Advanced Solid State

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Books: Richard Martin: Interacting Electrons
Chapters 5 to 10

David Vanderbilt: Berry phases in Electronic Structure Theory
Chapters 3 and 4

3:20
ARC 108

①

Correlation Functions (R.M. Chapter 5)

1) Provide a way to characterize the system theoretically, and many of C.F. are directly measured in experiment:

a) $A(k,\omega) = -\frac{1}{\pi} \operatorname{Im} G_k(\omega)$ by ARPES

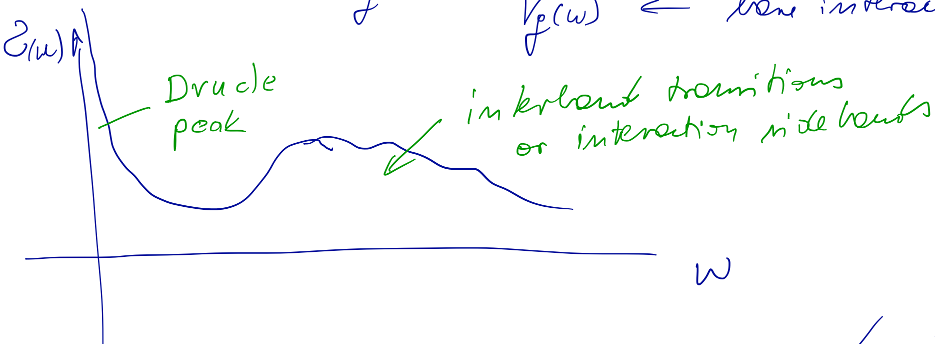
b) optical conductivity $\sigma_{q=0}(\omega) = \omega \operatorname{Im}\left(\varepsilon_q(\omega)\right)$ where ε is dielectric function

and $\frac{1}{\varepsilon_q(\omega)} = \frac{W_q(\omega)}{V_q(\omega)}$ ← screened interaction / ← bare interaction

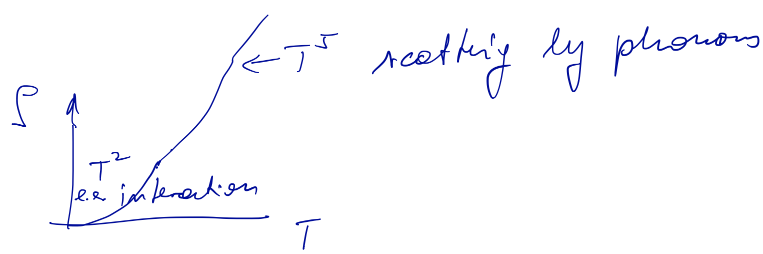
$\frac{1}{\varepsilon_q(\omega)} = 1 - V_q \chi_q(\omega)$

$\chi_c(\vec{r}_1\tau_1, \vec{r}_2\tau_2) = \langle \psi_1^+ \psi_2^+ \psi_2 \psi_1 \rangle$

$1 \equiv (\vec{r}_1, \tau_1)$
$2 \equiv (\vec{r}_2, \tau_2)$



c) resistivity: $\rho = \frac{1}{\sigma_{q=0}(\omega=0)}$

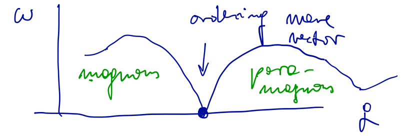


d) spin susceptibility

Inelastic neutron scattering measures $S(q,\omega) = \frac{\chi_s''(q,\omega)}{1 - e^{-\beta\omega}}$

where $\chi_s(\vec{r}_1\tau_1, \vec{r}_2\tau_2) = \langle \psi_{s_1}^+(\vec{r}_1\tau_1)\vec{\sigma}_{s_1 s_2}\psi_{s_2}(\vec{r}_1\tau_1)\, \psi_{s_3}^+(\vec{r}_2\tau_2)\vec{\sigma}_{s_3 s_4}\psi_{s_4}(\vec{r}_2\tau_2) \rangle$

$= \langle \vec{S}(\tau_1) \cdot \vec{S}(\tau_2) \rangle$



e) Single particle correlation function (main building block of many body)

b...d) Two particle correlation function (harder to compute, but clearly very important)

(2)

Short note on the grand canonical ensemble

At constant particle number use

$$Z = \mathrm{Tr}\left(e^{-\beta H}\right) = e^{-\beta F} \qquad dF(V,T,N) = -p\,dV - S\,dT + \mu\,dN$$

When the number of particles is not constant, we use Legendre transform

$$Z = \mathrm{Tr}\left(e^{-\beta(H-\mu\hat{N})}\right) = e^{-\beta\Omega} \qquad \text{where } \Omega = F - \mu N$$

$$d\Omega(V,T,\mu) = -p\,dV - S\,dT - N\,d\mu$$

In these lectures we will use

$\mathrm{Tr}\left(e^{-\beta H}\cdots\right)$ instead of $\mathrm{Tr}\left(e^{-\beta(H-\mu N)}\cdots\right)$ for short notation, hence H in such trace stands for $\hat{H} \to \hat{H} - \mu\hat{N}$.

(3) # Dynamic Correlation Function

Imaginary time & time ordered

$$\langle\langle A;B\rangle\rangle \equiv -\langle T_\tau A(\vec r_1,\tau_1)\, B(\vec r_2,\tau_2)\rangle = -\frac{1}{Z}\mathrm{Tr}\left(T_\tau e^{-\beta H}\, e^{H\tau_1} A(\vec r_1) e^{-H\tau_1}\; e^{H\tau_2} B(\vec r_2) e^{-H\tau_2}\right)$$

Heissenberg, in imaginary time

here $H \equiv \hat H - \mu \hat N$ if working with grand canonical ensemble.

where $\langle T_\tau A(\tau_1) B(\tau_2)\rangle = \Theta(\tau_1>\tau_2)\langle A(\tau_1)B(\tau_2)\rangle \mp \Theta(\tau_2>\tau_1)\langle B(\tau_2)A(\tau_1)\rangle$ (fermions: upper sign; bosons: lower sign)

most useful for calculation

Real time & time ordered

$$\langle\langle A;B\rangle\rangle^T = -i\frac{1}{Z}\mathrm{Tr}\left(T_\sim\, e^{-\beta H} e^{iHt_1} A(\vec r_1) e^{-iHt_1} e^{iHt_2} B(\vec r_2) e^{-iHt_2}\right)$$

useful for $T=0$ calculations

Retarded C.F.

$$\langle\langle A;B\rangle\rangle^R = -i\Theta(t_1-t_2)\langle [A(\vec r_1 t_1), B(\vec r_2,t_2)]_\pm\rangle$$

fermionic ($+$), bosonic ($-$)

measured in experiment

Can be obtained from Matsubara by analytic continuation

Fourier transform

$$\langle\langle A;B\rangle\rangle(\omega) = \int_{-\infty}^{\infty} e^{i\omega t}\langle\langle A(t);B(0)\rangle\rangle dt \qquad \text{real time}$$

$$\langle\langle A;B\rangle\rangle(i\omega) = \int_0^\beta e^{i\omega\tau}\langle\langle A(\tau);B(0)\rangle\rangle d\tau \qquad \text{imaginary time \& imaginary frequency}$$

What is relation between them?

$$\langle\langle A;B\rangle\rangle^R = -i\Theta(t_1-t_2)\frac{1}{Z}\mathrm{Tr}\left(e^{-\beta H}\{e^{iHt_1} A\, e^{-iH(t_1-t_2)} B\, e^{-iHt_2} \pm e^{iHt_2} B\, e^{-iH(t_2-t_1)} A\, e^{-iHt_1}\}\right)$$

$$= -i\Theta(t_1-t_2)\frac{1}{Z}\sum_{m,M} e^{E_m(-\beta+it_1)}\langle m|A|M\rangle e^{-iE_M(t_1-t_2)}\langle M|B|m\rangle e^{-iE_m t_2} \pm e^{E_m(-\beta-it_2)}\langle m|B|M\rangle e^{-iE_M(t_2-t_1)}\langle M|A|m\rangle e^{-iE_m t_1} =$$

(m, M: many body eigenstates)

$$= -i\Theta(t_1-t_2)\sum_{m,M}\langle m|A|M\rangle\langle M|B|m\rangle e^{i(E_m-E_M)(t_1-t_2)}\left(\frac{e^{-\beta E_m}}{Z} \pm \frac{e^{-\beta E_M}}{Z}\right)$$

$$\langle\langle A;B\rangle\rangle^R(\omega) = -i\int_0^\infty dt\, e^{i(\omega+i\delta)t}\sum_{m,M}\langle m|A|M\rangle\langle M|B|m\rangle e^{i(E_m-E_M)t}\left(\frac{e^{-\beta E_m}}{Z} \pm \frac{e^{-\beta E_M}}{Z}\right) =$$

($i\delta$: to make it converge)

$$= \sum_{mM}\frac{\langle m|A|M\rangle\langle M|B|m\rangle}{(\omega+E_m-E_M+i\delta)}\left(\frac{e^{-\beta E_m} \pm e^{-\beta E_M}}{Z}\right)$$

(Lehmann representation)

Define $A(\omega) \equiv \sum_{mM}\delta(\omega+E_m-E_M)\langle m|A|M\rangle\langle M|B|m\rangle \times \left(\frac{e^{-\beta E_m}}{Z} \pm \frac{e^{-\beta E_M}}{Z}\right)$

$$\langle\langle A;B\rangle\rangle^R(\omega) = \int \frac{A(x)}{\omega - x + i\delta}dx \qquad \text{(spectral representation)}$$

Now for Matsubara equivalent:

$$\langle\langle A;B\rangle\rangle(i\omega) = -\int_0^\beta d\tau\, e^{i\omega\tau}\left\{\Theta(\tau>0)\frac{1}{Z}\mathrm{Tr}\left(e^{-\beta H}e^{H\tau}\overset{|m\rangle\langle m|}{\underset{\uparrow}{A}}\, e^{-H\tau}\overset{|m\rangle\langle m|}{\underset{\uparrow}{B}}\right) \mp \Theta(\tau<0)\frac{1}{Z}\mathrm{Tr}\left(e^{-\beta H}B\, e^{H\tau}A\, e^{-H\tau}\right)\right\}$$

($A(\tau)$, $B(0)$)

$$= -\sum_{m,n}\int_0^\beta d\tau\, e^{i\omega\tau}\langle m|A|n\rangle\langle n|B|m\rangle\left\{\Theta(\tau>0)\frac{1}{Z}e^{E_m(-\beta+\tau)-E_n\tau} \mp \Theta(\tau<0)\frac{1}{Z}e^{E_n(-\beta-\tau)+E_m\tau}\right\}$$

$$= -\sum_{m,n}\langle m|A|n\rangle\langle n|B|m\rangle\frac{e^{-\beta E_m}}{Z}\int_0^\beta e^{\tau(E_m-E_n)+i\omega}\,d\tau = \sum_{m,n} -\frac{\langle m|A|n\rangle\langle n|B|m\rangle}{i\omega+E_m-E_n}\frac{e^{-\beta E_m}}{Z}\left(e^{\beta i\omega+\beta(E_m-E_n)}-1\right)$$

$$= \sum_{m,n}\frac{\langle m|A|n\rangle\langle n|B|m\rangle}{i\omega+E_m-E_n}\frac{e^{-\beta E_m}}{Z}\left(\pm e^{\beta(E_m-E_n)}+1\right) =$$

$$\beta i\omega = \begin{cases}\text{fermion} & (2n+1)\pi\\ \text{boson} & 2n\pi\end{cases}\qquad e^{\beta i\omega} = \begin{cases}-1\\ +1\end{cases}$$

$$= \sum_{m,n}\frac{\langle m|A|n\rangle\langle n|B|m\rangle}{i\omega+E_m-E_n}\left(\frac{e^{-\beta E_m}\pm e^{-\beta E_n}}{Z}\right)$$

We can also integrate $\int_{-\beta}^{0} d\tau\left(\pm\frac{1}{Z}\right)e^{-\beta E_n+\tau(E_m-E_n+i\omega)}\langle m|A|n\rangle\langle n|B|m\rangle = \pm\frac{\langle m|A|n\rangle\langle n|B|m\rangle}{i\omega+E_m-E_n}e^{-\beta E_n}\left(1-e^{-\beta(i\omega+E_m-E_n)}\right)$

$$= \pm\left(e^{-\beta E_n}\pm e^{-\beta E_m}\right)\frac{\langle m|A|n\rangle\langle n|B|m\rangle}{i\omega+E_m-E_n}$$

equal

Conclusion: $\langle\langle A;B\rangle\rangle^R(\omega) = \langle\langle A;B\rangle\rangle(i\omega\to\omega+i\delta)$

Analytic continuation

It is much easier to work with Matsubara $i\omega$ than real time/frequency. No need to take care of convergence, poles, (limit $\beta\to\infty$, $V\to\infty$).

It turns out $T=0$ calculation can be wrong because the correct order of limits is ($\beta\to\infty$, $V\to\infty$), which is done in Matsubara, while $T=0$ calculation corresponds to ($V\to\infty$, $\beta\to\infty$), which can be different.

Conclusion: Matsubara method is "safer" and easier.

(I)

Properties of correlation functions

back to Lehman representation

$$\langle\langle A; B\rangle\rangle^R_{(\omega)} = \sum_{m M} \frac{\langle m|A|M\rangle\langle M|B|m\rangle}{(\omega + E_m - E_M + i\delta)} \left(\frac{e^{-\beta E_m} \pm e^{-\beta E_M}}{Z} \right)$$

if $B = A^+$ like $G^R = -\langle T_\tau \psi(\tau)\psi^+(0)\rangle$

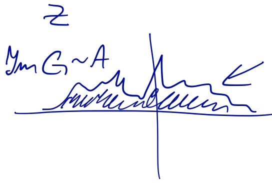
or $\chi_s = -\langle T_\tau \vec{S}(\tau)\cdot\vec{S}(0)\rangle$

or $\chi_c = -\langle T_\tau \rho(\tau)\rho(0)\rangle$

then $\langle m|A|M\rangle\langle M|A^+|m\rangle = |\langle m|A|M\rangle|^2 > 0$

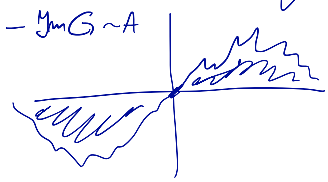
$$\mathrm{Im}\left(\langle\langle A; A^+\rangle\rangle^R(\omega)\right) = \sum_{m,M} -\pi\, \delta(\omega + E_m - E_M)|\langle m|A|M\rangle|^2 \; \frac{e^{-\beta E_m} \pm e^{-\beta E_M}}{Z}$$

for fermions $\mathrm{Im}\left(\langle\langle A; A^+\rangle\rangle^R(\omega)\right) < 0$



causality requires positive spectral function

for bosons $\mathrm{Im}\left(\langle\langle A; A^+\rangle\rangle^R(\omega)\right) = -\mathrm{sign}(\omega)$



$E_M > E_m \Rightarrow \omega > 0 \Rightarrow -\pi \cdot$ positive

$E_M < E_m \Rightarrow \omega < 0 \Rightarrow$

What about real part? From spectral representation

$$\langle\langle A; B\rangle\rangle^R(\omega) = \int \frac{A(x)}{\omega - x + i\delta} dx$$

$$G(\omega) = \int_{-\infty}^{\infty} \frac{-\frac{1}{\pi}\mathrm{Im}\, G(x)}{\omega - x + i\delta} dx$$

$$\mathrm{Re}\, G(\omega) = \frac{1}{\pi} P \int_{-\infty}^{\infty} \frac{\mathrm{Im}\, G(x)}{x - \omega} dx$$ Kramers-Kronig relations

Sum Rules for spectra.

Back to its definition $A(\omega) \equiv \sum_{mM} \delta(\omega + E_m - E_M)\langle m|A|M\rangle\langle M|B|m\rangle\left(\frac{e^{-\beta E_m}}{Z} \pm \frac{e^{-\beta E_M}}{Z}\right)$

$$\int_{-\infty}^{\infty} A(\omega)\, d\omega = \sum_{m,M} \langle m|A|M\rangle\langle M|B|m\rangle \frac{e^{-\beta E_m}}{Z} \pm \langle m|B|M\rangle\langle M|A|m\rangle \frac{e^{-\beta E_m}}{Z} = \langle AB \pm BA\rangle = \langle [A, B]_\pm \rangle$$

For fermionic $G = -\langle T_\tau \psi(\tau)\psi^+(0)\rangle \Rightarrow [\psi, \psi^+]_+ = 1 \Rightarrow \int A(\omega)\, d\omega = 1$

For bosons $\Rightarrow [\psi, \psi^+]_- = 1 \Rightarrow \int A(\omega)\, d\omega = 1$

For susceptibility $A = B = \begin{cases} S \\ \rho \end{cases} \Rightarrow \begin{matrix} [S, S]_- = 0 \\ [\rho, \rho]_- = 0 \end{matrix} \Rightarrow \int \chi''(\omega)\, d\omega = 0$

(6) For bosons it is convenient to rewrite:

$$A(\omega) \equiv \sum_{m n} \delta(\omega+E_m-E_n)\langle n|A|m\rangle\langle m|B|n\rangle\left(\frac{e^{-\beta E_n}}{Z}-\frac{e^{-\beta E_m}}{Z}\right)=\sum_{m n} \delta(\omega+E_m-E_n)\langle n|A|m\rangle\langle m|B|n\rangle \frac{e^{-\beta E_n}}{Z}\left(1-e^{-\beta(E_m-E_n)}\right)$$

$$A(\omega)=\left(1-e^{-\beta\omega}\right)\underbrace{\sum_{m,n} \delta(\omega+E_m-E_n)\langle n|A|m\rangle\langle m|B|n\rangle \frac{e^{-\beta E_n}}{Z}}_{\text{positive}}$$

Complex representation

Back to spectral representation: $\langle\langle A;B\rangle\rangle^R(\omega)=\int \frac{A(x)}{\omega-x+i\delta}dx$

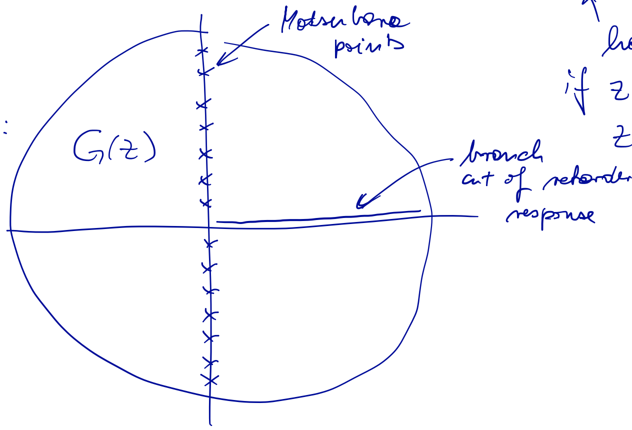
Matsubara: $\langle\langle A;B\rangle\rangle(i\omega)=\int \frac{A(x)}{i\omega-x}dx$

Complex quantity defined in the entire plane for convenient integration: $\langle\langle A;B\rangle\rangle(z)=G(z)=\int \frac{A(x)}{z-x}dx$

↑ has poles when z is on real axis

if $z=\omega+i\delta \Rightarrow$ retarded G

$z=\omega-i\delta \Rightarrow$ advanced G



(7) Response functions from linear response (Kubo)

External field $S \to S + \int dx\, \hat{M}(x) \cdot h(x)$ or $S \to S + \int d\tau\, \Delta H$ with ΔH perturbation

$x = (\vec{r}, \tau)$; $\hat{M}$ is observable $= \psi^{+}_{(\vec{r}\tau)} \hat{M}\, \psi_{(\vec{r}\tau)}$

h is external field

e) Magnetic susceptibility $M(x) = \vec{M}(\vec{r}, \tau) = \psi^{+}_{s}(\vec{r},\tau)\, \vec{\sigma}_{ss'}\, \psi_{s'}(\vec{r}\tau)$. The external field $h = -\vec{B}$

b) Optical conductivity $M(x) = \frac{1}{c}\vec{j}(\vec{r},\tau)$ and $h(x) = \vec{A}(\vec{r},\tau)$ vector potential

Recall

$$H = \int \psi^{+}(\vec{r}) \frac{1}{2m}(\underbrace{-i\hbar\vec{\nabla}}_{\vec{p}} - e\vec{A})^2 \psi(\vec{r})\, d^3r + \mu_B \vec{B} \cdot \int \psi^{+}_{s} \vec{\sigma}_{ss'} \psi_{s'} + H_{int}$$

$$= H^0 + \frac{ie\hbar}{2m} \int \psi^{+} (\vec{\nabla}\cdot\vec{A} + \vec{A}\cdot\vec{\nabla}) \psi\, d^3r + \text{small terms} \left(\frac{1}{\alpha}\right)$$

by parts

$$(\psi^{+}\psi\vec{A})\Big| - \int (\vec{\nabla}\psi^{+})\, \vec{A}\, \psi\, d^3r$$

boundary vanishes

$$H = H^0 - \int \vec{A} \cdot \frac{e i\hbar}{2m} \{(\vec{\nabla}\psi^{+})\psi - \psi^{+}(\nabla\psi)\} d^3r = H^0 - \int \vec{A}\cdot\vec{j}\, d^3r$$

$$\vec{j} = \frac{e\hbar}{2mi}(\psi^{+}\nabla\psi - (\nabla\psi^{+})\psi)$$

Need to find change of the observable M at point x_1 due to disturbance at earlier time $x_2 = (r_2, t_2)$

First sloppy derivation of the response:

$$\langle M(x_1)\rangle = \frac{1}{Z}\int D[\psi^{+}\psi]\, e^{-S_0 - \int dx\, M(x) h(x)} M(x_1) \approx \frac{\int D[\psi^{+}\psi]\, e^{-S_0}\left(M(x_1) - \int dx_2\, M(x_2) M(x_1) h(x_2)\right)}{\int D[\psi^{+}\psi]\, e^{-S_0}\left(1 - \int dx_2\, M(x_2) h(x_2)\right)}$$

$$\langle M(x_1)\rangle \approx \frac{Z_0\{\langle M(x_1)\rangle^0 - \int dx_2\, h(x_2) \langle T_\tau M(x_2) M(x_1)\rangle^0\}}{Z_0\{1 - \int dx_2\, h(x_2) \langle M(x_2)\rangle^0\}} = \langle M(x_1)\rangle^0 + \int dx\, h(x_2)\{\langle M(x_2)\rangle^0 \langle M(x_1)\rangle^0 - \langle M(x_2) M(x_1)\rangle^0\}$$

$$\langle M(x_1)\rangle \approx \langle M(x_1)\rangle^0 + \int dx_2\, h(x_2)\, \chi(x_2 x_1) \; ; \; \chi(x_2,x_1) = \langle M(x_2)\rangle^0 \langle M(x_1)\rangle^0 - \langle M(x_2) M(x_1)\rangle^0$$

connected correlation function

(8) # More careful real time derivation of causal response

$$\langle M(t)\rangle^0 = \frac{Tr(e^{-\beta H^0} M(t))}{Tr(e^{-\beta H^0})}$$

We will work in the interaction representation

- Operators have time dependence $O(t) = e^{iH^0 t}\, O\, e^{-iH^0 t}$
- Wave function have the rest of time dependence $|\Psi(t)\rangle = e^{iH_0 t} e^{-i(H_0+\Delta H)t} |\Psi(0)\rangle$

So that $\langle\Psi(t)|O(t)|\Psi(t)\rangle = \langle\Psi(0)| e^{i(H_0+\Delta H)t} \underbrace{e^{-iH_0 t} e^{iH_0 t}}_{=1} O \underbrace{e^{-iH_0 t} e^{iH_0 t}}_{=1} e^{-i(H_0+\Delta H)t} |\Psi(0)\rangle$

$$\frac{\partial}{\partial t}|\Psi(t)\rangle = e^{iH_0 t}[iH_0 - i(H_0+\Delta H)] e^{-i(H_0+\Delta H)t} |\Psi(0)\rangle = -i\Delta H(t)|\Psi(t)\rangle$$ therefore

formally $|\Psi(t)\rangle = T_t e^{-i\int_0^t \Delta H(t')dt'} |\Psi(0)\rangle$ i.e., $U(t,0) = T_t\, e^{-i\int_0^t \Delta H(t')dt'}$

Why?

Because of causality the response is after the cause.

$$\frac{\partial}{\partial t} U(t) = -i\Delta H(t)\, U(t)$$

$$U(t) - U(0) = -i\int_0^t \Delta H(t')\, U(t')\, dt'$$ where $U(0)=1$

recursively inverting $U(t)$ back, we get

$$U(t) = 1 - i\int_0^t dt_1\, \Delta H(t_1) + (-i)^2\int_0^t dt_1\, \Delta H(t_1)\int_0^{t_1} dt_2\, \Delta H(t_2) + \cdots = \sum_{m=0}^{\infty} (-i)^m \int_0^t dt_1\, \Delta H(t_1)\int_0^{t_1} dt_2\, \Delta H(t_2)\cdots\int_0^{t_{m-1}} dt_m\, \Delta H(t_m)$$

$$= \sum_{m=0}^{\infty}\frac{(-i)^m}{m!} T_t \int_0^t dt_1\, \Delta H(t_1)\int_0^t dt_2\, \Delta H(t_2)\cdots\int_0^t dt_m\, \Delta H(t_m)$$

$$= T_t\, e^{-i\int_0^t dt_1\, \Delta H(t_1)}$$

Now we say that at $t=-\infty$ there was no external force, but was gradually switched on, so that at time t we have:

$$\langle M(t)\rangle = \frac{1}{Z} Tr\left(e^{-\beta H^0}\, U(-\infty,t)\, M(t)\, U(t,-\infty)\right)$$

where $U(t,-\infty) = T_t\, e^{-i\int_{-\infty}^t dt_1\, \Delta H(t_1)}$

and $M(t) = e^{iH_0 t} M e^{-iH_0 t}$

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$$\langle M(t)\rangle = \frac{1}{Z} Tr\left(e^{-\beta H^0} T_t\, e^{+i\int_{-\infty}^{t} dt_1\, \Delta H(t_1)} M(t)\, e^{-i\int_{-\infty}^{t} dt_2\, \Delta H(t_2)}\right)$$

$$\langle M(t)\rangle \approx \frac{1}{Z} Tr\left(e^{-\beta H_0}\left(1+i\int_{-\infty}^{t} dt_1\, \Delta H(t_1)\right) M(t)\left(1-i\int_{-\infty}^{t} dt_2\, \Delta H(t_2)\right)\right)$$

$$\approx \frac{1}{Z} Tr\left(e^{-\beta H_0}\left(M(t) - i\int_{-\infty}^{t} [M(t), \Delta H(t_1)]\, dt_1\right)\right)$$

$$= \langle M(t)\rangle^0 - i\int_{-\infty}^{\infty} \Theta(t_1<t)\langle [M(t), \Delta H(t_1)]\rangle^0 dt_1 = \langle M(t)\rangle^0 - i\int_{-\infty} dt_1\, h(t_1)\, \Theta(t_1<t)\langle [M(t), M(t_1)]\rangle^0$$

since $\Delta H(t) = M(t)\, h$

$$\langle M(t)\rangle - \langle M(t)\rangle^0 \approx \int_{-\infty}^{\infty} dt_1\, \chi(t,t_1)\, h(t_1)$$

where $\chi(t,t_1) = -i\Theta(t-t_1)\langle [M(t), M(t_1)]\rangle_0$

Conclusion: The measurable response function is the retarded susceptibility:

$\chi_M = \langle\langle M; M\rangle\rangle^R$ i.e., $\chi_M(t,t_1) = -i\Theta(t-t_1)\langle [M(t), M(t_1)]\rangle_0$

It can be obtained from Matsubara $\chi(i\omega) = -\int_0^\beta \langle T_\tau M(\tau) M(0)\rangle e^{i\omega\tau} d\tau$

by analytic continuation $\chi^R(\omega) = \chi(i\omega \to \omega + i\delta)$

Examples: Optical conductivity

$\Delta H = -\vec{A}\cdot\vec{j}$

$\Delta H = \frac{1}{i\omega}\vec{E}\cdot\vec{j}$

from Maxwell in Coulomb gauge ($\vec{\nabla}\cdot\vec{A}=0$ and $\vec{E} = -\frac{\partial \vec{A}}{\partial t}$)

$\vec{E} = -i\omega\vec{A}$

$h = \vec{E}$

$M = -\frac{i}{\omega}\vec{j}$

$$\langle j\rangle = \int_{-\infty}^{t} \sigma(t,t_1)\, \vec{E}(t_1)\, dt_1$$

$$\langle -\tfrac{i}{\omega} j\rangle = \left(-\tfrac{i}{\omega}\right)^2 \langle\langle j; j\rangle\rangle E$$

$$\sigma_{\vec{q}}(\omega) = -i\int_{-\infty}^{t} \Theta(t-t_1)\langle [j(\vec{r},t), j(\vec{r}_1,t_1)]\rangle\, e^{i\omega(t-t_1) - i\vec{q}(\vec{r}-\vec{r}_1)}\, dt_1\, d^3r_1 \left(-\frac{i}{\omega}\right)$$

$$\sigma_q(\omega) = \frac{1}{\omega}\int_0^{\infty} \Theta(t)\langle [j(\vec{r},t), j(0,0)]\rangle\, e^{i\omega t - i\vec{q}\vec{r}}\, dt\, d^3\vec{r}$$

(10)

Example charge response

start with: $\Delta H = -\int V_{ext}(\vec{r})\, M(\vec{r})\, d^3 r$

($V_{ext}(\vec{r})$: associate with h; $M(\vec{r})$: M)

Recall: $\langle M(x_1)\rangle \approx \langle M(x_1)\rangle^0 + \int dt_2\, h(x_2)\, \chi(x_2 x_1)$; $\chi(x_2,x_1) = \langle M(x_2)\rangle^0 \langle M(x_1)\rangle^0 - \langle M(x_2) M(x_1)\rangle^0$

connected correlation function

In this case:

$$M([V_{ext}]\, \vec{r}, \tau) = M([V_{ext}=0], \vec{r}, \tau) - \int V_{ext}(\vec{r}'\tau')\, \chi(\vec{r}'\tau', \vec{r}, \tau) \Rightarrow \delta M(\vec{r},\tau) = -\int V_{ext}(\vec{r}', \tau')\, \chi(\vec{r}'\tau', \vec{r}\tau)$$

with $\chi(\vec{r}'\tau', \vec{r}\tau) = -\langle T_\tau M(\vec{r}'\tau')\, M(\vec{r}\tau)\rangle^0 + \langle M(\vec{r}, \tau)\rangle^0 \langle M(\vec{r},\tau)\rangle^0$

How is this related to dielectric constant? We usually want to express charge response in terms of

$$\delta V_{tot}(x_1) \equiv \int \varepsilon^{-1}(x_1, x_2)\, V_{ext}(x_2)\, dt_2 \qquad \text{(definition)}$$

- δV_{tot}: interaction that charged particle feels
- $\equiv$: definition
- ε^{-1}: screening by dielectric function of the material
- V_{ext}: external potential (electric field)

$$\delta V_{tot}(x_1) = \delta V_{ext}(x_1) + \int V_c(x_1, x_3)\, \delta M(x_3)\, dx_3 = \delta V_{ext} - \int V_c(x_1 x_3)\, \chi(x_3, x_2)\, V_{ext}(x_2)\, dt_2\, dt_3$$

- V_c: bare interaction between electrons $= \frac{1}{|\vec{r}_1 - \vec{r}_2|}$
- $\delta M(x_3)$: electrons rearrange in the solid, and contribute to the potential change

Hence:

$$\delta V_{tot}(x_1) = \int \left[\delta(x_1 - x_2) - \int V_c(x_1 x_3)\, \chi(x_3, x_2)\, dt_3\right] V_{ext}(x_2)\, dt_2$$

Finally using definition (definition) we get:

$$\varepsilon^{-1}(x_1, x_2) = \delta(x_1 - x_2) - \int V(x_1, x_3)\, \chi(x_3, x_2)\, dt_3$$

By Fourier transform: $\varepsilon^{-1}_{q\omega} = 1 - V_q\, \chi_q(\omega)$ where $\chi_q(i\omega) = -\int\int_0^\beta \langle T_\tau M(\vec{r}, \tau) \cdot M(0,0)\rangle\, e^{i\omega\tau - i\vec{q}\cdot\vec{r}}\, d^3r\, d\tau$

Note that from Maxwell relations we also have

$$\varepsilon = \varepsilon_0 + 4\pi i \frac{\sigma(\omega)}{\omega}$$

- ε: dielectric constant
- $\sigma(\omega)$: optical conductivity

(11)

Back to the Single particle Green's function

Very important because:

It is the lowest order correlation function with the simplest analytic structure
It appears as the basic building block of Feynman diagrammatic technique.

$$\langle\langle A; B\rangle\rangle^R = -i\Theta(t_1-t_2)\langle [\overset{\psi}{A}(\vec r_1,t_1), \overset{\psi^\dagger}{B}(\vec r_2,t_2)]_+\rangle$$

$$G^R_{\vec k}(\omega) = \iint_0^\infty dt\,(-i)\langle[\psi(\vec r,t),\psi^\dagger(0,0)]\rangle\, e^{i\omega t - i\vec k\cdot\vec r} d^3r$$

$$G_{\vec k}(i\omega) = \iint_0^\beta d\tau\, e^{i\omega\tau}(-1)\langle T_\tau \psi(\vec r,\tau)\psi^\dagger(0,0)\rangle\, e^{i\omega\tau - i\vec k\cdot\vec r} d^3r$$

We proved $\int G^R_{\vec k}(\omega)\,d\omega = 1$ and $G_{\vec k}(z) = \int \frac{A_{\vec k}(\omega)}{z-\omega}d\omega$ where $A_{\vec k}(\omega) = -\frac{1}{\pi}\mathrm{Im}\,G_{\vec k}(\omega)$
and $A_{\vec k}(\omega)$ is positive spectral function.

Noninteracting system: $\boxed{A_{\vec k}(\omega) = \delta(\omega-\varepsilon_{\vec k})}$ and $\boxed{G^R_{\vec k}(\omega) = \frac{1}{\omega-\varepsilon_{\vec k}+i\delta}}$

From definition $A(\omega) \equiv \sum_{mn}\delta(\omega+E_m-E_n)\langle m|c_{\vec k}|n\rangle\langle n|c^\dagger_{\vec k}|m\rangle\left(\frac{e^{-\beta E_m}}{Z}+\frac{e^{-\beta E_n}}{Z}\right) \to \delta(\omega-\varepsilon_{\vec k})$

$|m\rangle = \prod_{k_i} c^\dagger_{k_i}|0\rangle \qquad E_n = E_m + \varepsilon_{\vec k}$

$|n\rangle = c^\dagger_{\vec k}\prod_{k_i\neq k} c^\dagger_{k_i}|0\rangle \qquad \langle n|c^\dagger_{\vec k}|m\rangle = 1$

(12)

Which quantities can be computed from $G_2(\omega)$?

1) Density $n(\vec r) = \lim_{\substack{\tau\to 0^-\\ \vec r_1 \to \vec r_2 = \vec r}} G(\vec r_1 \tau; \vec r_2 0) \equiv G(\vec r, \vec r; 0^-)$

from definition: $G(\vec r_1 \tau_1, \vec r_2 0) = -\langle T_\tau \psi(\vec r_1 \tau_1)\psi^+(\vec r_2 0)\rangle \Rightarrow \langle \psi^+(r_2, 0)\psi(r_1 0)\rangle$

because $\tau_1 < 0$

2) Density matrix $n(\vec r_1, \vec r_2) = \lim_{\tau\to 0^-} G(\vec r_1 \tau, r_2 0)$

3) Kinetic energy $\langle \hat T\rangle = \lim_{\vec r' \to \vec r} \int \frac{\vec\nabla_{\vec r}^2}{2m} G(\vec r, \vec r'; 0^-)\, d^3r \equiv Tr(h^0 G)$

$$\lim_{\vec r' \to \vec r} \int \frac{\vec\nabla_{\vec r}^2}{2m}\langle \psi^+(\vec r')\psi(\vec r)\rangle = \langle \psi^+(\vec r)\frac{\nabla^2}{2m}\psi(\vec r)\rangle = \langle T\rangle \checkmark$$

4) Potential energy $\langle V_{ee}\rangle = \frac{1}{2}Tr(\Sigma G) \approx \frac{1}{2}Tr((i\omega - h^0)G)$

$\frac{1}{2}Tr((i\omega - h^0)G - 1)$

It should depend on two body density matrix:

$$\langle V_{ee}\rangle = \frac{1}{2}\iint V_c(\vec r - \vec r')\langle \psi^+(\vec r)\psi^+(\vec r')\psi(\vec r')\psi(\vec r)\rangle d^3r\, d^3r'$$

$$\approx \langle n(\vec r)\, n(\vec r')\rangle \neq \langle n(\vec r)\rangle\langle n(\vec r')\rangle$$

$\langle n(\vec r)\rangle\langle n(\vec r')\rangle$ ← needs single particle G.

$n(\vec r)\, n(\vec r')$ needs charge response function χ_c

Trick: Use equation of motion:

$$\frac{\partial}{\partial\tau_1}\hat\psi(\tau_1) = \frac{\partial}{\partial\tau_1}\left(e^{iH\tau_1}\hat\psi\, e^{-iH\tau_1}\right) = [H, \psi(\tau_1)] = -h_0(1)\hat\psi(1) - \int d2\, V(2,1)\hat\psi^+_{(2)}\hat\psi(2)\hat\psi(1)$$

evaluation of commutator:

> Note here we use $\int 1 \equiv \int d^3r_1$ but not $\int 1 = \int d^3r_1 \int d\tau_1$

$$H = \int d1\, \psi_1^+ h_0(1)\psi_1 + \frac{1}{2}\int \psi_1^+\psi_2^+ V(2-1)\psi_2\psi_1\, d1\, d2$$

$$[H, \psi(1)] = \int d2\, h_0(2)[\psi^+(2)\psi(2), \psi(1)] + \frac{1}{2}\int d2\, d3\, V(2,3)[\psi^+(2)\psi^+(3)\psi(3)\psi(2), \psi(1)]$$

$$= -h_0(1)\psi(1) - \int d2\, V(2,1)\psi^+_{(2)}\psi(2)\psi(1)$$

$$\psi^\dagger(1)\frac{\partial}{\partial\tau_1}\psi(1) = -\psi^\dagger(1)h_0(1)\psi(1) - \int d2\, V(2,1)\psi^\dagger(1)\psi^\dagger(2)\psi(2)\psi(1)$$

$$\int d1 \langle \psi^\dagger(1)\left[\frac{\partial}{\partial\tau_1} + h_0(1)\right]\psi(1)\rangle = -2\langle V_{ee}\rangle$$

$$G(1) = -\langle T_\tau \psi(1)\psi^\dagger(0)\rangle$$

$$\lim_{\tau_1\to 0^-}\frac{\partial}{\partial\tau_1}G(1) = \langle\psi^\dagger(0^-)\frac{\partial}{\partial\tau_1}\psi(0)\rangle$$

$$\lim_{\tau_1\to 0^-} G(1) = \langle\psi^\dagger(0^-)\psi(0)\rangle$$

$$\langle V_{ee}\rangle = -\frac{1}{2}\lim_{\tau\to 0^-}\int d1\left(\frac{\partial}{\partial\tau} + h_0\right)G(1) = -\frac{1}{2}\frac{1}{\beta}\sum_{i\omega}\int(-i\omega + h_0)G(\vec{r}_1, i\omega)\,d^3r_1$$

$$G(\vec{r}_1\tau) = \frac{1}{\beta}\sum_{i\omega} e^{-i\omega\tau}G(\vec{r}_1 i\omega)$$

$$\frac{\partial}{\partial\tau}G(\vec{r}_1\tau) = \frac{1}{\beta}\sum_{i\omega}\left[(-i\omega)e^{-i\omega\tau}G(\vec{r}_1 i\omega) + 1\right]$$

need to add proper constant to make it converge at $\tau\to 0$

$$\langle V_{ee}\rangle = \frac{1}{2}\frac{1}{\beta}\sum_{i\omega}\left[\int d^3r\,(i\omega - h_0)G(\vec{r}_1 i\omega) - 1\right]$$

Definition: $\mathrm{Tr}(\hat{O}G) \equiv \frac{1}{\beta}\sum_{i\omega}\int d^3r\,\hat{O}\,G(\vec{r}_1 i\omega)$

We can use Dyson : $G^{-1} = i\omega - h_0 - \Sigma$

$$\langle V_{ee}\rangle = \frac{1}{2}\mathrm{Tr}((G^{-1}+\Sigma)G - 1) = \frac{1}{2}\mathrm{Tr}(\Sigma G)$$

← this converges $G \sim \frac{1}{\omega_n}$, $\Sigma \sim \frac{1}{\omega_n}$

5) Total energy : $\langle T\rangle + \langle V_{ee}\rangle = \mathrm{Tr}((h_0 + \frac{1}{2}\Sigma)G)$

↑ $\frac{1}{2}$ comes from two body interaction

6) Grand canonical partition function

But only if willing to integrate over coupling constant strength.

It contains entropy $S = -k_B T\,\mathrm{Tr}(\hat{\rho}\ln\hat{\rho})$ which measures "disorder"

When density matrix has eigenvalues 1 and 0, there is no entropy. When all eigenvalues are equal (and not 0 or 1) the entropy is maximal.

Can be directly computed by Luttinger-Ward approach (will see later).

(16)

$\hat{H}_\lambda = \hat{H}_0 + \lambda \hat{V}_{ee}$ and λ will be set to unity at the end.

Then

$$\frac{\partial}{\partial \lambda} \ln Z = \frac{\partial}{\partial \lambda} Tr\left(e^{-\beta(H_0+\lambda V_{ee} - \mu N)}\right) = -\frac{\beta}{\lambda}\langle \lambda V_{ee}\rangle_\lambda$$

$$\text{where } \langle \lambda V_{ee}\rangle = \frac{Tr\left(e^{-\beta(H_0+\lambda V_{ee}-\mu N)}\cdot \lambda V_{ee}\right)}{Tr\left(e^{-\beta(H_0+\lambda V_{ee}-\mu N)}\right)}$$

$\Omega = -\frac{1}{\beta}\ln Z$

$$\frac{\partial}{\partial\lambda}\Omega = -\frac{1}{\beta}\frac{\partial}{\partial\lambda}\ln Z = \frac{1}{\lambda}\langle\lambda V_{ee}\rangle_\lambda$$

hence

$$\Omega = \Omega_0 + \int_0^1 \frac{d\lambda}{\lambda}\langle\lambda V_{ee}\rangle_\lambda = \Omega_0 + \frac{1}{2}\int_0^1 \frac{d\lambda}{\lambda} Tr_\lambda(\Sigma_\lambda G_\lambda)$$

↑ interacting system; ↑ non-interacting system; ↑ like slowing turning on interactions. Should work in the absence of phase transitions.

Link to Experiment

$A_k(\omega) = -\frac{1}{\pi} Im\, G_k(\omega)$ is the spectra, which usually assumed to be measured by ARPES.

Conservation of momentum

$$\frac{h\vec{\nu}}{c_{light}} \approx 0 = -\vec{k}_i + (\vec{k}_d + \vec{K})$$

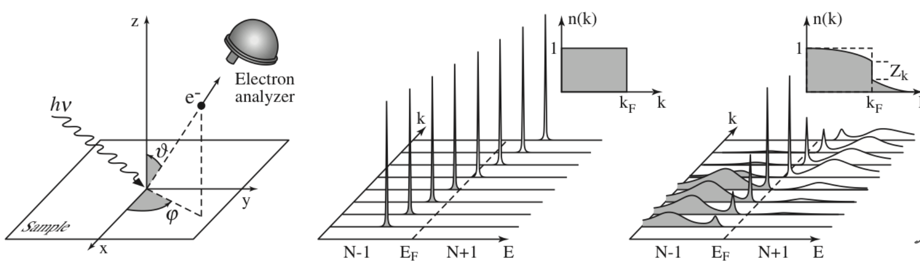
↑ initial in material; ↑ detected; ↖ reciprocal

Conservation of energy

$$h\nu + E_k = \frac{k_d^2}{2m} - \phi$$

$E_k = -|\omega|$

photon energy; detected by detector; work function



Photoemission geometry — Non-interacting electron system — Fermi liquid system

But this is really based on sudden approximation. In reality one needs to add matrix elements because the outgoing electron is plane wave, not just a hole in the solid

$$G_k^R(-\omega) = \iint dt\, i\langle[\psi_k^+(\vec{r},t), \psi(0,0)]\rangle e^{+i\omega t - i\vec{k}\vec{r}}$$

↑ measures negative energies; ↖ create a hole in the material, and see how it propagates.

$$G_k^R(-\omega) = \iint dt\, i\langle[\psi_k^+(t), \psi(0,0)]\rangle e^{i\omega t}$$

↑ into which (k,ω) will hole relax

But here we do not care about outgoing electron: propagating hole described by G → e^- goes to detector

Need to add matrix elements: basis for electrons in the solid $|\langle \varphi_{ik}(\vec{r})| e^{i\vec{k}\vec{r}}\rangle|^2$ — plane waves

(15)

The two particle Green's function

$$G_2(\vec r_1\tau_1, \vec r_2\tau_2, \vec r_2{}'\tau_2{}', \vec r_1{}'\tau_1{}') = -\langle T_\tau\, \psi(\vec r_1\tau_1)\,\psi(\vec r_2\tau_2)\,\psi^+(\vec r_2{}'\tau_2{}')\,\psi^+(\vec r_1{}'\tau_1{}')\rangle$$

Short:

$$G_2(1,2,2',1') = -\langle T_\tau\, \psi(1)\psi(2)\psi^+(2')\psi^+(1')\rangle$$

Can express all other susceptibilities with G_2:

$$\chi_{charge}(1,2) = -\langle T_\tau\, n(1)\, n(2)\rangle = G_2(1,2,2^+,1^+)$$

$$\chi_{spin}(1,2) = -\langle T_\tau\, \vec S(1)\, \vec S(2)\rangle = -\langle T_\tau\, \psi^+_{s_1}(1)\,\vec\sigma_{s_1 s_1'}\,\psi_{s_1'}(1)\,\psi^+_{s_2}(2)\,\vec\sigma_{s_2 s_2'}\,\psi_{s_2'}(2)\rangle$$

$$= \vec\sigma_{11'}\,\vec\sigma_{22'}\, G_2(1,2,2^+,1^+)$$

Retarded Equivalent

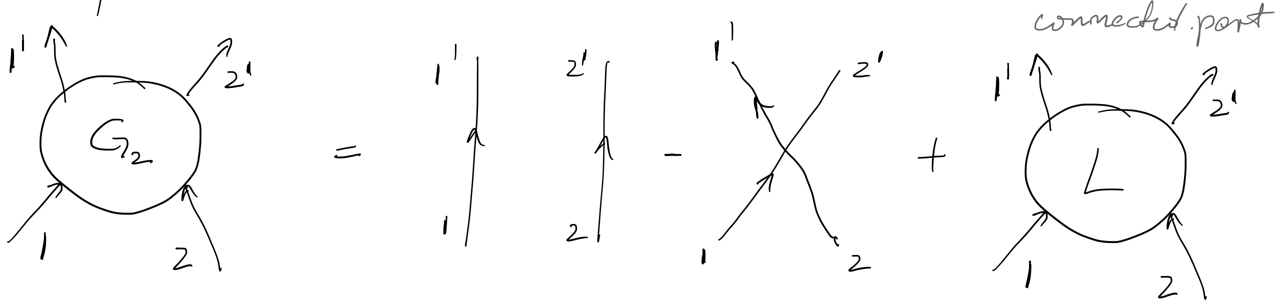
$$G_2^R(\vec r_1 t_1, \vec r_2 t_2, \vec r_2{}' t_2{}', \vec r_1{}' t_1{}')\Big|_{\substack{t_1'=t_1^+\\ t_2'=t_2^+}} = -\Theta(t_1-t_2)\langle \psi^+(\vec r_1{}'\tau_1^+)\psi(\vec r_1\tau_1)\psi^+(\vec r_2{}'\tau_2^+)\psi(\vec r_2\tau_2) - \psi^+(\vec r_2{}'\tau_2^+)\psi(\vec r_2\tau_2)\psi^+(\vec r_1{}'\tau_1^+)\psi(\vec r_1\tau_1)\rangle + 1\leftrightarrow 2$$

The general case is a mess with 12 terms!

Homework:

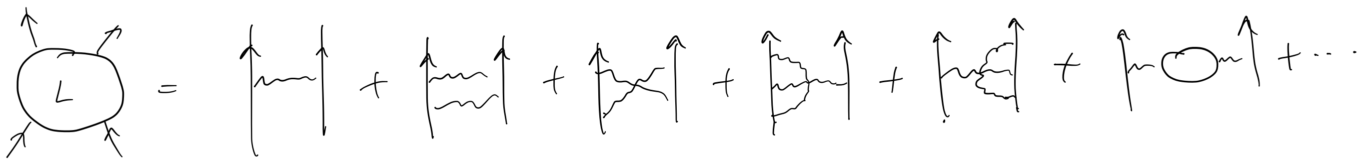
Using Lehman representation show that G_2^R is analytically continued equivalent of G_2

Usually we calculate so-called connected part:



$$G_2(1,2,2',1') = G(1,1')G(2,2') - G(1,2')G(2,1') + L(1,2,2',1')$$

Note: every book seems to define the signs and orders of simple slightly differently.



(R. M. Chapter 6)

Now detour to alternative representation

Correlation functions ⟷ wave function

Some basic properties of the many body W.F.

Most of physical observables can be described by correlation functions. However W.F. carries much more information and is very useful in proving many basic theorems.

If we know the W.F. we can calculate any correlation function.

(Succesfull examples: • Laughlin W.F. for fractional quantum Hall effect
• BCS W.F. for superconductors)

If we know all two particle (and single particle) correlation functions we still can not write down the wave function

How hard is to tabulate the W.F. for N electrons?

3N dimensional function. Assume each dimension requires 100 basis functions then $(100)^{3N}$ complex numbers.

Lets write $\Phi(\vec{r}_1 z_1, \vec{r}_2 z_2, \vec{r}_3 z_3, \dots \vec{r}_N z_N) = \Phi(x_1, x_2, \dots x_N) \equiv \Phi(X)$

Here we will use $(\vec{r}_i, z_i) \equiv x_i$ and $X = \{x_1, x_2, \dots x_N\}$

Below we will list basic properties of the multiparticle wave function.

Properties of multiparticle Φ for fermions

1) Antisymmetry : $\Phi(x_2, x_1, \ldots) = -\Phi(x_1 x_2, \ldots)$
2) Obeys symmetry of the associate space group

- normally group of H, if no broken symmetry.

Operator A: If $[H, A] = 0$ then

$$H\Phi = E\Phi$$ simultaneously eigenfunction of

and $$A\Phi = a\Phi$$ both, a is a good quantum number

3) Continuity: Wave function and all of their derivatives $\left(\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \ldots\right)$ are continuous at all points, except at points of coincidence. These are points where $\vec{r}_i = \vec{r}_j$ (for two electrons) or $\vec{r}_i = \vec{R}_j$ (electron at a nucleous).

4) At points of coincidence, the wave function satisfies the "Cusp condition". (Non-analytic points in space, which cause very slow convergence of most basis sets)

We can fix all points $\vec{r}_3, \vec{r}_4, \ldots \vec{r}_N$ except $\vec{r}_1$ and $\vec{r}_2$. We express the relevant part of the Hamiltonian in terms of in terms of $\vec{r}_1, \vec{r}_2$ and $r_{12} = |\vec{r}_1 - \vec{r}_2|$

After long calculation, one can obtain:

(usual ∇^2 in spherical coordinates)

$$(\vec{\nabla}_1^2 + \vec{\nabla}_2^2) = \left(\frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1}\frac{\partial}{\partial r_1} + \frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2}\frac{\partial}{\partial r_2} + 2\,\hat{r}_1\cdot\hat{r}_{12}\frac{\partial^2}{\partial r_1 \partial r_{12}} + 2\,\hat{r}_2\cdot\hat{r}_{12}\frac{\partial^2}{\partial r_2 \partial r_{12}} + \frac{4}{r_{12}}\frac{\partial}{\partial r_{12}} + 2\frac{\partial^2}{\partial r_{12}^2}\right)$$

= diverges when $r_1 \to 0$

= diverges when $r_{12} \to 0$

$$H = -\frac{1}{2}(\nabla_1^2 + \nabla_2^2) + \frac{e^2}{r_{12}} - \frac{Ze^2}{r_1} - \frac{Ze^2}{r_2} + \ldots$$

$$H = \ldots\ldots \quad -\frac{1}{2}\frac{2}{r_1}\frac{\partial}{\partial r_1} - \frac{Ze^2}{r_1} \quad - \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}} + \frac{e^2}{r_{12}} + \ldots$$

We must have $H\Phi \lneq \infty$ Therefore

$$\frac{1}{r_1}\left(\frac{\partial}{\partial r_1} + Ze^2\right)\Phi = \text{const}$$

$$\frac{1}{r_{12}}\left(\frac{\partial}{\partial r_{12}} - \frac{e^2}{2}\right)\Phi = \text{const}$$

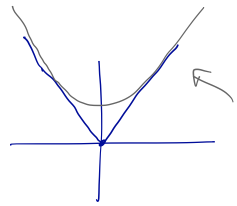
Cusp condition is a) $\frac{\partial \Phi}{\partial r_1} = -Ze^2 \Phi \Big|_{r_1 = R_1}$ $\Rightarrow$ $\Phi(\vec{r}_1, \vec{r}_2 \ldots) \approx e^{-Ze^2|\vec{r}_1 - \vec{R}_1|}\, \Phi(\vec{R}_1, \vec{r}_2 \ldots)$

we set $R_1 = 0$ above

b) $\frac{\partial \Phi}{\partial r_{12}} = \frac{e^2}{2} \Phi \Big|_{r_1 = r_2}$ $\Rightarrow$ $\Phi(\vec{r}_1, \vec{r}_2, \ldots) \approx \frac{e^2}{2}|\vec{r}_1 - \vec{r}_2|\, \Phi(\vec{r}_1, \vec{r}_1, \ldots)$ ← cusp, non-analytic

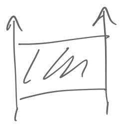
check $\Phi\big|_{r_1 = r_2} \approx \frac{e^2}{2} r_{12} \Phi^0$

$\frac{\partial \Phi}{\partial r_{12}} \approx \frac{e^2}{2} \Phi^0$



← very hard to approximate with any finite basis set.

Also the two particle response function are affected by cusp



$\chi(\vec{r}_1, \vec{r}_2) \equiv \chi(\vec{r}_1 - \vec{r}_2)$ in homogeneous system

$\chi(|\vec{r}_1 - \vec{r}_2|)$ non-analytic in r_{12}.

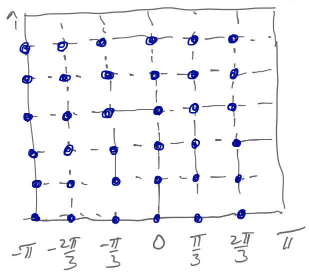
$\chi(q) \sim \frac{1}{q^2} \Rightarrow \chi(r_{12}) \sim \frac{1}{r_{12}}$ very slow fall-off.

5) If no SOC and no B field then Φ can be choosen real. Otherwise Φ is complex. However, complex Φ might have better convergence properties. So called "twisted boundary condition" can make finite system a better approximation for infinite system. It is also crucial if the system has finite polarization ("Modern theory of polarization" is based on the Berry phase)

(19)

Example: uniform electron gas with spherical fermi surface and 6×6 - sites in 2D. The first BZ would look like:

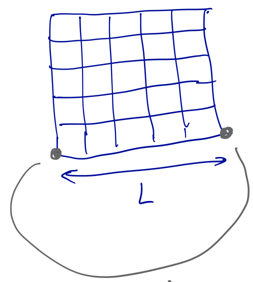
periodic boundary conditions



36 k-points

$$\vec{k} = \left(\frac{M_1}{N_1} 2\pi, \frac{M_2}{N_2} 2\pi\right)$$

real space



differ for phase e^{ik_xL}

periodic boundary conditions

$$\phi(\vec{r}_1 + L\vec{e}_{x}, \vec{r}_2, \dots) = \phi(\vec{r}_1, \vec{r}_2, \dots)$$

twisted boundary condition

$$\phi_{\vec{k}}(\vec{r}_1 + L\vec{e}_x, \vec{r}_2 \dots) = e^{i(k_x L)}\phi(\vec{r}_1, r_2, \dots) \qquad k_xL = \vartheta_x$$

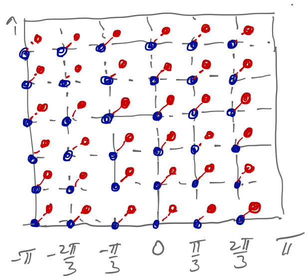
where $\vartheta \in [-\pi, \pi]$ freedom

Condition for periodicity

$$L \cdot k_1 = 2M\pi + \vartheta$$

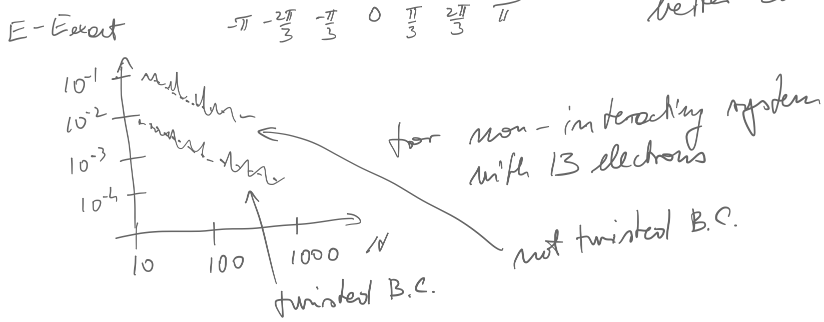
$$L = a \cdot N$$

$$k_1 a = \frac{2M\pi + \vartheta}{N}$$



shifted mesh for $\vartheta_x = \frac{\pi}{2}$ and $\vartheta_y = \frac{\pi}{2}$

Used in electronic structure calculations for better convergence.



(22) There is a more important property associated with the twisted phase. It can distinguish metals from insulators.

Kohn proposed: a) In insulators the energy is independent of the twist (because electrons are localized)

We can define the "center of mass" $\langle R_{cm} \rangle$ which is well defined, and gives polarization of the system.

$$\langle R_{cm}^2 \rangle - \langle R_{cm} \rangle^2 < \infty$$

b) In metals the energy increases with the twist

$E_t = 2 D V^{1/3} \cdot \vartheta$ where D is the Drude weight.

and $\langle R_{cm} \rangle$ is not well defined so that

$\langle R_{cm}^2 \rangle - \langle R_{cm} \rangle^2 = \infty$ and the system has net velocity.

The center of mass is proportional to polarization of the system, and is given by the Berry phase. It was first derived by David Vanderbilt in his "modern theory of polarization."

$$\langle \Delta R_{cm}^{\alpha} \rangle = \frac{2 V_{cell}}{(2\pi)^3} \int d^3 k \, \mathrm{Im} \left\{ \langle u_k^f | \frac{\partial}{\partial k_\alpha} | u_k^f \rangle - \langle u_k^i | \frac{\partial}{\partial k_\alpha} u_k^i \rangle \right\}$$

$\alpha = x, y, z$; f = final, i = initial

Here $u_k(\vec{r}_1, \vec{r}_2, \ldots) = e^{-i \sum_j \vec{k} \vec{r}_j} \phi(\vec{r}_1, \vec{r}_2, \ldots)$ (phase factor; eigenstate of H)

in complete analogy with non-interacting system, where $\psi_k(\vec{r}) = e^{-i \vec{k} \vec{r}} u_k(\vec{r})$ with $u(\vec{r})$ periodic in V_{cell}

with $u_k(\vec{r}_1, \vec{r}_2, \ldots)$ periodic in V_{cell}.

$$\langle (\Delta R_{cm}^{\alpha})^2 \rangle = \frac{V_{cell}}{(2\pi)^3} \int d^3 k \, \mathrm{Re} \left\{ \langle \frac{\partial}{\partial k_\alpha} u_k | \frac{\partial}{\partial k_\alpha} u_k \rangle - \langle u_k | \frac{\partial}{\partial k_\alpha} u_k \rangle \langle \frac{\partial}{\partial k_\alpha} u_k | u_k \rangle \right\}$$

(21) # Modern theory of polarization (MTP) David's book

All equations are going to be derived for non-interacting Hamiltonian $H\psi_\mathbf{k} = \varepsilon_\mathbf{k}\psi_\mathbf{k}$, where $\langle \vec{r}|\psi_\mathbf{k}\rangle = \psi_\mathbf{k}(\vec{r})$ is wave function for a single particle.

All final equations translate to multy particle system with "trivial" modifications, like $u_\mathbf{k}(\vec{r}_1) \Rightarrow u_\mathbf{k}(\vec{r}_1, \vec{r}_2, \ldots \vec{r}_N)$.

However, the MTP is defined only through the wave function and its phase, i.e., Berry phase. No formulation of polarization in terms of response functions exists. Knowing $G(\vec{r}_1, \vec{r}_2)$ seems not sufficient. Probably $\chi(\vec{r}_1, \vec{r}_2, \vec{r}_3, \vec{r}_4)$ not enough either? Open problem!

Short intro to problems in defining polarization

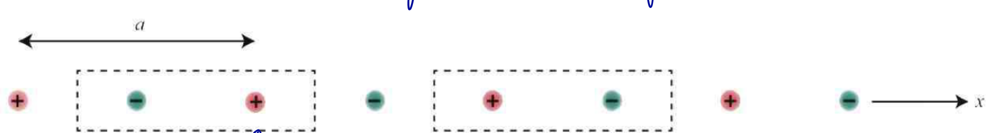
Naive expectation: $P_{NV} = \frac{1}{V_{cell}} \int_{cell} d^3r\, \vec{r}\rho(\vec{r})$

Misserably fails:
1) Answer depends on the choice of the unit cell.
2) For solids it is diverging

1) Non-uniqueness of polarization.

Consider NaCl 1D analog but with completely localized charges.

For completely localized charges we can use P_{NV}.



↑ unit cell ↑ $\frac{a}{4}$ $\frac{3a}{4}$ ↑ $\frac{a}{4}$ ↑ $\frac{3a}{4}$

$P = \frac{e}{V_{cell}}\left(-\frac{a}{4} + \frac{3a}{4}\right) = \frac{e}{V_{cell}} \cdot \frac{a}{2}$ | $P = \frac{e}{V_{cell}}\left(\frac{a}{4} - \frac{3a}{4}\right) = \frac{e}{V_{cell}}\left(-\frac{a}{2}\right)$

Which one is correct? It turns out P is defined up to $P \pm \frac{ea}{V_{cell}}$.

Given a system, we can not define it more precisely than up to $\pm\frac{ea}{V_{cell}}$. David calls such quantity "lattice valued vector", which can take values

$$P = \left(p_0 - \frac{Mea}{V_{cell}}, p_0 - \frac{(M-1)ea}{V_{cell}}, \ldots, p_0, p_0 + \frac{Mea}{V_{cell}}, \ldots\right)$$

$M \to \infty$

This is not a problem, because in experiment we always care about the change of polarization and not the absolute value.

The change $\frac{dP}{dt} = \vec{J}$ is current that flows through a unit cell

Imagine we take our original system of charges and transport one unit of charge from atom $1 \to 2 \to 3 \to \cdots$

after that operation, the charges of the system are the same, hence the same polarization. But we transported an entire quant of polarization, hence large current. Polarization actually changed from

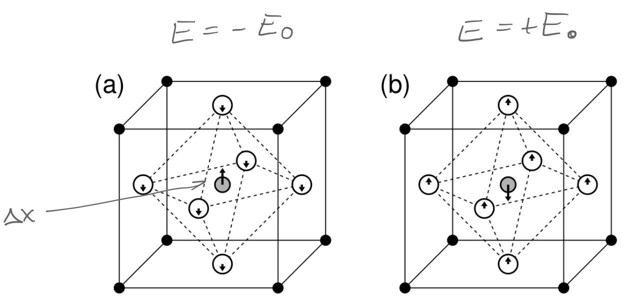
$$P_1 = \left(p_0 - \frac{Mea}{V_{cell}},\ p_0 - \frac{(M-1)ea}{V_{cell}},\ \cdots,\ p_0,\ p_0 + \frac{Mea}{V_{cell}}\right) \cdots \qquad M \to \infty$$

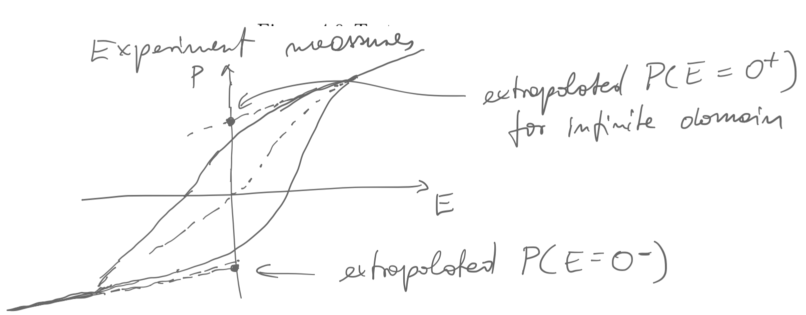
to

$$P_2 = \left(p_0 + \frac{ea}{V_{cell}} - \frac{Mea}{V_{cell}},\ p_0 + \frac{ea}{V_{cell}} - \frac{(M-1)ea}{V_{cell}},\ \cdots\right) \qquad M \to \infty$$

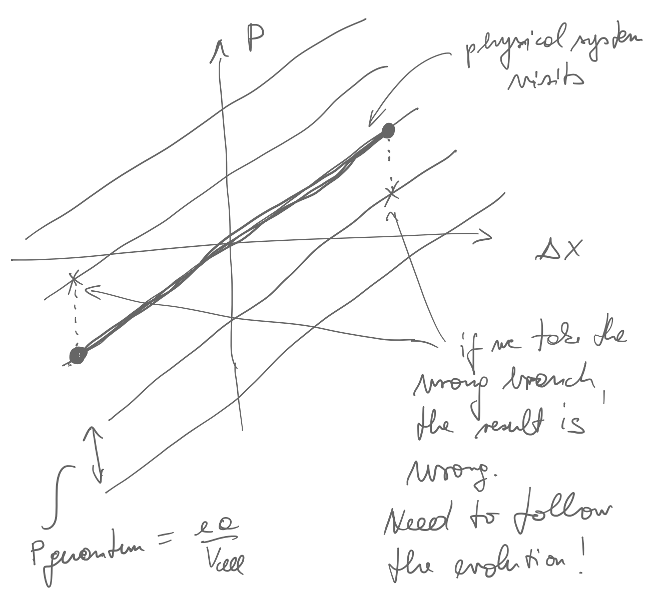
but $P_1 = P_2$ hence we see no change of the system.

Hence to calculate polarization, we need to follow the evolution of the system with external field

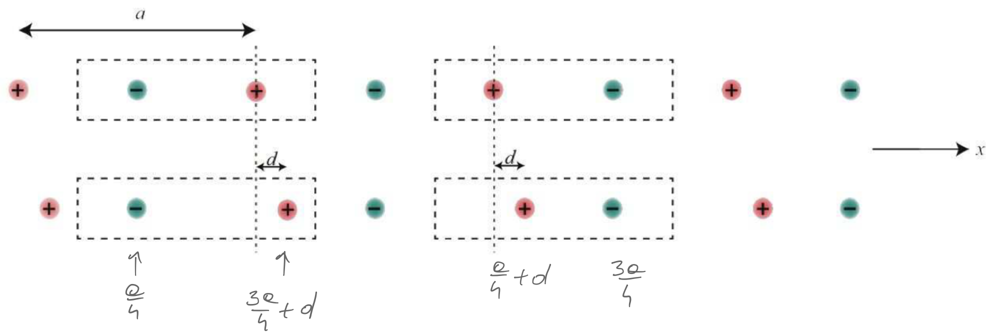




Theoretical calculation should give



Now we know that the charge with displacement should be measurable.
Let's calculate it



$$P_2 = \frac{e}{V_{cell}}\left(-\frac{a}{4} + \frac{3a}{4} + d\right) \qquad P_2 = \frac{e}{V_{cell}}\left(\frac{a}{4} + d - \frac{3a}{4}\right)$$

$$= P_1 + \frac{e}{V_{cell}} \cdot d \qquad P_2 = P_1 + \frac{e}{V_{cell}} \cdot d$$

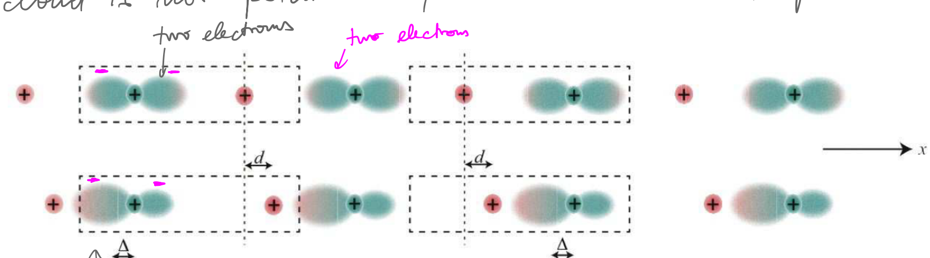
$P_2 - P_1 = \frac{e}{V_{cell}} \cdot d$ as expected and is unique.

Why is P not zero when there is no displacement?
If the system has inversion symmetry, then P has to commute with inversion

$$I \cdot P = P$$

If $P = \frac{ea}{V_{cell}}\left(-M, -M+1, \ldots, -1, 0, 1, \ldots, M-1, M\right)$ $\lim M \to \infty$
then $I \cdot P = P$
If $P = \frac{ea}{V_{cell}}\left(-M+\frac{1}{2}, -M+\frac{3}{2}, \ldots -\frac{3}{2}, -\frac{1}{2}, \frac{1}{2}, \frac{3}{2}, \ldots M-\frac{3}{2}, M-\frac{1}{2}\right)$ $\lim M \to \infty$
then $I \cdot P = P$
These are the only two possibilities. Either integer or half-integer quantum.

More realistic system would look like that Fig below, because electronic cloud is not point-like, but it moves and spreads.



Wannier function with center at $\frac{a}{4} - \Delta$.

It turns out that the details of the Wannier function do not matter. Only it's center of mass plays the role of displacement.
If we calculate $\langle r \rangle_W = \int dx\, W^*(x)\, x\, W(x) = \frac{a}{4} - \Delta$

Then: $P_2 = \frac{e}{V_{cell}}\left(\frac{a}{4} - 2\left(\frac{a}{4} - \Delta\right) + \frac{3a}{4} + d\right) = P_1 + \frac{e}{V_{cell}}\left(d + 2\Delta\right)$

extra charge due to movement of Wannier functions.

What if we do not want to construct Wannier functions. Can we compute P?

Yes, there is formula in terms of Bloch states, which can be used:

$$\langle \vec{r} \rangle = \sum_{m \in band} \int d^3r\, W_m(\vec{r}) \cdot \vec{r}\, W_m(\vec{r}) = \frac{V_{cell}}{(2\pi)^3} \sum_{m=band} \int d^3k \left\langle u_{mk} \middle| i \frac{\partial u_{mk}}{\partial \vec{k}} \right\rangle \qquad (1)$$

$$\psi_{mk}(\vec{r}) = e^{i\vec{k}\vec{r}} u_{mk}(\vec{r})$$

(ψ_{mk}: Bloch w.f., solution of S.E.; u_{mk}: periodic part, $u_{mk}(\vec{r}+\vec{R}) = u_{mk}(\vec{r})$)

We will first prove this identity (1), and later introduce more rigorously the polarization operator in Q.M. formulation.

Proof of (1):

Wannier functions for an isolated band $W_m(\vec{r}-\vec{R}) = \frac{V_{cell}}{(2\pi)^3} \int_{BZ} d^3k\, e^{-i\vec{k}\cdot\vec{R}} \psi_{mk}(\vec{r})$

Note also that
$$\int_{BZ} d^3k\, e^{i\vec{k}(\vec{R}-\vec{R}')} = \delta_{\vec{R},\vec{R}'} \frac{(2\pi)^3}{V_{cell}}$$
(reciprocal)
$$\sum_{\vec{R}} e^{-i(\vec{k}-\vec{k}')\vec{R}} = \delta^3(\vec{k}-\vec{k}') \frac{(2\pi)^3}{V_{cell}}$$
(reciprocal)

Let's check

- $$\langle u_{m\vec{k}} | u_{m\,\vec{k}+\vec{b}} \rangle = \int_{cell} d^3r \langle u_{m\vec{k}} | \vec{r} \rangle \langle \vec{r} | u_{m\,\vec{k}+\vec{b}} \rangle = \int_{cell} d^3r \left(\psi_{mk}(\vec{r}) e^{-i\vec{k}\vec{r}}\right)^* \left(\psi_{m\,\vec{k}+\vec{b}}\, e^{-i(\vec{k}+\vec{b})\vec{r}}\right)$$
$$= \int_{cell} d^3r\, e^{-i\vec{b}\cdot\vec{r}} \psi^*_{mk}(\vec{r}) \psi_{mk}(\vec{r})$$

- $$W_m(\vec{r}-\vec{R}) = \frac{V_{cell}}{(2\pi)^3} \int_{BZ} d^3k\, e^{-i\vec{k}\cdot\vec{R}} \psi_{mk}(\vec{r}) \Rightarrow \sum_{\vec{R}} W_m(\vec{r}-\vec{R}) e^{i\vec{k}\vec{R}} = \psi_{mk}(\vec{r})$$

- $$\langle u_{m\vec{k}} | u_{m\,\vec{k}+\vec{b}} \rangle = \int_{cell} d^3r\, e^{-i\vec{b}\cdot\vec{r}} \sum_{\vec{R},\vec{R}'} \underbrace{e^{-i\vec{k}\vec{R}} W^*_m(\vec{r}-\vec{R})\, e^{i\vec{k}\vec{R}'} W_m(\vec{r}-\vec{R}')}_{\text{depends only on } \vec{R}'-\vec{R}}$$
hence we can set $\vec{R}'=0$ and cancel $\frac{1}{N}$.
$$= \int_{cell} d^3r\, e^{-i\vec{b}\cdot\vec{r}} \sum_{\vec{R}} e^{-i\vec{k}\vec{R}} W^*_m(\vec{r}-\vec{R}) W_m(\vec{r}) = \sum_{\vec{R}} e^{-i\vec{k}\cdot\vec{R}} \underbrace{\int_{cell} d^3r\, W^*_m(\vec{r}-\vec{R}) e^{-i\vec{b}\cdot\vec{r}} W_m(\vec{r})}_{\langle W_m(\vec{R}) | e^{-i\vec{b}\vec{r}} | W_m(0) \rangle}$$

- expand both sides for small $\vec{b}$:

$$\left\langle u_{m\vec{k}} \middle| u_{m\vec{k}} + \vec{b}\cdot\frac{\partial}{\partial \vec{k}} u_{m\vec{k}} + \frac{1}{2}\left(\vec{b}\cdot\frac{\partial^2}{\partial \vec{k}^2}\right) u_{mk} + \ldots \right\rangle = \sum_{\vec{R}} e^{-i\vec{k}\cdot\vec{R}} \langle W_m(\vec{R}) | 1 - i\vec{b}\cdot\vec{r} - \frac{1}{2}(\vec{b}\cdot\vec{r})^2 + \ldots | W_m(0) \rangle$$

Previous equation is valid for any $\vec{b}$, hence

$$\langle u_{n\vec{k}} | u_{n\vec{k}} \rangle = \sum_{\vec{R}} e^{-i\vec{k}\cdot\vec{R}} \langle W_n(\vec{R}) | W_n(0) \rangle = 1$$

$$i \langle u_{n\vec{k}} | \frac{\partial}{\partial \vec{k}} u_{n\vec{k}} \rangle = \sum_{\vec{R}} e^{-i\vec{k}\cdot\vec{R}} \langle W_n(\vec{R}) | \vec{r} | W_n(0) \rangle \Rightarrow \frac{V_{cell}}{(2\pi)^3} \int e^{i\vec{k}\cdot\vec{R}} \langle u_{n\vec{k}} | i \frac{\partial}{\partial \vec{k}} u_{n\vec{k}} \rangle d^3k = \langle W_n(\vec{R}) | \vec{r} | W_n(0) \rangle$$

$$-\langle u_{n\vec{k}} | \frac{\partial^2}{\partial \vec{k}^2} | u_{n\vec{k}} \rangle = \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \langle W_n(\vec{R}) | r^2 | W_n(0) \rangle \Rightarrow -\frac{V_{cell}}{(2\pi)^3} \int e^{i\vec{k}\cdot\vec{R}} \langle u_{n\vec{k}} | \frac{\partial^2}{\partial \vec{k}^2} u_{n\vec{k}} \rangle d^3k = \langle W_n(\vec{R}) | r^2 | W_n(0) \rangle$$

Finally for the home cell $\bar{r} = \langle W_n(R=0) | \vec{r} | W_n(R=0) \rangle = \frac{V_{cell}}{(2\pi)^3} \int d^3k \langle u_{n\vec{k}} | i \frac{\partial}{\partial \vec{k}} u_{n\vec{k}} \rangle$ as promised.

This is well defined only for insulators

$$\overline{r^2} = \langle W_n(0) | r^2 | W_n(0) \rangle = \frac{V_{cell}}{(2\pi)^3} \int d^3k \langle u_{nk} | -\frac{\partial^2}{\partial k^2} | u_{nk} \rangle$$

Fluctuations of the Wannier centers.

We have a recipy to compute P, and we know that only ΔP makes sense, which is:

$$\langle r \rangle_{final} - \langle r \rangle_{initial} = \frac{V_{cell}}{(2\pi)^3} \int d^3k \left[\langle u^f_{n\vec{k}} | i \frac{\partial}{\partial \vec{k}} u^f_{n\vec{k}} \rangle - \langle u^i_{n\vec{k}} | i \frac{\partial}{\partial \vec{k}} u^i_{n\vec{k}} \rangle \right]$$

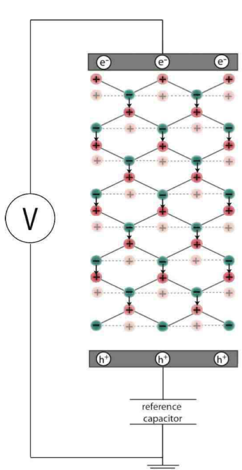
But we do not have real understanding of why P is not uniquely defined and how is this connected to the Berry phase.

How this follows from general laws of Q.M.?

Back to the question of why P is not a simple correlation function.

We expect: $P_W = \frac{1}{V_{cell}} \int_{cell} d^3r \, \vec{r} \rho(\vec{r})$ and for

current we know: $\vec{J}(t) = \frac{1}{V_{cell}} \int_{cell} d^3r \, j(\vec{r}, t)$ where we have in mind slow adiabatic change with time, so that we are always in quasi equilibrium.



When we slowly turn on voltage, the positive ions slowly move to new positions, which allows the current to flow.

Then: $\delta P = J\,\delta t$ should be obeyed

$$\delta P(t) = \frac{1}{V_{cell}} \int d^3r\, \vec{r}\, \frac{\delta \rho}{\delta t}\, \delta t$$

$$= -\frac{1}{V_{cell}} \int d^3r\, \vec{r}\,(\vec{\nabla}\cdot\vec{j})\, \delta t$$

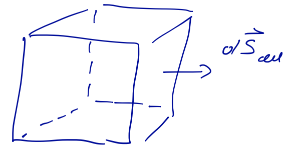
continuity $\frac{\delta \rho}{\delta t} = -\vec{\nabla}\cdot\vec{j}$

local charge conservation in a unit cell.

$$\vec{\nabla}(\vec{r}\cdot\vec{j}) = \vec{j} + \vec{r}\cdot(\vec{\nabla}\cdot\vec{j})$$

$$\int_{V_{cell}} d^3r\, \vec{\nabla}(\vec{r}\cdot\vec{j}) = \int_{V_{cell}} d^3r\, \vec{j} + \int_{V_{cell}} d^3r\, \vec{r}\cdot(\vec{\nabla}\cdot\vec{j})$$

$$\int_{S_{cell}} \vec{r}\,(\vec{j}\cdot d\vec{S}) = \int_{V_{cell}} d^3r\, \vec{j} + \int_{V_{cell}} d^3r\, \vec{r}\cdot(\vec{\nabla}\cdot\vec{j})$$



$$\int \vec{\nabla} f\, d^3r = \int_{\partial V} f \cdot d\vec{S}$$

$$\delta P(t) = -\frac{1}{V_{cell}} \int_{S_{cell}} \vec{r}\,(\vec{j}\cdot d\vec{S})\,\delta t + \frac{1}{V_{cell}} \int d^3r\, \vec{j}\, \delta t$$

(surface term:) non-zero during adiabatic evolution, because current flows through the sample ($\int_{S_{cell}} \vec{j}\cdot d\vec{S} = 0$ but $\int \vec{r}\,(\vec{j}\cdot d\vec{S})$ is not)

(second term:) The true current we observe in experiment

But we need to have $\frac{\delta P}{\delta t} = \frac{1}{V_{cell}} \int d^3r\, \vec{j} = \frac{I}{V_{cell}}$ for E.M. to be valid.

The culprint is the P formula with ill defined $\vec{r}$ in the equation that grows and diverges, is not cell periodic.

In treating isolated molecules, where boundary is insulating, we can use $P = \int d^3r\, \vec{r}\, \rho(\vec{r})$ because the surface term vanishes. But in solids it would have the form $P = \sum_{i \in occupied} \int d^3r\, \vec{r}\, |\psi_{ik}(\vec{r})|^2 = \sum_{i \in occupied} \langle \psi_{ik} | \vec{r} | \psi_{ik} \rangle$ which is ill defined for infinite solid.

Conclusion: We need to start from observable we know how to handle, the current $\vec{j}$ and derive $\vec{P}$ to satisfy $I = \frac{dP}{dt}$

$$\vec{j} = \frac{d\vec{P}}{dt} = \frac{d\vec{P}}{d\lambda}\frac{d\lambda}{dt} = \dot\lambda \frac{d\vec P}{d\lambda} = \dot\lambda \frac{e}{V_{cell}} \frac{d\langle \vec r\rangle}{d\lambda}$$

Need $\frac{d\langle\vec r\rangle}{d\lambda}$!

$$\hat{\vec v} = \frac{d}{dt} e^{iHt}\hat{\vec r} e^{-iHt} = i[H,\hat{\vec r}]$$

Heisenberg operators

$$\langle \psi_{n\vec k}|\vec v|\psi_{m\vec k}\rangle = i\left(\langle\psi_{n\vec k}|H\vec r|\psi_{m\vec k}\rangle - \langle \psi_{n\vec k}|\vec r H|\psi_{m\vec k}\rangle\right)$$
$$= i(E_n - E_m)\langle\psi_{n\vec k}|\vec r|\psi_{m\vec k}\rangle$$

(note $E_n = E_n(\vec k)$)

Hence: $$\langle\psi_{n\vec k}|\vec r|\psi_{m\vec k}\rangle = -i \frac{\langle\psi_{n\vec k}|\vec v|\psi_{m\vec k}\rangle}{E_n-E_m}$$ valid for $m\neq n$

well defined object because $\vec v = \frac{\vec P}{m} = -\frac{i}{m}\frac{\partial}{\partial \vec r}$

Use Bloch's theorem $\psi_{n\vec k}(\vec r) = e^{i\vec k\vec r} u_{n\vec k}(\vec r)$ where $u_{n\vec k}$ is cell periodic. Then

$$\langle\psi_{n\vec k}|\vec v|\psi_{m\vec k}\rangle = \int d^3r\, u^*_{n\vec k}(\vec r)\, \underbrace{e^{-i\vec k\vec r}\,\vec v\, e^{i\vec k\vec r}}_{\equiv\, \vec v_{\vec k}}\, u_{m\vec k}(\vec r)$$

$\vec v_{\vec k}$ because it is now cell periodic; also cell periodic

Idea: Replace $\vec v_{\vec k}$ by $\frac{\partial H_{\vec k}}{\partial \vec k}$.

Check: $$\frac{\partial}{\partial\vec k}\left(e^{-i\vec k\vec r}He^{i\vec k\vec r}\right) = -i\, e^{-i\vec k\cdot\vec r}(\vec r H - H\vec r)e^{i\vec k\cdot\vec r} = i\, e^{-i\vec k\vec r}[H,\vec r]e^{i\vec k\vec r} = e^{-i\vec k\cdot\vec r}\,\vec v\, e^{i\vec k\vec r}$$

There is no term $\frac{\partial H}{\partial \vec k}$ because in this representation $H = \sum_i \frac{(i\nabla_i)^2}{2m} + \sum_i V_{ext}(\vec r_i) + \sum_j V_c(\vec r_i - \vec r_j)$

Note that $e^{-i\vec k\vec r}He^{i\vec k\vec r}$ is cell periodic, because

therefore: $$\langle\psi_{n\vec k}|\vec v|\psi_{m\vec k}\rangle = \int d^3r\, u^*_{n\vec k}(\vec r)\frac{\partial}{\partial\vec k}\left(e^{-i\vec k\vec r}He^{i\vec k\vec r}\right)u_{m\vec k}(\vec r) = \langle u_{n\vec k}|\frac{\partial}{\partial \vec k}\left(e^{-i\vec k\vec r}He^{i\vec k\vec r}\right)|u_{m\vec k}\rangle$$

$$\langle\psi_{n\vec k}|\vec r|\psi_{m\vec k}\rangle = -i\frac{1}{E_n-E_m}\langle u_{n\vec k}|\frac{\partial}{\partial \vec k}\big(\underbrace{e^{-i\vec k\vec r}He^{i\vec k\vec r}}_{H_{\vec k}}\big)|u_{m\vec k}\rangle \qquad m\neq n$$

Note $H_{\vec k}|u_{n\vec k}\rangle = \varepsilon_{\vec k}|u_{n\vec k}\rangle$

For polarization $P = \frac{e}{V_{cell}}\langle\vec r\rangle$ we would need $\langle\psi_{n\vec k}|\vec r|\psi_{n\vec k}\rangle$ which we do not have. However, for the change of P ($\frac{dP}{d\lambda}$) only off-diagonal matrix elements contribute, and we can definitely compute $\frac{dP}{d\lambda}$ due to movement of atoms. To do that, we need to repeat perturbation theory, i.e., how to compute the change of the W.F. under adiabatic change: $\frac{\partial}{\partial\lambda}|n(\lambda)\rangle$

Linear response through ordinary perturbation theory

We have a variable λ, which changes the system adiabatically
(like electric field moves atoms in the unit cell, or momentum changes $u_{n\vec{k}}$)

How do eigenstates change as a function of λ?

$|n(\lambda)\rangle$ eigenstates for current value of λ

$$H(\lambda)\,|n(\lambda)\rangle = E_n(\lambda)\,|n(\lambda)\rangle$$

depend on λ smoothly

Examples:
- $H_{\vec{k}}|u_{n\vec{k}}\rangle = \varepsilon_{\vec{k}}|u_{n\vec{k}}\rangle$ smooth dependence on $\vec{k}$ required!
- $H(\lambda)|u_{n\vec{k}}(\lambda)\rangle = \varepsilon_{\vec{k}}(\lambda)|u_{n\vec{k}}(\lambda)\rangle$ smooth dependence on λ.

First order derivative:

$$\frac{\partial H}{\partial \lambda}|n\rangle + H\left|\frac{\partial n}{\partial \lambda}\right\rangle = \frac{\partial E_n}{\partial \lambda}|n\rangle + E_n\left|\frac{\partial n}{\partial \lambda}\right\rangle$$

$$\frac{\partial E_n}{\partial \lambda} = \frac{\partial}{\partial \lambda}\langle n|H|n\rangle = \langle n|\frac{\partial H}{\partial \lambda}|n\rangle + \underbrace{\left\langle\frac{\partial n}{\partial \lambda}\right|H|n\rangle + \langle n|H\left|\frac{\partial n}{\partial \lambda}\right\rangle}$$

$E_n\frac{\partial}{\partial \lambda}\langle n|n\rangle = 0$ because states are kept normalized!

$$(E_n - H)\left|\frac{\partial n}{\partial \lambda}\right\rangle = \left(\frac{\partial H}{\partial \lambda} - \langle n|\frac{\partial H}{\partial \lambda}|n\rangle\right)|n\rangle$$

$$\sum_m \underbrace{|m\rangle\langle m|}_{= I}\frac{\partial H}{\partial \lambda}|n\rangle - |n\rangle\langle n|\frac{\partial H}{\partial \lambda}|n\rangle$$

$$\boxed{(E_n - H)\left|\frac{\partial n}{\partial \lambda}\right\rangle = \sum_{m\neq n}|m\rangle\langle m|\frac{\partial H}{\partial \lambda}|n\rangle} \qquad (1)$$

if $m \neq n$ then:

$$\left|\frac{\partial n}{\partial \lambda}\right\rangle = (E_n - H)^{-1}\sum_{m\neq n}|m\rangle\langle m|\frac{\partial H}{\partial \lambda}|n\rangle = \sum_{m\neq n}\frac{1}{E_n - E_m}|m\rangle\langle m|\frac{\partial H}{\partial \lambda}|n\rangle$$

covers Hilbert space orthogonal to $|n\rangle$

but there must be a term also in the direction of $|n\rangle$.
It is an arbitrary value, here designated by iA_n

$$\boxed{\left|\frac{\partial n}{\partial \lambda}\right\rangle = -iA_n|n\rangle + \sum_{m\neq n}\frac{1}{E_n - E_m}|m\rangle\langle m|\frac{\partial H}{\partial \lambda}|n\rangle} \qquad (2)$$

We can check the correctness by plugging it back to Eq (1).

(29) check: $(E_n - H)\left[-iA_n|n\rangle + \sum_{m\neq n} \frac{1}{E_n-E_m} |m\rangle\langle m|\frac{\partial H}{\partial x}|n\rangle\right] \stackrel{?}{=} \sum_{m\neq n} |m\rangle\langle m|\frac{\partial H}{\partial \lambda}|n\rangle$

$$-i(E_n-E_n)A_n|n\rangle + \sum_{m\neq n} \frac{E_n-E_m}{E_n-E_m} |m\rangle\langle m|\frac{\partial H}{\partial x}|n\rangle$$

$\parallel$ 0

$$\sum_{m\neq n} |m\rangle\langle m|\frac{\partial H}{\partial x}|n\rangle = \checkmark$$

Recall:
$$\boxed{|\frac{\partial n}{\partial x}\rangle = -iA_n|n\rangle + \sum_{m\neq n}\frac{1}{E_n-E_m}|m\rangle\langle m|\frac{\partial H}{\partial x}|n\rangle} \quad (2)$$

check that if H does not depend on x we get:

$$|\frac{\partial n}{\partial x}\rangle = -iA_n|n\rangle \implies |n(\lambda)\rangle = e^{-iA_n\lambda}|n(0)\rangle$$

When H does not depend on x, we do not expect eigenfunctions to change, hence $A_n \in$ Real, change of "irrelevant" phase. Most often this term is dropped because of "irrelevant phase"!

But note that this is a Berry phase, because multiplying by $\langle n|$ we get:

$$\langle n|\frac{\partial n}{\partial x}\rangle = -iA_n$$

For now we will avoid this term, and write:

$$\boxed{\hat{Q}_n|\frac{\partial n}{\partial x}\rangle = \sum_{m\neq n}\frac{1}{E_n-E_m}|m\rangle\langle m|\frac{\partial H}{\partial \lambda}|n\rangle} \quad (3)$$

where $\hat{Q}_n = 1 - |n\rangle\langle n|$ is projector to the rest of the Hilbert space.

How do observables change with λ? $\langle n|O|n\rangle$?
We have in mind an operator O that does not depend on λ explicitely: (like $\vec{r}, \vec{p}, \cdots$)

The positions of nuclei change $R_i(t)$, but $\vec{p} = -i\vec{\nabla}$ does not change it's form.

H is changing because it depends on nuclei $R(t)$.

$$\frac{\partial}{\partial x}\langle n|O|n\rangle = \langle\frac{\partial n}{\partial x}|O|n\rangle + \langle n|O|\frac{\partial n}{\partial x}\rangle$$

$\hat{O}$ hermitian, then $\langle\frac{\partial n}{\partial x}|O|n\rangle^* = \langle n|O^+|\frac{\partial n}{\partial x}\rangle = \langle n|O|\frac{\partial n}{\partial x}\rangle$

and
$$\frac{\partial}{\partial \lambda}\langle n|O|n\rangle = 2\,\mathrm{Re}\left(\langle\frac{\partial n}{\partial \lambda}|O|n\rangle\right)$$

(30) We can also insert identity I

$$2\,\mathrm{Re}\left(\langle \tfrac{\partial m}{\partial\lambda} | I\, O | m\rangle\right) = 2\,\mathrm{Re}\Big(\sum_{n\neq m} \langle \tfrac{\partial m}{\partial\lambda} | n\rangle\langle n|O|m\rangle + \underbrace{\langle \tfrac{\partial m}{\partial\lambda} | m\rangle}_{i A_m}\underbrace{\langle m|O|m\rangle}_{\in \text{Real}}\Big)$$

$i A_m \in \mathrm{Im}$ — Im can be dropped

We get:

$$\boxed{\frac{\partial}{\partial\lambda}\langle m|O|m\rangle = 2\,\mathrm{Re}\left(\langle \tfrac{\partial m}{\partial\lambda} | Q_m\, O | m\rangle\right)} \qquad (4)$$

Next if $|m\rangle$ is an occupied state, we want to replace Q_m by more convenient

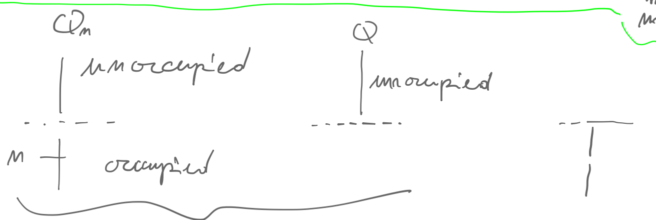
$$Q = \sum_{n\in \text{unoccupied}} |n\rangle\langle n| = 1 - \sum_{n\in\text{occupied}} |n\rangle\langle n|$$

which is independent of m.

$$\boxed{\sum_{m\in occ} \frac{\partial}{\partial\lambda}\langle m|O|m\rangle = \sum_{m\in occ} 2\,\mathrm{Re}\left(\langle \tfrac{\partial m}{\partial\lambda} | Q\, O | m\rangle\right)} \qquad (5)$$

We will prove that the difference (4)−(5) vanishes when summing over all occupied states.

$$X_m = \mathrm{Re}\left(\langle \tfrac{\partial m}{\partial\lambda} | (Q_m - Q)\, O | m\rangle\right) = \mathrm{Re}\Big(\sum_{\substack{n\neq m \\ n\in occ}} \langle \tfrac{\partial m}{\partial\lambda} | n\rangle\langle n|O|m\rangle\Big) = \sum_{\substack{n\neq m \\ n\in occ}} \Big\{ \langle \tfrac{\partial m}{\partial\lambda} | n\rangle\langle n|O|m\rangle + \langle n | \tfrac{\partial m}{\partial\lambda}\rangle\langle m|O|n\rangle \Big\}$$



$$Q_m - Q = \sum_{\substack{m'\neq m \\ m'\in \text{occupied}}} |m'\rangle\langle m'|$$

Then $\frac{\partial}{\partial\lambda}\langle n|m\rangle = 0$ therefore

$$\langle \tfrac{\partial n}{\partial\lambda} | m\rangle + \langle n | \tfrac{\partial m}{\partial\lambda}\rangle = 0$$

$$X_m = \sum_{\substack{n\neq m \\ n\in occ}} -\langle m | \tfrac{\partial n}{\partial\lambda}\rangle\langle n|O|m\rangle + \langle n | \tfrac{\partial m}{\partial\lambda}\rangle\langle m|O|n\rangle$$

$$\text{If } \sum_{m\in occ} X_m = \sum_{\substack{n,m\in occ \\ n\neq m}} \langle m|O|n\rangle\langle n | \tfrac{\partial m}{\partial\lambda}\rangle - \langle n|O|m\rangle\langle m | \tfrac{\partial n}{\partial\lambda}\rangle = 0$$

$n \leftrightarrow m$ dummy variables

(31) Polarization derivation (continuation)

We derived before:

$$\langle \psi_{n\vec{k}} | \vec{r} | \psi_{m\vec{k}} \rangle = -i \frac{1}{E_n - E_m} \langle u_{n\vec{k}} | \frac{\partial}{\partial \vec{k}} \big(\underbrace{e^{-i\vec{k}\vec{r}} H e^{i\vec{k}\vec{r}}}_{H_k} \big) | u_{m\vec{k}} \rangle \qquad n \neq m$$

Note $H_k | u_{mk} \rangle = \varepsilon_k | u_{mk} \rangle$

Multiply by $|u_{n\vec{k}}\rangle$ and sum over n:

$$\sum_{n \neq m} |u_{n\vec{k}}\rangle \langle u_{n\vec{k}} | \underbrace{e^{-i\vec{k}\vec{r}} \vec{r} e^{i\vec{k}\vec{r}}}_{\vec{r}} | u_{m\vec{k}} \rangle = -i \sum_{n \neq m} \frac{1}{E_n - E_m} |u_{n\vec{k}}\rangle \langle u_{n\vec{k}} | \frac{\partial}{\partial \vec{k}} H_k | u_{m\vec{k}} \rangle$$

$\parallel$

We derived by perturbation theory

$$\hat{Q}_m \left| \frac{\partial m}{\partial \lambda} \right\rangle = \sum_{n, n \neq m} \frac{1}{E_m - E_n} |n\rangle \langle n | \frac{\partial H}{\partial \lambda} | m \rangle \qquad (3)$$

identify $|n\rangle = |u_{n\vec{k}}\rangle$, $\lambda = \vec{k}$

Then:

$$\langle u_{n\vec{k}} | \sum_{n \neq m} |u_{n\vec{k}}\rangle \langle u_{n\vec{k}} | \vec{r} | u_{m\vec{k}} \rangle = +i \hat{Q}_m \left| \frac{\partial u_{m\vec{k}}}{\partial \vec{k}} \right\rangle$$

$$\langle u_{n\vec{k}} | \vec{r} | u_{m\vec{k}} \rangle = +i \langle u_{n\vec{k}} | \hat{Q}_m \left| \frac{\partial u_{m\vec{k}}}{\partial \vec{k}} \right\rangle \quad \text{valid for any } u_{n\vec{k}} \neq u_{m\vec{k}}$$

Then: $\hat{Q}_m \vec{r} | u_{m\vec{k}} \rangle = +i \hat{Q}_m \left| \frac{\partial u_{m\vec{k}}}{\partial \vec{k}} \right\rangle$

hence it looks like we can replace $\vec{r} \rightarrow i \frac{\partial}{\partial \vec{k}}$ in matrix element of $|u_{\vec{k}}\rangle$

Just like $\vec{k} = -i \frac{\partial}{\partial \vec{r}}$.

→ Matrix elements of $\vec{r}$ operator are: $\langle u_{n\vec{k}} | \vec{r} | u_{m\vec{k}} \rangle = \langle u_{n\vec{k}} | (i \frac{\partial}{\partial \vec{k}}) | u_{m\vec{k}} \rangle$ as long as $n \neq m$!

We previously derived:

$$\sum_{m \in occ} \frac{\partial}{\partial \lambda} \langle m | O | m \rangle = \sum_{m \in occ} 2 \,\mathrm{Re} \left(\langle \frac{\partial m}{\partial \lambda} | Q_m O | m \rangle \right) \qquad (5)$$

($m \in$ occup; Q_m: unoccupied; $|m\rangle$: occupied)

To calculate the change of $\frac{\partial \langle O \rangle}{\partial \lambda}$ for occupied states we need matrix elements of O only between occupied and unnoccupied states, i.e.,

$\frac{\partial \langle \vec{r} \rangle}{\partial \lambda}$ needs only matrix elements : $\langle u_{n\vec{k}} | \vec{r} | u_{m\vec{k}} \rangle$ hence $n \neq m$!

($u_{n\vec{k}}$: unoccupied; $u_{m\vec{k}}$: occupied)

which is simply given by: $\vec{r} = \left(i \frac{\partial}{\partial \vec{k}} \right)$

(32)

Repeat: $$\sum_{m\in occ} \frac{\partial}{\partial\lambda}\langle m|O|m\rangle = \sum_{m\in occ} 2\,\mathrm{Re}\left(\langle \frac{\partial m}{\partial\lambda}|Q\,O|m\rangle\right) \qquad (5)$$

($m \in$ occup; Q: unoccupied; $|m\rangle$: occupied)

Next:

Insert $|m\rangle \to |u_{m\vec{k}}\rangle$ and $O = -i\frac{\partial}{\partial\vec{k}}$

$\sum_m \to \frac{V_{cell}}{(2\pi)^3}\int d^3k \sum_m$

$$\frac{\partial}{\partial\lambda}\langle\vec{r}\rangle \equiv \frac{V_{cell}}{(2\pi)^3}\int d^3k \sum_{m\in occ}\frac{\partial}{\partial\lambda}\langle u_{m\vec{k}}|\vec{r}|u_{m\vec{k}}\rangle = \frac{V_{cell}}{(2\pi)^3}\int d^3k \sum_{m\in occup} 2\,\mathrm{Re}\left(\langle\frac{\partial u_{mk}}{\partial\lambda}|Q\,(i)\frac{\partial}{\partial\vec{k}}|u_{m\vec{k}}\rangle\right)$$

(sum over all states in the crystal) (all states of e crystal)

Finally:

$$\frac{d}{d\lambda}P = \frac{e}{V_{cell}}\frac{\partial}{\partial\lambda}\langle\vec{r}\rangle = \frac{e}{(2\pi)^3}\sum_{m\in occ}\int_{BZ} d^3k\; 2\,\mathrm{Im}\langle\frac{\partial u_{mk}}{\partial\lambda}|Q\frac{\partial}{\partial\vec{k}}|u_{m\vec{k}}\rangle$$

We want to drop $Q = 1-P$. We will show that $\langle\cdots|P|\cdots\rangle$ is purely real, hence Q can be dropped.

$$\sum_{m\in occ}\langle\frac{\partial u_{mk}}{\partial\lambda}|P\frac{\partial}{\partial\vec{k}}|u_{m\vec{k}}\rangle = \sum_{\substack{m\in occ\\ m'\in occ}}\underbrace{\langle\frac{\partial u_{mk}}{\partial\lambda}|u_{m'k}\rangle}_{a}\underbrace{\langle u_{m'k}|\frac{\partial u_{m\vec{k}}}{\partial\vec{k}}\rangle}_{a^*} \in \text{Real}. \quad (= |a|^2)$$

Finally:

$$\frac{dP}{d\lambda} = \frac{e}{(2\pi)^3}\sum_{m\in occ}\int_{BZ} d^3k\; 2\,\mathrm{Im}\langle\frac{\partial u_{mk}}{\partial\lambda}|\frac{\partial u_{m\vec{k}}}{\partial\vec{k}}\rangle$$

Next we want to compute P for each state of the crystal, i.e., we need a two point formula for change of $\Delta P = P_{final} - P_{initial}$. Formally we just write $\Delta P = \int_i^f \frac{dP}{d\lambda}d\lambda = \int_0^1 \frac{dP}{d\lambda}d\lambda$ hence:

$$\Delta P = \int_0^1 \frac{dP}{d\lambda}d\lambda = \frac{2e}{(2\pi)^3}\sum_{m\in occ}\int_0^1 d\lambda\int_{BZ} d^3k\;\mathrm{Im}\langle\frac{\partial u_{m\vec{k}}}{\partial\lambda}|\frac{\partial u_{m\vec{k}}}{\partial\vec{k}}\rangle$$

(33) Lets see what this means for 1D crystal like we discussed in the intro:

$$\Delta P = \frac{2e}{2\pi} \sum_{n \in occ} \underbrace{\int_0^1 d\lambda \int_0^{2\pi/a} dk}_{\text{2D space}} \, \mathrm{Im} \left\langle \frac{\partial u_{nk}}{\partial \lambda} \Big| \frac{\partial u_{nk}}{\partial k} \right\rangle$$

Define a vector quantity $\vec{A} \equiv \begin{pmatrix} A_n^{(\lambda)} \\ A_n^{(k)} \\ 0 \end{pmatrix} = \begin{pmatrix} i \langle u_{nk} | \frac{\partial u_{nk}}{\partial \lambda} \rangle \\ i \langle u_{nk} | \frac{\partial u_{nk}}{\partial k} \rangle \\ 0 \end{pmatrix}$

<u>Then</u>

$$\left(\vec{\nabla} \times \vec{A}\right)_3 = \frac{\partial}{\partial \lambda} A_n^{(k)} - \frac{\partial}{\partial k} A_n^{(\lambda)} = i \left\langle \frac{\partial u_{nk}}{\partial \lambda} \Big| \frac{\partial u_{nk}}{\partial k} \right\rangle + i \left\langle u_{nk} \Big| \frac{\partial^2}{\partial \lambda \partial k} u_{nk} \right\rangle$$

$$- i \left\langle \frac{\partial}{\partial k} u_{nk} \Big| \frac{\partial u_{nk}}{\partial \lambda} \right\rangle - i \left\langle u_{nk} \Big| \frac{\partial^2}{\partial k \partial \lambda} u_{nk} \right\rangle$$

$$= i \left(\left\langle \frac{\partial u_{nk}}{\partial \lambda} \Big| \frac{\partial u_{nk}}{\partial k} \right\rangle - \left\langle \frac{\partial u_{nk}}{\partial \lambda} \Big| \frac{\partial}{\partial k} u_{nk} \right\rangle^* \right)$$

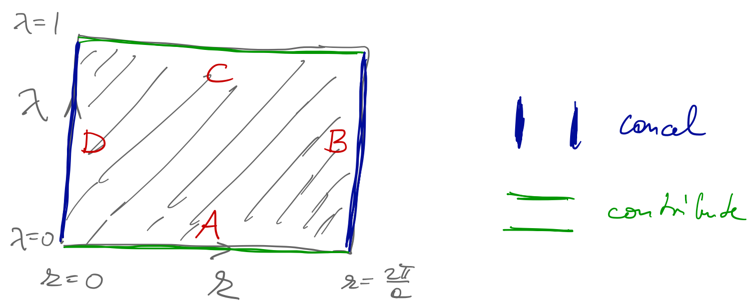
$$= -2 \, \mathrm{Im} \left(\left\langle \frac{\partial u_{nk}}{\partial \lambda} \Big| \frac{\partial u_{nk}}{\partial k} \right\rangle \right)$$

<u>Stokes theorem</u>:

$$\int_{\text{shape}} dS \left(\vec{\nabla} \times \vec{A}\right) = \int_{\partial \text{shape}} d\vec{l} \cdot \vec{A}$$

Here $dS = d\lambda \cdot dk$

Define 2D space



$$-\Delta P \cdot \left(\frac{2\pi}{e}\right) = \int \vec{\nabla} \times \vec{A} \, d\lambda \, dk = \underbrace{\int_0^{2\pi/a} \left[\vec{A}(\lambda=0, k)\right]_k dk}_{A} + \underbrace{\int_0^1 d\lambda \left[\vec{A}(\lambda, k=\tfrac{2\pi}{a})\right]_\lambda}_{B} + \underbrace{\int_{2\pi/a}^0 \left[\vec{A}(\lambda=1, k)\right]_k dk}_{C} + \underbrace{\int_1^0 d\lambda \left[\vec{A}(\lambda, k=0)\right]_\lambda}_{D}$$

$\Delta P = -\frac{e}{2\pi} \cdot X$

$\Delta P \left(\frac{2\pi}{e}\right)$

$$\int_0^{2\pi/a} \left[A^{(k)}(\lambda=0) - A^{(k)}(\lambda=1)\right] dk + \int_0^1 \left[A^{(\lambda)}(k=\tfrac{2\pi}{a}) - A^{(\lambda)}(k=0)\right] d\lambda$$

(A, C; B, D)

Crucial point $u_{nk}\big|_{k=0} = u_{nk}\big|_{k=\frac{2\pi}{a}}$ because this is the same point.

Hence B and D segments cancel

$$\int_0^1 \left(\left\langle u_n(k=\tfrac{2\pi}{a}) \Big| \frac{\partial}{\partial \lambda} u_n(k=\tfrac{2\pi}{a}) \right\rangle - \left\langle u_n(k=0) \Big| \frac{\partial}{\partial \lambda} u_n(k=0) \right\rangle \right) d\lambda = 0$$

(33) Then $\Delta P = -\frac{e}{2\pi}\sum_{n\in occ}\int_0^{2\pi/a} dk \left[A^{(k)}(\lambda=1) - A^{(k)}(\lambda=0)\right] = -\frac{ei}{2\pi}\sum_{n\in occ}\int_0^{2\pi/a} dk \left[\langle u_{nk}|\frac{\partial u_{nk}}{\partial k}\rangle\Big|_{\lambda=1} - \langle u_{nk}|\frac{\partial u_{nk}}{\partial k}\rangle\Big|_{\lambda=0}\right]$

Important: We need to substract value at $\lambda=1$ and $\lambda=0$. Hence P is a property of the state (up to a quantum).

Finally we can generalized this to 3D (straighforward) to get:

$$\Delta P^{\alpha} = -\frac{e}{(2\pi)^3}\sum_{n\in occ}\int_{BZ} d^3k\,(i)\left[\langle u_{n\vec{k}}|\frac{\partial u_{n\vec{k}}}{\partial k_\alpha}\rangle\Big|_{\lambda=1} - \langle u_{n\vec{k}}|\frac{\partial u_{n\vec{k}}}{\partial k_\alpha}\rangle\Big|_{\lambda=0}\right] = -\frac{e}{(2\pi)^3}\int d^2k_\beta \sum_{n\in occ} \Phi_n^{\alpha}(1,k_\beta) - \Phi_n^{\alpha}(1,k_\beta)$$

$P \propto$ Berry phase

Here we introduce Berry connection: $\vec{A}_{n\vec{k}} = i\langle u_{n\vec{k}}|\frac{\partial u_{n\vec{k}}}{\partial \vec{k}}\rangle$

Berry phase: $\Phi_n^{\alpha}(\lambda, k_\beta) = \oint A^{\alpha}_{n\vec{k}}\, dk_\alpha$

Berry curvature: $\Omega_n^{(\lambda,\alpha)} = -2\,\mathrm{Im}\langle \frac{\partial u_{n\vec{k}}}{\partial \lambda}|\frac{\partial u_{n\vec{k}}}{\partial k_\alpha}\rangle$

Some of these quantities are not gauge invariant $\Rightarrow$ P is lattice vector quantity (defined up to quantum of $P = \frac{e\cdot a}{V_{cell}}$)

Let's redefine $\tilde{u}_{n\vec{k}}(\vec{r}) = e^{-i\beta(\vec{k})}\, u_{n\vec{k}}(\vec{r})$

$e^{-i\beta(\vec{k})}$ periodic function of $\vec{k}$ in BZ, hence $\beta(\vec{k}=0) - \beta(\vec{k}=(\pi,\pi,\pi)) = 2\pi m$

$$\tilde{A}^{\alpha}_{n\vec{k}} = i\langle u_{n\vec{k}}\, e^{i\beta(\vec{k})}\left[\frac{\partial}{\partial k_\alpha}\right] e^{-i\beta(\vec{k})}|u_{n\vec{k}}\rangle$$

$$= i\langle u_{n\vec{k}}\, e^{i\beta(\vec{k})}\, e^{-i\beta(\vec{k})}\left[-i\frac{d\beta}{dk_\alpha} + \frac{\partial}{\partial k_\alpha}\right]|u_{n\vec{k}}\rangle = \frac{d\beta}{dk_\alpha} + A^{\alpha}_{n\vec{k}}$$

Conclusion: $\vec{A}_{nk}$ is not gauge invariant (like vector potential $\vec{A}$ for B field ($\vec{B} = \vec{\nabla}\times\vec{A}$))

What about Berry phase?

$$\tilde{\Phi}^{\alpha}_n = \int_0^{2\pi/a} dk_\alpha\left(\frac{d\beta}{dk_\alpha} + A^{\alpha}_{n\vec{k}}\right) = \Phi^{\alpha}_n + \underbrace{\left[\beta\left(\tfrac{2\pi}{a}\right) - \beta(0)\right]}_{2\pi m}$$

$2\pi m$ with m integer

Conclusion: Berry phase unique up to $2\pi m$ quantum.

If $\Phi^{\alpha}_n \Rightarrow \Phi^{\alpha}_n + 2\pi m$ then $\Delta P^{\alpha} \Rightarrow \Delta P^{\alpha} - \frac{e}{(2\pi)^3}\left(\frac{2\pi}{a_\beta}\frac{2\pi}{a_\gamma}\right) 2\pi m = \Delta P^{\alpha} - \frac{e\, a_\alpha}{V_{cell}}\cdot m$

P quantum

Berry phase

Geometry and topology in quantum mechanics give B.P.

It is based on adiabatic evolution of Hamiltonian $H(\lambda)$, where λ is some external parameter, like position of atoms in the unit cell or external field.

If we change λ slowly enough, we can derive how the eigenstates change with λ, provided that:

- the states are non-degenerate (unique)

  [Can be exact many-body eigenstates, not just single particle states]

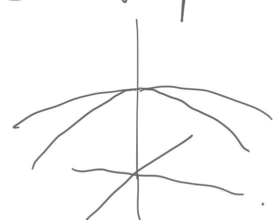
  [If degeneracy is known (p) we can generalize the concept to arbitrary p, but this will give rise to different quantum (instead of $2\pi M \to 2\pi p \cdot M$)]

  integer Q.H.F → fractional Q.H.F

- the parameter λ is varied slowly enough

  It has to be slow enough so that the system is never excited to the neighboring state. This means that there has to be a gap in the excitation spectrum. This is therefore not valid for metals.

In electronic structure there is a lot of level crossings at high symmetry points:



To take care of such situation we need to treat the group of bands as a common unit and arrange a "smooth gauge" through the crossings.

We vary parameter λ in $H(\lambda)$ but eventually we go back to the initial state (like $k = 0 \dots 2\pi$ in BZ, and 2π is the same point as 0)

If we go around in the phase space $\lambda_0 \to \lambda_1 \to \lambda_2 \dots \to \lambda_N = \lambda_0$, we must arrive to the same wave function, but only up to a phase

$$|\psi\rangle \to e^{i\gamma} |\psi\rangle \quad \text{(geometric part of } \gamma \text{ is Berry phase)}$$

γ is important when we look at interference effects.

If adiabatic theorem is satisfied! $H(\lambda)|m(\lambda)\rangle = E_m(\lambda)|m(\lambda)\rangle$

the state of the system is parametrized by the ansatz $|\psi(t)\rangle = \underbrace{C(t)}_{\text{extra phase}} \underbrace{e^{-i\int_0^t E_m(t')dt'}}_{U} |m(t)\rangle$

S.E. satisfied at each time: $\left(i\frac{\partial}{\partial t} - H\right)|\psi(t)\rangle = 0$

remember $|m\rangle = |m(t)\rangle$ and $C(t)$ and $E_m(t)$, ---

$$i\left(\dot{C}U|m\rangle - iE_m(t)CU|m\rangle + CU|\tfrac{dm}{dt}\rangle\right) - H\underbrace{CU}_{\text{numbers}}|m\rangle = 0$$

$$i\dot{C}U|m\rangle + E_m(t)CU|m\rangle + iCU|\tfrac{dm}{dt}\rangle - CUE_m|m\rangle = 0$$

$$\langle m| \;/\; \dot{C}|m\rangle + C|\tfrac{dm}{dt}\rangle = 0$$

$$\dot{C} + C\langle m|\tfrac{dm}{dt}\rangle = 0 \implies C = e^{i\phi(t)} = e^{-\int_0^t \langle m(t')|\frac{\partial m}{\partial t'}\rangle dt'}$$

$$\text{with } \phi(t) = i\int_0^t \langle m(t')|\frac{\partial m(t')}{\partial t'}\rangle dt'$$

but $|m(t)\rangle = |m(\lambda(t))\rangle$ hence

$$|\tfrac{\partial m}{\partial t}\rangle = |\tfrac{\partial m}{\partial \lambda}\rangle \frac{d\lambda}{dt} \quad \text{and} \quad \langle m(t')|\frac{\partial m(t')}{\partial t'}\rangle = \langle m(\lambda)|\frac{\partial m}{\partial \lambda}\rangle \dot{\lambda}$$

Hence

$$\phi(t) = i\int_{\lambda(0)}^{\lambda(t)} \langle m(\lambda)|\frac{\partial m}{\partial \lambda}\rangle d\lambda$$

ϕ depends only on λ and not on type of time evolution (details of t. evolution)

We conclude that $|\psi(t)\rangle = e^{i\phi(\lambda(t))} e^{-i\int_0^t E_m(t')dt'} |m(t)\rangle$

If $\lambda_{final} = \lambda(0)$ then $\phi = i \oint \langle M(\lambda) | \frac{\partial M}{\partial \lambda} \rangle d\lambda$

where adiabatic evolution gives: $|\psi(t)\rangle = e^{i\phi(\lambda(t))} e^{-i\int_0^t E_n(t')dt'} |M(t)\rangle$

Again define Berry connection: $A^{\mu}(\lambda) = \langle M(\lambda) | i \frac{\partial M(\lambda)}{\partial \lambda_\mu} \rangle$

Berry phase: $\phi = \sum_{\mu} \int d\lambda_\mu A^{\mu}(\lambda)$ (like $\oint \vec{A} \cdot d\vec{l}$)

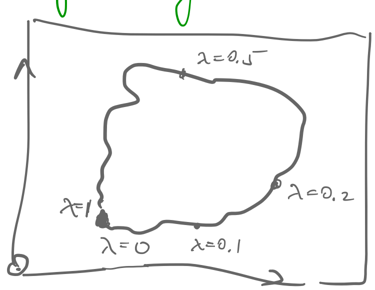
Berry curvature: $\Omega^{\mu\nu} = \left(\frac{\partial}{\partial \mu} A^{\nu}(\lambda) - \frac{\partial}{\partial \nu} A^{\mu}(\lambda) \right)$ (like $\vec{\nabla} \times \vec{A}$)

Note: $\Omega^{\mu\nu} = i \left[\frac{\partial}{\partial \lambda_\mu} \left(\langle M | \frac{\partial}{\partial \lambda_\nu} M \rangle \right) - \frac{\partial}{\partial \lambda_\nu} \left(\langle M | \frac{\partial}{\partial \lambda_\mu} M \rangle \right) \right]$

$= i \left(\langle \frac{\partial M}{\partial \lambda_\mu} | \frac{\partial M}{\partial \lambda_\nu} \rangle - \langle \frac{\partial M}{\partial \lambda_\nu} | \frac{\partial M}{\partial \lambda_\mu} \rangle \right)$

$\Omega^{\mu\nu} = -2 \, \text{Im} \langle \frac{\partial M}{\partial \lambda_\mu} | \frac{\partial M}{\partial \lambda_\nu} \rangle$

Gauge transformation is freedom in choosing initial $|M(\lambda_0)\rangle$. We could choose $|\tilde{M}(\lambda_0)\rangle = e^{-i\beta(\lambda)} |M(\lambda_0)\rangle$ and require that $\beta(\lambda=1) - \beta(\lambda=0) = 2\pi M$ when $\lambda_f = \lambda_i$ and the system goes around a closed loop



Then $\tilde{A}^{\mu}(\lambda) = A^{\mu}(\lambda) + \frac{d\beta}{d\lambda_\mu}$ $\quad$ $\vec{A}$ is not gauge invariant (like potential $\vec{A}$)

$\tilde{\phi} = \oint \tilde{A}(\lambda) d\lambda + \beta(\lambda=1) - \beta(\lambda=0) = \phi + 2\pi M$ $\quad$ ϕ is unique up to a quantum

$\tilde{\Omega}^{\mu\nu} = \frac{\partial \tilde{A}^{\nu}}{\partial \lambda_\mu} - \frac{\partial \tilde{A}^{\mu}}{\partial \lambda_\nu} = \Omega^{\mu\nu} + \underbrace{\frac{d^2\beta}{d\lambda_\mu \partial \lambda_\nu} - \frac{d^2\beta}{d\lambda_\nu d\lambda_\mu}}_{=0} = \Omega^{\mu\nu}$ $\quad$ Ω is gauge invariant and unique.

(like magnetic field B)

Cern theorem says:

$$\frac{1}{2\pi}\iint \Omega^{\mu\nu} d\lambda_\mu d\lambda_\nu = C \quad \in \text{Integer}$$

Consider 2D space λ_1 and λ_2.

We see that $\phi = \int d\lambda_1 A^1(x) + \int d\lambda_2 A^2(x)$

and then $\Omega^{12} = \frac{\partial}{\partial\lambda_1} A^2 - \frac{\partial}{\partial\lambda_2} A^1 = (\vec{\nabla}\times\vec{A})_3$

Stokes theorem says $\int \Omega^{12} d\lambda_1 d\lambda_2 = \int (\vec{\nabla}\times\vec{A})_3 d\lambda_1 d\lambda_2 = \oint \vec{A}\cdot d\vec{l} = \phi(f) - \phi(i) = 2\pi C$

closed path

but this is the same state, hence $2\pi C$

Other forms of Chern theorem:

$$-2\iint \text{Im}\left\langle \frac{\partial M}{\partial\lambda_\mu} \middle| \frac{\partial M}{\partial\lambda_\nu}\right\rangle d\lambda_\mu d\lambda_\nu = 2\pi C$$

What can happen to ϕ?

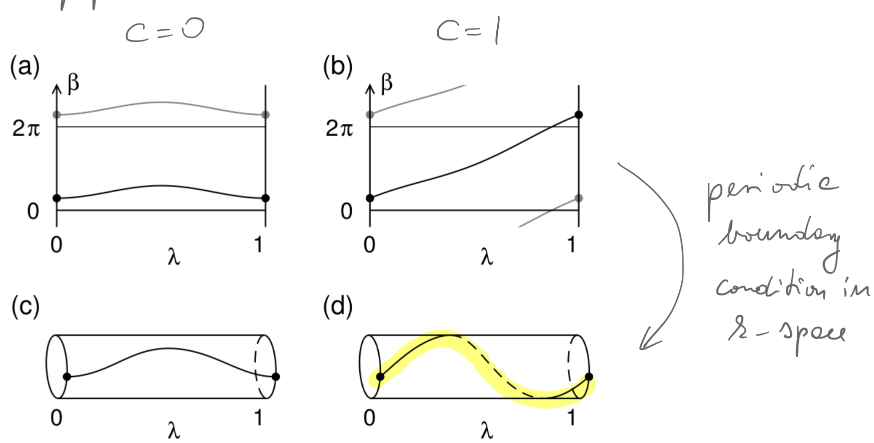
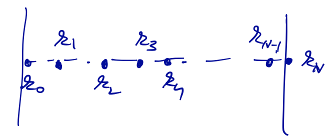


Figure 3.5 Possible behaviors of the function $\beta(\lambda)$ defining a gauge transformation through Eq. (3.15). (a-b) Conventional plots of "progressive" (a) and "radical" (b) gauge transformations, for which β returns to itself or is shifted by a multiple of 2π at the end of the loop, respectively. Shaded lines show 2π-shifted periodic images. (c-d) Same as (a-b) but plotted on the surface of a cylinder to emphasize the nontrivial winding of the radical gauge transformation in (b) and (d).

Practical calculations use formula:

$$\phi = -\operatorname{Im} \ln\left(\langle u_{\lambda_0}|u_{\lambda_1}\rangle\langle u_{\lambda_1}|u_{\lambda_2}\rangle \cdots \langle u_{\lambda_{N-1}}|u_{\lambda_N}\rangle\right)$$

λ for k-space



but $|u_{\lambda_N}\rangle$ in closed loop is $e^{i2\pi m}|u_{\lambda_0}\rangle$

$$\phi = -\operatorname{Im} \ln\left(\langle u_{\lambda_0}|u_{\lambda_1}\rangle\langle u_{\lambda_1}|u_{\lambda_2}\rangle \cdots \langle u_{\lambda_{N-1}}|u_{\lambda_0}\rangle\right)$$

Why is this the same?

$$\langle u_\lambda|u_{\lambda+\delta\lambda}\rangle = \langle u_\lambda|u_\lambda + \frac{\partial u_\lambda}{\partial\lambda}\delta\lambda + \cdots\rangle = 1 + \langle u_\lambda|\frac{\partial u}{\partial\lambda}\rangle\delta\lambda$$

$$\ln\langle u_\lambda|u_{\lambda+\delta\lambda}\rangle \approx \ln\left(1+\delta\lambda\langle u_\lambda|\frac{\partial u}{\partial\lambda}\rangle\right) \approx \langle u|\frac{\partial u}{\partial\lambda}\rangle\delta\lambda$$

Note that: $2\operatorname{Re}\langle u|\frac{\partial u}{\partial\lambda}\rangle = \langle u|\frac{\partial u}{\partial\lambda}\rangle + \langle u|\frac{\partial u}{\partial\lambda}\rangle^* = \langle u|\frac{\partial u}{\partial\lambda}\rangle + \langle\frac{\partial u}{\partial\lambda}|u\rangle = \frac{\partial}{\partial\lambda}\langle u|u\rangle = 0$

hence $\langle u|\frac{\partial u}{\partial\lambda}\rangle$ is purely imaginary and

$$\phi = -\operatorname{Im}\ln\prod_{i=0}^{N}\langle u_{\lambda_i}|u_{\lambda_{i+1}}\rangle = -\operatorname{Im}\int\langle u|\frac{\partial u}{\partial\lambda}\rangle d\lambda = \int i\langle u|\frac{\partial u}{\partial\lambda}\rangle d\lambda$$

Why do we use the discrete formula?

Every eigenstate $|u_{\lambda_i}\rangle$ has an arbitrary phase $|\tilde{u}_{\lambda_i}\rangle = e^{i\beta}|u_{\lambda_i}\rangle$ and using numerically determined eigenvectors $|u_{\lambda_i}\rangle$ the phase will never be a smooth function of λ. But adiabatic theorem requires smoothness.

The discrete formula is gauge free, because each $|u_{\lambda_i}\rangle$ appears exactly twice, once as bra, and once as ket:

$$\phi = -\operatorname{Im}\ln\left(\langle u_{\lambda_0}|u_{\lambda_1}\rangle\langle u_{\lambda_1}|u_{\lambda_2}\rangle\langle u_{\lambda_2}| \cdots \langle u_{\lambda_{N-1}}|u_{\lambda_0}\rangle\right)$$

simple phase $e^{i\beta_j}|u_{\lambda_j}\rangle$ cancels

$$\cdots e^{+i\beta_j}|u_{\lambda_j}\rangle\langle u_{\lambda_j}|e^{-i\beta_j}\cdots$$

We need to use u_{λ_0} rather than u_{λ_N}!

Example of Berry phase: Spin 1/2 particle in a magnetic field $\vec{B}=B\vec{n}$

where $\vec{n}$ is slowly (adiabatically) varies with time.

$$H = -\mu_B B\, \vec{n}\cdot\vec{\sigma}$$

Here x is $\vec{n}(x)$ and changes with time.

The ground state is spinor pointing in the direction of $\vec{n}$, i.e., instantaneous σ_z.

From Q.M. course we know that $|\psi_\uparrow\rangle = \begin{pmatrix}\cos\theta/2 \\ \sin\theta/2\, e^{i\varphi}\end{pmatrix}$ where (θ,φ) are determined from $\vec{n} = \begin{pmatrix}\sin\theta\cos\varphi \\ \sin\theta\sin\varphi \\ \cos\theta\end{pmatrix}$.

Note that when $\theta=\pi$, we have $|\psi_\uparrow\rangle = \begin{pmatrix}0 \\ e^{i\varphi}\end{pmatrix}$ and any φ will give different phase. This will make $\theta=\pi$ a special point with singularity of Ω, and consequently nontrivial Berry phase.

We can compute $\vec{A} = i\langle\psi_\uparrow|\frac{\partial\psi_\uparrow}{\partial\vec{n}}\rangle$ in spherical coordinates. We have

$$A_\theta = \langle\psi_\uparrow|\frac{\partial}{\partial\theta}|\psi_\uparrow\rangle = i\left(\cos\theta/2,\ \sin\theta/2\, e^{-i\varphi}\right)\cdot\frac{\partial}{\partial\theta}\begin{pmatrix}\cos\theta/2 \\ \sin\theta/2\, e^{i\varphi}\end{pmatrix} = 0$$

$$A_\varphi = \langle\psi_\uparrow|\frac{1}{\sin\theta}\frac{\partial}{\partial\varphi}|\psi_\uparrow\rangle = -\frac{\sin^2\theta/2}{\sin\theta}$$

$$\vec{\Omega} = \vec{\nabla}\times\vec{A} = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(A_\varphi\sin\theta\right)\vec{e}_r + \cdots = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin^2\frac{\theta}{2}\right)\vec{e}_r = -\frac{1}{2}\frac{2\sin\frac{\theta}{2}\cos\frac{\theta}{2}}{\sin\theta}\vec{e}_r = -\frac{1}{2}\vec{e}_r$$

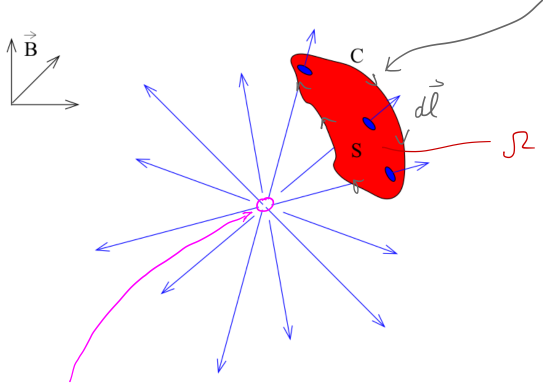
Berry curvature is constant on the sphere and looks like a magnetic monopole.

The Berry phase $\Phi = \oint\vec{A}\cdot d\vec{l} = \int\vec{\Omega}\cdot\frac{d\vec{S}}{r^2} = -\frac{1}{2}\int d\Omega = -\frac{\Omega}{2}$

quarter of the sphere $\Omega = \frac{4\pi}{4}\left(-\frac{1}{2}\right) = -\frac{\pi}{4}$

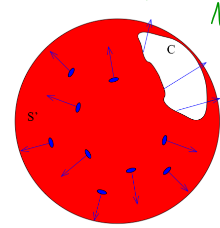
half the sphere $\Omega = -\frac{\pi}{2}$

entire sphere $\Phi = -2\pi \Rightarrow$ chern number $= -1$



Singularity of Ω gives nonzero Chern number.

We could equally well use this surface in Stokes. We would get



$$\Phi = -(4\pi-\Omega)\left(-\frac{1}{2}\right) = 2\pi-\frac{\Omega}{2}$$

because opposite orientation in integration

equivalent!

Example 2: We have a molecule, which goes through a sequence of transformations (a) → (b) → (c) → (d) = (a)

See picture.

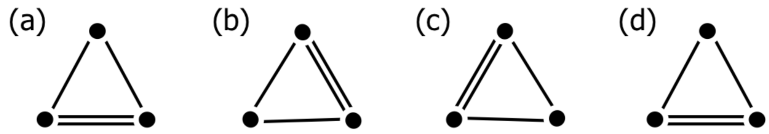


Figure 3.2 Triangular molecule going though a sequence of distortions in which first the bottom, then the upper-right, then the upper-left bond is the shortest and strongest of the three. The configurations in panels (a) and (d), representing the beginning and end of the loop, are identical.

Let's suppose that the wave functions are $u_a = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$ $u_b = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\e^{2\pi i/3}\end{pmatrix}$

$u_c = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\e^{4\pi i/3}\end{pmatrix}$ $u_d = u_a$

What is Berry's phase?

The discrete formula is $\phi = -\operatorname{Im}\ln \langle u_a|u_b\rangle\langle u_b|u_c\rangle\langle u_c|u_a\rangle = -\pi$

$(e^{\pi i/3}\cos\frac{\pi}{3})\,(e^{\pi i/3}\cos\frac{\pi}{3})(e^{\pi i/3}\cos\frac{\pi}{3})$

Berry phase in the Brillouine zone

Here we take $x_1 = k_x$ $x_2 = k_y$ and $x_3 = k_z$ and evolve our system through the Brillouine zone (like what we need for polarization).

$$\vec{A}_{n\vec{k}} = i\langle u_{n\vec{k}}|\frac{\partial}{\partial\vec{k}} u_{n\vec{k}}\rangle$$

$$\vec{\Omega}_{n\vec{k}} = \vec{\nabla}\times\vec{A}_{n\vec{k}}$$

$$\phi_n = \oint \vec{A}_{n\vec{k}}\cdot d\vec{k} = \int_{\text{inside the loop}} (\vec{\nabla}\times\vec{A}_{n\vec{k}})\cdot d\vec{S}_k = \int_{\text{inside the loop}} \vec{\Omega}_{nk}\cdot d\vec{S}_k$$

Note $\Omega_{n\vec{k}}$ is uniquelly defined (gauge invariant) and has the following properties:

1) If the crystal has inversion symmetry I, then $\Omega(\vec{k}) = \Omega(-\vec{k})$.
1) If the crystal has time reversal symmetry (TR) then $\Omega(\vec{k}) = -\Omega(-\vec{k})$
2) If the crystal has some other symmetry, $\Omega(\vec{k})$ inherits it.
3) If the crystal has

consequence If we have I + TR ⇒ $\Omega(\vec{k}) = 0$! No Berry phase or chern number.

(the same symmetries as $\vec{B}$ has, because is $\vec{\nabla}\times\vec{A}$).

How to see that these concepts survive interactions?

Bloch's theorem is valid only for non-interacting electrons. Once interaction is switched on, bands are not well defined, and therefore Bloch theorem is not valid.

Thouless introduced a trick with the twisted boundary condit. [Q. Niu, D.J. Thouless, Y-Shi Wu, PRB 31, 3372 (1985)]

Let the many body wave function $\Phi(\vec{r}_1,\vec{r}_2,\ldots\vec{r}_N)$ have the following boundary conditions

$$\Phi\left(\vec{r}_1+\begin{pmatrix}L_x\\0\\0\end{pmatrix},\vec{r}_2,\ldots\right)=e^{i\theta_x L_x}\,\Phi(\vec{r}_1,\vec{r}_2,\ldots)$$

$$\Phi\left(\vec{r}_1+\begin{pmatrix}0\\L_y\\0\end{pmatrix},\vec{r}_2\ldots\right)=e^{i\theta_y L_y}\,\Phi(\vec{r}_1,\vec{r}_2,\ldots)$$

If the system size is large, the precise form of the boundary condition should not matter, as long as it satisfies basic laws. Such B.C. are used to derive Berry phase formula for the interacting system.

To derive it, we will use Kubo formula for electric conductivity. We will compute Hall effect σ_{xy}, which is a current response $\langle j_x\rangle$ due to magnetic field in z-direction. The action in the presence of the B-field is $S=S_0-\int \vec{j}\cdot\vec{A}\,dt$.

The derivation for polarization is analogous, except that the coupling for polarization is $S=S_0+\int \frac{\partial H}{\partial x}\,\dot{x}\,dt$

Reminder:

$$H=\int d^3r\,\psi^\dagger(\vec{r})\left[\frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial\vec{r}}-e\vec{A}\right)^2+V_{ext}(\vec{r})\right]\psi(\vec{r})\;+V_{int}[\psi^\dagger,\psi]$$

$$-\frac{\hbar^2}{2m}\nabla^2+\frac{ie\hbar}{2m}\left(\frac{\partial}{\partial\vec{r}}\vec{A}+\vec{A}\frac{\partial}{\partial\vec{r}}\right)+\frac{e^2}{2m}A^2$$

(the $\frac{e^2}{2m}A^2$ term is crossed out)

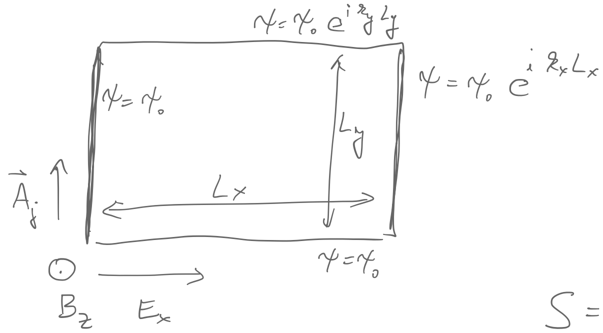
$$H=\underbrace{\int d^3r\,\psi^\dagger(\vec{r})\left[-\frac{\hbar^2}{2m}\nabla^2+V_{ext}(\vec{r})\right]\psi(\vec{r})+V_{int}[\psi^\dagger\psi]}_{H_0}+\underbrace{\frac{ie\hbar}{2m}\int\vec{A}(\vec{r})\left[\psi^\dagger(\vec{r})\frac{\partial}{\partial\vec{r}}\psi(\vec{r})-\left(\frac{\partial}{\partial\vec{r}}\psi^\dagger\right)\psi(\vec{r})\right]}_{-\int\vec{A}(\vec{r})\cdot\vec{j}(\vec{r})\,d^3r}$$

by parts

because $\vec{j}=\frac{e\hbar}{2mi}\left[\psi^\dagger\vec{\nabla}\psi-(\nabla\psi^\dagger)\psi\right]$

Hence:

$$S=S_0-\int\vec{A}\cdot\vec{j}\,dt$$



$$\vec{B}=\vec{\nabla}\times\vec{A}=\begin{pmatrix}\partial_x\\ \partial_y\\ \partial_z\end{pmatrix}\times\underbrace{\begin{pmatrix}0\\ Bx\\ 0\end{pmatrix}}=\begin{pmatrix}0\\0\\B\end{pmatrix}$$

This choice is called Landau gage

and $\vec{E}=-\frac{\partial\vec{A}}{\partial t}$

$E_y=-i\omega A_y$

$$S=S_0-\int\vec{A}\cdot\vec{j}\,d^4$$

$$\langle j_x(x)\rangle=\frac{1}{Z}\int\mathcal{D}[\psi^+\psi]\,e^{-S_0+\int\vec{A}\cdot\vec{j}\,d4'}j_x(x)\approx\frac{1}{Z_0}\int\mathcal{D}[\psi^+\psi]\,e^{-S_0}\left(j_x(x)+\int\vec{A}(x')\,\vec{j}(x')\,j_x(x)\,d4'\right)=\int d4'\,A_y(x')\langle j_y(x')j_x(x)\rangle$$

note $\langle j_x\rangle_0=0$

$$\sum_{\vec{q},i\omega}\underbrace{\langle j_x(\vec{q},\omega)\rangle}_{\sigma^{xy}_q E_y(q,\omega)}e^{i\omega\tau-i\vec{q}\vec{r}}=\sum_{\vec{q},i\omega}\underbrace{A_y(\vec{q},\omega)}_{\frac{E_y(q,\omega)}{\omega}}\int e^{i\omega\tau'-i\vec{q}\vec{r}'}\langle j_y(\vec{r}',\tau')\,j_x(\vec{r},\tau)\rangle\,d^3r'\,d\tau'$$

Tricky issue:

real axis	imag. axis
$A_y(\omega)=\frac{E_y(\omega)}{-i\omega}$	$A_y(i\omega)=\frac{E_y(i\omega)}{-i(i\omega)}$
	$A_y(i\omega)=\frac{E_y(i\omega)}{\omega}$

$$\sigma^{xy}_q(i\omega)\,e^{i\omega\tau-i\vec{q}\vec{r}}=\frac{1}{\omega}\int e^{i\omega\tau'-i\vec{q}\vec{r}'}\langle j_y(\vec{r}',\tau')\,j_x(\vec{r},\tau)\rangle\,d^3r'\,d\tau'$$

$$\sigma^{xy}_q(i\omega)=\frac{1}{\omega}\int e^{i\omega\tau-i\vec{q}\vec{r}}\langle j_y(\vec{r},\tau)\,j_x(0,0)\rangle\,d^3r\,d\tau$$

; $\vec{J}=e\vec{v}$ where

$\vec{v}=\frac{1}{m}(\vec{p}-e\vec{A})$

$q\to 0$

$$\sigma^{xy}(i\omega)=\frac{e^2}{\omega}\int e^{i\omega\tau}\frac{1}{Z}\mathrm{Tr}\Big(e^{-\beta H}e^{H\tau}\underbrace{\int j_y(\vec{r})\,d^3r}_{J_y}\,e^{-H\tau}\underbrace{j_x(0)}_{\frac{1}{V}J_x}\Big)d\tau$$

$$\sigma^{xy}(i\omega)=\frac{e^2}{\omega V}\sum_{\substack{m\\M}}\underbrace{\langle m|v_y(\vec{r})|M\rangle}_{(v_y)_{mM}}\underbrace{\langle M|v_x(0)|m\rangle}_{(v_x)_{Mm}}\frac{e^{-\beta E_m}}{Z}\underbrace{\int_0^\beta e^{\tau(E_m-E_M+i\omega)}d\tau}_{\frac{e^{\beta E_m-E_M}-1}{i\omega+E_m-E_M}}$$

$$\sigma^{xy}(i\omega)=\frac{e^2}{\omega V}\sum_{mM}\frac{(v_y)_{mM}(v_x)_{Mm}}{i\omega+E_m-E_M}\left(\frac{e^{-\beta E_M}}{Z}-\frac{e^{-\beta E_m}}{Z}\right)$$

first $T\to 0$

$$\sigma^{xy}(i\omega)=\frac{e^2}{\omega V}\sum_M\Bigg[\frac{(v_x)_{0M}(v_y)_{M0}}{\underbrace{i\omega+E_M-E_0}_{\frac{1}{E_M-E_0}\left(1+\frac{i\omega}{E_M-E_0}\right)}}-\frac{(v_y)_{0M}(v_x)_{M0}}{\underbrace{i\omega+E_0-E_M}_{-\frac{1}{E_M-E_0}\left(1-\frac{i\omega}{E_M-E_0}\right)}}\Bigg]$$

(for $M=0$ vanishes, hence $M>0$)

next $\omega\to 0$

$$\sigma^{xy}=\frac{e^2}{\omega V}\sum_{M>0}\Bigg[\underbrace{\frac{(v_x)_{0M}(v_y)_{M0}+(v_y)_{0M}(v_x)_{M0}}{(E_M-E_0)}}+i\omega\frac{(v_x)_{0M}(v_y)_{M0}-(v_y)_{0M}(v_x)_{M0}}{(E_M-E_0)^2}\Bigg]$$

From gauge invariance we can prove that it vanishes (Otherwise diverges)

$$\sigma^{xy}=\frac{ie^2}{V}\sum_{M>0}\frac{(v_x)_{0M}(v_y)_{M0}-(v_y)_{0M}(v_x)_{M0}}{(E_M-E_0)^2}$$

$$\hat{v}_x = \frac{1}{m}\left(-i\frac{\partial}{\partial x}\right)$$
$$\hat{v}_y = \frac{1}{m}\left(-i\frac{\partial}{\partial y} - eBx\right)$$

at $T=0$ we have the ground state $|0\rangle \equiv |\phi_0\rangle$ and expectation values:

$$(v_x)_{00} = \langle \phi_0 | \hat{v}_x | \phi_0 \rangle \quad \text{and} \quad (v_y)_{00} = \langle \phi_0 | \hat{v}_y | \phi_0 \rangle$$

Next we make a unitary transformation $|\phi\rangle = e^{-i\sum_i \vec{\varkappa}\cdot\vec{r}_i} |\phi_0\rangle$ which twists the boundary condition. We see $\phi(r_1 + L_x, \ldots) = e^{-i\varkappa_x L_x} \phi_0(r_1 + L_x, \ldots)$ and we require $\varkappa_x L_x \in [-\pi, \pi]$, hence the change of momentum is really small for large crystal, i.e., $\varkappa_x \sim \frac{\pi}{L_x}$. If we have insulator (no gap closing while adding the twist) we expect equivalently good solution).

ϕ is a function of many variables $\phi(r_1, r_2, \ldots r_N)$ but let's concentrate on r_1 only:

$$\phi(r_1 + L_x) = e^{-i\varkappa_x L_x} e^{-i\varkappa_x r_1} \phi_0(r_1 + L_x) = e^{-i\varkappa_x L_x + i k_x L_x} e^{-\varkappa_x r_1} \phi_0(r_1) = e^{i(k_x - \varkappa_x)L_x} \phi(r_1)$$

Hence, we see a slight change of phase through the crystal.

What is momentum in this new state compared to $|\phi_0\rangle$?

$$(v_x)_{00} = \langle \phi | e^{-i\sum \vec{\varkappa}\vec{r}_i} v_x e^{i\sum \vec{\varkappa}\vec{r}_i} |\phi\rangle \quad \text{hence}$$

$$(v_x)_{00} = \langle \phi | e^{-i\sum \vec{\varkappa}\vec{r}_i} \frac{1}{m}\left(-ii\varkappa_x - i\frac{\partial}{\partial x}\right) e^{i\sum \vec{\varkappa}\vec{r}_i} |\phi\rangle = \langle \phi | \frac{1}{m}\left(-i\frac{\partial}{\partial x} + \varkappa_x\right) |\phi_0\rangle$$

$$(v_y)_{00} = \langle \phi | e^{-i\sum \vec{\varkappa}\vec{r}_i} \frac{1}{m}\left(-i\frac{\partial}{\partial y} + \varkappa_y - eBx\right) e^{i\sum_i \vec{\varkappa}\vec{r}_i} |\phi\rangle = \langle \phi | \frac{1}{m}\left(-i\frac{\partial}{\partial y} - eBx + \varkappa_y\right) |\phi_0\rangle$$

This transformation is thus equivalent to transforming operators

$$\left.\begin{array}{l} -i\frac{\partial}{\partial x} \to -i\frac{\partial}{\partial x} + \varkappa_x \\ -i\frac{\partial}{\partial y} \to -i\frac{\partial}{\partial y} + \varkappa_y \end{array}\right\} \text{hence the Hamiltonian is } \tilde{H} =$$

The corresponding transformed Hamiltonian is thus:

$$\tilde{H} = \sum_i \frac{\left(-i\frac{\partial}{\partial x_i} + \varkappa_x\right)^2}{2m_i} + \frac{\left(-i\frac{\partial}{\partial y_i} + \varkappa_y - eBx_i\right)^2}{2m_i} + V_{int}$$

and therefore:
$$\frac{\partial \tilde{H}}{\partial \varkappa_x} = \sum_i \frac{\left(-i\frac{\partial}{\partial x_i} + \varkappa_x\right)}{m_i} = v_x \quad \text{and} \quad \frac{\partial \tilde{H}}{\partial \varkappa_y} = \sum_i \frac{\left(-i\frac{\partial}{\partial y_i} + \varkappa_y - eBx_i\right)}{m_i} = v_y$$

Finally we can write conductivity for the state with twisted B.C.:

$$\sigma^{xy} = \frac{ie^2}{V} \sum_{m>0} \frac{(v_x)_{0m}(v_y)_{m0} - (v_y)_{0m}(v_x)_{m0}}{(E_m-E_0)^2}$$

$$\Rightarrow \frac{ie^2}{V} \sum_{m>0} \frac{\langle\phi_0|\frac{\partial \tilde{H}}{\partial \theta_x}|\phi_m\rangle\langle\phi_m|\frac{\partial \tilde{H}}{\partial \theta_y}|\phi_0\rangle - \langle\phi_0|\frac{\partial \tilde{H}}{\partial \theta_y}|\phi_m\rangle\langle\phi_m|\frac{\partial \tilde{H}}{\partial \theta_x}|\phi_0\rangle}{(E_m-E_0)^2}$$

Next we try to simplify the products!

$$\frac{\partial}{\partial \theta_x}\langle\phi_0|\tilde{H}|\phi_m\rangle = \langle\frac{\partial \phi_0}{\partial \theta_x}|\tilde{H}|\phi_m\rangle + \langle\phi_0|\tilde{H}|\frac{\partial \phi_m}{\partial \theta_x}\rangle + \langle\phi_0|\frac{\partial \tilde{H}}{\partial \theta_x}|\phi_m\rangle$$

$$\frac{\partial}{\partial \theta_x} E_0 \delta_{m0} = 0 = E_m \langle\frac{\partial \phi_0}{\partial \theta_x}|\phi_m\rangle + \underbrace{E_0\langle\phi_0|\frac{\partial \phi_m}{\partial \theta_x}\rangle}_{} + \langle\phi_0|\frac{\partial \tilde{H}}{\partial \theta_x}|\phi_m\rangle$$

but $\langle\phi_0|\frac{\partial \phi_m}{\partial \theta_x}\rangle = \underbrace{\frac{\partial}{\partial \theta_x}\langle\phi_0|\phi_m\rangle}_{=0} - \langle\frac{\partial \phi_0}{\partial \theta_x}|\phi_m\rangle$

Finally we simplified to:

$$m \neq 0: \quad \langle\phi_0|\frac{\partial \tilde{H}}{\partial \theta_x}|\phi_m\rangle = -(E_m - E_0)\langle\frac{\partial \phi_0}{\partial \theta_x}|\phi_m\rangle$$

Similarly we can get (just conjugating and replacing $\theta_x \to \theta_y$)

$$\langle\phi_m|\frac{\partial \tilde{H}}{\partial \theta_y}|\phi_0\rangle = -(E_m - E_0)\langle\phi_m|\frac{\partial \phi_0}{\partial \theta_y}\rangle$$

We plug this back to σ^{xy} to get

$$\sigma^{xy} = \frac{ie^2}{V}\sum_{m>0} \frac{(E_m-E_0)^2\left[\langle\frac{\partial \phi_0}{\partial \theta_x}|\phi_m\rangle\langle\phi_m|\frac{\partial \phi_0}{\partial \theta_y}\rangle - \langle\frac{\partial \phi_0}{\partial \theta_y}|\phi_m\rangle\langle\phi_m|\frac{\partial \phi_0}{\partial \theta_x}\rangle\right]}{(E_m-E_0)^2}$$

$$\sigma^{xy} = \frac{ie^2}{V}\left[\langle\frac{\partial \phi_0}{\partial \theta_x}|\left(\sum_m |\phi_m\rangle\langle\phi_m|\right)|\frac{\partial \phi_0}{\partial \theta_y}\rangle - \langle\frac{\partial \phi_0}{\partial \theta_y}|\left(\sum_m |\phi_m\rangle\langle\phi_m|\right)\frac{\partial \phi_0}{\partial \theta_x}\rangle\right]$$

$$\sigma^{xy} = \frac{ie^2}{V}\left[\langle\frac{\partial \phi_0}{\partial \theta_x}|\frac{\partial \phi_0}{\partial \theta_y}\rangle - \langle\frac{\partial \phi_0}{\partial \theta_y}|\frac{\partial \phi_0}{\partial \theta_x}\rangle\right]$$

The result should be insensitive to this twist in the B.C. as long as there is a gap in the spectrum for any choice of θ_x, θ_y. We will average over the twist $\in [0, 2\pi]$:

$$\theta_x L_x = \tilde{\theta}_x \in [0, 2\pi] \quad \text{and} \quad \theta_y L_y = \tilde{\theta}_y \in [0, 2\pi]$$

$$\sigma^{xy} = \frac{ie^2}{V}\frac{L_x L_y}{(2\pi)^2}\int_0^{2\pi} d\tilde{\theta}_x \int_0^{2\pi} d\tilde{\theta}_y \left[\underbrace{\langle\frac{\partial \phi_0}{\partial \tilde{\theta}_x}|\frac{\partial \phi_0}{\partial \tilde{\theta}_y}\rangle - \langle\frac{\partial \phi_0}{\partial \tilde{\theta}_y}|\frac{\partial \phi_0}{\partial \tilde{\theta}_x}\rangle}_{}\right]$$

Chern theorem has something to do with it!

We recall the Chern theorem:

$$-2\iint \text{Im}\left\langle \frac{\partial M}{\partial \lambda_\mu} \middle| \frac{\partial M}{\partial \lambda_\nu}\right\rangle d\lambda_\mu \, d\lambda_\nu = 2\pi c$$

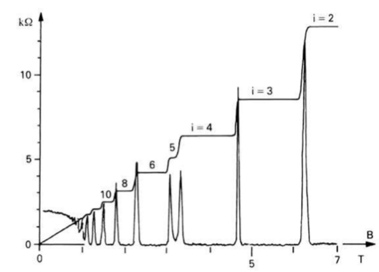
Which here mean that when we change the twist $\tilde{\theta}_x$ or $\tilde{\theta}_y$ for 2π, we should get the same state, hence the twist of $2\pi c$ (for arbitrary c) should give the same answer.

We hence recognize:

$$\sigma^{xy} = \frac{ie^2}{V}\frac{L_x L_y}{(2\pi)^2}\int_0^{2\pi} d\tilde{\theta}_x \int_0^{2\pi} d\tilde{\theta}_y \underbrace{\left[\left\langle \frac{\partial \phi_0}{\partial \tilde{\theta}_x} \middle| \frac{\partial \phi_0}{\partial \tilde{\theta}_y}\right\rangle - \left\langle \frac{\partial \phi_0}{\partial \tilde{\theta}_y} \middle| \frac{\partial \phi_0}{\partial \tilde{\theta}_x}\right\rangle\right]}_{2i\,\text{Im}\left\langle \frac{\partial \phi_0}{\partial \tilde{\theta}_x} \middle| \frac{\partial \phi_0}{\partial \tilde{\theta}_y}\right\rangle} = e^2 \frac{L_x L_y}{V} \frac{2\pi}{(2\pi)^2} c = \frac{e^2}{2\pi}\cdot c$$

for 2D system $\frac{L_x L_y}{V} = 1$

This is Thouless's proof of 2D quantization of the integer quantum Hall effect.



He also prove fractional quantum Hall effect.

Key point: The ground state $|\phi_0\rangle$ is degenerate p-times.

Then we need an extra sum over degenerate ground states:

$$\sigma^{xy} = \frac{ie^2}{V}\sum_{0\in p}\left[\left\langle \frac{\partial \phi_0}{\partial \tilde{\theta}_x} \middle| \frac{\partial \phi_0}{\partial \tilde{\theta}_y}\right\rangle - \left\langle \frac{\partial \phi_0}{\partial \tilde{\theta}_y} \middle| \frac{\partial \phi_0}{\partial \tilde{\theta}_x}\right\rangle\right]$$

↑ degenerate ground states.

Assumption: There is no coupling between these states, so the system is in one of those states, and we can not reach different $|\phi_0\rangle$ by single particle (low energy) excitations.

Key point: When we twist the B.C. we are allowed to switch from one state of the set to another, hence in the worse case scenario it might be necessary to twist the phase up to $2\pi\cdot p\cdot c$ to get to the same state! (p: degeneracy)

Thouless therefore argued that the correct averaging for degenerate set is

$$\sigma^{xy} = \frac{ie^2}{V}\frac{L_x L_y}{(2\pi)^2}\,\frac{1}{p}\int_0^{2\pi p} d\tilde{\theta}_x \int_0^{2\pi} d\tilde{\theta}_y \left[\left\langle \frac{\partial \Phi_0}{\partial \tilde{\theta}_x}\Big|\frac{\partial \Phi_0}{\partial \tilde{\theta}_y}\right\rangle - \left\langle \frac{\partial \Phi_0}{\partial \tilde{\theta}_y}\Big|\frac{\partial \Phi_0}{\partial \tilde{\theta}_x}\right\rangle\right]$$

we will get one of the p states when phase is changed for 2π, and we need $2\pi p$ phase to get back to original state.

The space to integrate for Chern theorem, which should be modified to:

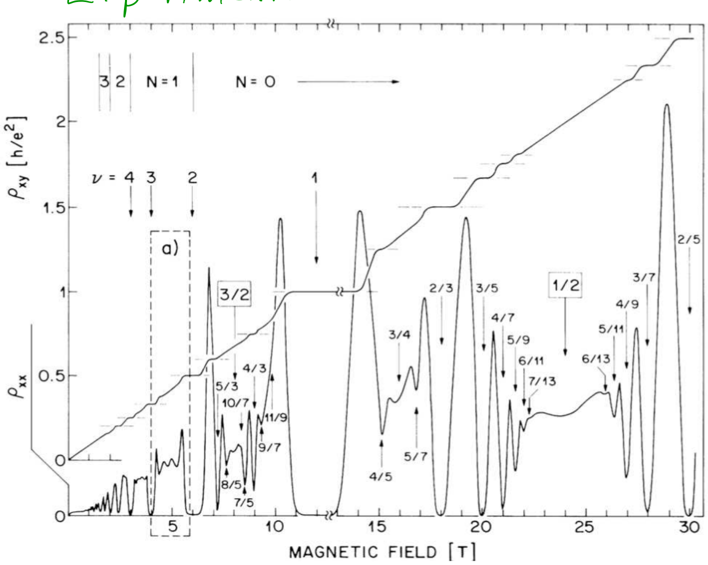
$$-2\int_0^{2\pi p}\int_0^{2\pi} \operatorname{Im}\left\langle \frac{\partial M}{\partial \lambda_\mu}\Big|\frac{\partial M}{\partial \lambda_\nu}\right\rangle d\lambda_\mu\, d\lambda_\nu = 2\pi C$$

Finally the result is:

$$\sigma^{xy} = \frac{e^2}{2\pi p}\cdot C$$

Laughlin wrote down a concrete wave function, which gives such conductivity (Both Laughlin and Thouless got Nobel prize.)

Experiment:



Note that if we started with $S = S_0 + \int \frac{\partial H}{\partial x}\dot{x}\,dt$ we could derive polarization. By playing with the twist B.C. we would then get:

$$\langle \Delta R^{\alpha}_{cm}\rangle = \frac{V_{cell}}{(2\pi)^3}\int_0^1 d\lambda \int_{BZ} d^3\theta \left\{\left\langle \frac{\partial \Phi_0}{\partial \lambda}\Big|\frac{\partial \Phi_0}{\partial \vec{\theta}}\right\rangle - \left\langle \frac{\partial \Phi_0}{\partial \vec{\theta}}\Big|\frac{\partial \Phi_0}{\partial \lambda}\right\rangle\right\} \qquad \alpha = x, y, z$$

After using Stokes theorem, as in non-interacting case, we would get

$$\langle \Delta R^{\alpha}_{cm}\rangle = \frac{2V_{cell}}{(2\pi)^3}\int_{BZ} d^3\theta\, \operatorname{Im}\left\{\left\langle \Phi_\theta(\lambda=1)\Big|\frac{\partial}{\partial \theta_\alpha}\Big|\Phi_\theta(\lambda=1)\right\rangle - \left\langle \Phi_\theta(\lambda=0)\Big|\frac{\partial}{\partial \theta_\alpha}\Big|\Phi_\theta(\lambda=0)\right\rangle\right\}$$

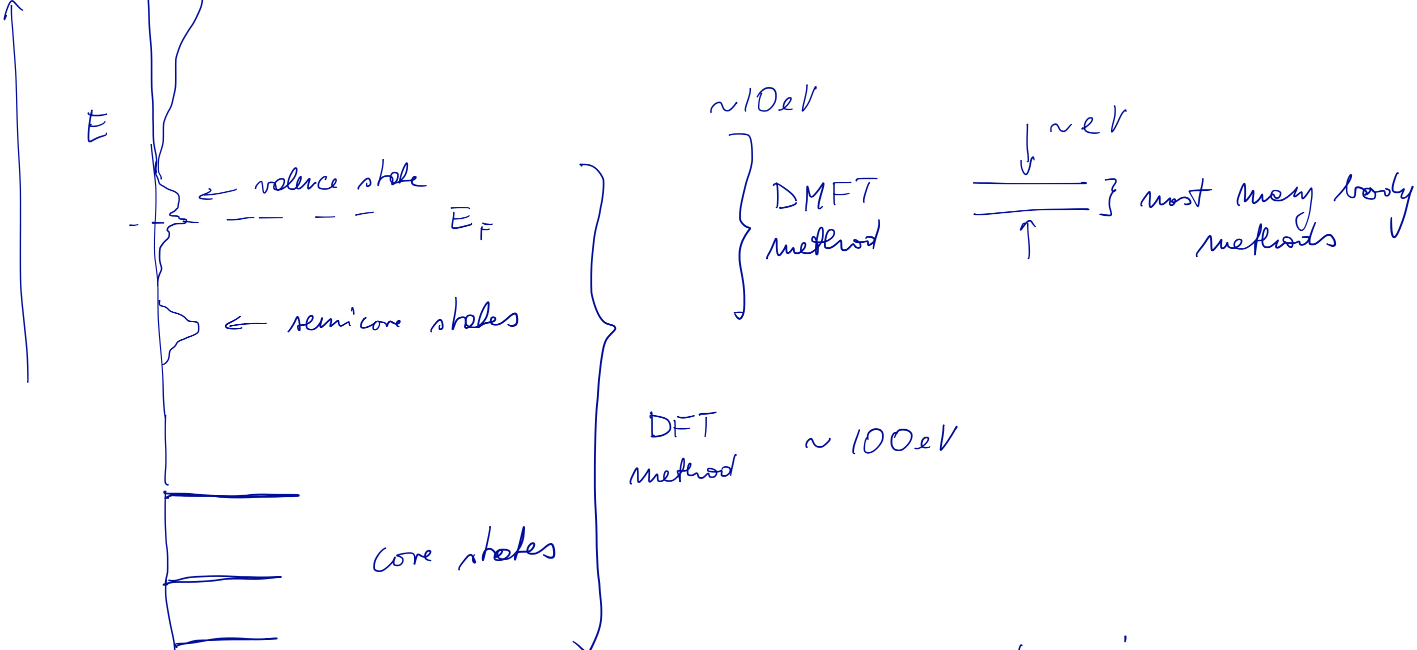
many body state with twisted B.C.

Quasiparticles (Richard Martin Chapter 7)

Origin of the frequency dependence of self energy.

We almost never treat all degrees of freedom in a solid, but almost always divide it into the "relevant" low energy degrees of freedom and the rest.

Exact theory would need to address extremely large energy window $\sim 10^4$ eV (10^8 K)



In practice it is convenient to write H in block form:

$$\begin{bmatrix} H_S , & H_{SR} \\ H_{RS} , & H_{RR} \end{bmatrix} \begin{bmatrix} \phi_S \\ \phi_R \end{bmatrix} = \omega \begin{bmatrix} \phi_S \\ \phi_R \end{bmatrix}$$

ϕ_S ← "relevant" degrees of freedom

ϕ_R ← the "rest"

ω ↑ energy

$$H_{RS}\,\phi_S + H_{RR}\,\phi_R = \omega\,\phi_R$$

$$H_{RS}\,\phi_S = (\omega - H_{RR})\,\phi_R$$

$$(\omega - H_{RR})^{-1} H_{RS}\,\phi_S = \phi_R$$

$$H_S\,\phi_S + H_{SR}\,\phi_R = \omega\,\phi_S$$

$$\left[H_S + H_{SR}(\omega - H_{RR})^{-1} H_{RS}\right]\phi_S = \omega\,\phi_S$$

$H_{SR}(\omega - H_{RR})^{-1} H_{RS}$: frequency dependent correction to low energy H_S due to the "rest".

$$\left[H_S + \Sigma_S(\omega)\right]\phi_S = \omega\,\phi_S$$

corrected equation for the low energy part only is always energy dependent.

If we concentrate on the single particle Green's function, it will also contain frequency dependent corrections to $\mathcal{G}^0$ if there are processes not included in $\mathcal{G}^0$.

$$\mathcal{G}^0 = \left(\omega + \frac{\nabla^2}{2m} - V_{ion}\right)^{-1}$$

What is missing?
- electron-electron interaction Σ_{ee}
- electron-phonon interaction Σ_{ep} } dynamic
- spin-orbit (is static)

We can write
$$\mathcal{G} = (\omega - H)^{-1} = \begin{pmatrix} \omega - H_S & -H_{SR} \\ -H_{RS} & \omega - H_{RR} \end{pmatrix}^{-1}$$

$$= \begin{pmatrix} \left(\omega - H_S - H_{SR}\frac{1}{\omega - H_{RR}} H_{RS}\right)^{-1} & \cdots \\ \cdots & \cdots \end{pmatrix}$$

$$\mathcal{G}_S = \left(\omega - H_S - \underbrace{H_{SR}\frac{1}{\omega - H_{RR}} H_{RS}}\right)^{-1}$$

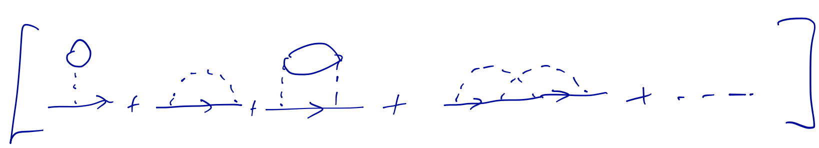
can be called $\Sigma_S(\omega)$

<u>Dyson Equation</u>:
$$\mathcal{G}(\omega) = \left(\mathcal{G}_0^{-1} - \Sigma(\omega)\right)^{-1}$$

↑ self energy describes interaction with the "rest"
- the real part describes the shifts and renormalization of the energy levels
- the imaginary part describes the lifetime of the quasiparticles.

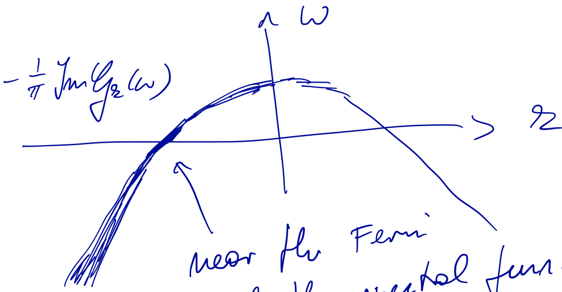
<u>In Feynman language</u>:

conclusion: Σ is the single particle irreducible part of $\mathcal{G}$: does not fall into two pices when cutting single $\mathcal{G}_0$



Now quasiparticles

$A_k(\omega) = -\frac{1}{\pi} \mathrm{Im}\, G_k(\omega)$



Note E_F corresponds $\omega = 0$.

near the Fermi level the spectral function in metals sharpen

We want to describe the "effective" quasiparticle

$$G_k \approx \frac{1}{\omega - \varepsilon_k - \Sigma_k(\omega)}$$

↑ because G is a matrix, and usually can not simply decouple bands

[Would require ε_k and $\Sigma_k(\omega)$ to be diagonal in the same basis which almost never happens]

near $\omega = 0$ we expand

$$\Sigma_k(\omega) = \Sigma_{k_F}(0) + \left(1 - \frac{1}{Z_k}\right)\omega + \frac{\partial \Sigma_k}{\partial k}(k - k_F) + \dots$$

$$-i\left[\frac{\omega^2 + \pi^2 T^2}{\varepsilon^*}\right] + \dots$$

↑ fermi liquid result

(follows from the Pauli ex. principle due to small phase space for the scattering)

$$1 - \frac{1}{Z_k} = \frac{\partial \Sigma_k}{\partial \omega} \quad \text{or} \quad Z_k = \left(1 - \frac{\partial \Sigma_k}{\partial \omega}\right)^{-1}_{\substack{\omega = 0 \\ k = k_F}}$$

Then $$G_k(\omega) \approx \frac{1}{\frac{\omega}{Z_k} - \varepsilon_k - \Sigma_k(\omega = 0)} = \frac{Z_k}{\omega - \underbrace{Z_k(\varepsilon_k + \Sigma_k(\omega=0))}_{\text{"effective dispersion"}}}$$

← weight is reduced i.e., quasiparticle

$$\varepsilon_k^{eff} = Z_k(\varepsilon_k + \Sigma_k(\omega = 0))$$

(Z_k) ↑ makes it narrower because $Z_k < 1$. (Σ_k) ↑ shift

Mass of the dispersion:

$$\varepsilon_k + \Sigma_k(\omega=0) \approx \left(\left.\frac{d\varepsilon_k}{dk}\right|_{k = k_F} + \left.\frac{d\Sigma_k(\omega=0)}{dk}\right|_{k = k_F}\right)(k - k_F) + \dots$$

Then $$G_k(\omega) \approx \frac{Z_k}{\omega - (k - k_F) Z_k \left(v_F + \frac{d\Sigma_k}{dk}\right)} = \frac{Z_k}{\omega - \frac{(k - k_F) v_F}{m^*/m_b}}$$

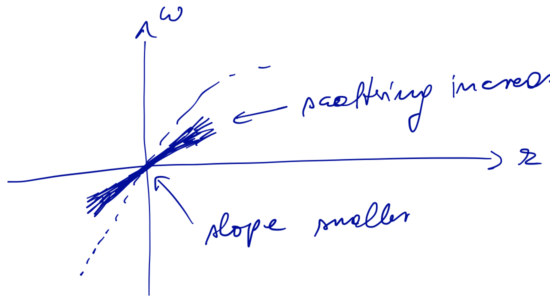
$$\frac{m^*}{m_b} = \frac{1}{Z_k}\left(1 + \frac{1}{v_F}\left.\frac{\partial \Sigma_k}{\partial k}\right|_{\substack{\omega = 0 \\ k = k_F}}\right)^{-1}$$

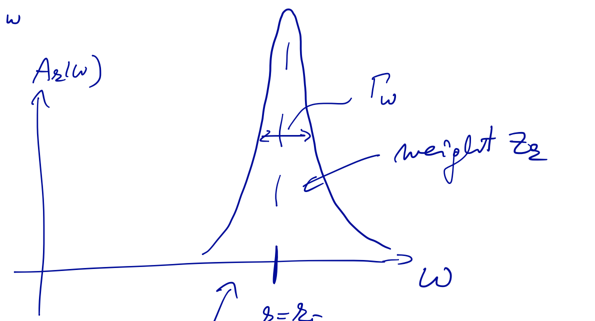
↑ typically the most important increases mass.

heavy fermions (~ 100 − 1000)

We thus have $\mathcal{G}_k(\omega) \approx \dfrac{z_k}{\omega - (k-k_F)v_F\, m_b/m^* + i\underbrace{z_k\left(\frac{\omega^2+\pi^2T^2}{\varepsilon^*}\right)}_{\Gamma_\omega}}$

$$A_k(\omega) \approx \frac{1}{\pi}\frac{z_k \Gamma_\omega}{\left(\omega - (k-k_F)v_F\, m_b/m^*\right)^2 + \Gamma_\omega^2}$$





$$\mathcal{G}^0_k(t) = -i\, e^{-i\varepsilon_k t}$$

then

$$\mathcal{G}_k(t) = -i\, z_k\, e^{-i(\varepsilon_k - i\Gamma)t} = -i\, z_k\, e^{-i\varepsilon_k - \Gamma_\omega t}$$

↖ finite lifetime of the quasiparticle

Functionals in many particle systems   Chapter 8

- Concise formulation of various useful approximation
  DFT, DMFT, GW, ...
- "Conserving functionals" conserve energy, momentum, particle number on provide "best" approximations.
- stationary functionals allow robust solution even when implementation is approximate

Most famous Functional theory is DFT. (chapter 4.3 in Z.M. book)

It is indirect approach in solving the many body problem, in which charge density $\rho(\vec{r})$ is the central quantity to be determined.

Total energy (at $T=0$) can be expressed by:

$$E = \langle\Psi|H|\Psi\rangle = \langle\Psi|T + V_{ee} + V_{nuc}|\Psi\rangle = \langle\Psi|\underline{T + V_{ee}}|\Psi\rangle + \underline{\int d^3r\, \rho(\vec{r})\, V_{nuc}(\vec{r})}$$

universal because it has explicit form

$$T = \sum_i -\frac{\nabla_i^2}{2m_i} \; ; \; V = \frac{1}{2}\sum_{i\neq j} V_c(\vec{r}_i - \vec{r}_j)$$

non-universal depends on the "material".

- Hohenberg and Kohn proved that H is a unique functional of the ground state charge density $\rho(\vec{r})$. In another words, there can not be two potentials $V^{(1)}_{nuc}(\vec{r})$ and $V^{(2)}_{nuc}(\vec{r})$ giving rise to the same ground state electron density $\rho(\vec{r})$. Hence if we know $\rho(\vec{r}) \Rightarrow$ we know $V_{nuc}(\vec{r}) \Rightarrow$ we know H.

If we know $H \Rightarrow$ there is unique ground state $|\Psi_0\rangle$ and corresponding $E = \langle\Psi_0|H|\Psi_0\rangle$ is uniquely determined from $\rho(\vec{r})$. Also all ground state properties are uniquely determined by $\rho(\vec{r})$.

Proof that H is unique functional of $\rho(\vec{r})$: Assume there exist two potentials $V_{nuc}^{(1)}(\vec{r})$ and $V_{nuc}^{(2)}(\vec{r})$ differing by more than a constant, and giving rise to the same g.s. density $\rho(\vec{r})$. We have

$$(T+V_{ee}+V_{nuc}^{(1)})|\psi^{(1)}\rangle = E^{(1)}|\psi^{(1)}\rangle$$
$$(T+V_{ee}+V_{nuc}^{(2)}|\psi^{(2)}\rangle = E^{(2)}|\psi^{(2)}\rangle$$

$|\psi^{(1)}\rangle$ and $|\psi^{(2)}\rangle$ are different. Then:

$$E^{(1)} = \langle\psi^{(1)}|H^{(1)}|\psi^{(1)}\rangle < \langle\psi^{(2)}|H^{(1)}|\psi^{(2)}\rangle$$

because of variational principle, any $|\psi^{(2)}\rangle$, which is not g.s. should give strictly higher energy.

We assumed $H^{(1)} = H^{(2)} + V_{nuc}^{(2)} - V_{nuc}^{(1)}$ therefore:

$$E^{(1)} = \langle\psi^{(1)}|H^{(1)}|\psi^{(1)}\rangle < \underbrace{\langle\psi^{(2)}|H^{(2)}|\psi^{(2)}\rangle}_{E^{(2)}} + \underbrace{\langle\psi^{(2)}|V_{nuc}^{(2)} - V_{nuc}^{(1)}|\psi_2\rangle}_{\int[V_{nuc}^{(2)}(\vec{r})-V_{nuc}^{(1)}(\vec{r})]\rho(\vec{r})d^3r}$$

exchange $(1)\Leftrightarrow(2)$

$$E^{(2)} = \langle\psi^{(2)}|H^{(2)}|\psi^{(2)}\rangle < E^{(1)} + \int[V_{nuc}^{(1)}(\vec{r})-V_{nuc}^{(2)}(\vec{r})]\rho(\vec{r})d^3r$$

sum the two equations:

$$E^{(1)}+E^{(2)} < E^{(2)}+E^{(1)}$$

which is absurd $\Rightarrow$ conclusion $V_{nuc}^{(1)} - V_{nuc}^{(2)} = 0$ or constant.

We just proved that if we are given ground state density $\rho(\vec{r})$ we can uniquely determine $V_{nuc}(\vec{r})$ and hence H. Since we have unique H, we could in principle find unique $|\psi^0\rangle$ and any ground state property.

Note: H.K. theorem breaks for degenerate ground states. In this case $|\psi^{(2)}\rangle$ and $|\psi^{(1)}\rangle$ have the same energy, but different density. Example "Mott insulator".

- H.K. also proved that $E[\rho]$ reaches <u>minimum</u> in the exact ground state density $\rho(\vec{r})$.

Proof: If $|\psi^{(2)}\rangle$ gives rise to density $\rho^{(2)}(\vec{r})$, which is different from g.s., we have

$$E[\rho] = \langle\psi^{(1)}|H|\psi^{(1)}\rangle < \langle\psi^{(2)}|H|\psi^{(2)}\rangle$$ because of the variational principle because $|\psi^{(2)}\rangle$ is not g.s. wave function, while $|\psi^{(1)}\rangle$ is.

Second step: Kohn-Sham auxiliary non-interacting system:

The exact g.s. density is represented in terms of some non-interacting set of orbitals, i.e., $\rho(\vec{r}) = \sum_{i \in occ} \psi_i^*(\vec{r})\, \psi_i(\vec{r})$

The kinetic energy is then expressed by $T_{ip}[\rho] = \sum_{i \in occ} \int \psi_i^*(\vec{r}) \left(-\frac{\nabla^2}{2m}\right) \psi_i(\vec{r})\, d^3r$

Therefore

$$E[\rho] = \sum_{i \in occ} \int \psi_i^*(\vec{r}) \left(-\frac{\nabla^2}{2m} + V_{nuc}(\vec{r})\right) \psi_i(\vec{r}) + E^H[\rho] + E^{xc}[\rho]$$

where $E^H[\rho] = \frac{1}{2} \iint \frac{\rho(\vec{r})\,\rho(\vec{r}\,')}{|\vec{r} - \vec{r}\,'|}\, d^3r\, d^3r'$ is the Hartree term.

$E^{xc}[\rho]$ is unknown functional. It's exact expression is

$$E^{xc}[\rho] = \langle T \rangle - T_{ip}[\rho] + \langle V_{ee} \rangle - E^H[\rho]$$ and is rather small

because $\langle T \rangle \approx T_{ip}[\rho]$ and $\langle V_{ee} \rangle \approx E^H[\rho]$

Moreover $E^{xc}[\rho]$ is universal functional $\Rightarrow$ can be computed in any simple interacting system. Idea: Solve the uniform electron problem and determine $E^{xc}[\rho]$ and use it in any material.

Unfortunately uniform electron gas is not solvable exactly, but we only know numerical value of $E^{xc}[\rho]$ where ρ is a constant density $\rho = n =$ constant in space.

Idea: Approximate $E^{xc}[\rho] = \int d^3r\, \rho(\vec{r})\, \varepsilon^{xc}[\rho(\vec{r})]$, i.e., to each point in space we can associate energy density $\varepsilon^{xc}[\rho(\vec{r})]$, and it's value depends on charge density at $\rho(\vec{r})$. [does not depend on $\rho(\vec{r}\,' \neq \vec{r})$].

This approximation is called "Local density approximation" LDA.

From solution of UEG we know $\varepsilon^{xc}[\rho]$ hence we can now solve DFT equations.

We are looking for the minimum of the functional $E[\rho]$ under constraint that K.S. orbitals are normalized. Hence we can perform constraint minimization:

$$\frac{\delta E}{\delta \rho} - \sum_i \varepsilon_i \left(\int \psi_i^*(\vec{r}) \psi_i(\vec{r}) d^3r - 1 \right) = 0$$

Note that $\frac{\delta}{\delta \rho}$ can be written as $\frac{\delta \psi_k^*(\vec{r})}{\delta \rho} \frac{\delta}{\delta \psi_k^*(\vec{r})}$

$$0 = \frac{\delta}{\delta \psi_k^*}\left(E[\rho] - \varepsilon_i \int \psi^* \psi\right) = \frac{\delta}{\delta \psi_k^*}\left\{ \sum_{i \in occ} \int \psi_i^*(\vec{r}) \left(-\frac{\nabla^2}{2m} + V_{nuc}(\vec{r}) - \varepsilon_i\right) \psi_i(\vec{r}) + E^H[\rho] + E^{xc}[\rho] \right\}$$

$$= \left(-\frac{\nabla^2}{2m} + V_{nuc}(\vec{r}) - \varepsilon_k\right) \psi_k(\vec{r}) + \left(\frac{\delta E^H[\rho]}{\delta \rho} + \frac{\delta E^{xc}[\rho]}{\delta \rho}\right) \frac{\delta \rho}{\delta \psi_k^*}$$

Define $\frac{\delta E^H[\rho]}{\delta \rho} \equiv V^H[\rho]$ $\qquad V^H[\rho] = \int \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|} d^3r'$

$\frac{\delta E^{xc}[\rho]}{\delta \rho} = V^{xc}[\rho]$ $\qquad V^{xc}[\rho] = \varepsilon^{xc}(\rho) + \rho \cdot \frac{\delta \varepsilon^{xc}}{\delta \rho}$

hence:

$$\left(-\frac{\nabla^2}{2m} + V_{nuc}(\vec{r}) + V^H_{(\vec{r})} + V^{xc}_{(\vec{r})} - \varepsilon_k\right) \psi_k(\vec{r}) = 0$$

This is Schroedinger equation for a non-interacting system. Note that DFT is "interacting theory" because $V^{xc}[\rho]$ has to be computed self-consistently. All correlations are hidden in this $V^{xc}(\vec{r})$ function.

Note that this is actually a Dyson equation for the Kohn-Sham green's function

$$\left.\begin{aligned} (G^0)^{-1} &\equiv \omega + \mu + \frac{\nabla^2}{2m} - V_{nuc}(\vec{r}) \\ \Sigma(\vec{r}, \vec{r}') &= [V^H(\vec{r}) + V^{xc}(\vec{r})]\, \delta(\vec{r} - \vec{r}') \\ G(\vec{r}, \vec{r}') &= \sum_k \psi_k(\vec{r}) \frac{1}{\omega + \mu - \varepsilon_k} \psi_k^*(\vec{r}') \end{aligned}\right\}$$

$$(G^{0-1} - \Sigma)\, G =$$

$$\sum_k \Big[\omega + \mu + \underbrace{\frac{\nabla^2}{2m} - V_{nuc}(\vec{r}) - V^H - V^{xc}}_{-\varepsilon_k}\Big] \psi_k(\vec{r}) \frac{1}{\omega + \mu - \varepsilon_k} \psi_k^*(\vec{r}')$$

$$\sum_k \psi_k(\vec{r}) \frac{\omega + \mu - \varepsilon_k}{\omega + \mu - \varepsilon_k} \psi_k^*(\vec{r}') = \delta(\vec{r} - \vec{r}')$$

because ψ_k are a complete basis.

We proved that $(\mathcal{G}_0^{-1}-\Sigma)\mathcal{G}=1 \implies \mathcal{G}^{-1}=\mathcal{G}_0^{-1}-\Sigma$ hence

this equation defines the Dyson equation for $\mathcal{G}=\sum_k \psi_k(\vec{r})\frac{1}{\omega+\mu-\varepsilon_k}\psi_k^*(\vec{r})$

One can define a functional of this green's function $\mathcal{G}(\vec{r},\vec{r}')$, which gives identical equations to DFT, but it becomes than an approximation for excitations, not just the ground state properties.

The functional is:

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

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

Optimizing the functional $\frac{\delta\Gamma}{\delta\mathcal{G}}=0$ gives

$$0=\frac{\delta\Gamma}{\delta\mathcal{G}} = \mathcal{G}^{-1}-\mathcal{G}_0^{-1}+\frac{\delta\rho}{\delta\mathcal{G}}\frac{\delta}{\delta\rho}\left(E^H[\rho]+E^{xc}[\rho]\right)$$

$$= \mathcal{G}^{-1}-\mathcal{G}_0^{-1}+(V^H+V^{xc})\,\delta(\vec{r}-\vec{r}')\,\delta(\tau-\tau')$$

hence $\Sigma(\vec{r}\tau,\vec{r}'\tau') = (V^H(\vec{r})+V^{xc}(\vec{r}))\,\delta(\vec{r}-\vec{r}')\,\delta(\tau-\tau')$ which exactly shows that $\Gamma[\mathcal{G}]$ delivers the same DFT equations and the same solution. But here we get $\mathcal{G}(\vec{r},\tau)$ as approximation to the single particle green's function (band structure), not just the ground state properties.

However, even if the exact $E^{xc}[\rho]$ is known this functional is still an approximation for the spectra. We will show later what is the exact $E^{xc}[\mathcal{G}]$ later in this chapter, and we will contrast it with $E^{xc}[\rho]$.

Most often used approximations include GGA and meta-GGA's, hybrids, DFT+U, DFT+DMFT, ...

- GGA: The functional is parametrized with more freedom, and $\varepsilon^{xc}(\vec{r})$ depends on $\rho(\vec{r})$ as well as $\nabla\rho(\vec{r})$, i.e.,

$$E^{xc}[\rho] = \int \varepsilon^{xc}[\rho(\vec{r}), \nabla\rho(\vec{r})]\, \rho(\vec{r})\, d^3r$$

A few conservation-laws and exact relation are used to determine unknown coefficients.

- meta-GGA: $\varepsilon^{xc}(\vec{r})$ is allowed to depend on the kinetic energy part $\varepsilon^{xc}(\rho(\vec{r}), \nabla^2\psi_k(\vec{r}))$

- DFT+U: Functional depends on the density matrix of the "correlated orbitals" of a heavy atom:

$$E^{xc}[\rho, N^{\vec{R}}_{LL'}]$$

where $N^{\vec{R}}_{LL'} = \sum_{k \in occ.} \int d^3r\, d^3r'\, \psi_k^*(\vec{r})\, Y_L(\widehat{r-R})\, \delta(r-r')\, Y_{L'}(\widehat{r'-R})\, \psi_k(\vec{r}')$

One obtains an Anderson-like impurity model, which is solved by the mean-field.

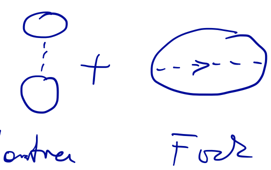
- DFT+DMFT: Functional depends on the single particle Green's function of the "correlated orbitals" or "correlated clusters".

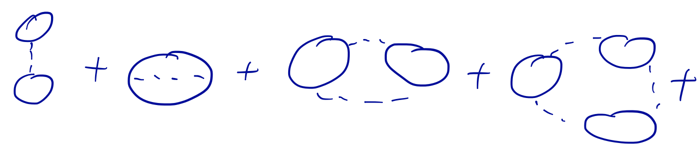
$$E^{xc}[\rho, \hat{P}\,\mathcal{G}(\vec{r}, \vec{r}')]$$

$\hat{P}\,\mathcal{G}(\vec{r}, \vec{r}') = \sum_{\alpha,\beta} \phi_\alpha(\vec{r})\, \mathcal{G}_{\alpha\beta}(\omega)\, \phi_\beta^*(\vec{r}')$ where α, β are the important degrees of freedom treated by DMFT. The generalized Anderson impurity model needs to be solved numerically by an impurity solver. A true many body problem remains to be solved.

Back to search for better functionals

- DFT probably is the most succesful functional, and is a functional of $\rho(\vec{r})$, therefore by the construction can give only ground state properties of the system. No excitation spectra available.
- Functionals of the Green's function can give the ground state, as well as the single particle excitation spectra. They can be defined by the Feynman diagrammatic technique.

  The simplest is the Hartree-Fock theory: $\Phi =$ 

  or GW : $\Phi =$ 

- Exact functional can be expressed in terms of Feynman diagrams and is known. But difficult to evaluate. In principle can give an exact solution to the many body problem.

Generating stationary functionals of physical observables

We will borrow the concept from statistical physics. We add the source term, and then perform the Legendre transform to obtain a stationary functional at constant value of the physical observable.

Example 1: Stationary functional at constant density is the free energy functional. If the particle number is not conserved, we work with Gibbs free energy (in this context it means in the presence of the source field $\mu \hat{N}$).

- Source field $H \to H - \mu \hat{N}$ where $\mu \hat{N}$ is the source field
- The free energy in the presence of the source term is the Gibbs free energy

$$\Omega[\mu] = F[N] - \mu N$$

— Legendre transform to eliminate the source (μ) in favor of observable N.

where

$$e^{-\beta \Omega[\mu]} = Z = \mathrm{Tr}\left(e^{-\beta(H-\mu N)}\right)$$

Then $$\frac{\delta \Omega}{\delta \mu} = -\frac{1}{\beta}\frac{\mathrm{Tr}\left(e^{-\beta(H-\mu N)}\hat{N}\right)\beta}{Z} = -\langle \hat{N} \rangle \equiv -N$$

- The functional $F[N]$ is the Legendre transform of the Gibbs free energy and is stationary at constant particle number.

$$F[N] = \Omega[\mu] + \mu N$$

$$\delta F[N] = \delta\Omega[\mu] + \delta\mu N + \mu \delta N = -N\delta\mu + N\delta\mu + \mu\delta N = \mu \delta N$$

hence $\frac{\delta F[N]}{\delta N} = \mu$ and vanishes when source term μN is absent.

$$\left(\frac{\delta F[N]}{\delta N} = 0\right)$$

Example 2: A single particle observable $\hat{O}$.

- Source field $H - \mu N \to H - \mu N + u\hat{O}$
  (u ↗ source, $\hat{O}$ ↑ observable)

- Free energy in the presence of the source term is the Gibbs free energy:

$$e^{-\beta\Omega[u]} = Z = \mathrm{Tr}\left(e^{-\beta(H-\mu N) - \beta u \hat{O}}\right)$$

$$\Omega[u] = F[\langle O\rangle] + u\langle O\rangle$$

Legendre transform to eliminate the source in favor of the observable.

Then $$\frac{\delta\Omega}{\delta u} = +\frac{\mathrm{Tr}(e^{\cdots}\cdot O)}{\beta Z}\beta = \langle O\rangle$$

- The stationary functional $F[O]$ at constant observable O is

$$F[\langle O\rangle] = \Omega[u] - u\langle O\rangle$$

and small variation $\delta F[O] = \delta\Omega[u] - u\,\delta O - O\,\delta u = -u\,\delta O$

hence F is functional of O and it is stationary when u is set to zero.

$$\left.\frac{\delta F}{\delta O}\right|_{u=0} = 0$$

Example 3: Introduce spatial and time dependent source term to get functional of the Green's function G.

- Source field: $S \to S + \int dx\, dx'\, \psi^+(x)\, j(x,x')\, \psi(x')$

  here x stands for $(\vec{r}, \tau)$

- The Gibbs free energy in the presence of the field is

$$e^{-\beta\Omega[j]} = Z = \int D[\psi^+\psi]\, e^{-S - \int dx\, dx'\, \psi^+(x)\, j(x x')\, \psi(x')}$$

$$\frac{\delta\Omega}{\delta j(x',x)} = -\frac{1}{\beta}\frac{1}{Z}\int D[\psi^+\psi]\, e^{-S-\int\cdots}\, \psi^+(x')\,\psi(x) = \frac{1}{\beta}\langle\psi(x)\,\psi^+(x')\rangle = -G(x\, x')\frac{1}{\beta}$$

- The stationary functional $\Gamma[\mathcal{G}]$ at constant physical observable $\mathcal{G}$ is

$$\Gamma[\mathcal{G}] = \beta\Omega[\mathcal{J}] + Tr(\mathcal{G}\cdot\mathcal{J}) = \beta\Omega[\mathcal{J}] + \int dx\, dx'\, \mathcal{G}(x,x')\, \mathcal{J}(x',x)$$

We eliminated the source $\mathcal{J}$ in favor of the observable $\mathcal{G}$ in the functional.

The variation of Γ is:

$$\delta\Gamma[\mathcal{G}] = \beta\,\delta\Omega[\mathcal{J}] + \int dx\, dx' \left[\delta\mathcal{G}(x,x')\,\mathcal{J}(x',x) + \mathcal{G}(x,x')\,\delta\mathcal{J}(x',x)\right]$$

$$\beta\,\delta\Omega[\mathcal{J}] = \frac{1}{\beta}\iint\left(-\mathcal{G}(x,x')\,\delta\mathcal{J}(x',x)\right)dx\,dx'$$

hence $\delta\Gamma[\mathcal{G}] = Tr(\mathcal{J}\,\delta\mathcal{G})$

and $\left.\frac{\delta\Gamma[\mathcal{G}]}{\delta\mathcal{G}}\right|_{\mathcal{J}=0} = 0$

Γ is a functional of $\mathcal{G}$! At $\mathcal{J}=0$ is stationary.
At $\mathcal{J}=0$ $\Gamma[\mathcal{G}]$ has a value of free energy.
The later is clear from the fact that at $\Omega[\mathcal{J}=0] = F = \frac{1}{\beta}\Gamma[\mathcal{G}]\Big|_{\mathcal{J}=0}$.

<u>Note on higher order correlation functions</u>

Higher order derivatives of Ω can give two-particle correlation function or free particle correlation functions...
If evaluated through derivative, they obey conservation laws.

$$\frac{\delta^2\Omega}{\delta\mathcal{J}(x_1,x_1')\,\delta\mathcal{J}(x_2,x_2')} = -\frac{\delta G(x_2',x_2)}{\delta\mathcal{J}(x_1,x_1')} = \frac{1}{\beta}\frac{\delta}{\delta\mathcal{J}(x_1,x_1')}\left(\frac{1}{Z[\mathcal{J}]}\int D[\psi^+\psi]\, e^{-S-\int dx\,dx'\,\psi^+(x)\mathcal{J}(x,x')\psi(x')}\,\psi(x_2')\psi^+(x_2)\right)$$

$$= \frac{1}{\beta}\frac{1}{Z[\mathcal{J}]}\int D[\psi^+\psi]\, e^{-S-\int dx\,dx'\,\psi^+(x)\mathcal{J}(x,x')\psi(x')}\,\psi(x_1')\psi^+(x_1)\,\psi(x_2')\psi^+(x_2)$$

$$-\frac{1}{\beta}\int D[\psi^+\psi]\, e^{-S-\cdots}\,\psi(x_2')\psi^+(x_2)\,\frac{1}{Z[\mathcal{J}]^2}\int D[\psi^+\psi]\, e^{-S\cdots}\,\psi(x_1')\psi^+(x_1)$$

$$= \langle T_\tau\psi(x_1')\psi^+(x_1)\,\psi(x_2')\psi^+(x_2)\rangle - \langle T_\tau\psi(x_2')\psi^+(x_2)\rangle\langle T_\tau\psi(x_1')\psi^+(x_1)\rangle$$

$\equiv L(1,2,1',2')$ the connected two particle correlation function

This is important to prove conservation laws.

One standard way of approximating functional $\Gamma[\mathcal{G}]$ is to use systematic expansion. (Thouless - Anderson - Palmer Eq. in spin glasses; chiral symmetry breaking in QCD)

We split the action in terms of the solvable part S^0 and the rest ΔS.

Then we write $S = S^0 + \lambda \Delta S + \iint \psi^{+} y \psi$

where λ is varied from 0 to 1.

At $\lambda=0$ we have solvable problem.

At $\lambda=1$ we have original interacting problem.

When we vary λ we keep $\mathcal{G}$ constant and add source field y so as to keep $\mathcal{G}$ fixed. At $\lambda=1$ we set $y=0$ so that $\mathcal{G}$ is the exact green's function of the interacting problem.

- At $\lambda=0$, we have $S = \underbrace{\iint \psi^{+} \mathcal{G}_0^{-1} \psi}_{S^0} + \iint \psi^{+} y_0 \psi = \iint \psi^{+} \underbrace{[\mathcal{G}_0^{-1} + y_0]}_{\mathcal{G}^{-1}} \psi$

The corresponding $\mathcal{G}^{-1} = \mathcal{G}_0^{-1} + y_0$

- At $\lambda=1$, we have $S = S^0 + \Delta S$ and we set $y_{\lambda=1} = 0$, so that $\Gamma_{\lambda=1}[\mathcal{G}]$ is the desired stationary functional.

At $\lambda=1$ we know that $\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \Sigma$, where Σ is the exact self-energy of the system.

To work at constant $\mathcal{G}$ we thus see that $y_0 = -\Sigma$

(y_0: source term at $\lambda=0$; $-\Sigma$: exact self energy)

Systematic expansion could be carried out:

$$\Gamma[G] = \Gamma_0[G] + \lambda \Gamma_1[G] + \cdots$$
$$\mathcal{Y}[G] = \mathcal{Y}_0[G] + \lambda \mathcal{Y}_1[G] + \cdots$$

We could use perturbation theory to determine order by order what is $\Gamma[G]$.

Alternatively, we can split

$$\Gamma[G] = \underbrace{\Gamma_0[G]}_{\Gamma_0 = \Gamma(\lambda=0)} + \underbrace{\Delta\Gamma[G]}_{\text{correction due to interactions.}}$$

<u>What is $\Gamma_0[G]$?</u>

$\Omega_0[\mathcal{Y}_0]$ can be calculated from:

$$e^{-\beta\Omega_0[\mathcal{Y}_0]} = \int D[\psi^\dagger,\psi]\, e^{-\iint \psi^\dagger [G_0^{-1} + \mathcal{Y}_0]\psi}$$ which is quadratic

and can be integrated by Gaussian integral

The result is $\int D[\psi^\dagger,\psi]\, e^{-\int \psi^\dagger G^{-1}\psi} = \operatorname{Det} G^{-1}$ therefore

$$-\beta\Omega_0[\mathcal{Y}_0] = \ln \operatorname{Det}(G_0^{-1} + \mathcal{Y}_0) = \operatorname{Tr}\ln G^{-1} = -\operatorname{Tr}\ln G$$

Indeed, for non-interacting system $\Omega_0 = -T\sum_{i\omega,\alpha} \ln(-i\omega + \varepsilon_\alpha)$ with $G^{-1} = i\omega - \varepsilon_\alpha$

Then we have

$$\Gamma_0[G] = \beta\Omega_0[\mathcal{Y}_0] + \operatorname{Tr}(G\mathcal{Y}_0) = \operatorname{Tr}\ln G - \operatorname{Tr}(\Sigma G)$$

(↑ because $\mathcal{Y}_0 = -\Sigma$)

<u>Finally at $\lambda = 1$ we write:</u> <u>$\Gamma[G] = \operatorname{Tr}\ln G - \operatorname{Tr}(\Sigma G) + \Delta\Gamma[G]$</u>

We will call $\Delta\Gamma[G] \equiv \Phi[G]$

At $\lambda=1$ we thus have: $\Gamma[\mathcal{G}] = \mathrm{Tr}\ln\mathcal{G} - \mathrm{Tr}(\Sigma\mathcal{G}) + \Phi[\mathcal{G}]$

where Φ is what is being added due to interactions.

We previously defined that at $\lambda=1$ $j=0$ (because $\mathcal{G}$ is the exact $\mathcal{G}$)

and therefore $\left.\frac{\delta\Gamma}{\delta\mathcal{G}}\right|_{\lambda=1} = 0$

Then: $\frac{\delta\Gamma}{\delta\mathcal{G}} = \underbrace{\frac{\delta}{\delta\mathcal{G}}(\mathrm{Tr}\ln\mathcal{G})}_{\mathcal{G}^{-1}} - \frac{\delta\Sigma}{\delta\mathcal{G}}\mathcal{G} - \Sigma + \frac{\delta\Phi}{\delta\mathcal{G}} = 0$

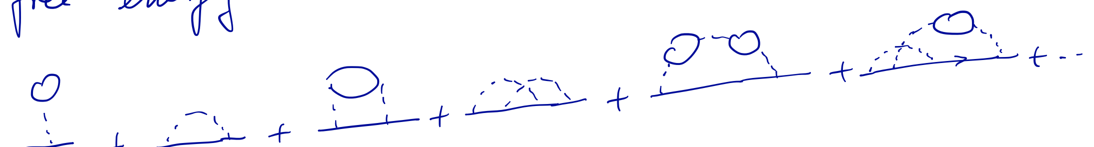
At $\lambda=1$ $\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \Sigma$ and hence: $\mathcal{G}^{-2} = +\frac{\delta\Sigma}{\delta\mathcal{G}}$ therefore:

$$0 = \frac{\delta\Gamma}{\delta\mathcal{G}} = \mathcal{G}^{-1} - \mathcal{G}^{-1} - \Sigma + \frac{\delta\Phi}{\delta\mathcal{G}} \quad \text{or} \quad \boxed{\Sigma = \frac{\delta\Phi[\mathcal{G}]}{\delta\mathcal{G}}}$$

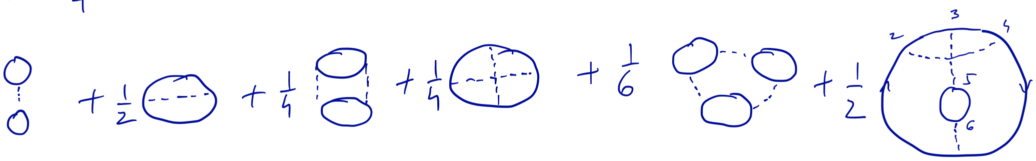
We just proved that $\Phi[\mathcal{G}]$ is generating functional for Σ, i.e., Σ is obtained by cutting $\mathcal{G}$ propagators in all possible ways.

Since Σ contains all skeleton diagrams, Φ has to contain all skeleton diagrams for the free energy.

Example: $\Sigma =$



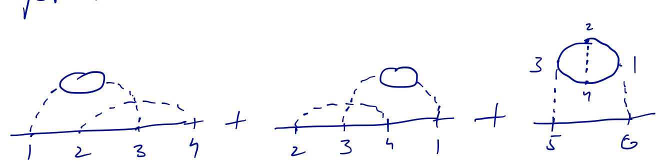
$\Phi =$



$\uparrow$ ϕ^0

Note that $\frac{\delta\phi^0}{\delta\mathcal{G}}$ generates several terms:

$\frac{\delta\phi^0}{\delta\mathcal{G}} =$



Alternative derivation with power counting (Chapter 8.8, R.M.)

We start with coupling constant integration

$$\hat{H} = \hat{H}_0 + \lambda \hat{V}_{int}$$

and $$e^{-\beta F} = Tr\left(e^{-\beta(H_0 + \lambda V_{int})}\right)$$

$$\frac{\delta F}{\delta \lambda} = +\frac{\beta}{\beta}\frac{1}{Z} Tr\left(e^{-\beta H}\hat{V}_{int}\right) = \langle V_{int} \rangle = \frac{1}{\lambda}\langle \lambda V_{int} \rangle$$

On page 13 we derived $\langle V_{int} \rangle = \frac{1}{2} Tr(\Sigma \mathcal{G})$ for general interacting system.

We can then write:

$$\frac{\delta F}{\delta \lambda} = \frac{1}{\lambda}\frac{1}{2} Tr(\Sigma_\lambda \mathcal{G}_\lambda)$$

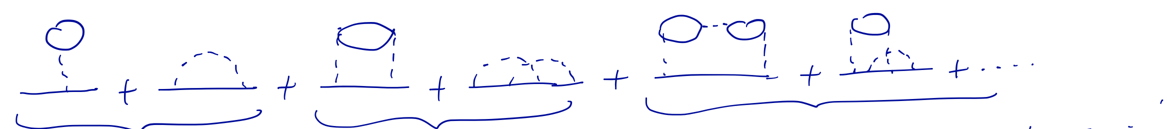
where both Σ and $\mathcal{G}$ need to be evaluated for each λ.

and $$F = F(\lambda=0) + \int_0^1 \frac{1}{2\lambda} Tr(\Sigma_\lambda \mathcal{G}_\lambda)$$

Power expansion of $\Sigma_\lambda[\mathcal{G}_\lambda, V_c]$ as derived by Baym-Kadanoff.

Using Feynman diagrams technique, one can expand self energy in powers:

$\Sigma =$



$n=1$: $\propto \lambda V_c$, $\lambda \Sigma^{(1)}[\mathcal{G}_\lambda, V_c]$

$n=2$: $\propto \lambda^2 V_c^2$, $\lambda^2 \Sigma^{(2)}[\mathcal{G}_\lambda, V_c]$

$n=3$: $\propto \lambda^3 V_c^3$, $\lambda^3 \Sigma^{(3)}[\mathcal{G}_\lambda, V_c]$

$+ \ldots$

Summary: $$\Sigma = \sum_{n=1}^{\infty} \lambda^n \Sigma^{(n)}[\mathcal{G}_\lambda, V_c].$$ Note Σ is functional of $\mathcal{G}_\lambda$ and V_c.

$$\Sigma' = \sum_{n=1}^{\infty} \lambda^n \Sigma^{(n)}[\mathcal{G}_\lambda, v_c]$$

by parts

$$\text{Then}: \Delta F = \frac{1}{2}\int_0^1 d\lambda \, \frac{\lambda^n}{\lambda} \, \mathrm{Tr}\left(\Sigma^{(n)}[\mathcal{G}_\lambda, v_c]\cdot \mathcal{G}_\lambda\right) = \sum_{n=1}^{\infty} \frac{\lambda^n}{2n} \mathrm{Tr}\left(\Sigma^{(n)}[\mathcal{G}_\lambda, v_c]\cdot\mathcal{G}_\lambda\right) - \sum_{n=1}^{\infty}\int_0^1 d\lambda \, \frac{\lambda^n}{2n} \frac{d}{d\lambda} \mathrm{Tr}\left(\Sigma^{(n)}[\mathcal{G}_\lambda, v_c]\cdot\mathcal{G}_\lambda\right)$$

by parts

$dv = d\lambda \, \frac{\lambda^{n-1}}{2}$ $\quad u = \mathrm{Tr}(\ldots)$

$v = \frac{\lambda^n}{2n}$ $\quad du = \frac{d}{d\lambda}\mathrm{Tr}(\ldots)$

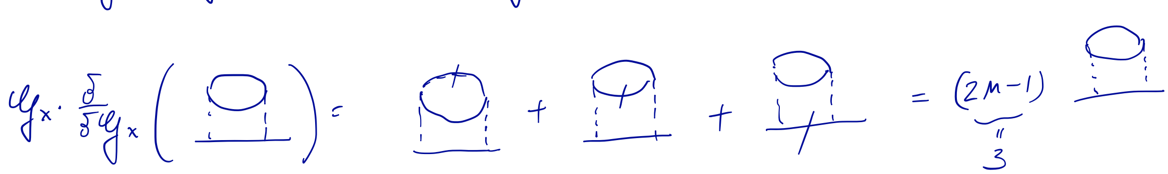
We define $\Phi[\mathcal{G}_\lambda] = \sum_{n=1}^{\infty} \frac{1}{2n} \mathrm{Tr}\left(\lambda^n \Sigma^n \cdot \mathcal{G}_\lambda\right)$ so that

$$\Delta F = \Phi[\mathcal{G}] - \sum_{n=1}^{\infty}\int_0^1 d\lambda \, \frac{\lambda^n}{2n} \mathrm{Tr}\left(\mathcal{G}_\lambda \frac{\delta \Sigma^{(n)}}{\delta \mathcal{G}^\lambda} \frac{\delta \mathcal{G}_\lambda}{\delta \lambda} + \Sigma^{(n)} \frac{\delta \mathcal{G}_\lambda}{\delta \lambda}\right)$$

Next we want to prove that $\frac{\delta \Phi}{\delta \mathcal{G}_\lambda} = \Sigma_\lambda$, i.e., Φ is the sum of skeleton free energy diagrams.

From definition follows: $\frac{\delta \Phi}{\delta \mathcal{G}_\lambda} = \sum_{n=1}^{\infty} \frac{\lambda^n}{2n}\left(\Sigma^n + \frac{\delta \Sigma^n}{\delta \mathcal{G}_\lambda}\cdot \mathcal{G}_\lambda\right) \stackrel{?}{=} \Sigma_\lambda$

Crucial point: $\frac{\delta \Sigma^n}{\delta \mathcal{G}_\lambda}\cdot \mathcal{G}_\lambda$ cuts one of the propagators and puts the same propagator back, hence we get back Σ^n. But there are many ways to cut, namely $(2n-1)$ ways.



It follows that: $\frac{\delta \Sigma^n}{\delta \mathcal{G}_\lambda}\cdot \mathcal{G}_\lambda = (2n-1)\,\Sigma^n$ and therefore $\frac{\delta \Phi}{\delta \mathcal{G}} = \sum_{n=1}^{\infty} \lambda^n \Sigma^n = \Sigma'$

as promised above.

Now continue with: $\Delta F = \Phi[\mathcal{G}] - \sum_{m=1}^{\infty} \int_0^1 d\lambda \frac{\lambda^m}{2m} \mathrm{Tr}\left(\underbrace{\underbrace{\mathcal{G}_\lambda \frac{\delta \Sigma^{(m)}}{\delta \mathcal{G}^\lambda}}_{(2m-1)\Sigma^{(m)}} \frac{\delta \mathcal{G}_\lambda}{\delta \lambda} + \Sigma^{(m)} \frac{\delta \mathcal{G}_\lambda}{\delta \lambda}}_{2m \Sigma^{(m)} \cdot \frac{\delta \mathcal{G}_\lambda}{\delta \lambda}} \right)$

hence $\Delta F = \Phi[\mathcal{G}] - \sum_{m=1}^{\infty} \int_0^1 d\lambda\, \lambda^m \mathrm{Tr}\left(\Sigma^{(m)} \frac{\delta \mathcal{G}_\lambda}{\delta \lambda}\right)$

which is

$$\Delta F = \Phi[\mathcal{G}] - \int_0^1 d\lambda\, \mathrm{Tr}\left(\Sigma_\lambda \frac{\delta \mathcal{G}_\lambda}{\delta \lambda}\right)$$

once more by parts! $F = \Phi[\mathcal{G}] - \mathrm{Tr}(\Sigma_\lambda \mathcal{G}_\lambda)\Big|_0^1 + \int_0^1 d\lambda\, \mathrm{Tr}\left(\frac{\delta \Sigma}{\delta \lambda} \mathcal{G}_\lambda\right)$

here $\Sigma(\lambda=0) = 0$ and $\Sigma(\lambda=1) \equiv \Sigma$ hence

$$\Delta F = \Phi[\mathcal{G}] - \mathrm{Tr}(\Sigma \mathcal{G}) + \int_0^1 d\lambda\, \mathrm{Tr}\left(\frac{\delta \Sigma}{\delta \lambda} \mathcal{G}_\lambda\right)$$

Now we guess the last integral $R(\lambda) = -\mathrm{Tr}(\ln(1 - \mathcal{G}_0 \Sigma_\lambda))$

$$\frac{dR(\lambda)}{d\lambda} = \mathrm{Tr}\left[(1 - \mathcal{G}_0 \Sigma_\lambda)^{-1} \mathcal{G}_0 \frac{\delta \Sigma_\lambda}{\delta \lambda}\right]$$

$$= \mathrm{Tr}\left[(\mathcal{G}_0^{-1} - \Sigma_\lambda)^{-1} \frac{\delta \Sigma_\lambda}{\delta \lambda}\right] = \mathrm{Tr}\left(\mathcal{G}_\lambda \frac{\delta \Sigma}{\delta \lambda}\right)$$

therefore $\int_0^1 d\lambda\, \mathrm{Tr}\left(\frac{\delta \Sigma}{\delta \lambda} \mathcal{G}_\lambda\right) = \int_0^1 \frac{dR}{d\lambda} d\lambda = R(1) - R(0) = -\mathrm{Tr}(\ln(1 - \mathcal{G}_0 \Sigma))$

Finally $F = F_0 + \Phi[\mathcal{G}] - \mathrm{Tr}(\Sigma \mathcal{G}) - \mathrm{Tr} \ln(\mathcal{G}_0 \mathcal{G}^{-1})$

and $F = \mathrm{Tr} \ln \mathcal{G} - \mathrm{Tr}(\Sigma \mathcal{G}) + \Phi[\mathcal{G}]$

To make it stationary functional of $\mathcal{G}$ we use $\Sigma = \mathcal{G}_0^{-1} - \mathcal{G}^{-1}$ to eliminate Σ in favor of $\mathcal{G}$:

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

Now we can check $\frac{\delta F}{\delta \mathcal{G}} = \mathcal{G}^{-1} - \mathcal{G}_0^{-1} + \frac{\delta \Phi}{\delta \mathcal{G}} = \mathcal{G}^{-1} - \mathcal{G}_0^{-1} + \Sigma = 0$

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 $\Phi[\mathcal{G}]$.

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

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

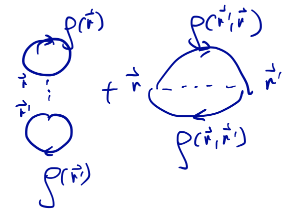
where ρ is diagonal part of $\mathcal{G}$ in space-time basis, i.e.,

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

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

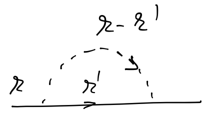
$$\rho(\vec r,\vec r') = \mathcal{G}(\vec r\tau, \vec r'\tau')\,\delta(\tau-\tau')$$

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

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



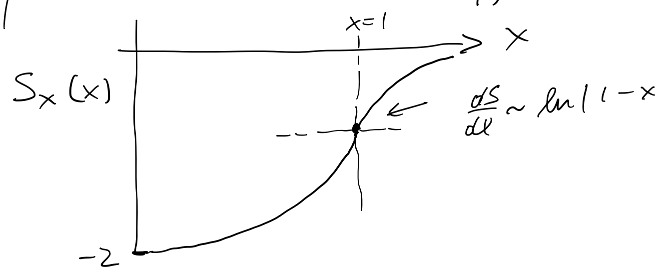
$$\Sigma_x^k = -\frac{1}{\beta}\sum_{k' i\omega} G_{k'}(i\omega)\, V_{k-k'} = -\int \frac{d^3k'}{(2\pi)^3} f(\varepsilon_{k'}) \frac{8\pi}{|\vec{k}-\vec{k}'|^2} = -\int \frac{dk'\, k'^2\, 2\pi}{(2\pi)^3} f(\varepsilon_{k'}) \int_{-1}^{1} \frac{dx\; 8\pi}{(k^2+k'^2-2kk'x)}$$

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

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

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

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



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 $\frac{d\Sigma}{d\omega}=0$

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

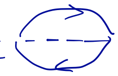
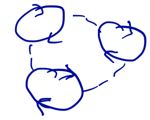
$$S_x'(x\sim 1) \approx \ln|1-x| + \text{const}\ldots \implies \frac{\partial \Sigma_k}{\partial k}\Big|_{k=k_F} \to \infty$$

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.

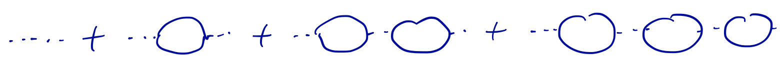
$$\Phi[\mathcal{G}] = E^H[\rho] + \frac{1}{2}$$  $$+\frac{1}{4}$$  $$+\frac{1}{6}$$  $$+ \cdots$$

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

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

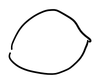
$$-\frac{1}{6}\mathrm{Tr}(v_c\cdot\mathcal{G}\cdot\mathcal{G}\cdot v_c\cdot\mathcal{G}\cdot\mathcal{G}\cdot v_c\cdot\mathcal{G}\cdot\mathcal{G}) - \cdots$$

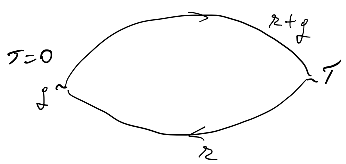
Can be rewriten in terms of the screened coulomb interaction W and $\mathcal{G}$:

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

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

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)



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

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

(2 ↑ spin deg.)

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

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

↑ 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 $P^0_{q\sim 0}(\tau) \simeq -2\int\frac{d^3k}{(2\pi)^3} f(\varepsilon_k)f(-\varepsilon_k)$

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

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

Conclusion: $W_q(\Omega\sim 0) \approx \dfrac{V_q}{1+V_q D(0)} = \dfrac{8\pi}{q^2 + 8\pi D(0)}$ 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: $V_q = \dfrac{8\pi}{q^2+\lambda}$

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

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

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

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

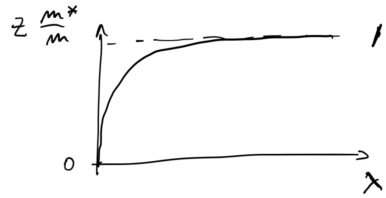
$$S_x\left(\frac{k}{k_F}\right) \equiv -\frac{1}{2kk_F}\int k'\,f(\varepsilon_{k'})\ln\left(\frac{(k+k')^2+\lambda}{(k-k')^2+\lambda}\right)dk'$$

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

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

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

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



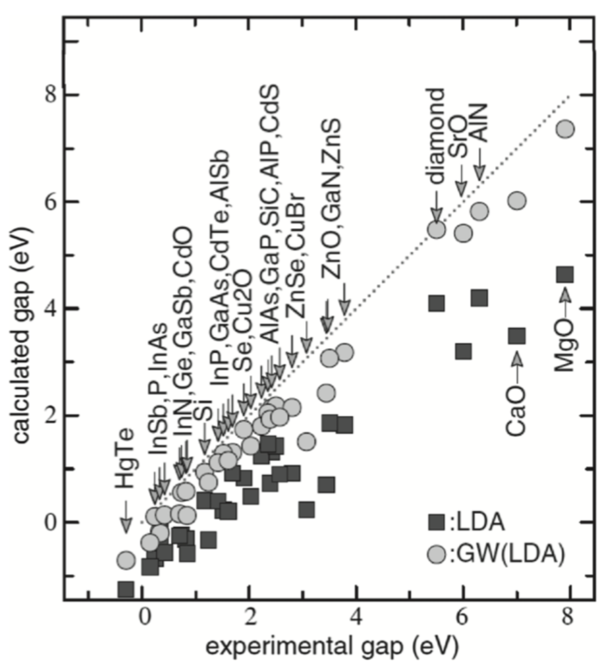
$$D(\lambda) = \frac{2+\lambda}{4}\ln\left(1+\frac{4}{\lambda}\right) - 1$$

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)

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

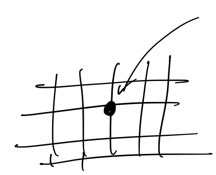
← sum over correlated ions at position $\vec{R}$ in solids. Needs projection of $\mathcal{G}$ to such a "correlated atom".

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

Example : single band Hubbard model :

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

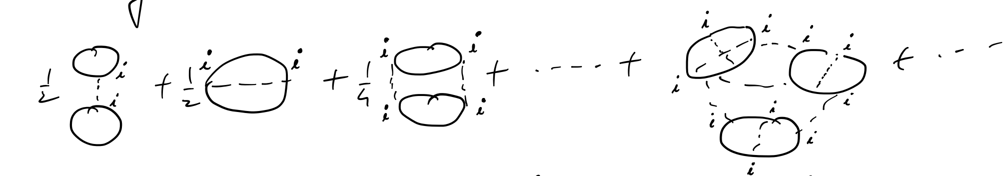
↑ lattice site



If the system is periodic $\mathcal{G}_{ii}(\omega) = \sum_k \mathcal{G}_k(\omega)$

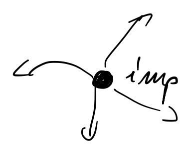
What is $\Phi^{exact}[\mathcal{G}_{ii}] = ?$

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



all possible Feynman diagrams.

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



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

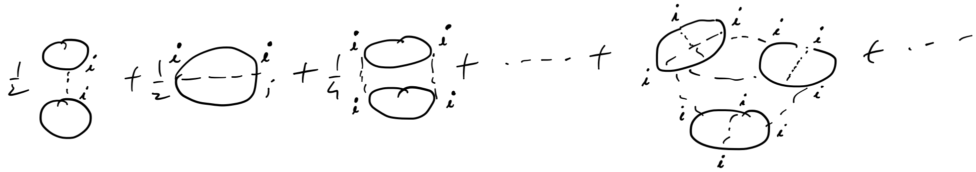
$$S = \int_0^\beta d\tau\, H_{local}(\tau) + \int_0^\beta d\tau \int_0^\beta d\tau'\, d^\dagger_{is}(\tau)\, \Delta_s(\tau-\tau')\, d_{is}(\tau')$$

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

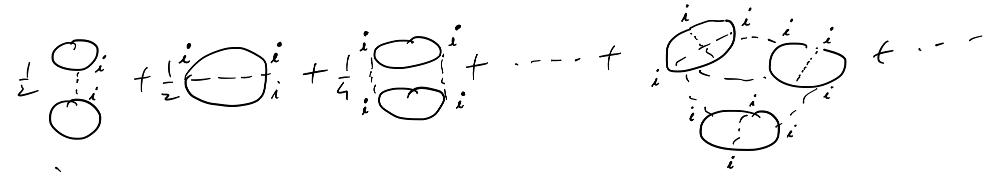
For the impurity we also have:

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

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



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



$i \equiv imp$

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 $E_{imp} = -\mu$

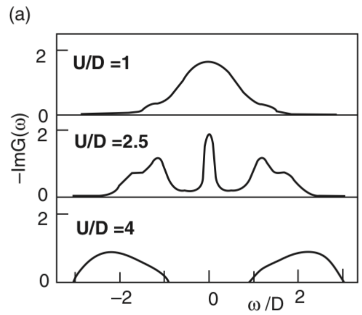
which delivers $\Sigma_{ii}(\omega)$, and can be plugged back to impurity solver.

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

$D \equiv$ half-bandwidth

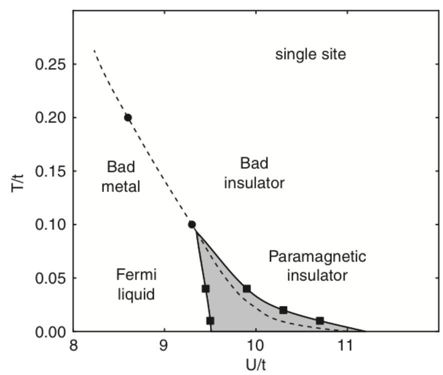
$U \equiv$ C.R.



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

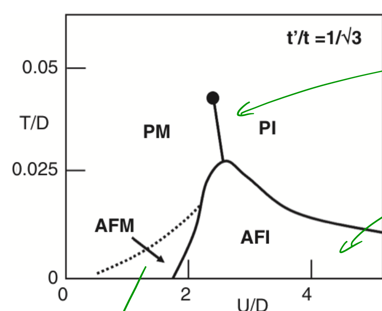
(2D = total bandwidth)

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

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:

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

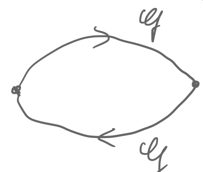
and the two particle response functions have to be calculated by

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

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

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

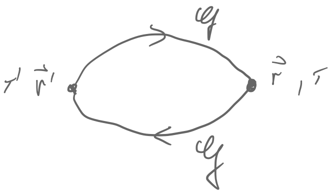
To understand what goes wrong with most approximations derived in different ways, we consider GW-like approximation, where the response function would be computed by the bubble, while the propagator $\mathcal{G}$ contains self-energy, i.e.,



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

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

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

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

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

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

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

conservation law requires

$$\partial_t\rho(\vec{r},\tau) + \vec{\nabla}_r\vec{j}(\vec{r},\tau) = 0$$

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

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

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

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

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

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

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

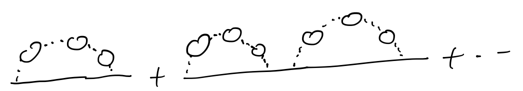
$$= 0$$

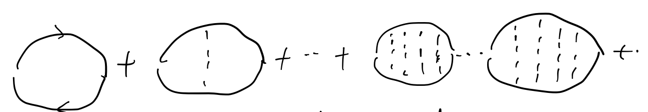
$$R_2(\vec r\tau,\vec r'\tau') = -\frac{1}{\beta^2}\int\frac{d^3k}{(2\pi)^3}\int\frac{d^3k'}{(2\pi)^3}\underbrace{\left(\Sigma_k(i\omega)-\Sigma_{k'}(i\omega')\right)\mathcal{G}_k(i\omega)\,\mathcal{G}_{k'}(i\omega')}_{\text{does not vanish for arbitrary }\Sigma\,!}\,e^{-i(\omega-\omega')(\tau-\tau')+i(\vec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

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

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 $\vec j$:

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

$$\langle\vec j(\vec r,t)\rangle = \frac{1}{2mi}\left\langle \psi^\dagger(r_2t_2)\,\vec\nabla_1\psi(r_1t_1) - \vec\nabla_2\psi^\dagger(r_2t_2)\,\psi(r_1t_1)\right\rangle = \frac{-i}{2mi}\left(\vec\nabla_1-\vec\nabla_2\right)G(1,2=1^+)$$

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 $\left.\begin{matrix} G_0^{-1}G = 1 + \Sigma G \\ G G_0^{-1} = 1 + G\Sigma \end{matrix}\right]$ hence $G_0^{-1}G - G G_0^{-1} = \Sigma G - G\Sigma$

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

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.

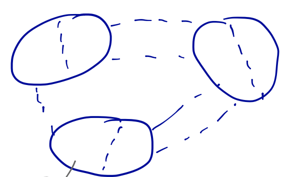
It turns out that this holds whenever $\Sigma(1,2) = \frac{\delta \Phi}{\delta G(2,1)}$ is the derived from the generating functional.

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

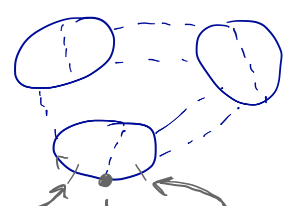


$\int d1 \int d2 \frac{\delta \Phi}{\delta G(2,1)} G(2,1)$ will cut one propagator and will put it back

↑ 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 $\Phi =$



$\int \frac{\delta \Phi}{\delta G(2,1)} G(2,1)$ — cuts one line

$\int G(1,2) \frac{\delta \Phi}{\delta G(1,2)}$ — cuts different line

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

Summary: If $\Sigma(1,2) = \frac{\delta \Phi}{\delta G(2,1)}$ 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 $\quad G\cdot G^{-1} = 1$

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

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

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

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

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

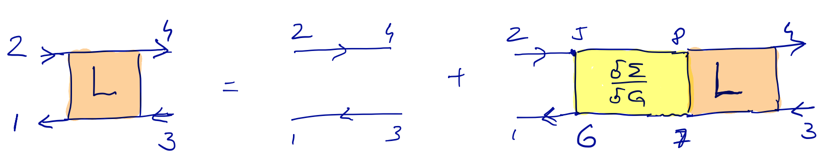
$$\frac{\delta \Sigma[G(y),v_c]}{\delta y} = \frac{\delta \Sigma}{\delta G}\frac{\delta G}{\delta y} : \quad \frac{\delta G(1,6)}{\delta y(3,4)} - G(1,3)\, G(4,6) - G(1,2)\frac{\delta \Sigma(2,5)}{\delta G(7,8)}\frac{\delta G(7,8)}{\delta y(3,4)} G(5,6) = 0$$

$6 \leftrightarrow 2$

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:

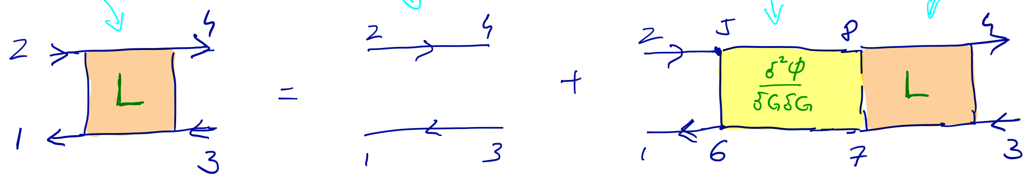


Note that $\frac{\delta \Sigma}{\delta G} = \frac{\delta^2 \Phi}{\delta G \delta G}$ is the second derivative of the generating functional. Hence Φ gives complete description of how to calculate the high-order correlation functions. In particular

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

Bethe Salpeter:

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

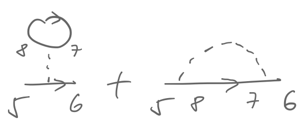


(1)

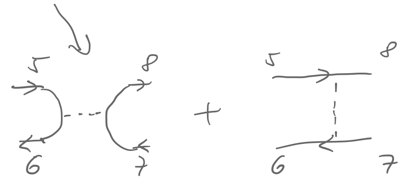
Example 1: Hartree-Fock for Σ

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

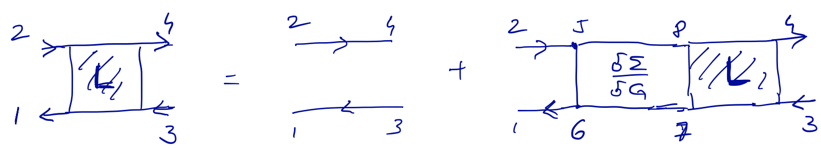
$\Sigma(6,5) =$



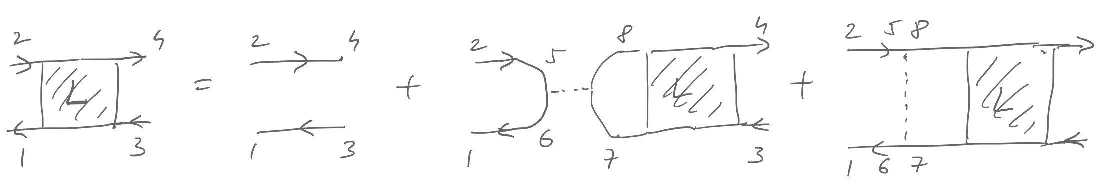
$\frac{\delta \Sigma(6,5)}{\delta G(78)} =$



General Bethe Salpeter:



For Hartree-Fock we get:



generates RPA bubbles

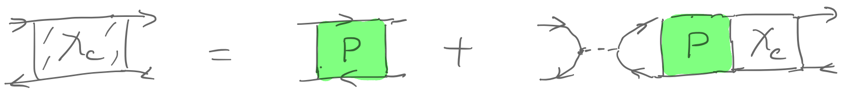
generates ladders

bubbles and ladders

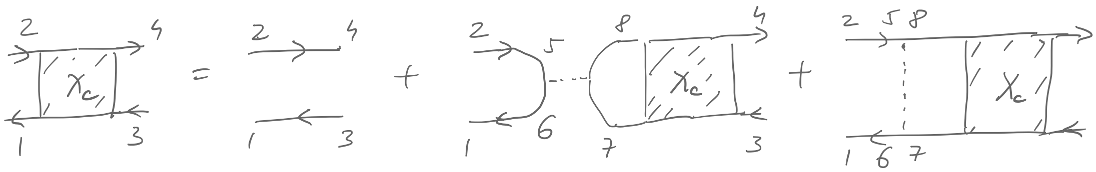
If we are interested in charge-charge correlation function χ_c, then the vertex is unity. We can then use a trick to pre-sum geometric series of diagrams by working with so-called polarization:

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

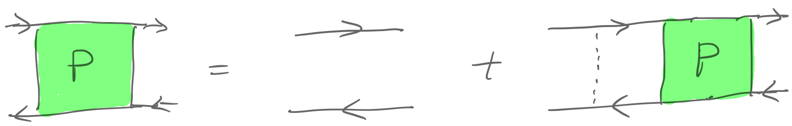
which is $\chi_c = P + v_c P \chi_c$ and diagrammatically



While



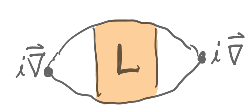
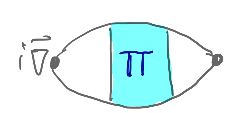
It should be clear that



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 $\frac{\delta \Phi^x}{\delta G}$.

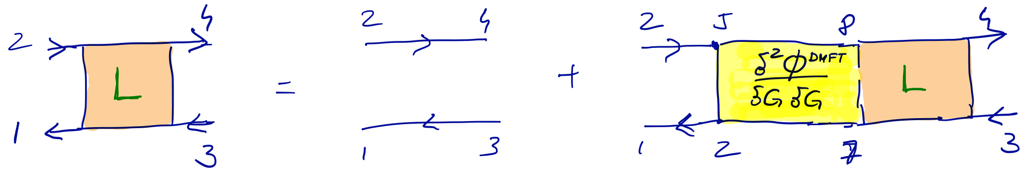
In another words, we manage to remove $\frac{\delta \Phi^H}{\delta G}$ from Bethe-Salpeter equation by concentrating on P rather than χ.

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.

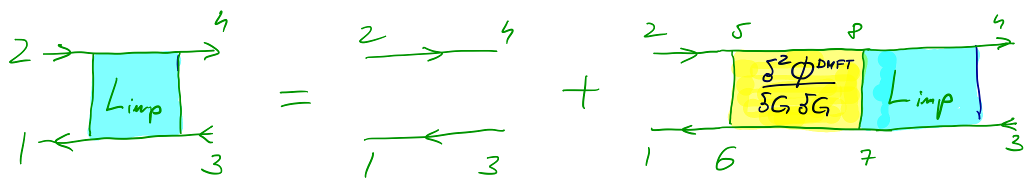
Note that this works for charge response, while optics (calculated by $\langle jj \rangle$ has extra vertices at the two ends  and requires slightly modified equations, involving the quantity !

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:



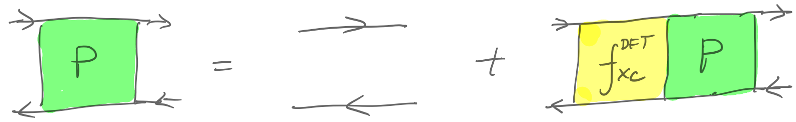
where: $L_{imp}(23,41) = -\langle T_\tau \psi_2^+ \psi_3^+ \psi_4 \psi_1 \rangle_{imp} + \langle T_\tau \psi_2^+ \psi_1 \rangle \langle T_\tau \psi_3^+ \psi_4 \rangle_{imp}$

and notice: G_{imp} (green arrow), $G_{lattice}$ (blue arrow)

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).

Note on constructing stationary functional of the Green's function

Definition of partition function: $Z = \int D[\psi^+\psi]\, e^{-S}$ where action $S = \int_0^\beta d\tau \left[\psi^+ \frac{\partial}{\partial\tau}\psi + H - \mu N\right]$

Definition of the Green's function (imaginary time) $G(\tau,\tau') = -\langle T_\tau \psi(\tau)\psi^+(\tau')\rangle$

1) Add source term to S: $S \to S + \int dx\, \psi^+(x)\, J(x,x')\, \psi(x')$

note $x = (\vec r, \tau)$ which is like conjugate field to "Landau order parameter".

Free energy in the presence of the field is a Gibbs free energy $\Omega[J] = F[G] - \mathrm{Tr}(G\cdot J)$ and can be calculated from the corresponding partition function Z

$$e^{-\beta\Omega[J]} = Z = \int D[\psi^+\psi]\, e^{-S - \int dx\, \psi^+(x) J(x,x')\psi(x')}$$

We then obtain:

$$\frac{\delta\Omega}{\delta J(x',x)} = -\frac{1}{\beta}\frac{1}{Z}\int D[\psi^+\psi]\, e^{-S-\int dx\, \psi^+ J \psi}(-\psi^+(x')\psi(x)) = \langle \psi(x)\psi^+(x')\rangle = -G(x,x')$$

The functional $F[G]$ is the Legendre transform of the Gibbs free energy and is $F[G] = \Omega[J] + \mathrm{Tr}(G\cdot J) \equiv \Omega[J] + \int dx\,dx'\, G(x,x')\, J(x'x)$

Then we have $\delta F[G] = \underbrace{\delta\Omega[J]}_{= -\mathrm{Tr}(G\delta J)} + \mathrm{Tr}(\delta G\, J + G\,\delta J) = \mathrm{Tr}(J\,\delta G)$

Then if source term is removed $J=0$, we have $\underline{\frac{\delta F}{\delta G} = J = 0}$

The free energy functional $F[G]$ is stationary with respect to G.