2)}\int d3\,\chi_s(1,3)v_{\rm xc}(3) = \int d3\,\frac{\delta\chi_s(1,3)}{\delta v_s(2)}v_{\rm xc}(3) + \int d3\chi_s(1,3)\frac{\delta v_{\rm xc}(3)}{\delta v_s(2)}$$

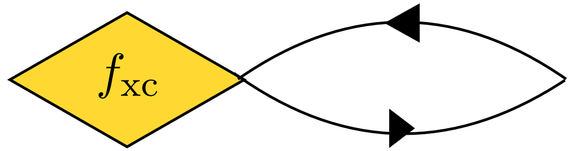
The two terms on the right can be worked out as

$$\chi_s^{(2)}(1,2,3) = \frac{\delta\chi_s(1,3)}{\delta v_s(2)} = -iG_s(1,2)G_s(2,3)G_s(3,1) - iG_s(1,3)G_s(3,2)G_s(2,1)$$



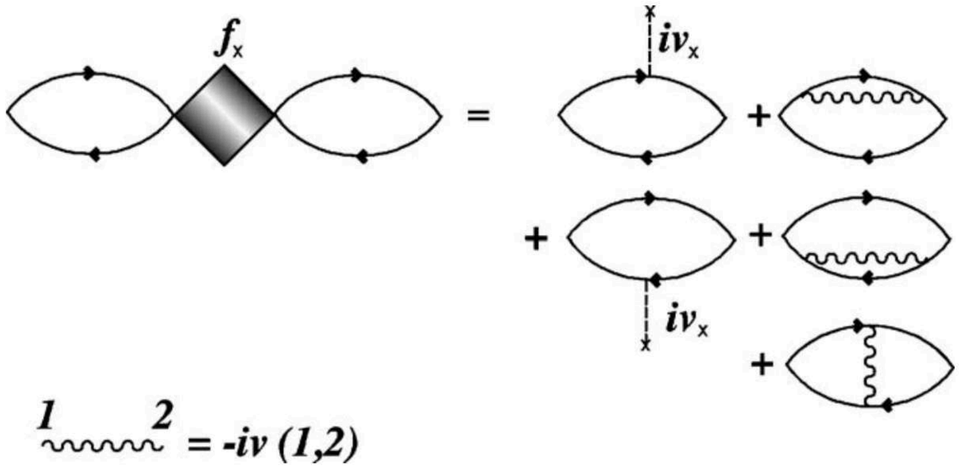


$$\frac{\delta v_{\rm xc}(3)}{\delta v_s(2)} = \int d4\frac{\delta v_{\rm xc}(3)}{\delta n(4)}\frac{\delta n(4)}{\delta v_s(2)} = \int d4\,f_{\rm xc}(3,4)\chi_s(4,2) \quad =$$



The term on the right hand side of the LSS equation depends on the choice of self energy and can be worked out in a similar way

In the x-only approximation we obtain the diagrammatic equation

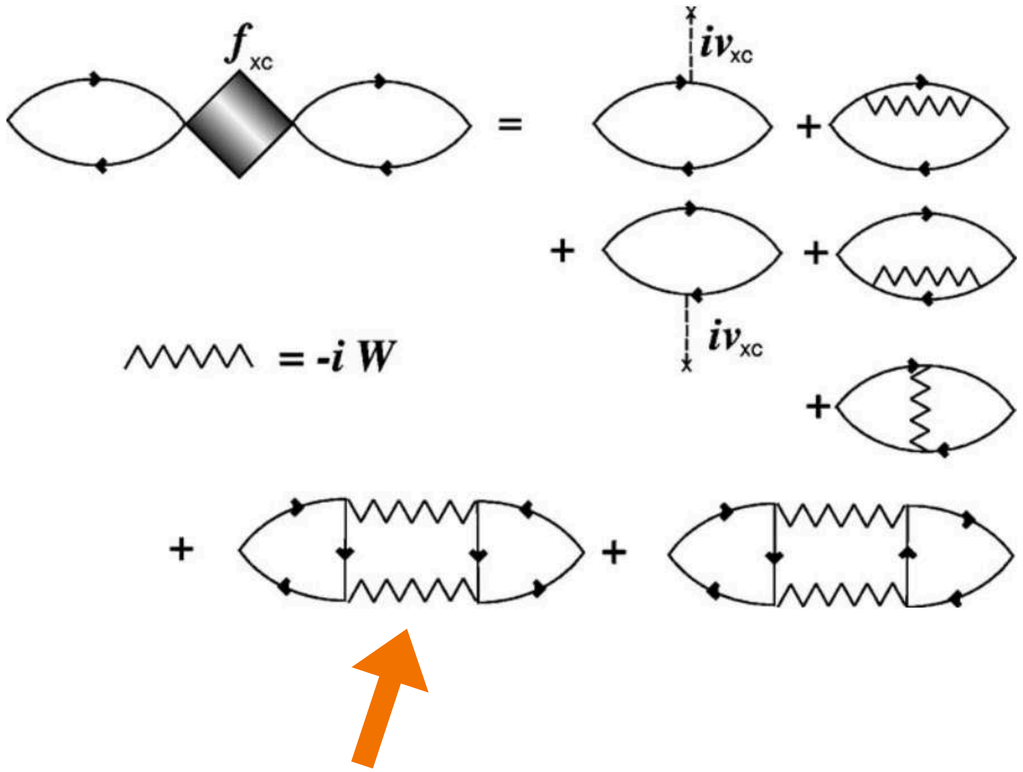


Ulf von Barth et al.
"Conserving approximations in TDDFT",
Phys.Rev.B72, 235109 (2005)

This equation has been usefully applied, for example, in Erhard, Bleiziffer, Görling, Phys.Rev.Lett. 117, 143002 (2016)

By choosing more sophisticated approximations to the self-energy we get more elaborate approximations for the xc-kernel

For example, using the GW approximation to the self-energy, we obtain the equation



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Connection to TDDFT: Take home message

- From the Dyson equation for the Kohn-Sham and the exact system we can derive the Sham-Schlüter equation which an exact equation for the xc-potential of TDDFT

- The linearised version is equivalent to the TDOEP method and can be used in a self-consistent manner for the construction of approximate xc-potentials in TD Kohn-Sham calculations

- By taking a functional derivative of the Sham-Schlüter equation we can derive diagrammatic equations for the xc-kernel of TDDFT