Comparison of many body methods within Baym-Kadanoff approach

All methods share the non-interacting part of the functional, and they differ only in what is included in $\Phi[\mathcal{G}]$.

$$\Gamma[\mathcal{G}] = \mathrm{Tr}\ln\mathcal{G} - \mathrm{Tr}((\mathcal{G}_0^{-1}-\mathcal{G}^{-1})\mathcal{G}) + \Phi[\mathcal{G}]$$

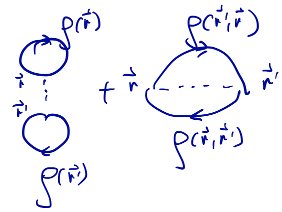
1) DFT : $\Phi[\mathcal{G}] = E_H[\rho] + E_{xc}[\rho]$

where ρ is diagonal part of $\mathcal{G}$ in space-time basis, i.e.,

$$\rho(\vec r) = \mathcal{G}(\vec r\tau, \vec r'\tau')\,\delta(\vec r-\vec r')\,\delta(\tau-\tau')$$

We previously verified that such setup gives DFT equations.

Also note that within LDA: $E_{xc}[\rho] \simeq \int d^3r\, \varepsilon^{xc}(\rho(\vec r))\,\rho(\vec r)$ is just a sum of local term, local to a point in 3D space.

2) Hartree-Fock $\Phi[\mathcal{G}] =$ 

$$\Phi[\mathcal{G}] = \frac{1}{2}\iint \rho(\vec r)\, v_c(\vec r-\vec r')\,\rho(\vec r')\, d^3r\, d^3r' - \frac{1}{2}\iint \rho(\vec r,\vec r')\, v_c(\vec r-\vec r')\,\rho(\vec r',\vec r)$$

connect different point in space

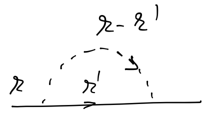
$$\rho(\vec r,\vec r') = \mathcal{G}(\vec r\tau, \vec r'\tau')\,\delta(\tau-\tau')$$

Hartree Fock is non-local approximation for E_{xc}, and is extremely succesfull in molecules. For infinite systems and solids it tends to exaggerate the size of band gaps, and makes metals unstable, i.e., metals have vanishing mass.

In periodic solids $v_c(\vec r-\vec r') \to v_q = \frac{8\pi}{q^2}$ in Galilean translation invariant system (like UEG)

Continue Hartree-Fock

$$V_q = \frac{8\pi}{q^2}$$



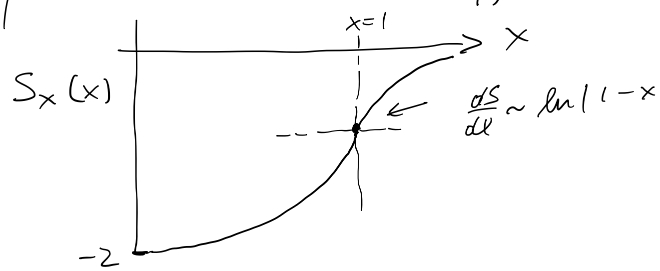
$$\Sigma_x^k = -\frac{1}{\beta}\sum_{k' i\omega} G_{k'}(i\omega)\, V_{k-k'} = -\int \frac{d^3k'}{(2\pi)^3} f(\varepsilon_{k'}) \frac{8\pi}{|\vec{k}-\vec{k}'|^2} = -\int \frac{dk'\, k'^2\, 2\pi}{(2\pi)^3} f(\varepsilon_{k'}) \int_{-1}^{1} \frac{dx\; 8\pi}{(k^2+k'^2-2kk'x)}$$

$$\Sigma_x^k = -\frac{2}{\pi k}\int dk'\, k'\, f(\varepsilon_{k'}) \int_{|k-k'|}^{|k+k'|} \frac{du}{u} = -\frac{1}{\pi k}\int dk'\, k'\, f(\varepsilon_{k'}) \ln\left(\frac{(k+k')^2}{(k-k')^2}\right) \underset{T=0}{=} -\frac{1}{\pi k}\int_0^{k_F} dk'\, k' \ln\left|\frac{k'+k}{k'-k}\right|$$

$k^2+k'^2-2kk'x = u^2$

$dx = -\frac{du\, u}{k k'}$

$$\Sigma_x^k = -\frac{2k_F}{\pi}\left(1+\frac{1-\left(\frac{k}{k_F}\right)^2}{2\left(\frac{k}{k_F}\right)}\ln\left|\frac{1+\frac{k}{k_F}}{1-\frac{k}{k_F}}\right|\right) \equiv \frac{2k_F}{\pi} S_x\left(\frac{k}{k_F}\right)$$



quasiparticles mass: $\frac{m^*}{m_b} = \frac{1}{Z_k}\left(1+\frac{1}{v_F}\frac{\partial \Sigma_k}{\partial k}\Big|_{\substack{\omega=0\\ k=k_F}}\right)^{-1}$

$Z_k = 1$ because $\frac{d\Sigma}{d\omega} = 0$

$$\frac{\partial \Sigma_k}{\partial k} = \frac{2}{\pi} S_x'\left(\frac{k}{k_F}\right) \; ; \quad S_x'(x) = \frac{2x-(1+x^2)\ln\left|\frac{1+x}{1-x}\right|}{2x^2}$$

$$S_x'(x\sim 1) \approx \ln|1-x| + \text{const}\ldots \Rightarrow \frac{\partial \Sigma_k}{\partial k}\Big|_{k=k_F} \to \infty$$

hence $\frac{m^*}{m} \to 0$ at $k = k_F$

Conclusion: metal unstable in H.F.

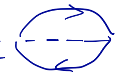
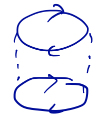
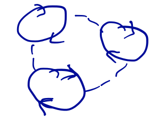
Specific heat diverges at $T=0$

This is wrong for simple metals, which H.F. might be able to describe (limit $V_q \to 0$)

The culprit is the long range Coulomb repulsion $V_q(q\sim 0)\to\infty$

Interaction is "over-emphasized" between very distant quasiparticles, which is physically wrong, because of screening effects in solids.

3) G.W.

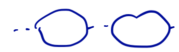
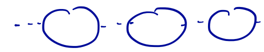
$\Phi[\mathcal{G}] = E^H[\rho] + \frac{1}{2}$  $+ \frac{1}{4}$  $+ \frac{1}{6}$  $+ \cdots$

$$\Phi[\mathcal{G}] = E^H[\rho] + \tfrac{1}{2}\mathrm{Tr}\ln(1 - v_c \cdot \mathcal{G}\cdot\mathcal{G})$$

check by expanding: $\Phi[\mathcal{G}] \approx E^H - \frac{1}{2}\mathrm{Tr}(v_c\cdot\mathcal{G}\cdot\mathcal{G}) - \frac{1}{4}\mathrm{Tr}(v_c\cdot\mathcal{G}\cdot\mathcal{G}\cdot v_c\cdot\mathcal{G}\cdot\mathcal{G})$

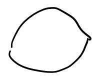
$$- \tfrac{1}{6}\mathrm{Tr}(v_c\cdot\mathcal{G}\cdot\mathcal{G}\cdot v_c\cdot\mathcal{G}\cdot\mathcal{G}\cdot v_c\cdot\mathcal{G}\cdot\mathcal{G}) - \cdots$$

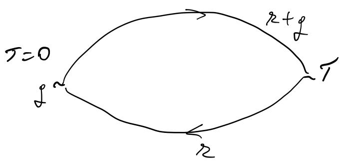
Can be rewriten in terms of the screened coulomb interaction W and $\mathcal{G}$:

$W =$  $= \cdots +$  $+$  $+$  $= \dfrac{v_q}{1 - v_q\,\mathcal{G}\cdot\mathcal{G}}$

$\Phi[\mathcal{G}, W] = E^H[\rho] + \frac{1}{2}$ 

Hence like H.F. but with screened interaction.

What is $P_q(\Omega) \equiv$  $= \mathcal{G}\cdot\mathcal{G}$ (hard to compute with $\mathcal{G}$ interacting, but easy with $\mathcal{G}\approx\mathcal{G}^0$, i.e.) RPA



$$\mathcal{G}^0_k(\tau) = -f(-\varepsilon_k)\,e^{-\varepsilon_k\tau}$$
$$\mathcal{G}^0_k(-\tau) = f(-\varepsilon_k)\,e^{-\varepsilon_k(\beta+\tau)} = f(\varepsilon_k)\,e^{-\varepsilon_k\tau}$$

$$P^0_q(\tau) = 2\int\frac{d^3k}{(2\pi)^3}\mathcal{G}^0_{k+q}(\tau)\,\mathcal{G}^0_k(-\tau) = -2\int\frac{d^3k}{(2\pi)^3} f(-\varepsilon_{k+q})f(\varepsilon_k)\,e^{\tau(\varepsilon_k - \varepsilon_{k+q})}$$

spin deg.

$$P^0_q(i\Omega) = \int_0^\beta d\tau\, e^{i\Omega\tau} P^0_q(\tau) = -2\int\frac{d^3k}{(2\pi)^3} f(\varepsilon_k)f(-\varepsilon_{k+q})\,\frac{\left[e^{(i\Omega+\varepsilon_k-\varepsilon_{k+q})\beta} - 1\right]}{i\Omega + \varepsilon_k - \varepsilon_{k+q}}$$

$$= -2\int\frac{d^3k}{(2\pi)^3}\frac{f(\varepsilon_k)f(-\varepsilon_{k+q})\left[e^{\beta\varepsilon_k}e^{-\beta\varepsilon_{k+q}} - 1\right]}{i\Omega + \varepsilon_k - \varepsilon_{k+q}} = -2\int\frac{d^3k}{(2\pi)^3}\underbrace{\frac{f(\varepsilon_{k+q}) - f(\varepsilon_k)}{i\Omega + \varepsilon_k - \varepsilon_{k+q}}}_{\uparrow\ \text{Lindhart formula}}$$

$$f(x)\,e^x = f(-x)$$

$$\frac{e^{\beta\varepsilon_k - \beta\varepsilon_{k+q}} - 1}{(1+e^{\beta\varepsilon_k})(1+e^{-\beta\varepsilon_{k+q}})} = \frac{e^{\beta\varepsilon_k} - e^{\beta\varepsilon_{k+q}}}{(1+e^{\beta\varepsilon_k})(1+e^{\beta\varepsilon_{k+q}})} = \frac{1}{1+e^{\beta\varepsilon_{k+q}}} - \frac{1}{1+e^{\beta\varepsilon_k}} = f(\varepsilon_{k+q}) - f(\varepsilon_k)$$

For general q, Ω is still a complicated formula. But at $q\approx 0$, which is relevant for stability of metals, we have $P^0_{q\sim 0}(\tau) \simeq -2\int\frac{d^3k}{(2\pi)^3} f(\varepsilon_k)f(-\varepsilon_k)$

$$P^0_{q\sim 0}(\tau) \simeq -2\int\frac{d^3k}{(2\pi)^3} f(\varepsilon_k) f(-\varepsilon_k) = -2T\int\frac{d^3k}{(2\pi)^3}\left(-\frac{df}{dx}\right)_{x=\varepsilon_k} \approx -T\underbrace{D(0)}$$

Density of states at the Fermi level

$$f(x)f(-x) = T\left(-\frac{df}{dx}\right) \quad ; \quad \left(-\frac{df}{dx}\right) \approx \delta(x)$$

$$D(\omega) = 2\int\frac{d^3k}{(2\pi)^3}\delta(\varepsilon_k - \omega)$$

Hence $\quad P_{q\sim 0}(i\Omega=0) = \int_0^\beta P^0_{q\sim 0}(\tau)\,d\tau = \beta P^0_{q\sim 0}(\tau) = -D(0)$

Conclusion: $\quad W_q(\Omega\sim 0) \approx \dfrac{V_q}{1+V_q D(0)} = \dfrac{8\pi}{q^2 + 8\pi D(0)}$ $\quad$ i.e. does not diverge at $q\approx 0$

$$W(\Omega\sim 0, r) \approx \frac{e^{-\sqrt{\lambda}\,r}}{r} \quad \text{with} \quad \lambda = 8\pi D(0)$$

Hence the method is "like" "screened Hartree Fock" and it's self-energy is approximately:

approximate form: $\quad V_q = \dfrac{8\pi}{q^2+\lambda}$

$$\Sigma_x^k = -\frac{1}{\beta}\sum_{k', i\omega} \mathcal{G}_{k'}(i\omega)\, V_{k-k'} = -\int\frac{d^3k'}{(2\pi)^3} f(\varepsilon_{k'})\frac{8\pi}{|\vec{k}-\vec{k}'|^2+\lambda} = -\int\frac{dk'\,k'^2\,2\pi}{(2\pi)^3} f(\varepsilon_{k'})\int_{-1}^{1}\frac{dx\;8\pi}{(k^2+k'^2-2kk'x)+\lambda}$$

$$\Sigma_x^k = -\frac{2}{\pi k}\int dk'\,k'\, f(\varepsilon_{k'})\int_{|k-k'|}^{|k+k'|} du\,\frac{u}{u^2+\lambda} = -\frac{1}{\pi k}\int dk'\,k' f(\varepsilon_{k'})\ln\left(\frac{(k+k')^2+\lambda}{(k-k')^2+\lambda}\right) \equiv \frac{2\pi}{k_F} S_x\left(\frac{k}{k_F}\right)$$

$$k^2 + k'^2 - 2kk'x = u^2$$

$$dx = -\frac{du\,u}{kk'}$$

$$S_x\left(\frac{k}{k_F}\right) \equiv -\frac{1}{2kk_F}\int k' f(\varepsilon_{k'})\ln\left(\frac{(k+k')^2+\lambda}{(k-k')^2+\lambda}\right)dk'$$

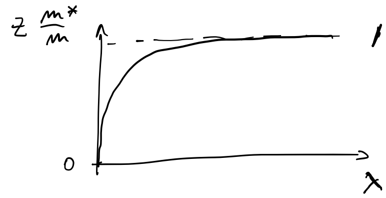
$$T\to 0: \quad S_x(y) = -\frac{1}{2y}\int_0^1 dx\, x\ln\left(\frac{(y+x)^2+\lambda k_F^2}{(y-x)^2+\lambda k_F^2}\right)$$

$$\Delta(\lambda) \equiv \left.\frac{dS_x(y)}{dy}\right|_{y=1} = \frac{2+\lambda}{4}\ln\left(1+\frac{4}{\lambda}\right) - 1 \quad ; \quad \begin{array}{l} \lambda\to 0 \Rightarrow \Delta(\lambda)\Rightarrow\infty \\ \lambda\to\infty \Rightarrow \Delta(\lambda)\Rightarrow \frac{2+\lambda}{4}\left(\frac{4}{\lambda}-\frac{1}{2}\left(\frac{4}{\lambda}\right)^2\right)-1 \approx \frac{4}{3\lambda^2}\end{array}$$

Summary for RPA (or GW): metal stable with mass:

$$\frac{m^*}{m_b} = \frac{1}{Z_k}\left(1+\frac{1}{v_F}\frac{\partial \Sigma_k}{\partial k}\Big|_{\substack{\omega=0\\ k=k_F}}\right)^{-1} \Rightarrow \frac{m^*}{m} = \frac{1/Z}{1+D(\lambda)}$$

$$D(\lambda) = \frac{2+\lambda}{4}\ln\left(1+\frac{4}{\lambda}\right) - 1$$

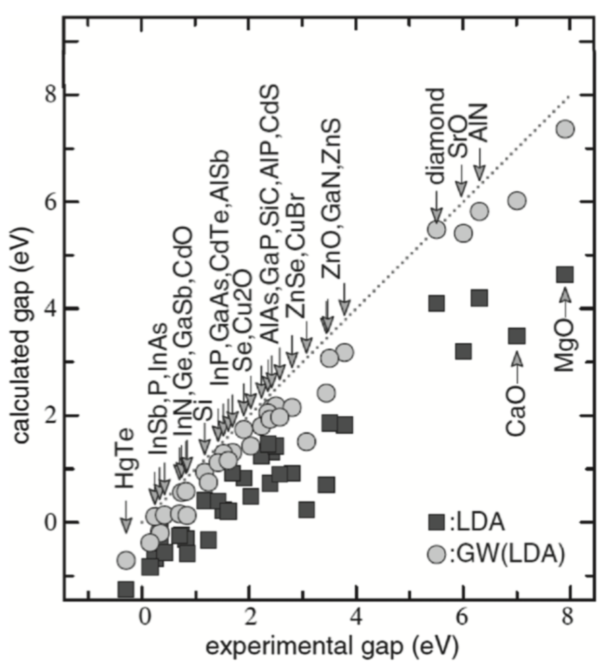


Frequency dependence increases mass, while momentum dependence of Σ_k reduces the effective mass.

Z tends to be close to unity when RPA or GW reliable, hence masses tend to be small.

It turns out RPA and GW are not very good in metals (LDA, GGA tend to agree better with experiment), but they predict better gaps in semiconductors than DFT based methods.

Band gaps in semiconductors:



4) Dynamical Mean Field Theory (DMFT)

$$\Phi[G] = \sum_{\vec{R}} \Phi[G_{local}^{\vec{R}}]$$

$\leftarrow$ sum over correlated ions at position $\vec{R}$ in solids. Needs projection of G to such a "correlated atom".

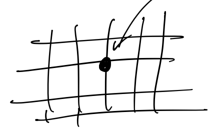
note similarity to LDA : $\Phi = \int d^3r\, \tilde{\varepsilon}_{xc}(\rho(r))$

Example : single band Hubbard model :

$$\Phi[G] = \sum_i \Phi[G_{ii}]$$

$\uparrow$ lattice site

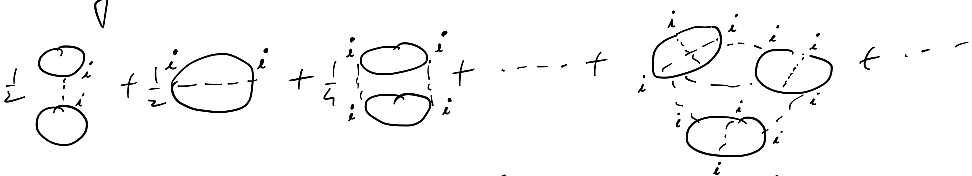
on-site G_{ii}



If the system is periodic $G_{ii}(\omega) = \sum_k G_k(\omega)$

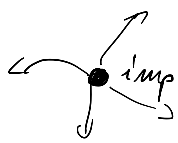
What is $\Phi^{exact}[G_{ii}] = ?$

$\Phi^{exact}[G_{ii}] =$



all possible Feynman diagrams.

Auxiliary problem of quantum impurity; which has a single interacting site



$$H = \underbrace{U\, n_{i\uparrow}\, n_{i\downarrow}}_{H_{local}} + \sum_k (V_k\, d_{is}^{+} c_{ki} + h.c.) + \underbrace{\sum_k c_{ki}^{+} c_{ki}\, \varepsilon_{ki}}_{\text{the infinite bath}}$$

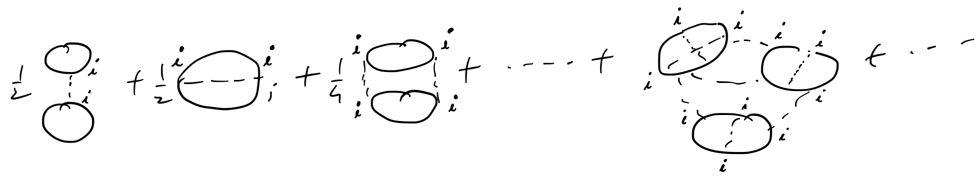
$$S = \int_0^\beta d\tau\, H_{local}(\tau) + \int_0^\beta d\tau \int_0^\beta d\tau'\, d_{is}^{+}(\tau)\, \Delta_s(\tau-\tau')\, d_{is}(\tau')$$

with $\Delta_s(i\omega) = \sum_k \frac{|V_k|^2}{i\omega - \varepsilon_k}$

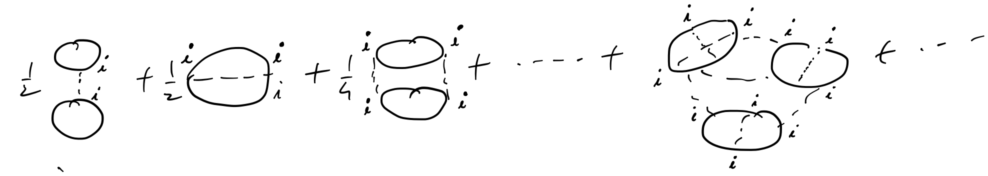
For the impurity we also have:

$$\Gamma_{imp}[G_{imp}] = \mathrm{Tr} \ln G_{imp} - \mathrm{Tr}(\Sigma_{imp} G_{imp}) + \Phi[G_{imp}]$$

$$\Phi^{DMFT}[\mathcal{G}_{ii}] =$$



$$\Phi^{imp}[\mathcal{G}_{imp}] =$$



$i \equiv imp$

They are identical, provided that we arrange $\mathcal{G}_{imp} = \mathcal{G}_{ii}$ of the lattice problem and $U_{imp} = U_{ii}$ of the lattice problem.

Then $$\Sigma_{imp} = \frac{\delta \Phi^{imp}}{\delta \mathcal{G}_{imp}} = \frac{\delta \Phi^{DMFT}[\mathcal{G}]}{\delta \mathcal{G}_{ii}} = \Sigma_{ii}$$

Then $$\mathcal{G}_{ii} = \sum_{k} \frac{1}{i\omega + \mu - \varepsilon_k - \Sigma_{ii}} = \mathcal{G}_{imp} = \frac{1}{i\omega - E_{imp} - \Sigma_{ii} - \Delta(\omega)}$$

lattice problem

impurity self-energy

Hence we need to solve impurity problem with hybridization

$$\Delta(\omega) = i\omega + \mu - \Sigma_{ii}(\omega) - \left(\sum_{k} \frac{1}{i\omega + \mu - \varepsilon_k - \Sigma_{ii}(\omega)}\right)^{-1}$$

and impurity level $E_{imp} = -\mu$

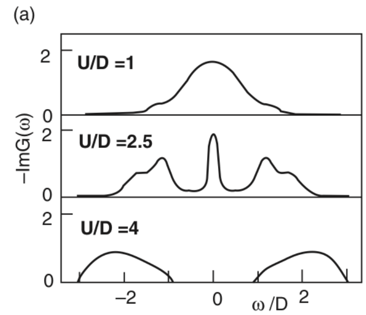
which delivers $\Sigma_{ii}(\omega)$, and can be plugged back to impurity solver.

Conclusion: The lattice problem solved with the solution on an auxiliary problem of Q.I.M.

DMFT solution of the simplest single band Hubbard model

D ≡ half-bandwidth

U ≡ C.R.

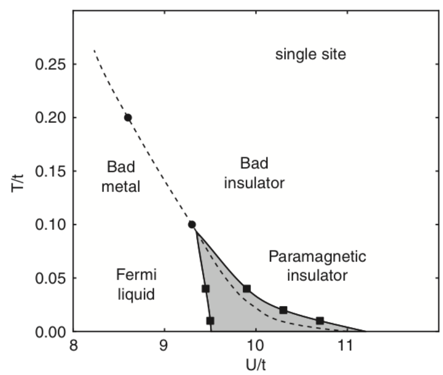


Mott state around $\frac{U}{D} \sim 3$ or $\frac{U}{2D} \sim 1.5$

total bandwidth

phase diagram in T and U plane for 2D Hubbard model with

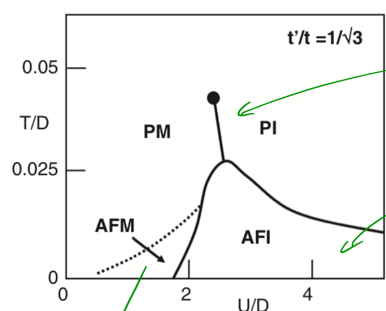
$D \sim 4t$



↑

$\frac{U}{D} \sim 1.25$

Allowing magnetic solutions and adding a bit of frustration $t' \sim \frac{t}{\sqrt{3}}$



Mott transition as above

antiferromagnetic insulator

Antiferromagnetic metal