The Hedin's equation

> Ref: http://wwwteor.mi.infn.it/~molinari/NOTES/hedin2017.pdf

In 1965, Lars Hedin derived the formally closed set of equations for propagator G, self-energy Σ_0, effective potential W, proper polarization Π_0 and dressed vertex Γ.

$$G(1,2) = G_0(1,2) + \int d1'2' G_0(1,1')\Sigma_0(1',2')G(2',2) \tag{1}$$

$$W(1,2) = V(1,2) + \int d1'2' V(1,1')\Pi_0(1',2')W(2',2) \tag{2}$$

$$\Sigma_0(1,2) = i\int d34 W(1,3)\Gamma(3;4,2)G(1,4) \tag{3}$$

$$\Pi_0(1,2) = -i\int d34 \Gamma(1;3,4)G(2,4)G(4,2) \tag{4}$$

$$\Gamma(1;2,3) = \delta(1,2)\delta(1,3) + \int d4567 \Gamma(1;4,5)G(6,4)G(5,7)\frac{\partial\Sigma_0(2,3)}{\partial G(6,7)} \tag{5}$$

Here, $1 = (x_1, t_1)$, $V(1,2) = V_0(x_1,x_2)\delta(t_1 - t_2)$ and G_0 is Green function with Hartree approximation ("tadpole" diagrams with **exact** particle density).

> In Landau's book, the self energy is decoupled to two parts. One is "branched" diagrams Σ_a, which is absorbed into G_0, and another is Σ_b, which is Σ_0 in our notation.
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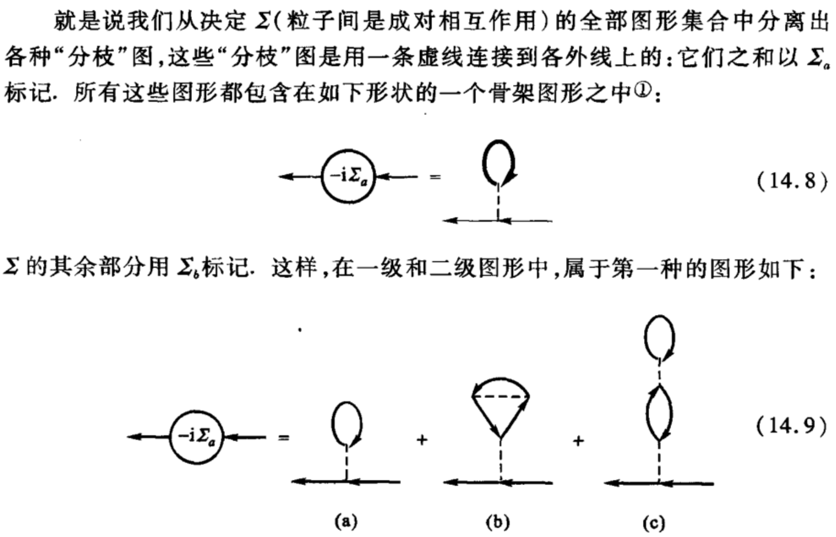
> 
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> 就是说我们从决定 Σ(粒子间是成对相互作用)的全部图形集合中分离出各种“分枝”图,这些“分枝”图是用一条虚线连接到各外线上的:它们之和以 Σ_a 标记. 所有这些图形都包含在如下形状的一个骨架图形之中①:
>
> (14.8)
>
> Σ 的其余部分用 Σ_b 标记. 这样,在一级和二级图形中,属于第一种的图形如下:
>
> (14.9)
>
> (a) (b) (c)

EQU1 and EQU2 are just Dyson's equation. EQU3 and EQU4 gives the skeleton diagram, and EQU5 contains a functional derivative, which is the main difficulty of many-body systems.

We now derive it from a field perspective. We assume that EQU1 is already proved.

Dyson-Schwinger equation

Consider adding a source term ϕ to the Hamiltonian:

$$H(t) = H_0 + U + \int d\vec{x}\phi(\vec{x}, t)n(\vec{x})$$

Where n is density operator. We will take $\phi = 0$ in the results. The Dyson-Schwinger equation show that

$$\frac{\delta}{\delta\phi(x)} \frac{\langle\Omega|\mathcal{T}SF|\Omega\rangle}{\langle\Omega|S|\Omega\rangle} = -i\frac{\langle\Omega|\mathcal{T}SF\delta n(x)|\Omega\rangle}{\langle\Omega|S|\Omega\rangle}$$

- F is product of field operators
- $\delta n = n - \langle n\rangle$
- Ω is ground state of $H_I = H_0 + U$
- $S = \mathcal{T} \exp \frac{1}{i\hbar} \int d^4x\phi(x)n(x)$ is the evolution operator
- $n(x) = n(\vec{x}, t) = e^{iH_I t} n(\vec{x}) e^{-iH_I t}$.
- $\langle n(x)\rangle = \frac{\langle\Omega|\mathcal{T}Sn(x)|\Omega\rangle}{\langle\Omega|S|\Omega\rangle}$

This equation is easily verified by

$$\frac{\delta\mathcal{T}[SF]}{\delta\phi(x)} = \sum_{k=1}^{\infty} \frac{(-i)^k k}{k!} \int d1' \dots k' n(1') \dots n(k')\delta(1-1')\phi(2') \dots \phi(k') = -i\mathcal{T}[SFn(x)]$$

and the definition of $\langle n\rangle$.

Derivation of Hedin's equation

The first equation is easiest to verify: because $G = g + g(\Sigma_H + \Sigma_0)G$ and $G_0 = g + g\Sigma_0 G_0$, then $G = G_0 + G_0\Sigma_0 G$. Σ_H is contribution from Hartree terms and g is Green function with no interaction.

We define the time-ordered propagator and full polarization as

$$G(1,2) = -i\frac{\langle\Omega|\mathcal{T}S\psi(1)\psi^\dagger(2)|\Omega\rangle}{\langle\Omega|S|\Omega\rangle}$$
$$\Pi(1,2) = -i\frac{\langle\Omega|\mathcal{T}S\delta n(1)\delta n(2)|\Omega\rangle}{\langle\Omega|S|\Omega\rangle}$$

Choosing $F = n$ in DS equation, we have

$$\frac{\delta}{\delta\phi(2)} \frac{\langle\Omega|\mathcal{T}Sn(1)|\Omega\rangle}{\langle\Omega|S|\Omega\rangle} = -i\frac{\langle\Omega|\mathcal{T}Sn(1)\delta n(2)|\Omega\rangle}{\langle\Omega|S|\Omega\rangle} = -i\frac{\langle\Omega|\mathcal{T}S\delta n(1)\delta n(2)|\Omega\rangle}{\langle\Omega|S|\Omega\rangle}$$

We express it in Green's function: because $\langle n(1)\rangle = -iG(1, 1^+)$, then

$$\Pi(1,2) = -i\frac{\delta G(1,1^+)}{\delta\phi(2)}$$

We define a "modified" local potential by adding in Hartree term:

$$v(1) = \phi(1) - i\int d2V(1,2)G(2,2^+)$$

Then

$$\frac{\delta}{\delta\phi(1)}=\int d2\frac{\delta v(2)}{\delta\phi(1)}\frac{\delta}{\delta v(2)}=\frac{\delta}{\delta v(1)}+\int d23V(2,3)\Pi(3,1)\frac{\delta}{\delta v(2)}$$

Impose this equation on $-iG$ and defining the proper polarization as $\Pi_0(1,2)=-i\frac{\delta G(1,1^+)}{\delta v(2)}$, we have the Dyson's equation for Π:

$$\Pi(1,2)=\Pi_0(1,2)+\int d34\Pi_0(1,3)V(3,4)\Pi(4,2)$$

Define the two-body effective potential as

$$\begin{aligned}W(1,3)&=\int d2\frac{\delta v(1)}{\delta\phi(2)}V(2,3)\\&=V(1,3)+\int d24V(1,4)\Pi(4,2)V(2,3)\\&=V(1,3)+\int d24V(1,4)\Pi_0(4,2)W(2,3)\end{aligned}$$

In the last equation, we used $\int d1V(4,1)\frac{\delta}{\delta\phi(1)}=\int d1W(4,1)\frac{\delta}{\delta v(1)}$. **This is the second Hedin's equation.**

We now define the inverse Green function

$$\int d3G^{-1}(1,3)G(3,2)=\delta(1,2)$$

The derivative of $v(4)$ gives

$$\begin{aligned}0&=\int d3\frac{\delta G^{-1}(1,3)}{\delta v(4)}G(3,2)+\int d3G^{-1}(1,3)\frac{\delta G(3,2)}{\delta v(4)}\\&=\int d13G(5,1)\frac{\delta G^{-1}(1,3)}{\delta v(4)}G(3,2)+\frac{\delta G(5,2)}{\delta v(4)}\end{aligned}$$

In the second equation, we inserted $\int d1G(5,1)$. Define vertex as

$$\Gamma(1;2,3)=-\frac{\delta G^{-1}(2,3)}{\delta\phi(1)}$$

Then let $2=5^+$:

$$\Pi_0(1,2)=-i\int d34\Gamma(1;3,4)G(3,2)G(4,2)$$

This is the fourth Hedin's equation.

Now because $G^{-1}(1,2)=G_0^{-1}(1,2)-\Sigma_0(1,2)$, and the equation of motion for G_0 is

$$(i\partial_{t_1}-h(1)-\phi(1)-\int d2V(1,2)n(2))G_0(1,2)=\delta(1,2)$$

Then $G_0^{-1}(1,2)=i\partial_{t_1}-h(1)-v(1)$, and

$$\Gamma(1;2,3)=\delta(1,2)\delta(1,3)+\frac{\partial\Sigma_0(2,3)}{\partial v(1)}$$

Because of Hohenberg-Kohn theorem, G is uniquely determined by V, then

$$\frac{\delta}{\delta v(5)} = \int d12 \frac{\delta G(1,2)}{\delta v(5)} \frac{\delta}{\delta G(1,2)} = \int d1234 G(1,4)\Gamma(5;4,3)G(3,2)\frac{\delta}{\delta G(1,2)}$$

Then

$$\Gamma(1;2,3) = \delta(1,2)\delta(1,3) + \int d4567 \Gamma(1;4,5)G(6,4)G(5,7)\frac{\partial \Sigma_0(2,3)}{\partial G(6,7)}$$

This is the fifth Hedin's equation.

Lastly, we consider the equation of motion for G. By expanding the time-derivative of the expression of G, we obtain

$$\begin{aligned}(i\partial_{t_1} - h(1) - v(1))G(1,2) &= \delta(1,2) + \int d3 V(1,3)\frac{\langle\Omega|\mathcal{T}S\psi(1)\psi^\dagger(2)\delta n(3)|\Omega\rangle}{\langle\Omega|S|\Omega\rangle} \\ &= \delta(1,2) + i\int d3 V(1,3)\frac{\delta G(1,2)}{\delta\phi(3)}\end{aligned}$$

Let $G = G_0 + G_0\Sigma_0 G$, we have

$$\int d3 \Sigma_0(1,3)G(3,2) = i\int d3 V(1,3)\frac{\delta G(1,2)}{\delta\phi(3)} = i\int d3 W(1,3)\frac{\delta G(1,2)}{\delta v(3)}$$

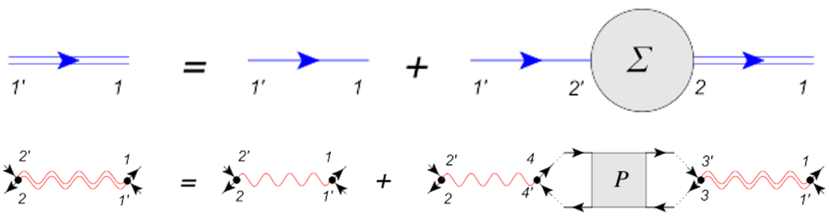
Inserting $\int d2 G^{-1}(2,4)$:

$$\begin{aligned}\Sigma_0(1,2) &= i\int d34 W(1,3)\frac{\delta G(1,4)}{\delta v(3)}G^{-1}(4,2) \\ &= -i\int d34 W(1,3)G(1,4)\frac{\delta G^{-1}(4,2)}{\delta v(3)} \\ &= i\int d34 W(1,3)\Gamma(3;4,2)G(1,4)\end{aligned}$$

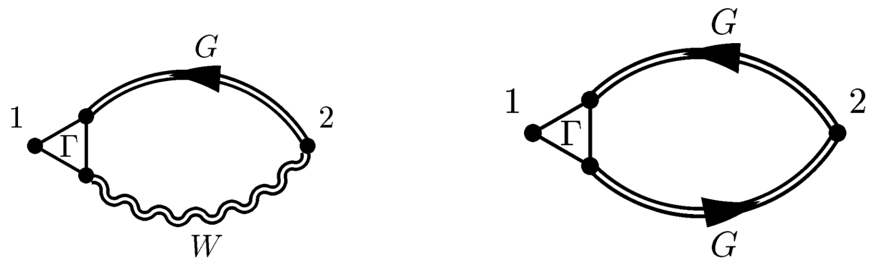
This is the third Hedin's equation.

Diagrammatic expression of Hedin's equation

EQU1 and EQU2:



EQU3 and EQU4 (the left is Σ_0 and the right is Π_0):

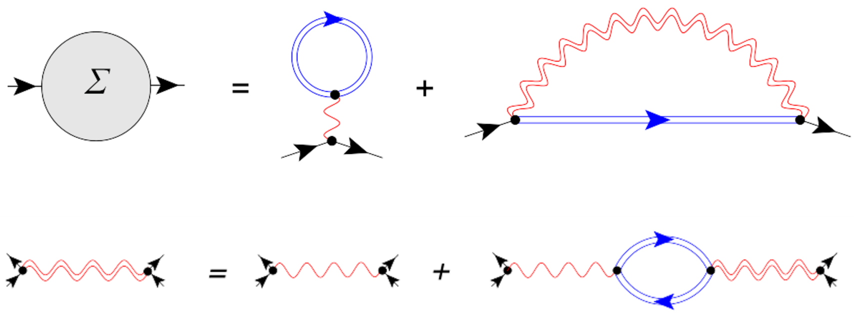


GW approximation

The second term in (5) can be neglected in GW, then

$$\Gamma(1;2,3)=\delta(1,2)\delta(1,3)$$
$$\Sigma_0(1,2)=iG(1,2)W(1,2)$$
$$\Pi_0(1,2)=-iG(1,2)G(2,1)$$

And W is determined by Π_0. This is like the RPA approximation:



(The first term in the first equation above is absorbed into G_0).

> Figures from https://www.cond-mat.de/events/correl11/manuscripts/held.pdf