Lect 5 Perturbation theory of fermions

§ Free fermions

We will use operator formalism and path integral in parallel for comparison. For the imaginary time Green's function

$$\mathcal{G}_k = - T_\tau \langle | \hat{\psi}_k(\tau)\, \psi_k^\dagger(\tau') | \rangle ,$$

and in the path integral: $\mathcal{G}_k = - \langle \psi_k(\tau) \bar{\psi}_k(\tau') \rangle$ based on the partition function:

$$Z_0 = \int D\bar{\psi}_k\, D\psi_k\, \exp\left[- \int_0^\beta d\tau\, \bar{\psi}_k(\tau) \left[\partial_\tau + \xi_k \right] \psi_k(\tau) \right]$$

Then $\mathcal{G}_k(\tau,\tau') = - (\partial_\tau + \xi_k)^{-1}_{\tau,\tau'}$ ← continous matrix

The continous matrix should be understood as

$$\boxed{\begin{array}{l} \text{identity } \delta(\tau-\tau'), \text{ and matrix product:} \\ \displaystyle\int_0^\beta d\tau' \, (\partial_\tau + \xi_k)_{\tau,\tau'}\, \mathcal{G}_k(\tau',\tau'') = -\sum_n \delta(\tau - \tau'' - n\beta)\, (-)^n \end{array}}$$

due to the anti-periodic boundary condition

what's $(\partial_\tau)_{\tau\tau'}$?

$$(\partial_\tau)_{\tau\tau'} = \lim_{\epsilon\to 0} \frac{\delta(\tau-\tau') - \delta(\tau-\epsilon-\tau')}{\epsilon} \quad \text{plug in}$$

$$(\xi_k)_{\tau\tau'} = \xi_k\, \delta(\tau-\tau')$$

$$\Rightarrow \boxed{(\partial_\tau + \xi_k)\, \mathcal{G}_k(\tau-\tau') = -\sum_n \delta(\tau-\tau'-n\beta)\, (-)^n}$$

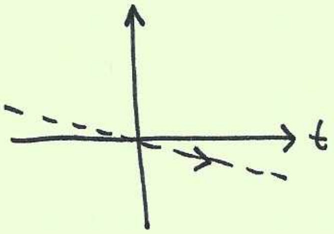
Fourier transform $\mathcal{G}_k(\tau-\tau') = \frac{1}{\beta} \sum_{i\omega_n} \mathcal{G}_k(i\omega_n)\, e^{-i\omega_n(\tau-\tau')}$

$$\Rightarrow \mathcal{G}_k(i\omega_n) = \frac{1}{i\omega_n - \xi_k}$$

$\longrightarrow$ real time / time ordered $\quad Z_0 = \int D\bar{\psi}_k(\tau)\, D\psi_k(\tau)\; e^{i\int dt\, \mathcal{L}_0}$

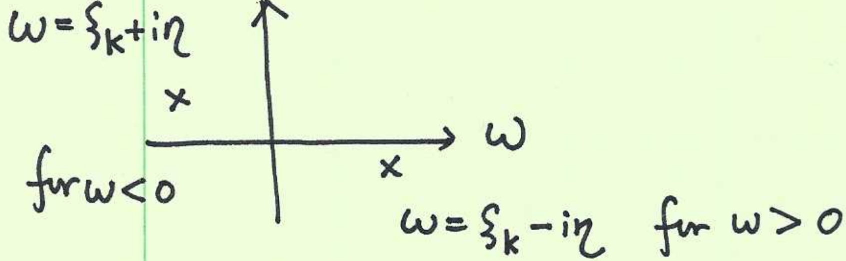
where $\mathcal{L}_0 = i\bar{\psi}_k(t)\,\partial_t \psi_k(t) - \bar{\psi}_k \xi_k \psi_k$

$$i G_k(t\,t') = T\langle |\hat{\psi}_k(t)\, \hat{\psi}^{\dagger}_k(t')| \rangle = \langle \psi_k(t)\, \bar{\psi}_k(t') \rangle = -\left(i(i\partial_t - \xi_k)\right)^{-1}_{t,t'}$$



$t \to t(1-i\eta) \;\to\; \omega \to \omega(1+i\eta)$

$$\to G_k(\omega) = \frac{1}{i(-i\omega(1+i\eta)) - \xi_k} = \frac{1}{\omega - \xi_k + i\,\mathrm{sgn}(\omega)\cdot\eta}$$



- Retarded $\quad i\omega_n \to \omega + i\eta$

$$i G^R(t,t') = \Theta(t-t')\langle |\{\psi_k(t)\, \psi^{\dagger}(t')\}| \rangle \Rightarrow G^R(\omega) = \frac{1}{\omega - \xi_k + i\eta}$$

§ Perturbation theory

Consider a system with Hamitonian H, we have defined time-ordered Green's function in the last lecture

$G(t_2,t_1) = -i\langle\Omega|T\hat{O}_2(t_2)\hat{O}_1(t_1)|\Omega\rangle$ where $|\Omega\rangle$ is the ground state of H. we have also showed that it can be expressed as path integrals as

$$iG(t_2,t_1) = \frac{\int D\bar{\psi}D\psi\ O_2(\bar{\psi}(t_2),\psi(t_2))\,O_1(\bar{\psi}(t_1),\psi(t_1))\,e^{i\int \mathcal{L}\,dt}}{\int D\bar{\psi}D\psi\ e^{i\int \mathcal{L}\,dt}}$$

[We extend to fermion and many-body system].

Now, we decompose $H = H_0 + H_I$, and assume H_I is small.

then $\mathcal{L} = \bar{\psi}(i\partial_t\psi - H = \bar{\psi}(i\partial_t)\psi - H_0 - H_I = \mathcal{L}_0 + \mathcal{L}_I$

where $\mathcal{L}_I = -H_I$. But remember that H_0 and H_I originally are operators, but when we write Lagrangian, operators become Complex field or grassman field. To simplify notation, we often do not distinguish carefully.

Now, we will develope a perturbation theory using $\mathcal{L}_I$ as small quantity.

we define $Z = \int D\bar{\Psi} D\psi \; e^{i\int dt\, \mathcal{L}} = \int D\bar{\Psi} D\psi \; e^{i\int dt\, \mathcal{L}_0 + \mathcal{L}_I}$

and $Z_0 = \int D\bar{\Psi} D\psi \; e^{i\int dt\, \mathcal{L}_0}$. Then

$$\frac{Z}{Z_0} = \frac{\int D\bar{\Psi} D\psi \; e^{i\int dt\, \mathcal{L}_0} \sum_{n=0}^{\infty} \frac{i^n}{n!}\left[\int dt\, \mathcal{L}_I\right]^n}{\int D\bar{\Psi} D\psi \; e^{i\int dt\, \mathcal{L}_0}} = \sum_{n=0}^{\infty} \frac{i^n}{n!} \left\langle \left(\int dt\, \mathcal{L}_I\right)^n \right\rangle_0$$

where $\langle \cdots \rangle_0$ means averging with respect to Z_0.

We can re-exponetialized

$$\frac{Z}{Z_0} = \left\langle e^{i\int dt\, \mathcal{L}_I} \right\rangle_0 = \exp\left[1 + \left\langle i\int dt\, \mathcal{L}_I \right\rangle_0 + \frac{1}{2!}\left\{ \left\langle \left(i\int dt\, \mathcal{L}_I\right)^2 \right\rangle - \left\langle i\int dt\, \mathcal{L}_I \right\rangle^2 \right. \right.$$

$$+ \cdots$$

$$\Rightarrow \ln \frac{Z}{Z_0} = 1 + \left\langle i\int dt\, \mathcal{L}_I \right\rangle_0 + \frac{1}{2!}\left\{ \left\langle \left(i\int dt\, \mathcal{L}_I\right)^2 \right\rangle_0 - \left(\left\langle i\int dt\, \mathcal{L}_I \right\rangle_0 \right)^2 \right\} + \frac{1}{3!} \cdots$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \left\langle \left(i\int dt\, \mathcal{L}_I\right)^n \right\rangle_{0,\text{ connected}}$$

$$= \left\langle e^{i\int dt\, \mathcal{L}_I} \right\rangle_{0,\text{ connected}}$$

$\longleftarrow$ Linked cluster expansion.

Let us assume the interaction takes the form of

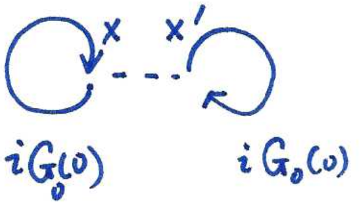
$$\int dt\, \mathcal{L}_I = \int dx\, dx'\; \bar{\psi}(x)\, \bar{\psi}(x')\, V(x-x')\, \psi(x')\, \psi(x)$$ here $x = (\vec{x}, t)$

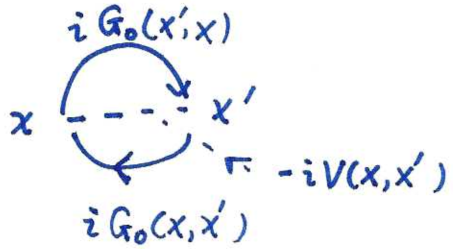
The first order contribution

$$\frac{Z}{Z_0} = 1 + \left\langle \int dx\, dx'\; \bar{\psi}(x)\bar{\psi}(x')\,(-i\, V(x-x'))\,\psi(x')\,\psi(x) \right\rangle_0 + \cdots$$

$$= 1 + \int dx\, dx' \;(-i\, G_0(0))\,(-i V(x,x'))\,(-i\, G_0(0))$$

$$+ \int dx\, dx' \;(-i\, G_0(x-x'))\,(-i V(x,x'))\,(i\, G_0(x'-x)) + \cdots$$





§ Self-energy and interaction:

$$i\, G_{\alpha\beta}(x,t) = \frac{\int D\bar{\psi} D\psi\;\; \psi_\alpha(x\,t)\, \bar{\psi}_\beta(0\,0)\; e^{i\int dt\, \mathcal{L}}}{\int D\bar{\psi} D\psi\;\; e^{i\int dt\, \mathcal{L}}},$$

restore electron spin index

where $\mathcal{L} = i\, \bar{\psi}_\alpha \partial_t \psi_\alpha - H$.

$$= \frac{\left[\int D\bar{\psi} D\psi\;\; \psi_\alpha(x,t)\, \bar{\psi}_\beta(0,0)\, e^{i\int dt\, \mathcal{L}_{int}}\; e^{i\int dt\, \mathcal{L}_0}\right] / Z_0}{\left[\int D\bar{\psi} D\psi\;\; e^{i\int dt\, \mathcal{L}_{int}}\;\; e^{i\int dt\, \mathcal{L}_0}\right] / Z_0}$$

$$= \langle \psi_\alpha(xt)\bar{\psi}_\beta(00)\, e^{i\int dt\, L_{int}} \rangle_0 \,/\, \langle e^{i\int dt\, L_{int}} \rangle_0$$

$$= \langle \psi_\alpha(x,t)\bar{\psi}_\beta(00)\, e^{i\int dt\, L_{int}} \rangle_{0,\ \text{connected}}$$

First order

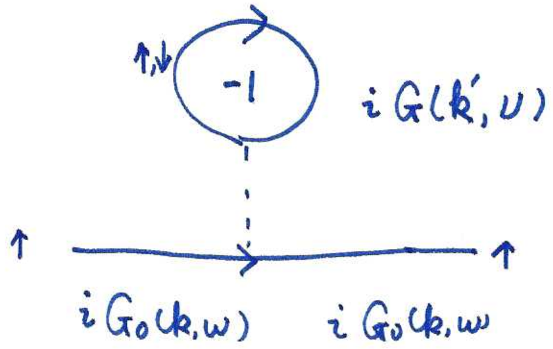
if spin is conserved

$$i G_{\alpha\beta}(xt)\,\delta_{\alpha\beta} = \langle \psi_\alpha(xt)\bar{\psi}_\beta(00)\rangle + \langle \psi_\alpha(xt)\bar{\psi}_\beta(00)\,(-i)\int dt'\, H_1(t') \rangle_{0,\ \text{connect}}$$

$\Rightarrow$

$$iG_{\alpha\beta}(k\omega) = i\,G_0(k,\omega) + (-)\,(i G_0(k,\omega))^2\,(-iV(0))\,\frac{1}{V}\sum_{k'\alpha'}\int\frac{d\nu}{2\pi}\, i\,G_0(k',\nu)\, e^{i0^+\nu}$$

$$+ (i\,G_0(k,\omega))\,\frac{1}{V}\sum_q\int\frac{d\nu}{2\pi}\, i\,G_0(k-q,\omega-\nu)\,(-iV(q))\, e^{-i0^+\nu}$$

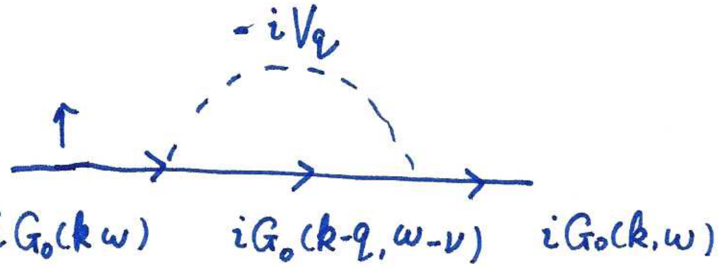


$$(-i)\quad \psi(k,t')\,\bar{\psi}(k,t)\,\frac{1}{2V}\sum \bar{\psi}(k_1+q,t'')\,\bar{\psi}(k_2-q,t'')\,V(q)\,\psi(k_2,t'')\,\psi(k,t'')$$

Four points: ① $q=0$, ② $\frac{1}{2}\times 2$, ③ spin summation, ④ overall $(-)$ sign

④ $$\langle \bar{\psi}(k_2, t'')\,\psi(k_2 t'')\rangle \longrightarrow -T\langle \psi(k_2, t''-0^+)\,\psi(k_2,t'')\rangle$$

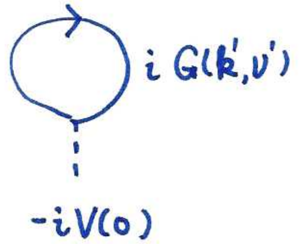
$$= -\int\frac{d\nu}{2\pi}\,\psi(k_2,\nu)\, e^{-i\nu(-0^+)}$$



$$iG(k,\omega) = iG_0(k,\omega) + \left[iG_0(k,\omega)\right]^2 \left(-i\,\Sigma(k,\omega)\right)$$

where
$$-i\Sigma(k,\omega) = (-)\,\frac{-iV(q=0)}{V} \sum_{k'\alpha'} \int \frac{d\nu}{2\pi}\, iG_0(k',\nu)\, e^{i0^+\nu}$$
$$+ \frac{1}{V} \sum_{q} \int \frac{d\nu}{2\pi}\, iG_0(k-q,\omega-\nu)\,(-iV_q)\, e^{-i0^+\nu}$$

$\Rightarrow -i\,\Sigma^{(1)}(k,\omega) =$



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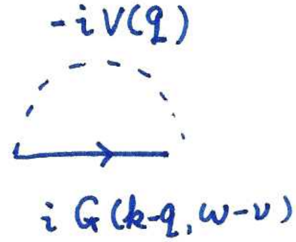
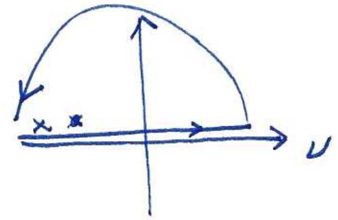


$$iG(k,\omega) = iG_0(k,\omega) \sum_{n=0}^{\infty} \left[(iG_0(k,\omega))(-i\,\Sigma(k,\omega))\right]^n$$
$$= \frac{1}{\left[iG_0(k,\omega)\right]^{-1} + (-i)\,\Sigma(k,\omega)}$$

$$G(k,\omega) = \frac{1}{G_0(k,\omega) - \Sigma(k,\omega)} = \frac{1}{\omega - \xi_k - \Sigma(k,\omega) + i\,\mathrm{sgn}(\omega)\,\eta}$$

HF level

$$\int \frac{d\nu}{2\pi}\, i\, G_0(k',\nu)\, e^{i0^+\nu} = i\int \frac{d\nu}{2\pi} \frac{1}{\nu - \xi_{k'} + i0^+ \mathrm{sgn}\,\nu}\, e^{i0^+\nu} = -\Theta(-\xi_{k'}) = -n_{k'}$$



$$\int \frac{d\nu}{2\pi}\, i\, G_0(k-q,\omega-\nu)\, e^{-i0^+\nu} = -\Theta(-\xi(k-q)) = -n_{k-q}$$

$$\boxed{\Sigma(k,\omega) = V_0\rho_0 + \frac{1}{V}\sum_q (-n_{k-q})\, V(q)}$$ ← H-F self-energy

cancel the background charge

For Coulumb potential $V(q) = \dfrac{4\pi e^2}{q^2}$

$$\Sigma_{Fock} = -\frac{1}{(2\pi)^3}\int_0^{\Theta(k'<k_F)} d\vec{k}'\, \frac{4\pi e^2}{|\vec{k}-\vec{k}'|^2},$$

define $\vec{q} = \vec{k}' - \vec{k}$

$k'^2 = k^2 + q^2 + 2kq\cos\theta$

$$= -\frac{4\pi e^2}{(2\pi)^3}\cdot 2\pi \int_0^{+\infty} dq \int_{-1}^{1} d\cos\theta\; \Theta(k_F^2 - (k^2+q^2+2kq\cos\theta))$$

$$= -\frac{2e^2}{\pi} k_f\, \frac{1}{2}\int_0^{\infty} dz \int_{-1}^{1} d\cos\theta\; \Theta(1-(x^2+z^2+2xz\cos\theta))$$

$$= -\frac{2e^2}{\pi} k_f\, F(x)$$, where $F(x) = \frac{1}{2}\int_0^{\infty} f(z)\,dz$, and

$$f(z) = \begin{cases} 2 & |x+z|<1 \\ \dfrac{1-(x-z)^2}{2x} & \text{otherwise} \\ 0 & |x-z|>1 \end{cases}$$

$$F(x) = \frac{1}{2} + \frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right|$$

where $z = \dfrac{q}{k_f}$, $x = \dfrac{k}{k_f}$.

Excerise: we can also use Matsubara representation

$$\mathcal{G}(k, ik_n) = \mathcal{G}^0(k, ik_n) + \mathcal{G}^0(k, ik_n)\,\Sigma(k, ik_n)\,\mathcal{G}(k, ik_n)$$

and then $\mathcal{G}(k, ik_n) = \dfrac{1}{ik_n - \xi_k - \Sigma(k, ik_n)}$

at HF level

$$\Sigma_{HF}(k, ik_n) = \frac{1}{V}\sum_{k', ik_n'} \frac{2V(0)}{ik_n' - \xi_{k'}} + \frac{1}{V}\sum_{q, q_n} \frac{1}{i(k_n - q_n) - \xi_{k-q}} V(q)$$

$$= \int \frac{d\vec{k}'}{(2\pi)^3} V(q=0)\, n_f(\xi_{k'}) - \int \frac{d\vec{q}}{(2\pi)^3} V(q)\, n_f(k-q)$$

which the same as before.

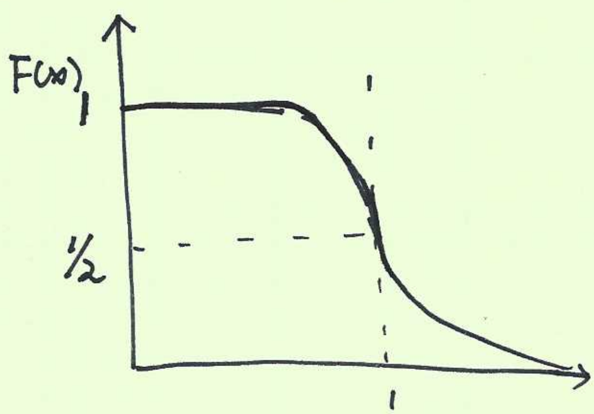
However, HF results have significant problem — artificial divergence of Fermi velocity

$$\delta \varepsilon_{HF}(k) \sim e^2 (k - k_f) \ln\left|\frac{k - k_f}{k_f}\right| ,$$

velocity shift $\delta v(k) = \hbar^{-1}\dfrac{\partial \delta\varepsilon}{\partial k} \sim \ln\left|\dfrac{k_f}{k - k_f}\right| \to \infty .$

→ suppression of density of states (DOS)

and $C \sim \dfrac{T}{\ln\left(\frac{T_F}{T}\right)}$ ← factor of DOS suppression.



More about HF: HF-method is to use <u>an optimized free fermion</u> wave function to approximate an interacting system!

$\underbrace{\text{wave function}}_{\text{(slater determinant-like WF)}}$

use $\Psi_{HF} = c^{+}_{i_1\sigma_1} c^{+}_{i_2\sigma_2} \cdots c^{+}_{i_\ell \sigma_\ell} |0\rangle$ to minimize

$$\langle \Psi_{HF} | H | \Psi_{HF} \rangle - \sum_{i\sigma} \lambda_{i\sigma} \int dr\, \phi^*_{i\sigma} \phi_{i\sigma}$$ ← basis of the operater $c^{+}_{i\sigma}$.

HF self-ansistent Eq

$$\left\{ -\frac{\hbar^2}{2m} \nabla_i^2 + \int d\vec{r}\, \frac{\left(\sum_{j\sigma'} n_{j\sigma'} |\phi_j(r')|^2\right)}{|\vec{r}-\vec{r}'|} \right\} \phi_{i\sigma}(r)$$

$$- \sum_j n_{j\sigma} \int d\vec{r}'\, \frac{\phi^*_{j\sigma}(\vec{r}')\, \phi_{j\sigma}(\vec{r})}{|\vec{r}-\vec{r}'|}\, \phi_{i\sigma}(\vec{r}') = \lambda_{i\sigma} \phi_{i\sigma}(r)$$

↑ HF-self energy

$$\lambda_{i\sigma} = \frac{\delta E}{\delta n_{i\sigma}}$$

For homogenous system, the HF wave function is the same as the free Fermi surface. In other words, HF wavefunction is a free fermion WF, <u>no correlation</u>. Any wave function which is not a slater determinat has <u>correlation effect!</u> (Say, Laughlin WF)

HF wavefunction correctly describes that electrons with the same spin avoid each other, but does not describle electron with opposite spin also have correlation!

Exchange hole

$$\langle HF|\, \rho_\sigma(r)\, \rho_{\sigma'}(r')\, |HF\rangle = \sum_{ij} n_{i\sigma} n_{j\sigma'} \left\{ |\varphi_{k_i}(r)|^2 |\varphi_{k_j}(r)|^2 - \delta_{\sigma\sigma'}\, \varphi^*_{k_i}(r)\, \varphi^*_{k_j}(r')\, \varphi_{k_j}(r)\, \varphi_{k_i}(r') \right\}$$

$$\langle HF|\, \rho_\sigma(r)\, \rho_{\sigma'}(r')\, |H_F\rangle - \langle HF|\, \rho_\sigma(r)\, |HF\rangle \langle HF|\, \rho_{\sigma'}(r')\, |H_F\rangle$$

$$= -\delta_{\sigma\sigma'} \sum_{ij} \cancel{\delta_{\sigma\sigma'}}\, \varphi^*_{k_i}(r)\, \varphi^*_{k_j}(r')\, \varphi_{k_j}(r')\, \varphi_{k_i}(r) = -\frac{1}{V^2} \sum_{kk'} e^{i(k-k')(r-r')}\, n_k n_{k'}$$

$$= -\delta_{\sigma\sigma'} \left| \frac{1}{(2\pi)^3} \int d\vec{k}\; e^{i\vec{k}\cdot(\vec{r}-\vec{r}')}\, \theta(k_F - k) \right|^2 = \underbrace{-}_{\delta_{\sigma\sigma'}} \left[\frac{+1}{2\pi^2 |r-r'|} \frac{d}{d|r-r'|} \left(\frac{\sin k_f |r-r'|}{|r-r'|} \right) \right]^2$$

$$= -\delta_{\sigma\sigma'} \left(\frac{n}{2}\right)^2 9 \left(\frac{x \cos x - \sin x}{x^3} \right)^2 \qquad \text{where} \quad x = k_f |r-r'|$$

Near an electron, it has less possibility to find another electron with the same spin!