Conservation Laws and conserving approximations (8.5. RM)

Continuity equation $\frac{\partial \rho}{\partial t} = -\vec{\nabla}\vec{j}$ ← does current conserves charge in an approximation?

↑ small disturbance creates current.

Baym-Kadanoff approach (1961, 1962)

They showed that conservation laws are satisfied if there exist a functional $\Phi[\mathcal{G}]$ such that:

$$\Sigma[\mathcal{G}] = \frac{\delta \Phi}{\delta \mathcal{G}}$$

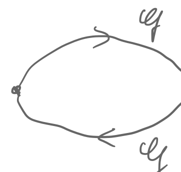
and the two particle response functions have to be calculated by

$$L(1,2;1'2') \equiv -\langle T_\tau \psi^+(x_1)\psi^+(x_2)\psi(x_1)\psi(x_2)\rangle - \langle T_\tau \psi^+(x_1)\psi(x_1)\rangle\langle\psi^+(x_2)\psi(x_2)\rangle$$

$$= -\frac{\delta \mathcal{G}(x_2' x_2)}{\delta \mathcal{J}(x_1 x_1')} = -\frac{\delta \mathcal{G}(x_1', x_1)}{\delta \mathcal{J}(x_2 x_2')}$$

When the source term $\mathcal{J}(x, x_1')$ is added to action $S \to S + \int \psi^+(x_1)\mathcal{J}(x, x_1')\psi(x_1')dx_1 dx_1'$

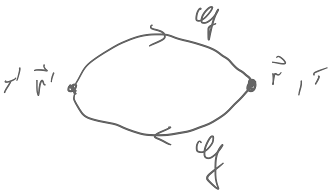
To understand what goes wrong with most approximations derived in different ways, we consider GW-like approximation, where the response function would be computed by the bubble, while the propagator $\mathcal{G}$ contains self-energy, i.e.,



where $\mathcal{G} = \left(i\omega + \mu - \frac{p^2}{2m} - \Sigma_p(i\omega)\right)^{-1}$

Using such bubble we might attempt to compute charge response, such as

$$\langle T_\tau \rho(\vec{r},\tau)\rho(\vec{r}',\tau')\rangle \text{ and } \langle T_\tau \vec{j}(\vec{r},\tau)\rho(\vec{r}',\tau')\rangle$$



We would get

$$\mathcal{G}(\vec{r},\tau) = \frac{1}{\beta}\sum_{i\omega} e^{-i\omega\tau + i\vec{k}\vec{r}}\, \mathcal{G}_k(i\omega)$$

$$\langle T_\tau\, \rho(\vec{r},\tau)\rho(\vec{r}',\tau')\rangle = \langle \psi^+(\vec{r},\tau)\psi(\vec{r},\tau)\psi^+(\vec{r}'\tau')\psi(\vec{r}'\tau')\rangle \approx -\langle \psi(\vec{r},\tau)\psi^+(\vec{r}'\tau')\rangle\langle \psi^+(\vec{r}'\tau')\psi(\vec{r}\tau)\rangle$$

$$= \mathcal{G}(\vec{r}-\vec{r}',\tau-\tau')\,\mathcal{G}(\vec{r}'-\vec{r},\tau'-\tau) = -\frac{1}{\beta^2}\int\frac{d^3k}{(2\pi)^3}\frac{d^3k'}{(2\pi)^3}\sum_{\substack{i\omega\\ i\omega'}} \mathcal{G}_k(i\omega)\,\mathcal{G}_{k'}(i\omega')\, e^{-i(\omega-\omega')(\tau-\tau') + i(\vec{k}-\vec{k}')(\vec{r}-\vec{r}')}$$

for the current we would get

$$\langle T_\tau\, \vec{j}(\vec{r},\tau)\,\rho(\vec{r}',\tau')\rangle = \frac{1}{2mi}\langle T_\tau[\psi^+(\vec{r},\tau)(\nabla\psi(\vec{r}\tau)) - (\vec{\nabla}\psi^+(\vec{r},\tau))\psi(\vec{r},\tau)]\,\psi^+(\vec{r}'\tau')\psi(\vec{r}'\tau')\rangle$$

$$\approx \frac{1}{2mi}\langle T_\tau\, \psi^+(\vec{r},\tau)\psi(\vec{r}'\tau')\rangle\langle T_\tau\, (\vec{\nabla}\psi(\vec{r},\tau))\psi^+(\vec{r}'\tau')\rangle$$

$$-\frac{1}{2mi}\langle T_\tau\, \vec{\nabla}\psi^+(\vec{r},\tau)\,\psi(\vec{r}',\tau')\rangle\langle T_\tau\, \psi(\vec{r},\tau)\,\psi^+(\vec{r}'\tau')\rangle$$

$$= -\frac{1}{2mi}\left\{\mathcal{G}(\vec{r}'-\vec{r},\tau'-\tau)\,\vec{\nabla}_{\vec{r}}\,\mathcal{G}(\vec{r}-\vec{r}',\tau-\tau') - \vec{\nabla}_{\vec{r}}\,\mathcal{G}(\vec{r}'-\vec{r},\tau'-\tau)\cdot\mathcal{G}(\vec{r}-\vec{r}',\tau-\tau')\right\}$$

$$= \frac{1}{\beta^2}\sum_{\substack{i\omega\\ i\omega'}}\int\frac{d^3k}{(2\pi)^3}\int\frac{d^3k'}{(2\pi)^3}\Big[-\frac{1}{2mi}\Big\{i\vec{k}\,\mathcal{G}_k(i\omega)\,e^{-i\omega'(\tau'-\tau)+i\vec{k}'(\vec{r}'-\vec{r})}\,\mathcal{G}_{k'}(i\omega')\,e^{-i\omega(\tau-\tau')+i\vec{k}(\vec{r}-\vec{r}')}$$

$$i\vec{k}'\,\mathcal{G}_k(i\omega)\,e^{-i\omega'(\tau'-\tau)+i\vec{k}(\vec{r}'-\vec{r})}\,\mathcal{G}_{k'}(i\omega')\,e^{-i\omega(\tau-\tau')+i\vec{k}(\vec{r}-\vec{r}')}\Big\}\Big]$$

$$= -\frac{1}{\beta^2}\int\frac{d^3k}{(2\pi)^3}\int\frac{d^3k'}{(2\pi)^3}\sum_{\substack{i\omega\\ i\omega'}}\frac{\vec{k}+\vec{k}'}{2m}\,\mathcal{G}_k(i\omega)\,\mathcal{G}_{k'}(i\omega')\,e^{-i(\omega-\omega')(\tau-\tau')+i(\vec{k}-\vec{k}')(\vec{r}-\vec{r}')}$$

<u>conservation law requires</u>

$$\frac{\partial}{\partial t}\rho(\vec{r},\tau) + \vec{\nabla}_{\vec{r}}\,\vec{j}(\vec{r},\tau) = 0$$

$\boxed{t \to -i\tau}$ because we are in imaginary time

real frequency $e^{i\omega t} = e^{i(i\omega_m)(-i\tau)} = e^{i\omega_m\tau}$
to imaginary frequency $\omega \to i\omega_m$, $t \to -i\tau$

$$\left\langle \frac{\partial}{\partial(-i\tau)}\rho(\vec{r},\tau)\,\rho(\vec{r}'\tau')\right\rangle + \langle \vec{\nabla}_{\vec{r}}\,\vec{j}(\vec{r},\tau)\,\rho(\vec{r}'\tau')\rangle =$$

$$= -\frac{1}{\beta^2}\int\frac{d^3k}{(2\pi)^3}\int\frac{d^3k'}{(2\pi)^3}\sum_{\substack{i\omega\\ i\omega'}}\underbrace{\left[(\omega-\omega') + \frac{(\vec{k}+\vec{k}')\,i(\vec{k}-\vec{k}')}{2m}\right]}_{-i\left[i\omega - i\omega' - \frac{k^2-k'^2}{2m}\right]}\mathcal{G}_k(i\omega)\,\mathcal{G}_{k'}(i\omega')\,e^{-i(\omega-\omega')(\tau-\tau')+i(\vec{k}-\vec{k}')(\vec{r}-\vec{r}')}$$

We have Dyson Eq.!

$$\mathcal{G}_k^{-1}(i\omega) = i\omega - \frac{k^2}{2m} - \Sigma_k(i\omega) \Rightarrow -i\left[\mathcal{G}_k^{-1}(i\omega) - \mathcal{G}_{k'}^{-1}(i\omega') + \Sigma_k(i\omega) - \Sigma_{k'}(i\omega')\right]\mathcal{G}_k(i\omega)\,\mathcal{G}_{k'}(i\omega')$$

$$-i\left[\mathcal{G}_{k'}(i\omega') - \mathcal{G}_k(i\omega) + (\Sigma_k(i\omega) - \Sigma_{k'}(i\omega'))\,\mathcal{G}_k(i\omega)\,\mathcal{G}_{k'}(i\omega')\right]$$

$$\left\langle \frac{\partial}{\partial(-i\tau)} \rho(\vec r,\tau)\, \rho(\vec r'\tau')\right\rangle + \left\langle \vec\nabla_{\vec r}\, \vec j(\vec r,\tau)\, \rho(\vec r'\tau')\right\rangle \equiv R(\vec r\tau, \vec r'\tau') \quad \text{should vanish}$$

$$R = R_1 + R_2$$

but we get

$$R_1(\vec r\tau, \vec r'\tau') = \frac{i}{\beta^2}\int\frac{d^3k}{(2\pi)^3}\int\frac{d^3k'}{(2\pi)^3}\left[\mathcal{G}_{k'}(i\omega') - \mathcal{G}_k(i\omega)\right] e^{-i(\omega-\omega')(\tau-\tau') + i(\vec k-\vec k')(\vec r-\vec r')}$$

$$= -i\left[\mathcal{G}(\vec r'-\vec r, \tau'-\tau)\,\delta(\tau-\tau')\,\delta^3(\vec r-\vec r') - \mathcal{G}(\vec r-\vec r', \tau-\tau')\,\delta(\tau-\tau')\,\delta^3(\vec r-\vec r')\right]$$

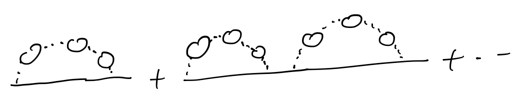
$$= 0$$

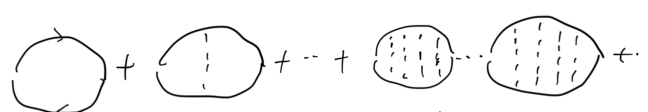
$$R_2(\vec r\tau, \vec r'\tau') = -\frac{1}{\beta^2}\int\frac{d^3k}{(2\pi)^3}\int\frac{d^3k'}{(2\pi)^3}\underbrace{\left(\Sigma_k(i\omega) - \Sigma_{k'}(i\omega')\right)\mathcal{G}_k(i\omega)\,\mathcal{G}_{k'}(i\omega')}_{\text{does not vanish for arbitrary }\Sigma\,!} e^{-i(\omega-\omega')(\tau-\tau') + i(\vec k-\vec k')(\vec r-\vec r')}$$

can be also written as

$$-\left[(\Sigma\mathcal{G})(\vec r-\vec r', \tau-\tau')\,\mathcal{G}(\vec r'-\vec r, \tau'-\tau) - (\Sigma\mathcal{G})(\vec r'-\vec r, \tau'-\tau)\,\mathcal{G}(\vec r-\vec r', \tau-\tau')\right] \neq 0$$

Conclusion: When we dress $\mathcal{G}$ by some self-energy Σ, we have to compute the charge-charge or current-charge correlation functions with vertex corrections included.

For GW, if $\Sigma =$  and $G =$ 

then $\langle \rho\rho\rangle \sim \frac{\delta^2 \ln Z}{\delta\phi\,\delta\phi} \sim \frac{\delta\mathcal{G}}{\delta\phi} \sim$ 

ladder vertex corrections

Derivation of Conservation laws

First derive the condition for the single particle $\mathcal{G}$

We will work on real axis this time, hence

$$G(\vec r t, \vec r' t') = i\langle \psi(\vec r t)\,\psi^\dagger(\vec r' t')\rangle$$

We want to make sure that $\left\langle \frac{\partial\rho}{\partial t} + \vec\nabla\vec j\right\rangle = 0$

First what is ρ and $\vec j$:

$$\langle \rho(\vec r_1 t)\rangle = \langle \psi^\dagger(\vec r t)\,\psi(\vec r t)\rangle = -\langle T_\tau\, \psi(\vec r_1 t_1)\,\psi^\dagger(r_2 t_2)\rangle\Big|_{2=1^+} = -i\,G(1, 2=1^+)$$

$$\langle \vec j(\vec r_1 t)\rangle = \frac{1}{2mi}\langle \psi^\dagger(r_2 t_2)\,\vec\nabla_1\psi(r_1 t_1) - \vec\nabla_2\psi^\dagger(r_2 t_2)\,\psi(r_1 t_1)\rangle = \frac{-i}{2mi}\left(\vec\nabla_1 - \vec\nabla_2\right)G(1, 2=1^+)$$

Next we need to work out derivatives of ρ and $\vec{j}$.

Time derivative of ρ: $\langle \rho \rangle = -i\, G(1, 2=1^+)$

$$\frac{\partial}{\partial t}\langle \rho(\vec{r}t)\rangle = \frac{\partial}{\partial t}\langle \psi^+(\vec{r}t)\,\psi(\vec{r},t)\rangle = \langle \frac{\partial \psi^+(\vec{r}t)}{\partial t}\psi(\vec{r},t)\rangle + \langle \psi^+(\vec{r},t)\frac{\partial \psi(\vec{r}t)}{\partial t}\rangle$$

$$= -\frac{\partial}{\partial t_2}\langle \underbrace{T_\tau\, \psi(\vec{r}_1 t_1)\,\psi^+(r_2 t_2)}_{iG(1,2)}\rangle\Big|_{2=1^+} - \frac{\partial}{\partial t_1}\langle \underbrace{T_\tau\, \psi(\vec{r}_1 t_1)\,\psi^+(r_2 t_2)}_{iG(1,2)}\rangle\Big|_{2=1^+}$$

$$= -i\left(\frac{\partial}{\partial t_2} + \frac{\partial}{\partial t_1}\right) G(1, 2=1^+) \qquad (a)$$

Space derivative of $\vec{j}$: $\langle \vec{j}\rangle = -\frac{1}{2m}(\vec{\nabla}_1 - \vec{\nabla}_2)\, G(1, 2=1^+)$

$$\langle \vec{\nabla}\vec{j}\rangle = (\vec{\nabla}_1 + \vec{\nabla}_2)\left(-\frac{1}{2m}\right)(\vec{\nabla}_1 - \vec{\nabla}_2)\, G(1, 2=1^+) \qquad (b)$$

We also know that: $G_0^{-1}(\vec{r}t, \vec{r}'t') = \left(i\frac{\partial}{\partial t} + \mu + \frac{\nabla^2}{2m}\right)\delta(\vec{r}-\vec{r}')\,\delta(t-t') \equiv \left(i\frac{\partial}{\partial t_1} + \mu + \frac{\nabla_1^2}{2m}\right)\delta(1,1')$

$G_0^{-1}(\vec{r}t, \vec{r}'t') = \left(-i\frac{\partial}{\partial t'} + \mu + \frac{\nabla'^2}{2m}\right)\delta(\vec{r}-\vec{r}')\,\delta(t-t') \equiv \left(-i\frac{\partial}{\partial t_1'} + \mu + \frac{\nabla_1'^2}{2m}\right)\delta(1,1')$

Hence from definition of G_0:

$$\left(i\frac{\partial}{\partial t_1} + \mu + \frac{\nabla_1^2}{2m}\right) G(1,2) = (G_0^{-1} G)(1,2) \qquad (c)$$

$$\left(-i\frac{\partial}{\partial t_2} + \mu + \frac{\nabla_2^2}{2m}\right) G(1,2) = (G\cdot G_0^{-1})(1,2) \qquad (d)$$

Subtract (c) and (d):

$$\left[i\left(\frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2}\right) + \frac{(\nabla_1^2 - \nabla_2^2)}{2m}\right] G(1,2) = (G_0^{-1}G - G G_0^{-1})(1,2)$$

$$\left[i\left(\frac{\partial}{\partial t_1} + \frac{\partial}{\partial t_2}\right) + (\vec{\nabla}_1 + \vec{\nabla}_2)\frac{(\vec{\nabla}_1 - \vec{\nabla}_2)}{2m}\right] G(1,2) = (G_0^{-1}\cdot G - G\cdot G_0^{-1})(1,2) \qquad (e)$$

Inserting (a) and (b) into (e) we get:

$$-\frac{\partial}{\partial t}\rho(1,1^+) - \vec{\nabla}\vec{j} = (G_0^{-1}G - G G_0^{-1})(1,1^+) = 0$$ for conservation law to hold

Dyson equation
$$\left.\begin{aligned} G_0^{-1} G &= 1 + \Sigma G \\ G G_0^{-1} &= 1 + G\Sigma \end{aligned}\right] \text{hence} \quad G_0^{-1}G - G G_0^{-1} = \Sigma G - G\Sigma$$

Hence we require $\underbrace{(\Sigma\cdot G - G\cdot\Sigma)}_{\text{like a condition of vanishing curl} \Rightarrow \text{exist functional } \Phi}(1,1^+) = 0$

explicitely: $\int d2\left[\Sigma(1,2)\,G(2,1^+) - G(1,2)\,\Sigma(2,1^+)\right] = 0$

Hence we want an approximation for which $\int d2 \left[\Sigma(1,2)\, G(2,1^+) - G(1,2)\, \Sigma(2,1^+) \right] = 0$ holds.

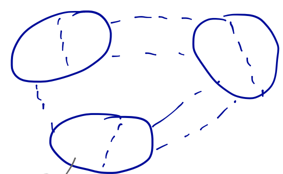
It turns out that this holds whenever $\Sigma(1,2) = \dfrac{\delta \Phi}{\delta G(2,1)}$ is the derived from the generating functional.

We want to prove that when $\Sigma(1,2) = \dfrac{\delta \Phi}{\delta G(2,1)}$ then:

$$\int d2 \left[\frac{\delta \Phi}{\delta G(2,1)}\, G(2,1^+) - G(1,2)\, \frac{\delta \Phi}{\delta G(1^+,2)} \right] = 0$$

The story of cutting the cake but not eating it:

Check arbitrary diagram $\Phi =$

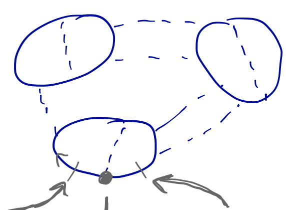


$$\int d1 \int d2\, \frac{\delta \Phi}{\delta G(2,1)}\, G(2,1)$$ will cut one propagator and will put it back

cuts one G puts it back

Result is: $2n\, \Phi$ because there are $2n$ propagators to cut.

If one fixes one time at 1, then $\Phi =$



$\int \dfrac{\delta \Phi}{\delta G(2,1)}\, G(2,1)$ $\int G(1,2)\, \dfrac{\delta \Phi}{\delta G(1,2)}$

cuts one line cuts different line

but it always puts it back, hence result is the same Φ in both cases. When subtracted, give zero!

Summary: If $\Sigma(1,2) = \dfrac{\delta \Phi}{\delta G(2,1)}$ then single particle G obeys conservation laws!

Conserving approximation for two particle response

chapter 10 & 14 in R.M.

Recall:

$$Z=\int D[\psi^+\psi]\, e^{-S-\int \psi_2^+ y_{21}\psi_1}$$

$$\frac{\delta \ln Z}{\delta y(2,1)} = \frac{1}{Z}\int D[\psi^+\psi]\, e^{-S}\,\psi(1)\psi^+(2) = -G(1,2)$$

$$\frac{\delta^2 \ln Z}{\delta y(2,1)\,\delta y(3,4)} = -\frac{\delta G(1,2)}{\delta y(3,4)} = \frac{1}{Z}\int D[\psi^+\psi]\, e^{-S}\,\psi_1\psi_2^+\psi_4\psi_3^+$$

$$=\langle T_\tau\, \psi_2^+\psi_3^+\psi_4\psi_1\rangle - \langle T_\tau\, \psi_2^+\psi_1\rangle\langle\psi_3^+\psi_4\rangle \equiv -L(23,41)$$

We want to compute

$$L(23,41)=\frac{\delta G(12)}{\delta y(34)}$$

start with matrix identity $\quad G\cdot G^{-1}=1$

$$G\cdot G^{-1}=1 \quad : \quad G(1,2)\,G^{-1}(2,5)=\delta(1,5)$$

$$\frac{\delta G}{\delta y}G^{-1}+G\frac{\delta G^{-1}}{\delta y}=0 \quad : \quad \frac{\delta G(1,2)}{\delta y(34)}\,G^{-1}(2,5)+G(1,2)\,\frac{\delta G^{-1}(2,5)}{\delta y(3,4)}=0$$

$$\frac{\delta}{\delta y}G^{-1}=\frac{\delta}{\delta y}(-y-\Sigma) \quad : \quad \frac{\delta G(1,2)}{\delta y(3,4)}\,G^{-1}(2,5)-G(1,2)\frac{\delta y(2,5)}{\delta y(3,4)}-G(1,2)\frac{\delta \Sigma(2,5)}{\delta y(3,4)}=0 \quad /\ G(5,6)$$

$$\frac{\delta G(1,2)}{\delta y(3,4)}\,\delta(2,6)-G(1,2)\,\delta(2,3)\,\delta(5,4)\,G(5,6)-G(1,2)\frac{\delta\Sigma(2,5)}{\delta y(3,4)}G(5,6)=0$$

$$\frac{\delta G(1,6)}{\delta y(3,4)}-G(1,3)\,G(4,6)-G(1,2)\frac{\delta\Sigma(2,5)}{\delta y(3,4)}G(5,6)=0$$

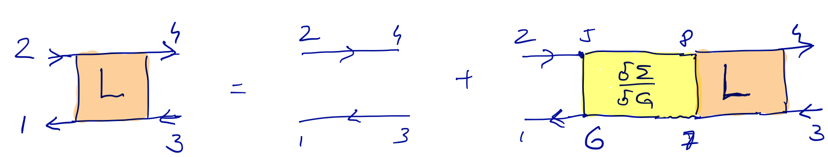
$$\frac{\delta\Sigma[G(y),v_c]}{\delta y}=\frac{\delta\Sigma}{\delta G}\frac{\delta G}{\delta y} \quad : \quad \frac{\delta G(1,6)}{\delta y(3,4)}-G(1,3)\,G(4,6)-G(1,2)\frac{\delta\Sigma(2,5)}{\delta G(7,8)}\frac{\delta G(7,8)}{\delta y(3,4)}G(5,6)=0$$

$6\leftrightarrow 2$

Finally:

$$\frac{\delta G(1,2)}{\delta y(3,4)}=G(1,3)\,G(4,2)+G(1,6)\frac{\delta\Sigma(6,5)}{\delta G(7,8)}\frac{\delta G(7,8)}{\delta y(3,4)}G(5,2)$$

Diagrammatically it corresponds to:

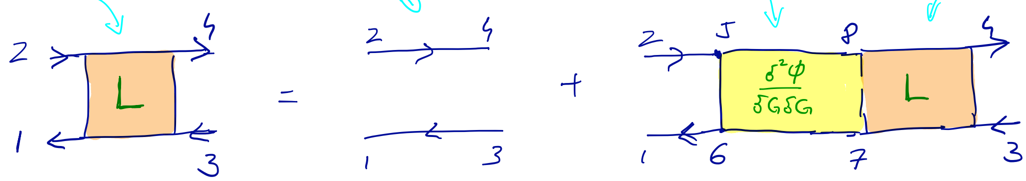


Note that $\frac{\delta \Sigma}{\delta G} = \frac{\delta^2 \Phi}{\delta G \, \delta G}$ is the second derivative of the generating functional. Hence Φ gives complete description of how to calculate the high-order correlation functions. In particular

$\frac{\delta \Phi}{\delta G \, \delta G}$ is the irreducible vertex for two particle G_2.

Bethe Salpeter:

$$\frac{\delta G(1,2)}{\delta y(3,4)} = G(1,3)\,G(4,2) + G(1,6)\left[\frac{\delta^2 \Phi}{\delta G(7,8)\,\delta G(5,6)}\right] G(5,2)\,\frac{\delta G(7,8)}{\delta y(3,4)}$$

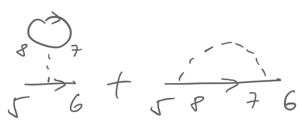


(1)

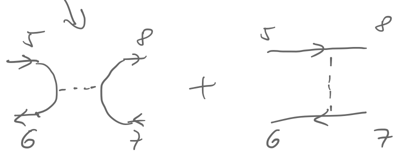
Example 1: Hartree-Fock for Σ

What is the corresponding $\langle \rho \rho \rangle$ or $\langle \vec{j}\, \vec{j} \rangle$?

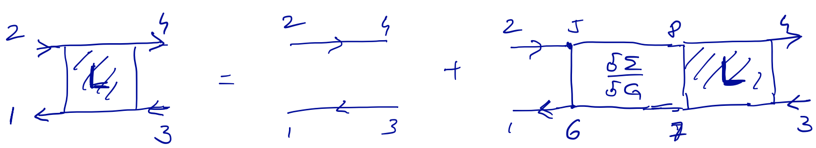
$\Sigma(6,5) =$



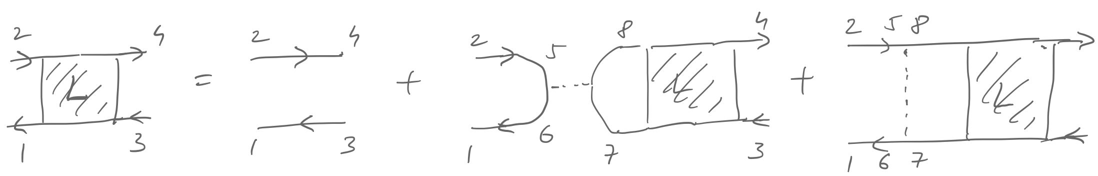
$\frac{\delta \Sigma(6,5)}{\delta G(7,8)} =$



General Bethe Salpeter:



For Hartree-Fock we get:



generates RPA bubbles

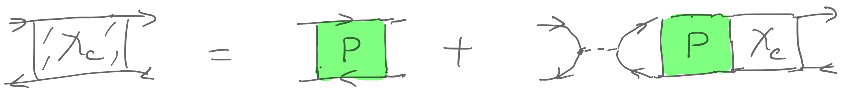
generates ladders

$\underbrace{\hspace{10em}}_{\text{bubbles and ladders}}$

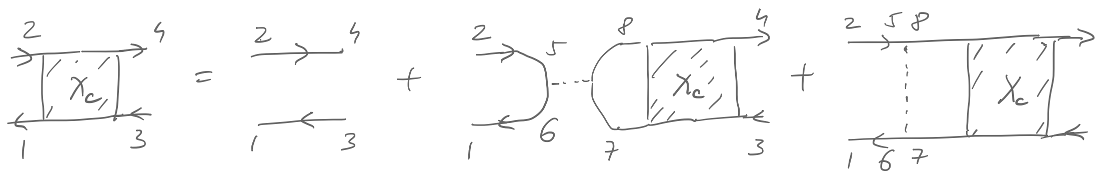
It we are interested in charge-charge correlation function χ_c, then the vertex is unity. We can then use a trick to pre-sum geometric series of diagrams by working with so-called polarization:

$$\chi_c = \frac{P}{1-v_c P} = P + P v_c P + P v_c P v_c P + \cdots$$

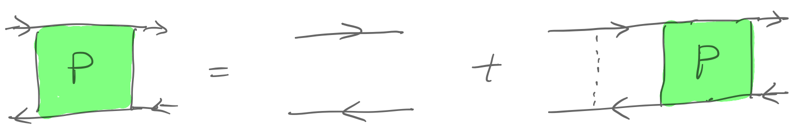
which is $\qquad \chi_c = P + v_c P \chi_c$ and diagrammatically



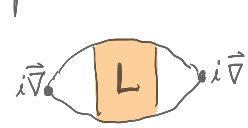
While

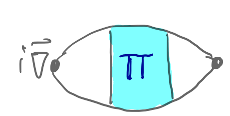


It should be clear that



Hence by writing equation for polarization P (which is related to $\chi_c = \frac{P}{1-v_c P}$) we keep only the exchange part of the functional derivative $\frac{\delta \Phi^x}{\delta G}$.
In another words, we manage to remove $\frac{\delta \Phi^H}{\delta G}$ from Bethe-Salpeter equation by concentrating on P rather than χ.
This can be generalized, so that in general case P contains irreducible vertex of $\frac{\delta^2 \Phi^{xc}}{\delta G \delta G}$ where $\Phi^{xc} = \Phi - \Phi^H$, i.e.

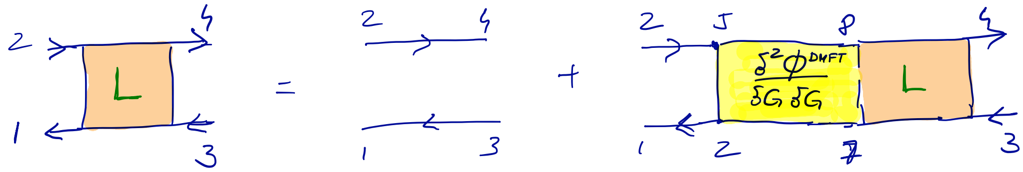
Note that this works for charge response, while optics (calculated by $\langle jj \rangle$ has extra vertices at the two ends 

and requires slightly modified equations, involving the quantity 

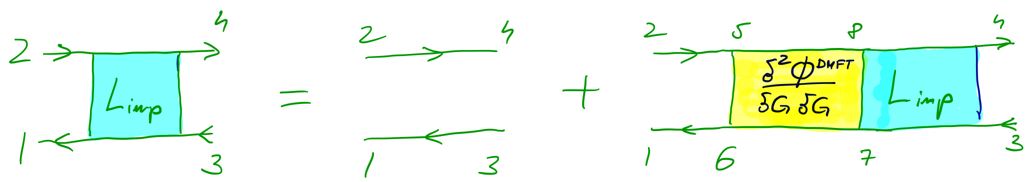
!

Finally, Baym-Kadanoff approach also shows how one should compute correlation functions within other methods, such as DMFT or DFT.

In particular according to Eq (1) in DMFT we should use:



Such irreducible vertex $\frac{\delta \Phi^{DMFT}}{\delta G \delta G}$ can be calculated by the impurity solver by computing the corresponding impurity quantities:



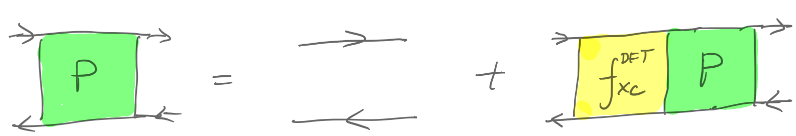
where: $L_{imp}(23,41) = -\langle T_\tau \psi_2^+ \psi_3^+ \psi_4 \psi_1 \rangle_{imp} + \langle T_\tau \psi_2^+ \psi_1 \rangle \langle T_\tau \psi_3^+ \psi_4 \rangle_{imp}$

and notice: $\xrightarrow{G_{imp}}$ $\xrightarrow{G_{lattice}}$

Within DFT, for example, the Hartree term is treated exactly, which can be absorbed by computing polarization P. The polarization should be however computed in the presence of exchange-correlation kernel:

$$f_{xc}^{DFT} = \frac{\delta^2 E_{xc}[\rho]}{\delta\rho\,\delta\rho}$$

and polarization should be



In practice f_{xc}^{DFT} is rather small and is almost always neglected, so that DFT response functions are usually calculated using formulas for the Hartree-interacting problem (RPA).