Oct. 18th. Green Function

classical Green Function:

$$\nabla_r^2 \phi = -\frac{1}{\varepsilon_0}\rho(r) \quad \phi: \text{certain boundary}$$

First we solve electron-dot-like $\phi$

$$\nabla_r^2 G(r) = \delta(r). \quad ①$$

So that original function is:

$$\phi(r) = -\frac{1}{\varepsilon_0}\int dr' G(r-r')\rho_e(r')$$

Function ① is solved as:

$$G(r) = -\frac{1}{4\pi r}$$

So that $\phi(r)$ can be solved as:

$$\phi(r) = \frac{1}{4\pi\varepsilon_0}\int dr' \frac{1}{|r-r'|}\rho(r')$$

For Schodinger Equation:

$$i\hbar\partial_t \psi(r.t) = \hat{H}\psi(r.t)$$

$$(-i\hbar\partial_t + \hbar^2/2m\,\nabla^2)\psi(r.t) = V(r.t)\psi(r.t).$$

First we solve Green Function like:

$$(-i\hbar\partial_t + \hbar^2/2m\,\nabla_r^2)G(r.t.r't') = \delta(r-r')\delta(t-t')$$

So that original function is:

$$\psi(r.t) = \int G_0(rtr't')\psi(r't')V(r'.t')\,dr'dt'$$

Altogether. Green Function has the form like

$$G = \langle r|e^{-i/\hbar H(t-t')}|r'\rangle$$

$$= \langle rt|r't'\rangle$$

In Eigenbasis $H|n\rangle = E_n|n\rangle$

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$$G(rtr't') = \sum_n \langle r | e^{-i/\hbar \mathcal{H}(t-t')} | n \rangle \langle n | r' \rangle$$
$$= \sum_n \varphi_n(r)\varphi_n^*(r) \exp[-i/\hbar E_n (t-t')]$$
$$G(r.r'.E) = \int G(rtr't') e^{i/\hbar E(t-t')} d(t-t')$$
$$= \sum_n \frac{\varphi_n(r)\varphi_n^*(r)}{E_n \cdots -}$$

Green Function for many-body systems:

First we introduce three representations:

① Schrodinger Representation: $\mathcal{H}$ irrelavant with $t$.

$$i\partial_t \varphi(t) = \hat{\mathcal{H}}\varphi(t) \qquad \varphi(t) = e^{-i\mathcal{H}t}\varphi(0)$$

② Heisenberg Representation: $O_H(t) = e^{i\mathcal{H}t} O_S(t) e^{-i\mathcal{H}t}$

$i\partial_t O_H(t) = [O_H(t).\mathcal{H}]$ with unchanged $\varphi(0)$

$$\langle \varphi(0) | O_H(t) | \varphi(0) \rangle = \langle \varphi(t) | O_S(0) | \varphi(t) \rangle$$

③ Interaction Representation:

$$\hat{\varphi}(t) = e^{i\mathcal{H}_0 t} e^{-i\mathcal{H}t} \varphi(0)$$
$$\hat{O}(t) = e^{i\mathcal{H}_0 t} O_S e^{-i\mathcal{H}_0 t}$$
$$\langle \hat{\varphi}(t) | \hat{O}(t) | \hat{\varphi}(t) \rangle = \langle \varphi(0) | O_H(t) | \varphi(0) \rangle \text{ unchanged}$$
$$\partial/\partial_t \hat{\varphi}(t) = -i \hat{V}(t) \hat{\varphi}(t)$$

Def. $\hat{U}(t) = e^{i\mathcal{H}_0 t} e^{-i\mathcal{H}t} \qquad \partial_t U(t) = -i V(t) U(t)$

$$U(t) - U(0) = -i\int_0^t dt_1 \cdot \hat{V}(t_1)\, \cancel{U(t_1)}\, \underbrace{U(t_1)}_{\to \left[1 - i\int_0^{t} dt_2 V(t_2)\right]}$$

Taylor Expand $t(1/n) \cdots$

$$U(t) = \sum_0^\infty (-i)^n \int_0^t dt_1 \int_0^{t_1} dt_2 \cdots \int_0^{t_{n-1}} dt_n\, \hat{V}(t_1) \cdots V(t_n).$$

Introduce time-ordering operator : $\hat{T}$

$$T(V(t_1)V(t_2)V(t_3)) = V(t_3)V(t_1)V(t_2) \quad t_3 > t_1 > t_2$$

Step Function

$$\theta(x) = \begin{cases} 1 & x > 0 \\ 1/2 & x = 0 \\ 0 & x < 0 \end{cases}$$

$$T[V(t_1)V(t_2)] = \theta(t_1 - t_2)V(t_1)V(t_2) + \theta(t_2 - t_1)V(t_2)V(t_1)$$

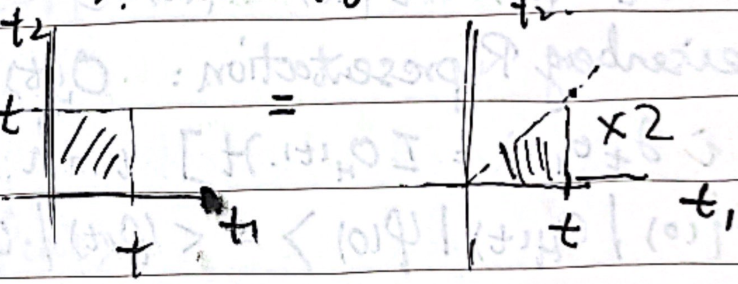
Therefore:

$$\frac{1}{2!}\int_0^t dt_1 \int_0^t dt_2 \hat{T}[V(t_1)V(t_2)]$$

$\Rightarrow \int_0^t dt_2\, \theta(t_1 - t_2)$ $\quad \int_0^{t_1}$ ✓ and $\int_{t_1}^{t_2}$ ✗ $\theta(t_1 - t_2)$ $t_2 > t_1$ is Ze

$$\Rightarrow \frac{1}{2!}\int_0^t dt_1 \int_0^{t_1} dt_2 \hat{V}(t_1)\hat{V}(t_2) + \frac{1}{2!}\int_0^t dt_2 \int_0^{t_2} dt_1 \hat{V}(t_2)\hat{V}(t_1)$$

$$= \int_0^t dt_1 \int_0^{t_1} dt_2 \hat{V}(t_1)\hat{V}(t_2)$$



Therefore

$$U(t) = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!}\left(\int_0^t dt_1 \cdots \int_0^t dt_n\right) T[V(t_1)\cdots V(t_n)]$$

$$= T\left[\exp\left(-i\int_0^t dt_1 V(t_1)\right)\right]$$

S-Matrix $\quad \varphi(t) = U(t)\varphi(0)$

$$\varphi(t') = S(t, t')\varphi(t')$$

$$\Rightarrow S(t, t') = U(t)U^{\dagger}(t')$$

① $S(t, t) = \hat{I}$

② $S^{\dagger}(t, t') = S(t', t)$

③ $S(t, t')S(t', t'') = S(t, t'')$

$\partial_t S(t.t') = -i\hat{V}(t) S(t.t')$

Therefore: $S(t.t') = T\left[\exp\left(-i\int_{t'}^{t} dt_1 V(t_1)\right)\right]$

$= 1 + \sum_{n=1} \frac{(-i)^n}{n!}\left(\int_{t'}^{t} dt_1 \int_{t'}^{t} dt_2 \cdots\right) T[V(t_1)\cdots V(t_n)]$

1) Further we Assume $\varphi_S(0) = \varphi_H(0) = \varphi_I(0) = |GS\rangle$ of $H$: $\varphi(0)$

2) Assume: Gell Mann ~~as~~ low theorem.

$\varphi(0) = S(0,-\infty)\phi_0 \rightarrow |GS\rangle$ of $\underline{\underline{H_0}}$

[At $V(t=0)$, is $\varphi(0)$]. [At $(-\infty)$ $V=0$], we introduce $V$ very slowly so that $\varphi$ can always be ground state. finally ~~until~~ we arrive $(t=0)$. similar to adiabatic theorem.

3) Assume: $\varphi(\infty) = S(\infty.0)\varphi(0) = \phi_0 e^{iL}$

V won't last long. very slowly it reduces to zero where system remains $|GS\rangle$, changed by a uniform transform $e^{iL}$.

$e^{iL} = \langle\phi_0|S(\infty,-\infty)|\phi_0\rangle$

Now we can have:

Green Function at $T=0$ for fermion:

$G(\lambda.t-t') = -i\langle T[C_\lambda(t) C_\lambda^\dagger(t')]\rangle$

$\lambda$: eg: lattice position $i$. $\langle|\rangle$ average over GS of $H$

$C_\lambda(t) =$ Heisenberg $e^{iHt} C_\lambda e^{-iHt}$

If $\lambda$ eigenenergy of $H$. ie:

$H C_\lambda^\dagger|GS\rangle = \varepsilon_\lambda C_\lambda^\dagger|GS\rangle$

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$$G(\lambda.\ t>t') = -i\ \langle GS|\ e^{iHt} C_\lambda e^{-iHt} e^{iHt'} C_\lambda^\dagger e^{-iHt'}\ |GS\rangle$$

$$= -i\ e^{-i(t-t')(\varepsilon_\lambda - \varepsilon_0)}$$

$$G(\lambda.\ t<t') = +i \langle GS|\ \underbrace{C_\lambda^\dagger(t')\ C_\lambda(t)}_{\text{Exchange Fermion } \times(-1)}\ |GS\rangle$$

We change to Interaction Representation

$$C_\lambda(t) = e^{iHt} e^{-iH_0t}\ \hat{C_\lambda}(t)\ e^{iH_0t} e^{-iHt}$$

$$= S(0.t)\ \hat{C_\lambda}(t)\ S(t.0)$$

$$G(\lambda.\ t\text{-}t') \qquad {}_{H_0}\langle GS| = {}_{H}\langle GS|\ S(-\infty.0) \cdots$$

$$= \cancel{i\theta(t-t')}\ {}_0\langle GS|\ S(-\infty,0)\ S(0.t)\ \hat{C_\lambda}(t)\ S(t.0)\ S(0.t')\ \hat{C}_\lambda^\dagger(t')\ S(t'.0)\ S(0$$

$$+ i\theta(t-t')\ {}_0\langle GS|\ S(-\infty.0)\ S(0.t')\ \hat{C}_\lambda^\dagger(t')\ S(t'.0)\ S(0.t)\ C_\lambda(t)$$

$$S(t.0)\ S(0,-\infty)\ |GS\rangle_0$$

where $\quad {}_{H_0}\langle GS|\ S(-\infty.0) = e^{-iL}\ {}_0\langle GS|\ S(\infty,-\infty)\ S(-\infty.0)$ $\qquad \varphi(-\infty) \quad \varphi(\infty)$

$$= {}_0\langle GS|\ \cancel{S(\infty,-\infty)} = \cancel{{}_0\langle GS|\ \ -\infty=+\infty\ \text{the same}}\ |GS$$

$$\Rightarrow \frac{{}_0\langle GS|\ S(\infty,0)}{{}_0\langle GS|\ S(\infty,-\infty)\ |GS\rangle_0}$$

$$\Rightarrow G(\lambda.\ t\text{-}t') = \frac{-i}{{}_0\langle GS|\ S(\infty,-\infty)\ |GS\rangle_0} \times \left[\ \overset{\theta(t-t')}{(\text{un})} - \overset{\theta(t'-t)\times}{(\text{un})}\ \right]$$

① ${}_0\langle GS|\ S(\infty.t)\ \hat{C_\lambda}(t)\ S(t.t')\ \hat{C}_\lambda^\dagger(t')\ S(t',-\infty)\ |GS\rangle_0$ First term.

② ${}_0\langle GS|\ S(\infty.t')\ \hat{C}_\lambda^\dagger(t')\ S(t'.t)\ \hat{C_\lambda}(t)\ S(t,-\infty)\ |GS\rangle_0$ Second term.

First term:

$$\theta(t-t')\ {}_0\langle Gs|T[C_\lambda(t)C^{+}_{\lambda'}(t')S(\infty,-\infty)]|Gs\rangle_0 \quad (t>t').$$

Second term can be also expressed under [T]. Therefore:

$$G(\lambda.t-t') = -i\frac{{}_0\langle Gs|T[C_\lambda(t)C_{\lambda'}(t')S(\infty,-\infty)]|Gs\rangle_0}{{}_0\langle Gs|TS(\infty,-\infty)|Gs\rangle_0}$$

We transfer $|Gs\rangle$ to $|Gs\rangle_{H_0}$ under free-fermion basis. with introducing $\hat{T}$, Green Function under $|Gs\rangle_{H_0}$ basis is much easier to solve without $\overset{\text{interaction}}{V_0}$, we calculate:

$$G^{(0)}(\lambda.t-t') = -i\,{}_0\langle Gs|T[\hat{C}_\lambda(t)\hat{C}^{+}_\lambda(t')]|Gs\rangle_0$$

We want to expand $G$ over $G^{(0)}$ where $S(V=0)=1$.

① Empty Band: $C_\lambda|Gs\rangle_0=0$ with No Fermi Seas Under.

$$G^{(0)}(\lambda.t-t') = -i\theta(t-t')e^{-i\varepsilon_\lambda(t-t')}$$

$$\Rightarrow G^{(0)}(\lambda.\omega) = \int_R dt\, e^{i\omega t}G(\lambda.t)$$

$$= \int_R dt\, -i\theta(t)e^{-i\varepsilon_\lambda t}e^{i\omega t} \longrightarrow$$

we introduce $\left[\lim_{\delta\to 0} e^{i(\omega-\varepsilon_\lambda+i\delta)t}\right]$ to solve the integral with $\delta$ a decay parameter.

$$= \frac{1}{\omega-\varepsilon_\lambda+i\delta}$$

Cauchy-主值 integral.

$\delta$ is a small positive. $G^{(0)}(\lambda.\omega) = \underbrace{P\left[\frac{1}{\omega-\varepsilon_\lambda}\right]}_{\text{主值}} \underbrace{-i\pi\delta(\omega-\varepsilon_\lambda)}_{\text{虚部}}$

for $f$: complex function:

$$\left[\lim_{\varepsilon\to 0}\right]\int_a^b \frac{f(x)}{x+i\varepsilon}dx = -i\pi f(0) + \overset{\text{主値}}{P}\left[\int_a^b \frac{f(x)}{x}dx\right]$$

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② Fermi Sea. Def: $\eta_K = \varepsilon_K - \mu$ $P_F$: Fermi Momentum.

$${}_0\langle GS| C_k^\dagger C_k |GS\rangle = \theta(P_F - k)$$

$${}_0\langle GS| C_k C_k^\dagger |GS\rangle = \theta(k - P_F).$$

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$$H = \sum_\lambda \varepsilon_\lambda C_\lambda^\dagger C_\lambda \text{ where } \varepsilon_\lambda = [\varepsilon_\lambda] - \mu$$

$$C_\lambda(t) = e^{iHt} C_\lambda e^{-iHt}.$$

$$G^{(0)}(\lambda, t-t') = -i[\theta(t-t')\theta(\varepsilon_\lambda) - \theta(t'-t)\theta(-\varepsilon_\lambda)] e^{-i\varepsilon_\lambda(t-t')}$$

$$= -i\,\theta(\varepsilon_\lambda)\int_0^\infty dt\, e^{it(\omega - \varepsilon_\lambda + i\delta)} - \theta(-\varepsilon_\lambda)\int_0^\infty e^{it(\omega - \varepsilon_\lambda - i\delta)}\, d$$

$$= \frac{\theta(\varepsilon_\lambda)}{\omega - \varepsilon_\lambda + i\delta} + \frac{\theta(-\varepsilon_\lambda)}{\omega - \varepsilon_\lambda + -i\delta}$$

$$= \frac{1}{\omega - (\varepsilon_\lambda - \mu) + i\delta_K} \qquad \delta_K = \delta \cdot \mathrm{sgn}(\underset{\varepsilon_\lambda - \mu}{\varepsilon_\lambda - \mu})$$

For phonons:

G: Def: $D(q, \lambda, t-t') = -i\, {}_0\langle GS| T \hat{A}_{q\lambda}(t) \hat{A}_{-q\lambda}(t') |GS\rangle_0$

$$A_{q\lambda} = a_{q\lambda} + a^\dagger_{-q\lambda} \quad \lambda: \text{polarization of phonons.}$$

$$D(q, t-t') = -i \frac{{}_0\langle T \hat{A}_q(t) \hat{A}_{-q}(t) S(\infty, -\infty) |\rangle_0}{{}_0\langle S(\infty, -\infty)\rangle_0}$$

$$D^0(q, t-t') = -i\, {}_0\langle | T \hat{A}_q(t) \hat{A}_{-q}(t) |\rangle_0$$

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similar as discussed above:

$$= -i\, {}_0\langle |(a_q e^{-i\omega_q t} + a_q^\dagger e^{i\omega t})(a_q e^{-i\omega_q t'} + a_q^\dagger e^{i\omega_q t'})| \rangle_0$$

At $T=0$. ${}_0\langle a_q^\dagger a_q \rangle_0 = 0$ ${}_0\langle a_q a_q^\dagger \rangle_0 = 1$

$$D^0(q.t-t') = -i[\theta(t-t')e^{-i\omega_q(t-t')} + \theta(t'-t)e^{i\omega_q(t-t')}]$$

$$D^0(q.\omega) = \int_R dt\, D^0(q.t) = \frac{2\omega_q}{\omega^2 - \omega_q^2 + i\delta}$$

Now we solve $G^{(0)}$ under non-interactive. expression ; we want to form $G$. in certain cases with $G^{(0)}$. firstly:

we introduce $S(\infty,-\infty) = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_R [dt_1 \cdots dt_n] T[V(t_1)\cdots V(t_n)]$.

into $G = -i\, \frac{{}_0\langle T| C_\lambda^\dagger(t) C_\lambda(t')\, S(\infty,-\infty) | \rangle_0}{{}_0\langle S(\infty,-\infty) \rangle_0}$

$$= \sum_{n=0}^{\infty} \frac{(-i)^{n+1}}{n!} \int_R [dt_1 \cdots dt_n] . \frac{{}_0\langle T[\hat{C_p}(t)\, \hat{V}(t_1) \cdots \hat{V}(t_n)\, \hat{C_p}(t')] \rangle_0}{{}_0\langle S(\infty,-\infty) \rangle_0}$$

we want to calculate:

$${}_0\langle GS| T\, \hat{C_p}(t)\, \hat{V}(t_1) \cdots \hat{V}(t_n)\, \hat{C}_p^\dagger(t') |GS\rangle_0$$

we introduce $\hat{V}(t)$ over plane-wave bases:

$$V(t_1)_{\text{Schodinger-representaton}} = \frac{1}{2} \sum_{kk'q} \sum_{ss'} \frac{4\pi e^2}{q^2} C_{k+q\,\sigma} C_{k'-q\,\sigma'} C_{k'\sigma'} C_{k\sigma}$$

$$\times e^{it_1(\eta_{k+q} + \eta_{k'-q} - \eta_k - \eta_{k'})}$$

$(\eta_k = \varepsilon_k - \mu)$

$\hat{V}(t_1)$ = interaction-representaton

$= e^{iH_0 t_1} V e^{-iH_0 t_1}$ ; $C_k(t) = e^{-i\eta_k t} C_k$

$\langle T \alpha \beta^{\dagger} \rangle_0$

we introduce.

① $-i\,{}_0\langle T[\hat{C}_\alpha(t)\hat{C}^{\dagger}_\beta(t')]\rangle_0 = \begin{cases} 0 & \alpha \neq \beta \\ G^0(0.\,t-t') & \alpha=\beta \end{cases}$  $\langle C_k C_{k'}\rangle_0 = 0 \quad k \neq k'$

② $-i\,{}_0\langle T\, \hat{C}_\alpha(t)\hat{C}^{\dagger}_\beta(t_1)\hat{C}_\gamma(t_2)\hat{C}^{\dagger}_\delta(t')\rangle_0 = \begin{cases} \text{nonzero if} \begin{cases} \alpha=\beta \ \gamma=\delta \\ \alpha=\delta \ \beta=\gamma \end{cases} \\ 0 \ \text{others.} \end{cases}$

We can introduce $\boxed{\text{Wick's theorem}}$ to calculate these terms.

① $C^{\dagger}, C$ pair $(\alpha_t\, \gamma_{t_2})$ with $(\beta_{t_1}\, \delta^{\dagger}_{t'})$ $^{\dagger}$在前无$^{\dagger}$在后

② 保留 T: $\langle T \alpha\beta\rangle_0 \langle T\gamma\delta\rangle_0$  $\langle T\alpha\beta^{\dagger}\gamma\delta^{\dagger}\rangle_0$

③ Fermion Sign $-\langle T\alpha\delta\rangle_0\langle T\gamma\beta\rangle_0$ // 形式一致可验

$= \delta_{\alpha\beta}\delta_{\gamma\delta}\, G^0(t-t_1)\, G^{(0)}(t_2-t')$.

$- \delta_{\alpha\delta}\delta_{\gamma\beta}\, G^{(0)}(t-t')\, G^{(0)}(t_2-t')$

④ electron commutes with phonon

${}_0\langle | T\, C_p(t) C^{\dagger}_{p_1}(t_1) A_{q_1}(t_1)\, C_{p_2}(t_2)\, C^{\dagger}_{p_3}(t_3)\, A_{q_2}(t_2)\rangle_0$

$(A_q = a_q + a_q^{\dagger})$

$= {}_0\langle T\, C_p(t) C^{\dagger}_{p_1}(t_1) C_{p_2}(t_2) C^{\dagger}_{p_3}(t_3)\rangle_0\, {}_0\langle T A_{q_1}(t_1) A_{q_2}(t_2)\rangle_0$

⑤ phonons

${}_0\langle | T\, A_{q_1}(t_1) A_{q_2}(t_2) A_{q_3}(t_3) A_{q_4}(t_4) | \rangle_0$

$= \langle q_1 q_2\rangle_0 \langle T q_3 q_4\rangle_0 \underset{\text{Boson}}{+} \langle T q_1 q_3\rangle\langle T q_2 q_4\rangle$

$\underset{\text{Boson}}{+} \langle T q_1 q_4\rangle \langle T q_2 q_3\rangle$

$\delta_{q_1,-q_2}\delta_{q_3,-q_4}\, D^{(0)}(t_1-t_2)\, D^{(0)}(t_3-t_4) + \delta_{q_1,-q_4}\delta_{q_2,-q_3}\, D^{(0)}(q_1 q_4)\, D^{(0)}(q_2 - q_3)$.

$\delta_{q_1,-q_3}\delta_{q_2,-q_4}\, D^{(0)}(t_1-t_3)\, D^{(0)}(t_2-t_4)$

定义: $n_F = \langle C^+(t_1) C(t_1) \rangle_0$

$1-n_F = \langle C(t_1) C^+(t_1) \rangle_0$

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⑥ if $t_2 = t_1$ $\quad {}_0\langle T (k_1 t_1)(k_2 t_2)^+ \rangle_0 = \delta_{k_1 k_2} \langle T t_1 t \rangle_0$

$= \delta_{k_1 k_2} \langle T \cdot k \rangle_0 = \langle k \rangle_0 \cdot \delta_{k_1 k_2}$

$= n_F (\varepsilon_\lambda - \mu) \delta_{k_1 k_2}$

定义 $G_0 = -i \langle \ \rangle_0$

⑦ $C$ before $C^+$: $\langle C C^+ \rangle_0 = i G^{(0)}$

$\langle C^+ C \rangle_0 = -i G^{(0)} (k, t_2 - t_1)$

$\langle T C(t_2) C^+(t_1) \rangle_0 = G^{(0)}(k, t_2 - t_1) \cdot (-i) \quad t(C) - t(C^+)$

Eg: For $G$: $\sum_{n=0}^{\infty}$ $n=0$ is $G^{(0)}$

$n=1$:

$$\frac{(-i)^2}{1!} \int_R dt_1 \, \frac{{}_0\langle T \, C_p(t) V(t_1) C_p^+(t') \rangle_0}{\text{分母} \langle S(R) \rangle_0}$$

$$+ \frac{(-i)^3}{2!} \int_R dt_1 dt_2 \, \frac{{}_0\langle T \, C_p(t) V(t_1) V(t_2) C_p^+(t') \rangle_0}{\text{分母} \, \langle S(R) \rangle}$$

If we insert interaction: $\boxed{V = \sum_{qks} M_q \hat{A}_q \cdot C^+_{k+q,\sigma} C_{k\sigma}}$

for $n=1$. $\langle C \cdot A \cdot C^+ \cdot C \cdot C^+ \rangle_0$ 奇数. 必零

so $n=1$ is $0$

for $n=2$. $\langle C \cdot A_{t_1} C^+_{t_1} C_{t_1} C^+ A_{t_2} C^+_{t_2} C_{t_2} C \rangle$ Exist

$$= \frac{(-i)^3}{2!} \int_R dt_1 dt_2 \sum_{q_1 q_2} M_{q_1} M_{q_2} \langle \hat{A}_{q_1}(t_1) \hat{A}_{q_2}(t_2) \rangle_0$$

separte fermion. phonon.

$$\times \sum_{\substack{k_1 k_2 \\ \sigma, s, s'}} {}_0\langle T \, C_{p\sigma}(t) \, C^+_{k_1+q_1,s}(t_1) \, C_{k_1 s}(t_1) \, C^+_{k_2+q_2,s'}(t_2) \, C_{k_2 s'}(t_2) \, C^+_{p\sigma}(t') \rangle_0$$

① Fermion 负号 X ② $\begin{cases} \langle t^{+} t \rangle_0 = \\ \langle t \cdot t \rangle_0 = n_F \end{cases}$ 则与 内部分符

DATE · · $G^{(0)} = -i\langle\ \rangle_0$ NOTE

First phonon term calculate:

$${}_0\langle T \hat{A}_{q_1}(t_1) \hat{A}_{q_2}(t_2) \rangle_0 = \underline{i\delta_{q_1,-q_2}} \cdot D^{(0)}(q_1, t_1-t_2)$$

Second term electron calculate. six term.

$${}_0\langle T C_{p\sigma}(t)\, C^{+}_{k_1+q_1}(t_1)\, C_{k_1}(t_1)\, C^{+}_{k_2+q_2}(t_2)\, C_{k_2}(t_2)\, C^{+}_{p\sigma}(t') \rangle_0$$

① (t) ② (t₁) ③ (t₁) ④ (t₂) ⑤ (t₂) ⑥ (t')

=

Step I: (① ③ ⑤) pair (② ④ ⑥)$^{+}$ [Sign]

[1] $\langle T ①(t) ②^{+}(t_1) \rangle_0 \langle T ③(t_1) ④^{+}(t_2) \rangle_0 \langle T ⑤(t_2) ⑥(t') \rangle_0$ Step II [×

[2] $\langle T ①(t) ②^{+}(t_1) \rangle_0 \langle T ③(t_1) ⑥^{+}(t') \rangle_0 \langle T ⑤(t_2) ④(t_2) \rangle_0$ 123654 ×(-1)少一个×(

[3] $\langle T ①(t) ④^{+}(t_2) \rangle_0 \langle T ③(t_1) ②^{+}(t_1) \rangle_0 \langle T ⑤(t_2) ⑥^{+}(t') \rangle_0$ 143256 ×(

[4] $\langle T ①(t) ④^{+}(t_2) \rangle_0 \langle T ③(t_1) ⑥^{+}(t') \rangle_0 \langle T ⑤(t_2) ②^{+}(t_1) \rangle_0$ 143652 × 1

[5] $\langle T ①(t) ⑥^{+}(t') \rangle_0 \langle T ③(t_1) ②^{+}(t_1) \rangle_0 \langle T ⑤(t_2) ④^{+}(t_2) \rangle_0$ 163254 × 1

[6] $\langle T ①(t) ⑥^{+}(t') \rangle_0 \langle T ③(t_1) ④^{+}(t_2) \rangle_0 \langle T ⑤(t_2) ②^{+}(t_1) \rangle_0$ 163452 ×(-

$= i^3 \delta_{p=k_2=k_1+q_1} \delta_{s=s'=\sigma} G^{(0)}(p, t-t_1) G^{(0)}(p-q_1, t_1-t_2) G^{(0)}(p, t_2-t')$ [1]

$+ i^3 \delta_{p=k_1=k_2-q_1} \delta_{s=s'=\sigma} G^{(0)}(p, t-t_2) G^{(0)}(p+q_1, t_2-t_1) G^{(0)}(p, t_1-t')$ [4]

少一个(i) 本身(-1)

$+ i^2 \delta_{q_1=0} \delta_{p=k_1} \delta_{s=\sigma}\ \underline{n_F(\varepsilon_{k_2}-\mu)} G^{(0)}(p, t-t_1) G^{(0)}(p, t_1-t')$ [2] 2

少一个(i) 本身(-1)

$+ i^2 \delta_{q_1=0} \delta_{p=k_1} \delta_{s'=\sigma}\ n_F(\varepsilon_{k_1}-\mu) G^{(0)}(p, t-t_2) G^{(0)}(p, t_2-t')$ [3] 5

少一个(-i)

步2个(一) 本征1 $\begin{cases} n_F = \langle C^{\dagger}(t_1) C(t_1)\rangle_0 \\ 1-n_F = \langle C(t_1) C^{\dagger}(t_1)\rangle_0 \end{cases}$

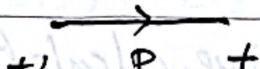


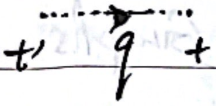
$+\ i^{-3}\delta_{q_1=0}\,\delta_{q_2=0}\, n_F(\varepsilon_{k_1}-\mu)\, n_F(\varepsilon_{k_2}-\mu)\, G^{(0)}(p.t-t')$ [5]

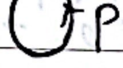
$(-)\ i^{-3}\,\delta_{k_1=k_2 q}\,\delta_{s'=s}\, G^{(0)}(p.t-t')\, G^{(0)}(k_1.t_1-t_2)\, G^{(0)}(\underbrace{k_1+q_1}_{k_2}, t_2-t_1)$, [6]

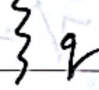
本征(一).

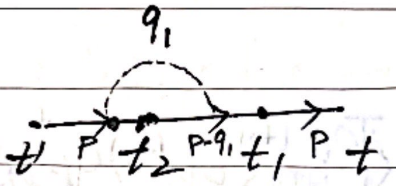
Feynman Diagram.

① $G^{(0)}(p.t-t')$ :  $t-t'$, $\vec{q}$

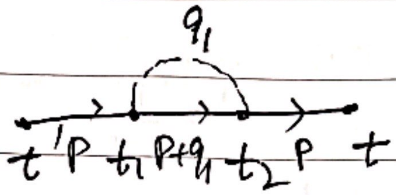
② $D^{(0)}(q.t-t')$  No ☒ Because $D^{(0)}(q.t-t')=D^{(0)}(-q.t'-t)$

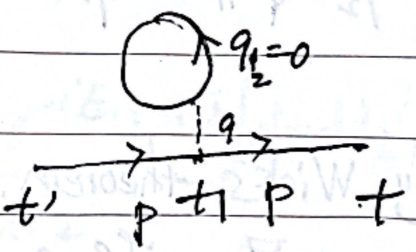
③ $_0\langle C^{\dagger}_{ps}(t) C_{ps}(t)\rangle_0 = n_F(\varepsilon_k-\mu)$ : 

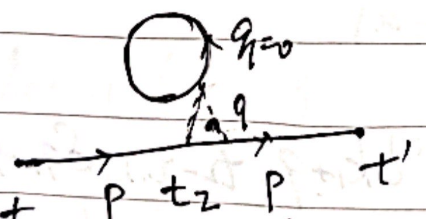
④ e-e interaction. $V_q =$ 

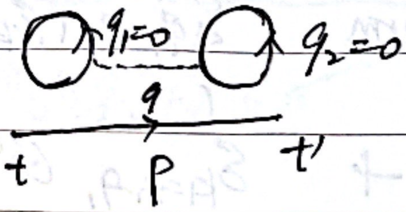
[1] 

$G^{(0)}(p.t-t_1)\, G^{(0)}(p-q_1, t_1-t_2)\, G^{(0)}(p.t_2-t')$ 向右延伸.

[4] 

[2]. 

[3] 

[5] 

[6] 

[1]: $\frac{1}{2!}\int_R dt_1 dt_2 \sum_q |M_q|^2 D^{(0)}(q, t_1-t_2)\, G^{(0)}(p, t-t_1)\, G^{(0)}(p-q, t_1-t_2)\, G^{(0)}(p, t_{\cdot}$

[4]. $\frac{1}{2!}\int_R dt_1 dt_2 \sum_q |M_q|^2 D^{(0)}(t_1-t_2)\, G^{(0)}(p, t-t_2)\, G^{(0)}(p+q, t_2-t_1)\, G^{(0)}(p, t_1-t')$

$t_1 \leftarrow t_2$ $q \longleftrightarrow -q$ 对 $D^{(0)}$ 等价. 故 [1] = [4]

We pause Here., we continue calculate:

$${}_0\langle S(\infty,-\infty)\rangle_0$$

vaccum polarization Graphs.

$$\langle S(\infty,-\infty)\rangle_0 = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!}\int_R [dt_1\cdots dt_n]\, {}_0\langle T[\hat V(t_1)\cdots \hat V(t_n)]\rangle_0$$

If we also use interaction $\hat V = \sum_{qks} M_q \hat A_{q_1} \hat C^{\dagger}_{k+q\, s} \hat C_{ks}$

$n=1$. also is zero is 1

$n=2$. ${}_0\langle T\, V(t_1) V(t_2)\rangle_0$

$$= \sum_{q_1 q_2} M_{q_1} M_{q_2} \langle T \hat A_{q_1}(t_1) \hat A_{q_2}(t_2)\rangle_0 \sum_{\substack{k_1 k_2\\ s's}} \langle T C^{\dagger}_{k_1+q_1 s}(t_1) C_{k_1 s}(t_1) C^{\dagger}_{k_2+q_2 s'}(t_2) C_{k_2 s'}(t_2)\rangle_0$$

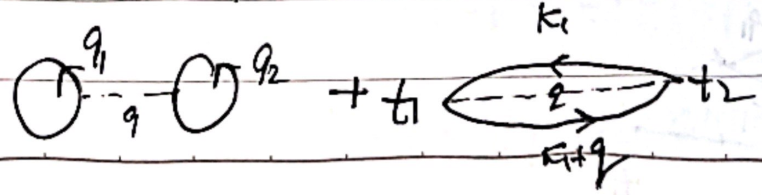
Also Apply Wick's theorem.

First term. $\delta_{q_1+q_2} D^{(0)}(q, t_1-t_2)$

Second term. $\delta_{q_1} n_F(\varepsilon_{k_1}-\mu)\, n_F(\varepsilon_{k_2}-\mu)$

$+\ \delta_{k_1=k_2-q_1} G^{(0)}(k_1, t_1-t_1)\, G^{(0)}(k_1+q, t_2-t_1)\, \delta_{q_1+q_2}$.

Graph:



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Nov. $1^{st}$.

如果 consider the distribution of $S$，分子中不连续图作用被抵消.

If we consider the connected Graph Among [1]~[6]

[1]~[2] consider. Now. [1] and [4] are similar. $G = \sum \frac{(-i)^n}{n!}(\cdots)$

term $\frac{1}{n!} = \frac{1}{2!} \times ([1]+[4]) = [1]$ for any $n!$. 抵消个数. we only consider [1].

Dyson Equation: In Energy space

$$G(p.E) = \int_R d(t-t') e^{-iE(t-t')} G(p.t-t')$$

we remember.

$$G^0(p.E) = \begin{cases} [E-\xi_p+i\delta]^{-1} & \text{for empty band.} \\ [E-\xi_p+i\delta_p]^{-1} & \text{for fermi sea.} \end{cases}$$

$$G(p.E) = -i\sum_{n=0}^{\infty}(-i)^n \int dt\, e^{-iE(t-t')} \int_R (dt_1 \cdots dt_n) \left\langle T\, C_p(t) V(t_1)\cdots V(t_n) C_p^+(t') \right\rangle_0$$

We also consider $n=2$

$$G(p.E) = \underbrace{G^0(p.E)}_{n=0} + i\sum_q |M_q|^2 \underbrace{\int_R dt\, e^{-iE(t-t')} \int dt_1 dt_2 \times}_{n=2}$$

($n=1$ 为0) $\quad G^0(p.t-t_1) G^{(0)}(p-q.t_1-t_1) G^{(0)}(p.t_2-t') D^{(0)}(q.t_1-t_2)$

For phonon term $D(q.\omega) = \int_R dt\, e^{it\omega} D(q.t)$ 用 $D^{(0)}(q.\omega)$ 取代

$$= [G^{(0)}(p.E)]^2 \times G^{(0)}(p-q.E-\omega) \, \backslash\backslash$$

$$G^{n=2} = \int_R dt\, e^{i(t-t_1)E} G^{(0)}(p.t-t_1) \int_R dt_1 e^{i(t_1-t_2)E} G^{(0)}(p-q.t_1-t_2) \int_R dt_2 e^{i(t_2-t')E} G^{(0)}(p.t_2-t')$$

$\int d\omega\, e^{\ldots} D(q.\omega) \times$

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NOTE

we arrive: 自能 Self-energy

$$\begin{cases} G(p.E) = G^{(0)}(p.E) + [G^{(0)}(p.E)]^2 \Sigma^{(1)}(p.E) \\ \Sigma^{(1)}(p.E) = i\int_R \frac{d\omega}{2\pi} \sum_q |M_q|^2 D^{(0)}(q.\omega) G^{(0)}(p-q, E-\omega) \end{cases}$$

combine G: n=0.2.4.

$$G(p.E) = G^{(0)}(p.E)\left(1 + G^{(0)}(\Sigma^{(1)} + \Sigma^{2a} + \Sigma^{2b} + \Sigma^{2c} + [G^{(0)}\Sigma^{(1)}]^2\right)$$

$(G^{0})^3(\Sigma^{1})^2$ n=4 有这项

Define:

$$G(p.E) = G^{(0)}(p.E)\frac{1}{1-G^{(0)}(p.E)\Sigma(p.E)}$$

where

$$\Sigma(p.E) = \sum_j \Sigma^j(p.E) = \Sigma^{(1)}(p.E) + \Sigma^{(2a)} + \Sigma^{2b} + \Sigma^{2c}$$

那么 $1/1-G^{(0)}(p.E)\Sigma(p.E)$ 自动出现高阶项

$$= G^{(0)} + G^{(0)2}\Sigma + G^{(0)(3)}\Sigma^2 + \cdots$$

So. the Result Arrives.

$$G(p.E) = \frac{1}{E-\varepsilon_p + i\delta - \Sigma(p.E)} \quad \text{Empty Band}$$

$$G(p.E) = \frac{1}{E-\xi_p + i\delta_p - \Sigma(p.E)} \quad \text{Fermi Sea.}$$

where $E>\mu$ $\mathrm{Im}\Sigma<0$

$E\le\mu$ $\mathrm{Im}\Sigma>0$

Feynman Diagram Rules:

① Self-Energy

② Line. $G^{(0)}(p.E) = \frac{1}{E-\xi_p+i\delta_p}$
with the same spin

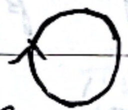
③ phonon: $D^{(0)}(q.\omega) = \frac{2\omega_q}{\omega^2-\omega_q^2+i\delta} |M_q|^2$

④ coulomb interaction: $\frac{4\pi e^2}{q^2}$

⑤ Conserve E-p at each vertex.

⑥ Sumover integral degrees of freedom. p. E. σ

⑦ factor $\frac{i^m}{(2\pi)^{4m}} \underbrace{(-1)}_{\text{spin}}{}^{F} \cdot \underbrace{(2S+1)}_{\text{sum spin}}{}^{F}$ F → closed Fermi Loop



$n_F(\xi_p)$

for electron self-energy. m = internal Lines and phonons.
for phonon self-energy. m = 1/2 (vertices) 点个数.

Finite temperature: G we used to $|GS\rangle_0$ Now in finite temperature. $e^{-\beta H}$ introduce.

$$G = \frac{Tr[e^{-\beta H} C_{p\sigma}(t) C^{+}_{p\sigma}(t')]}{Tr[e^{-\beta H}]} \qquad C_{p\sigma}(t) = e^{itH} C_{p\sigma}$$

$Tr(\hat{A}) = \sum_n \langle n|\hat{A}|n\rangle \qquad H = H_0 + V$

Multiple $e^{-\beta \vec{H}}$ expand too difficult!

~~Mas~~ Matsubara. real $t \to$ imaginary $\beta$.

$(e^{-\beta H} e^{iHt})$ $e^{\tau H} e^{-\beta H}$ satisfy commutation!

Firstly we make math preparations:

① sigularities of $n_F(\xi_p)$ if ~~$\beta$~~. $\xi_p = \varepsilon_p - \mu$

$1/(\beta\xi_p + 1) \xRightarrow{\text{Fermion}} \xi_p = \frac{2n+1}{\beta} \times i\pi$

$1/(\beta w_q - 1) \xRightarrow{\text{Phonon}} w_q = \frac{2n}{\beta} \times i\pi$

Residue $n_F(\xi_p)$ Also the same

亚纯函数(除孤立极点外皆解析)可写作全纯函数比值之形式.

$C + 1/\beta \sum_n \frac{1}{iw_n - w_q}$ or $C + 1/\beta \sum_n \frac{1}{iw_n - \xi_p}$ is the Residue.

for function $f(\tau)$ $(-\beta, \beta) \ni \tau$

we write its Fourier term

$$f(\tau) = \frac{1}{2} a_0 + \sum_{n=1}^{\infty} \left(a_n \cos\left(\frac{n\pi\tau}{\beta}\right) + b_n \sin\left(\frac{n\pi\tau}{\beta}\right)\right)$$

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where $a_n = \frac{1}{\beta} \cdot \int_{-\beta}^{\beta} d\tau\, f(\tau) \cos\left(\frac{n\pi\tau}{\beta}\right)$

$b_n = \frac{1}{\beta} \int_{-\beta}^{\beta} d\tau\, f(\tau) \sin\left(\frac{n\pi\tau}{\beta}\right)$

or we define

$f(i\omega_n) = \frac{1}{2}\beta(a_n + i b_n)$

$f(\tau) = \frac{1}{\beta} \sum_{-\infty}^{\infty} e^{-in\pi\tau/\beta} f(i\omega_n)$

$f(i\omega_n) = \frac{1}{2} \int_{-\beta}^{\beta} d\cancel{\phi}\tau\, f(\tau)\, e^{in\pi\tau/\beta}$

~~For Bosons~~ $\int_{-\beta}^{\beta} \to \int_{0}^{\beta}$. works out: where if $f(i\omega_n) = 0$

$f(i\omega_n) = \frac{1}{2}(1 + e^{in\pi}) \int_0^{\beta} d\tau\, f(\tau)\, e^{in\pi/\beta}$

For Bosons:
$$\begin{cases} f(i\omega_n) = \int_0^{\beta} d\tau\, e^{i\omega_n \tau} f(\tau) \\ f(\tau) = \frac{1}{\beta} \sum_n e^{-i\omega_n \tau} f(i\omega_n) \\ \omega_n = 2n\pi k_B T \end{cases}$$
$f(i\omega_n) = 0$ $n$: odd

For Fermions:
$$\begin{cases} f(i\omega_n) = \int_0^{\beta} d\tau\, e^{i\omega_n \tau} f(\tau) \\ f(\tau) = \frac{1}{\beta} \sum_n e^{-i\omega_n \tau} f(i\omega_n) \\ \omega_n = (2n+1)\pi k_B T \end{cases}$$
$f(i\omega_n) = 0$ $n$: even.

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Definition of Matsubara Green's Function.

$$G(p,\tau-\tau') = -\langle T_\tau c_{p\sigma}(\tau) c^\dagger_{p\sigma}(\tau') \rangle$$

$$= -\mathrm{Tr}[e^{-\beta(H-\mu N-\Omega)} \times T_\tau [e^{\tau(H-\mu N)} c_{p\sigma} \times e^{-(\tau-\tau')(H-\mu N)} \times c^\dagger_{p\sigma} \times e^{-\tau'(H-\mu N)}]]$$

$$c^\dagger_{p\sigma}(\tau) \neq [c_{p\sigma}(\overset{(it)}{\tau})]^\dagger$$

$\exp[\beta\Omega] = \mathrm{Tr}[e^{-\beta(H-\mu N)}]$ 分母

Also we can use $\theta(\tau-\tau')$ express $T_\tau$.

① Using $\mathrm{Tr}[\hat{A}\hat{B}] = \mathrm{Tr}[\hat{B}\hat{A}]$ $e^{-\beta\hat{H}}$ can't exchange. $\mathrm{Tr}(ABCD) = \mathrm{Tr}(DA$

② Setting $\tau'=0$ $G(p,\tau) = -\langle T_\tau c_{p\sigma}(\tau) c^\dagger_{p\sigma}(0) \rangle$ $K = H-\mu N$

$$G(p,\tau) = -\theta(\tau)\mathrm{Tr}[e^{-\beta(K-\Omega)} e^{\tau K} c_{p\sigma} e^{-\tau K} c^\dagger_{p\sigma}]$$

$$+\theta(-\tau)\mathrm{Tr}[e^{-\beta(K-\Omega)} e^{-\tau K} c^\dagger_{p\sigma} e^{\tau K} c_{p\sigma}]$$

For $\tau<0$,

$$G(p,\tau) = \mathrm{Tr}[e^{-\beta(K-\Omega)} e^{(\tau+\beta)K} c_{p\sigma} e^{-(\tau+\beta)K} c^\dagger_{p\sigma}]$$

$$= -G(p,\tau+\beta)$$

with properties $f(\tau) = -f(\tau+\beta)$.

So that we can apply Fourier transform:

$$G(p,i\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n\tau} G(p,\tau)$$

$$G(p,\tau) = \frac{1}{\beta}\sum_n e^{-i\omega_n\tau} G(p,i\omega_n).$$

$$\omega_n = (2n+1)\pi/\beta.$$

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Homework:

colomb potential: $V=\sum_{\substack{kk'q\\ \sigma\sigma'}} V_q\, C^{+}_{k+q.\sigma}\, C^{+}_{k'-q\sigma'}\, C_{k'\sigma'} C_{k\sigma}$

Feynman Diagram $n=1$

$$\frac{(-i)^2}{1!}\int_R dt_1 \frac{\langle T(C_{ps}(t)\, V(t_1)\, C^{+}_{ps}(t'))\rangle_0}{分母}$$

分子 $\langle \sum_{kk'q\sigma\sigma'} V_q\, T\, C_{ps}(t)\, C^{+(t_1)}_{k+q\sigma}\, C^{+(t_1)}_{k'-q\sigma'}\, C^{(t_1)}_{k'\sigma'}\, C^{(t_1)}_{k\sigma}\, C^{+}_{ps}(t')\rangle_0$

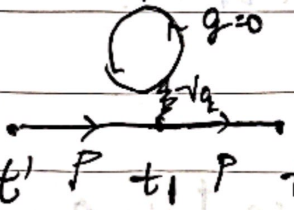
① ② ③ ④ ⑤ ⑥

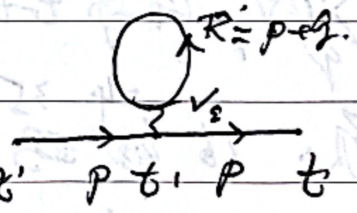
第一项: 1 2 3 4 5 6 $\times(1)$

$= \langle C_{ps}(t) C^{+}_{k+q\,\sigma}(t_1)\rangle_0 \langle \underbrace{C^{+}_{k'-q\sigma'}(t_1)\, C_{k'\sigma'}(t_1)}_{\delta_{q=0}}\rangle_0 \langle C_{k\sigma}(t_1)\, C^{+}_{ps}(t')\rangle_0$

$= i^2 \delta_{p.k+q}\, \delta_{s\sigma}\, G^{(0)}(p.t-t_1)\, \delta_{q0}\, n_F(\varepsilon_{k'}-\mu)\, \delta_{kp}\delta_{\sigma s}\, G^{(0)}(p.t_1-t')$

$= i^2 \sum_{\substack{pk'\sigma\\ \sigma\sigma'}} V_{q=0}\, G^{(0)}(p.t-t_1)\, n_F(\varepsilon_{k'}-\mu)\, G^{(0)}(p.t_1-t')$

(一): 


(二): 


第二项: 12 46 ~~5~~ 35 $\times(-1)$

$= \langle C_{ps}(t)\, C^{+}_{k+q\,\sigma}(t_1)\rangle_0 \langle C_{k'\sigma'}(t_1)\, C_{ps}(t')\rangle_0 \langle C^{+}_{k'-q.\sigma'}(t_1)\, C_{k\sigma}(t_1)\rangle_0$

$= i^2 \times \delta_{p.k+q}\, \delta_{s\sigma}\, G^{(0)}(p.t-t_1)\, \delta_{k'p}\, \delta_{\sigma' s}\, G^{(0)}(p.t_1-t')\, n_F(\varepsilon_k-\mu)$.

$s=\sigma=\sigma'$

$p=k'=k+q$.

$k=k'-q$.

$-i^2 \sum_{\substack{q\\ \sigma}} V_q\, G^{(0)}(p.t-t_1)\, G^{(0)}(p.t_1-t')\, n_F(\varepsilon_k-\mu)$.

第三项: 13 46 $\overset{25}{\cancel{52}}$ $\times 1$

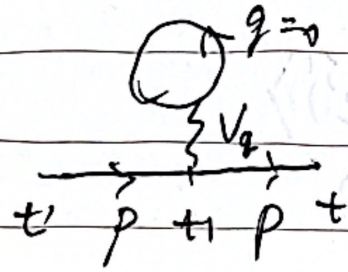
$$\langle C_{ps}(t) C^{+}_{k'q\sigma}(t_1)\rangle_0 \langle C_{k\sigma'}(t_1) C^{+}_{ps}(t')\rangle_0 \langle C^{+}_{k+q\sigma}(t_1) C_{k\sigma}(t_1)\rangle_0 .$$

$$= i^2 \times \delta_{p.k'q}\delta_{s\sigma} G^{(0)}(p.t-t_1)\delta_{kp}\delta_{\sigma s} G^{(0)}(p.t_1-t')\delta_{q=0}\, n_F(\varepsilon_k -$$

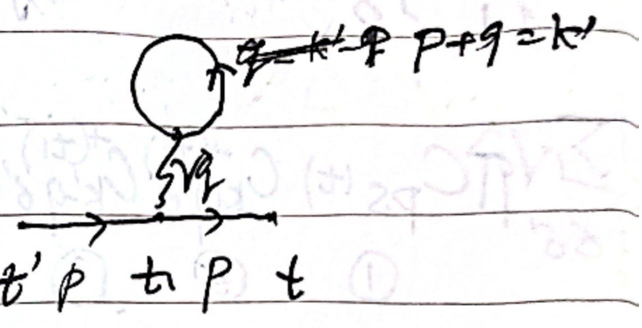
$$= i^2 \sum_{\sigma} V_{q=0} G^{(0)}(p.t-t_1) G^{(0)}(p.t_1-t')\, n_F(\varepsilon_k-\mu).$$

(s.p).

(三)




(四)




第四项 13 $\overset{24}{\cancel{46}}$ $\overset{35}{\cancel{52}}$.56 $\times(-1)$

$$\langle C_{ps}(t) C_{k'q\sigma}(t_1)\rangle_0 \langle C_{k\sigma'}(t_1) C_{ps}(t')\rangle_0 \langle C^{+}_{kq\sigma}(t_1) C_{k\sigma'}(t_1)\rangle_0$$

$$= i^2 \delta_{p.k'q}\delta_{s\sigma} G^{(0)}(p.t-t_1) G^{(0)}(p.t_1-t')\delta_{k'p}\delta_{\sigma\sigma'}\delta_{k',k+q}\, n_F(\varepsilon_k-\mu).$$

$p=k=k'-q;\ \sigma=\sigma'=s$

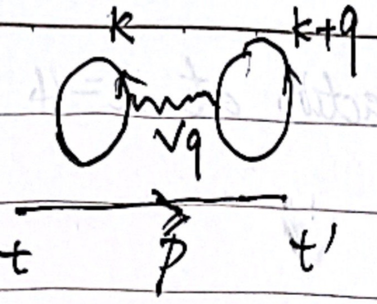
$$= -i^2 \sum_{q} V_q G^{(0)}(p.t-t_1) G^{(0)}(p.t_1-t')\, n_F(\varepsilon_k-\mu).$$

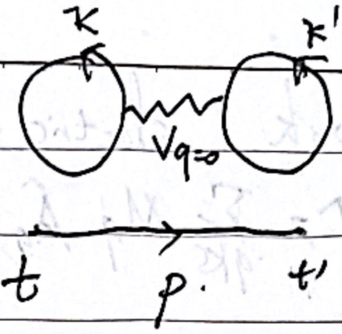
第五项: 16 $\overset{24}{\cancel{42}}$ $\overset{35}{\cancel{53}}$ $\times(-1)$

$$\langle C_{ps}(t) C^{+}_{ps}(t')\rangle_0 \langle C^{+}_{k+q\sigma}(t_1) C_{k'\sigma'}(t_1)\rangle_0 \langle C^{+}_{k'q\sigma}(t_1) C_{k\sigma}(t_1)\rangle_0$$

$$= i\, G^{(0)}(p.t-t')\, \underset{\delta_{\sigma\sigma'}}{\delta_{k',k+q}}\, n_F(\varepsilon_{k'}-\mu)\, \underset{\delta_{s\sigma}}{\delta_{k,k'-q}}\, n_F(\varepsilon_k-\mu)$$

$$= \sum_{qk\sigma} -i\, G^{(0)}(p.t-t') V_q\, n_F(\varepsilon_{kq}-\mu)\, n_F(\varepsilon_k-\mu).$$

五. 


六.. 

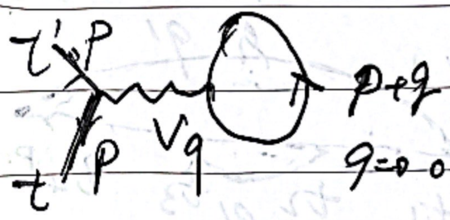

第六项: 16 34 25 ×1

$$\langle C_{ps}(t) C^{\dagger}_{ps}(t')\rangle_0 \langle C^{\dagger}_{k'+q\sigma'}(t_1) C_{k'\sigma'}(t_1)\rangle_0 \langle C^{\dagger}_{k+q\sigma}(t_1) C_{k\sigma}(t_1)\rangle_0.$$

$$= i\times 1\times G^{(0)}(p,t-t')\,\delta_{k',k'+q}\, n_F(\varepsilon_{k'}-\mu)\,\delta_{k,k+q}\, n_F(\varepsilon_k-\mu).$$

$$= i\sum_{\substack{\sigma\sigma'\\ kk'}} V_{q=0}\, G^{(0)}(p,t-t')\, n_F(\varepsilon_{k'}-\mu)\, n_F(\varepsilon_k-\mu)$$

(五)(六) disconnect. cancelled.

Remains $1\sim4 \times \frac{1}{2!}$ → 

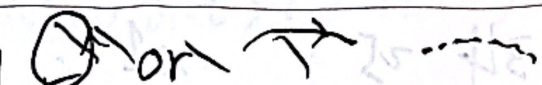

$q=0$ or $q\neq0$.

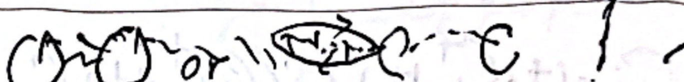
DATE · · NO·

Homework electric - phonon interaction at $n=4$

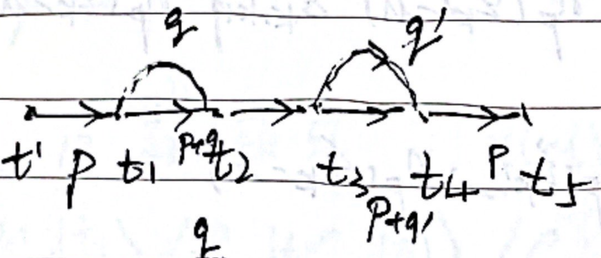
$$V=\sum_{qk\sigma} M_q \hat{A}_q C^{+}_{k+q\sigma} C_{k\sigma}$$

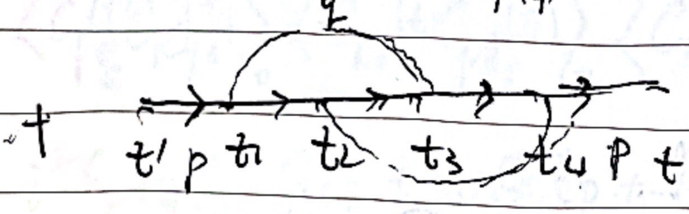
$n=4.$ $t.$ $t_1$ $t_2$ $t_3$ $t_4$ $t'$

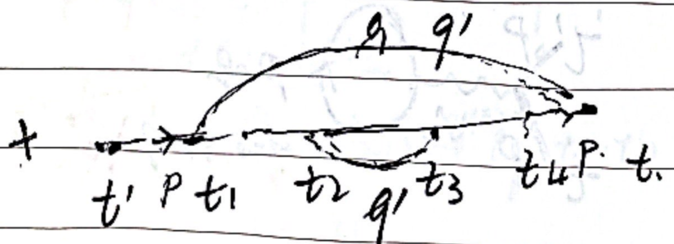
A part. $\langle\ \rangle_0$ 为  or

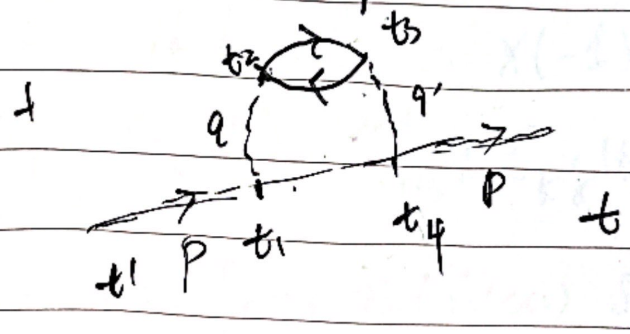
$\langle\ \rangle_0 \langle\ \rangle_0$ 为  or

Fermion part 十费米子. 五线 二虚线.



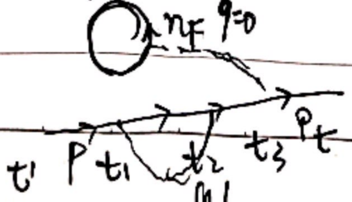




为 connected

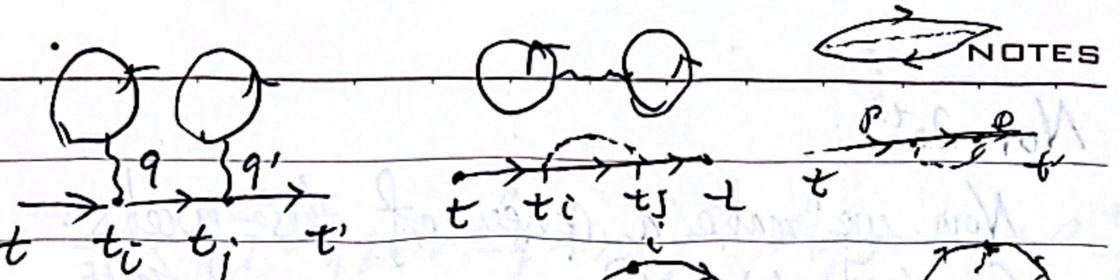
出现 $n_F$ 之图非 connect.



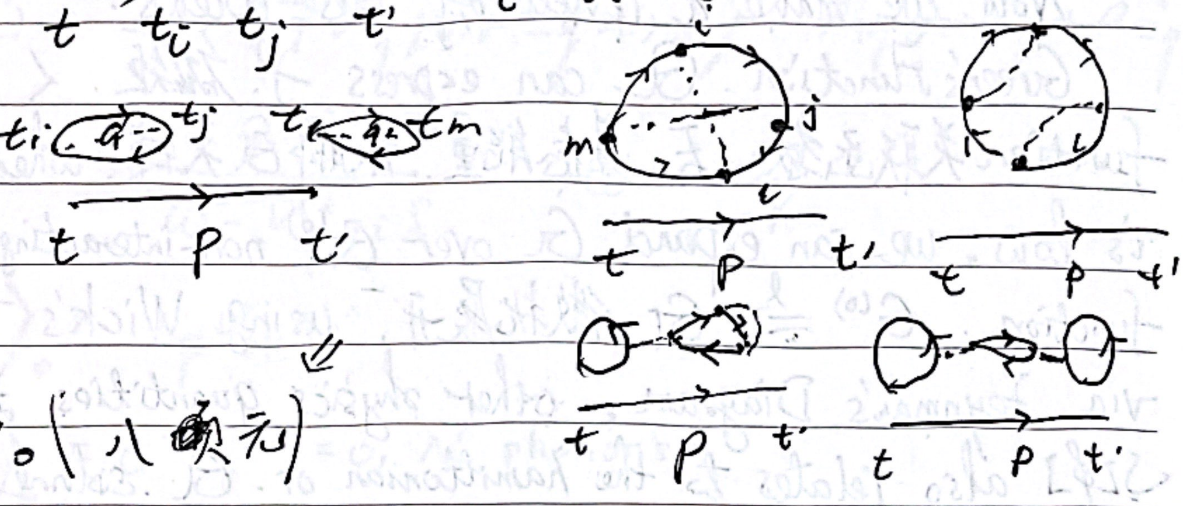

① $t_1.t_2.t_3.t_4$ 之图.

DATE NOTES

② 两个圈



③ 四个圈



$\Downarrow$

$\langle C_p^{\dagger}(t) C_p(t') \rangle_0$ (八项之)

DATE

Nov. 20th.

Now, we make a review of these weeks:

Green's Function. $G$ can express 子.磁矩. $\langle\ \rangle$ correl[ation] function 关联函数, $E_0$ 基态能量. 求解 $G$ 关键. when interact[ion] is low, we can expand $G$ over $G^{(0)}$ non-interacting Green's function. $G^{(0)} \Rightarrow G$ 微扰展开, using Wick's Theorem. [...] via Feynman's Diagram, other physics quantities $Z = \int DZ[\phi] S[\phi]$ also relates to the hamiltonian or. $G$. solving $G$. much can be solved.

$\boxed{\text{Formulas}}$: $V$ as pertubation $H_0$ non-interaction

$$G(k, t-t') = -i\langle|\hat{T}\hat{C}_K(t)\hat{C}_K^\dagger(t')|\rangle$$

$$\hat{C}_K(t) = e^{iH_0 t}C_K e^{-iH_0 t} \qquad H_0 \to \varepsilon_K$$

$$G^{(0)}(k, t-t') = -i\,{}_0\langle|C_K(t)C_K^\dagger(t')|\rangle_0 = -i\exp[-i\varepsilon_k(t-t')] \times\theta(t-t')$$

$$G^{(0)}(k, E) = \begin{cases} \dfrac{1}{E-\varepsilon_K+i\delta} & \text{Empty Band. At } T=0 \\[2ex] \dfrac{1}{E-\xi_K+i\delta_K} & \text{Fermi Sea. } \xi_K = \varepsilon_K-\mu \\ & \delta_K : \delta\,\mathrm{sgn}\,\xi_K \end{cases}$$

$$G(p, t-t') = \sum_{n=0}\frac{(-i)^{n+1}}{n!}\int_R dt_1\cdots dt_n \times \frac{\langle|T\,\hat{C}_p(t)V(t_1)\cdots V(t_n)\hat{C}_p^\dagger(t')}{\langle|S(\infty,-\infty)|\rangle_0}$$

$$\langle S\rangle_0 = \sum_{n=0}^{\infty}\int_R(dt_1\cdots dt_n)\,{}_0\langle|T\,V(t_1)\cdots V(t_n)|\rangle_0\frac{(-i)^n}{n!}$$

phonons:

$$D(q, t-t') = -i\langle|\hat{T}\hat{A}_q(t)\hat{A}_{-q}(t')|\rangle \qquad A_q = a_q + a^+_{-q}$$

$$D^{(0)}(q,\omega) = \frac{2\omega_q}{\omega^2-\omega_q^2+i\delta} \qquad H_0 \to \omega_q$$

$$_0\langle|c_K^+ c_K|\rangle_0 = n_F(\xi_K)$$

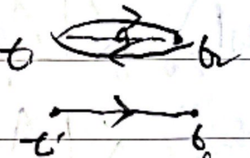
$$_0\langle|a_q^+ a_q|\rangle_0 = 0 \quad (T=0.\ \text{No phonons})$$

Attention; Rules:

① $M_q$ for $q=0$ electron-phonon interaction form like.

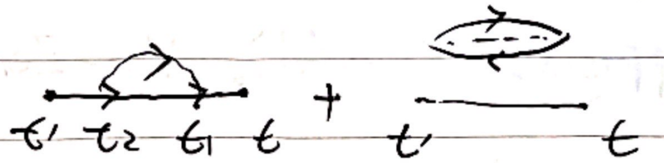
$[\frac{1}{q}(\ )]$ So $q\neq 0$ Graphs $q=0$ is Zero.

② such terms $G^0(t-t')F_1(t_1,t_2)$ if $(t,t')(t_1,t_2)$ seperated. called disconnected Graphs. like




cancelled under vaccum polarization Graphs.

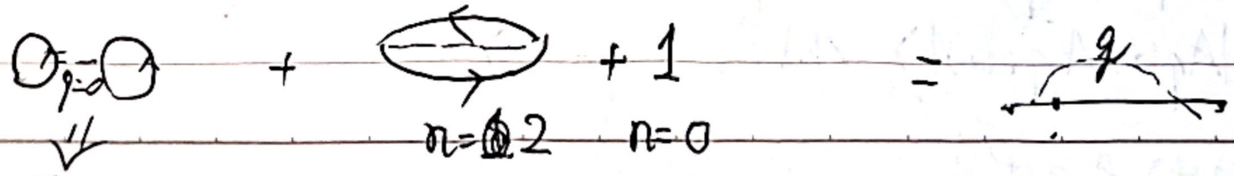
$\langle S(\infty,-\infty)\rangle_0$




$n=2$

$G^0 \times (1 + \ )$

$= G^0(t'-t)\,D^0$




$n=2$ $n=0$

Zero

$n=1 \to$ Zero Ters:

Exercise. Mahan. chapter. 2.

1. $\frac{1}{3!}\int^{t}dt_1\int^{t}dt_2\int^{t}dt_3\left[T\,V(t_1)V(t_2)V(t_3)\right]$

$\Rightarrow$ eg: $t_1>t_2>t_3$: $\int^{t}dt_1\int^{t}dt_2\int^{t}dt_3\,V(t_1)V(t_2)V(t_3)$

Therefore: $(t_2)_{max}=t_1$ $\quad\int^{t}dt_2\rightarrow\int^{t_1}dt_2$.

$(t_3)_{max}=t_2$ $\quad\int^{t}dt_3\rightarrow\int^{t_2}dt_3$

$=\int^{t}dt_1\int^{t_1}dt_2\int^{t_2}dt_3\,V(t_1)V(t_2)V(t_3)$.

共计六项 $t_1>t_2>t_3$ $t_1>t_3>t_2$ $t_2>t_1>t_3$ $t_2>t_3>t_1$ $t_3>t_1>t_2$ $t_3>t_2>$

此六项换元与 $\frac{1}{3!}$ 抵消 得.

$=\int^{t}dt_1\int^{t}dt_2\int^{t}dt_3\,V(t_1)V(t_2)V(t_3)$.

2. $D(q.\,t-t')$ $n=2$. $V=\sum_{qk} M_q A_q\, C^{\dagger}_{k+q} C_k$

D part: ${}_0\langle|\hat{A}_q(t)\,\hat{A}_{q_1}(t_1)\,\hat{A}_{q_2}(t_2)\,\hat{A}_{-q}(t')|\rangle_0$

$=\delta_{q+q_1=0}\,\delta_{q_2+(-q)=0}\;{}_0\langle|\hat{A}_q(t)\hat{A}_{q_1}(t_1)|\rangle_0\;{}_0\langle|\hat{A}_{q_2}(t_2)\hat{A}_{-q}(t')|\rangle_0$

$+\delta_{q+q_2=0}\,\delta_{q_1-q=0}\;{}_0\langle|\hat{A}_q(t)\hat{A}_{q_2}(t_2)|\rangle_0\;{}_0\langle|\hat{A}_{q_1}(t_1)\hat{A}_{-q}(t')|\rangle_0$

$+\delta_{q-q=0}\,\delta_{q_1+q_2=0}\;{}_0\langle|\hat{A}_q(t)\hat{A}_{-q}(t')|\rangle_0\;{}_0\langle|\hat{A}_{q_1}(t_1)\hat{A}_{q_2}(t_2)|\rangle_0$

Because only two wave vectors opposite $\langle|AA|\rangle_0$ Non-Zero.

$\Rightarrow\langle|\hat{A}_q(t)\hat{A}_{-q}(t_1)|\rangle_0\,\langle|\hat{A}_q(t_2)\hat{A}_q(t')|\rangle_0$

$+{}_0\langle|A_q(t)A_{-q}(t_2)|\rangle_0\,\langle|\hat{A}_q(t_1)A_{-q}(t')|\rangle_0$

$+\langle|A_q(t)\,A_{-q}(t')|\rangle_0\;{}_0\langle|\hat{A}_{q_1}(t_1)\hat{A}_{-q_1}(t_2)|\rangle_0$

$$\Rightarrow\ iD^{(0)}(q, t-t_1)\, iD^{(0)}(q, t_2-t')$$
$$+\ iD^{(0)}(q, t-t_2)\, iD^{(0)}(q, t_1-t')$$
$$+\ iD^{(0)}(q, t-t')\, iD^{(0)}(q, t_1-t_2)$$

~~Graph~~: Fermion Part:

$$\langle c_{q_1+k_1}(t_1)\, c^{+}_{k_1}(t_1)\, c^{+}_{q_2+k_2}(t_2)\, c_{k_2}(t_2) \rangle_0$$

$$= i^2 G^{(0)}\, \delta_{q_1+k_1,k_1}\, \delta_{q_2+k_2,k_2}\, \underbrace{G^{(0)}(q_1+k_1, t_1-t_1)}_{n_F}\ \underbrace{\quad}_{n_F}$$

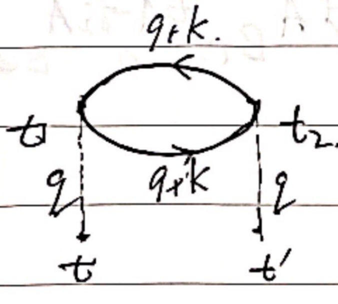
$$-\ i^2 G^{(0)}\, \delta_{q_1+k_1,q_2+k_2}\, \delta_{k_1,k_2}\, G^{(0)}(q_1+k_1, t_1-t_2)\, G^{(0)}(q_2+k_1, t_2-t_1)$$

$$= i^2 \delta_{q_1=q_2=0}\, n_F(k_1)\, n_F(k_2) - i^2 \delta_{\substack{k_1=k_2\\ q_1=q_2}}\, G^{(0)}(q+k, t_1-t_2)\, G^{(0)}(q+k, t_2-t_1)$$

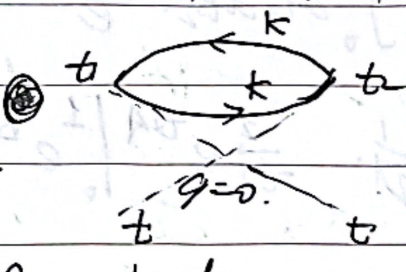
两者相乘共计六项：$3\times 2$.

$(q_1=q_2=q)$ $(k_1=k_2)$

$\delta(q_1=q, q_2=-q, q_1=q_2) \Rightarrow q=0$.

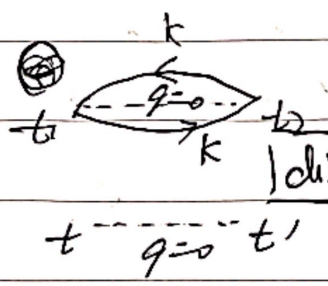



$\boxed{\text{Connect}}$ $\boxed{\text{connect}}$



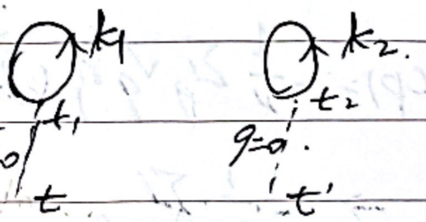

$(q_1=-q_2, q_1=q_2)\ q=0$

$q_1=q_2=q=0.\ k_1=k_2.$

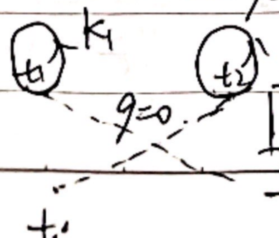



$\boxed{\text{disconnect}}$

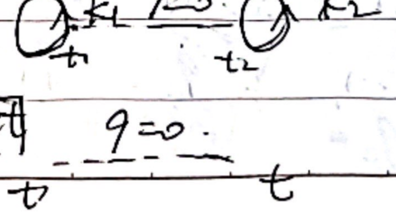
$\boxed{\text{disconnect}}$




$q=0.\ k_1, k_2.$




$\boxed{\text{disconnect}}$ $\boxed{\text{disconnect}}$



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3. Pf $e^{A+B}=e^{A}e^{B}e^{-\frac{1}{2}[A\cdot B]}$ ($[A\cdot B]$.) A and B commutes

Pf: $e^{-it_0 H_0} T\exp\left(-i\int_0^t dt_1 (\hat{V}(t_1))\right)$

$[A\cdot B]$ commutes Both $A\cdot B$ 保证没有二阶项 $[A\cdot[A\cdot B]]$

$e^{A}e^{B}e^{-\frac{1}{2}[A\cdot B]}e^{-it_0}$ → 没有之后的了.

因此保留 1st Order ie: $T\left[\int \hat{V}(t_1)\hat{V}(t_2)\right] \to e^{iH_0}V^2 e^{-iH_0}$ $H_0V-VH_0$

$\Rightarrow e^{-it_0(H_0+V)} = e^{-it_0 H_0} e^{-it_0 V} e^{\frac{1}{2} i[H_0\cdot V]} V[H_0V-V\ldots$

即 $e^{A+B}=e^{A}e^{B}e^{-1/2[A\cdot B]}$ 可以 $t_1>t_2$ or $t_2>t_1$ 保留一半出 1/2.

即计算1阶项: $\int_0^{t\times t} dt_1 dt_2\, V(t_1)V(t_2)$

$=\int_0^1 dt_1 dt_2\, e^{it[AB-BA]} = \int_0^1 dt_1 dt_2\, e^{-t_1 A} B e^{t_1 A} e^{-t_2 A} B$

$=\frac{1}{2!}\frac{1}{t_1} e^{t_1 A}\Big|_0^1 e^{B}$ 引入 $\eta$: $\frac{1}{-B+A+i\eta} e^{A}e^{B}$

4. $\Sigma_x(p) = -\frac{1}{V}\sum_q V_q\, n_F(\xi_{p+q})$ $T=0$

$T=0 \rightarrow -\frac{1}{V}\sum_{q\cdot(p+q<\mu_p)} V_q \times 1$

$= -\frac{1}{V^2}\sum_q \frac{4\pi e^2}{q^2} = \frac{-1}{V}\int_q d\vec{q}_{\,q\to 0} = \frac{1}{V}\frac{e^2}{q_F - i\delta}$

费米波矢: $q_F =$ $(p+q)<\mu_F$

# Nov. 22nd. Linear Response Theory:

when $t<t_0$, only $H_0$:

$$\langle A\rangle = \frac{1}{Z_0}\mathrm{Tr}(\rho_0 A) = \frac{1}{Z_0}\sum_n \langle n|A|n\rangle e^{-\beta E_n}$$

$$\rho_0 = e^{-\beta H_0} = \sum_n |n\rangle\langle n| e^{-\beta E_n}$$

$$Z_0 = \mathrm{Tr}(\rho_0) = \sum_n e^{-\beta E_n}$$

when at $t_0$ apply $\mathcal{H}'(t)$ pertubation.

$$\mathcal{H}(t) = H_0 + \mathcal{H}'(t)\,\Theta(t-t_0)$$

$$\langle A(t)\rangle = \frac{1}{Z_0}\sum_n \langle n(t)|A|n(t)\rangle e^{-\beta E_n} = \frac{1}{Z_0}\mathrm{Tr}[\rho(t) A]$$

$$\rho(t) = \sum_n |n(t)\rangle\langle n(t)| e^{-\beta E_n}$$

In Interaction Representation

$$|\hat{n}(t)\rangle = e^{iH_0 t}|n(t)\rangle$$

$$|\hat{n}(t)\rangle = \hat{U}(t,t_0)|\hat{n}(t_0)\rangle$$

Linear Assumption: only keep $\hat{U}$ 1st order.

$$\hat{U}(t,t_0) = 1 - i\int_{t_0}^{t} dt'\,\underbrace{\hat{\mathcal{H}}'(t')}$$

$$\overset{\text{pertubation}}{\hat{\mathcal{H}}'(t)} = e^{iH_0(t)}\,\overset{\text{pertubation}}{\mathcal{H}'(t)}\,e^{-iH_0(t)}\,\Theta(t-t_0)$$

$$\langle A(t)\rangle = \frac{1}{Z_0}\sum_n \langle n|U^{\dagger}(t,t_0)\,e^{iH_0 t} A e^{-iH_0 t}\,U(t,t_0)|n\rangle e^{-\beta E_n}$$

$\langle A \rangle_0 = \sum_n \cancel{\langle n|\ \ |n\rangle} A\, e^{-\beta E_n}$.
$\langle n|A|n\rangle$

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NOTES

↓ include $e^{-\beta E_n}$

内部为: Inside:

$$f(n) = \underbrace{\frac{1}{Z_0}\langle n|A|n\rangle}_{\langle A_0\rangle} - i\int_{t_0}^{t} dt' \langle [\hat{A}(t), \hat{H}'(t')]\rangle_0\, dt'$$

Interaction Representation $|\ \rangle_0$ $H_0$ eigen.

Defined the pertubation As:

$$C^R_{AH'}(t,t') = -i\theta(t-t')\langle[\hat{A}(t), \hat{H}'(t')]\rangle$$

$H'(t)$ Decay at $R(\infty)$. $\eta \to 0$

$$\delta\langle A(t)\rangle = \int_{t_0}^{\infty} dt'\, C^R_{AH'}(t,t')\, e^{-\eta(t-t')}$$

Fourier: $= -i\theta(t-t')\int \langle[\hat{A}(t), H'_{\omega}]\rangle e^{-i\omega t'}\, d\omega$

$\Rightarrow C_{AH'\omega}(t-t')$ 吸收 $\theta(t-t')$

Def:

$$C_{AH'\omega}(\omega) = \int_R e^{i\omega t} e^{-\eta t}\, C^R_{AH'\omega}(t)\, dt$$

$$\cancel{C^R_{AH}(t)}\ \delta\langle A(t)\rangle = \int_R \frac{d\omega}{2\pi} \cdot e^{-i\omega t}\, C_{AH'\omega}(\omega)$$

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Example: Fano-Anderson Model:

$$\mathcal{H} = \underbrace{\varepsilon_c b^+ b}_{\text{impurity}} + \sum_k \left[ \varepsilon_k c_k^+ c_k + A_k (b^+ c_k + c_k^+ b) \right]$$

we introduce $\{d_k\} \Rightarrow \{b_k\} \{c_k\}$.

$b = \sum_k V_k d_k$ if: $\sum_k V_k^2 = 1$ satisfy fermion $\{b_k, b_{k'}^+\}$

$c_k = \sum_{k'} \eta_{kk'} d_{k'}$ if: $\delta_{kk'} = \sum_{k''} \eta_{kk''} \eta_{k'k''}$ satisfy $\{c_k, c_k^+\}$

$\forall k$, if: $\sum_{k'} \eta_{kk'} V_{k'} = 0$ satisfy $\{b, c_k^+\}$

So that we can set

$$\mathcal{H} = \sum_k \varepsilon_{k\,New} \, d_k^+ d_k$$

We TRY TO SOLVE $\varepsilon_{k\,New}$

$$[b, H] \overset{old}{=} b\varepsilon_c + \sum_k A_k c_k$$

$$\overset{New}{=} \sum_k \varepsilon_{k\,New} V_k d_k$$

$$\Rightarrow \varepsilon_c \sum_k V_k d_k + \sum_{kk'} A_k \eta_{kk'} d_{k'} = \sum_k \varepsilon_{k\,New} V_k d_k$$

$$V_k (\varepsilon_{k\,New} - \varepsilon_c) = \sum_{k'} A_{k'} \eta_{k'k}$$

$$[c_k, H] \overset{old}{=} \varepsilon_k c_k + A_k b$$

$$\overset{New}{=} \sum_{k'} \eta_{kk'} \varepsilon_{k'} d_{k'}$$

$$\Rightarrow \eta_{kk'} = \frac{-A_k V_{k'}}{\varepsilon_{k'\,New} - \varepsilon_k} + \delta_{kk'} Z_k V_k A_k$$

so that we Arrive:

$$V_k(\mathcal{E}_{k\,new}-\mathcal{E}_c) = \sum_{k'}\left(A_{k'}\frac{-A_{k'}V_k}{\mathcal{E}_{k'new}-\mathcal{E}_k} - \delta_{kk'}A_k Z_k V_k\right)$$

Introduce Self-Energy.

$$\Sigma(\mathcal{E}_k) = \sum_{k'}\frac{A_{k'}^2}{\mathcal{E}_{k\,new}-\mathcal{E}_{k'}} \quad Z_k = \frac{1}{A_k^2}(\mathcal{E}_{k\,new}-\mathcal{E}_c-\Sigma(\mathcal{E}_k)).$$

Finally can solve

$$V_k = \frac{A_k^2}{(\mathcal{E}_k-\mathcal{E}_c-\Sigma(\mathcal{E}_k))^2 - 1(LA_k^2/2V_k)^2} \quad V_k = \frac{\partial \mathcal{E}_k}{\partial k}$$

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Dec. $4^{th}$. self-energy in energy space.

We write out final Result for $n=2$ + $n=0$ term in $t$ space with $H = \sum_q M_q A_q C^{+}_{k+q} C_k$ $G(p.t-t')$ then using fourier transform to $E$ space

$$G(p.E) = \int_R G(p.t-t') e^{-i(t-t')E} d(t-t')$$

$G^{(0)}$ 自带 $\theta(t-t')$ 故 $dt$ 即可保留 $t'$ 与 $\theta$ 自消

$$G(p.E) = G^{(0)}(p.E) + \qquad dt \Leftrightarrow d(t-t')$$

$$\cancel{(-i)^3 \sum_q M_q^2 \times \int_R dt\, G(p.t-t_1) e^{i(t-t_1)E} \int_R dt_2 e^{i(t_1-t_2)(E-\omega)} G^{(0)}(p-q. \ t_1-t)}$$

$$D^{(0)}(q.t_1-$$

$$(-i)^3 \sum_q M_q^2 \int_R dt\, e^{iE(t-t')} \int_R dt_1 dt_2\, G^{(0)}(p.t-t_1) G^{(0)}(p-q.t_1-t_2) G^{(0)}(p.t_2-$$

$$D^{(0)}(q.t_1-t_2) = \int_R \frac{d\omega}{2\pi} e^{-i\omega(t_1-t_2)} D^{(0)}(q.\omega)$$

$$\Rightarrow (-i)^3 \sum_q M_q^2 \times \iiint_{\boxed{4}} dt\, e^{iE(t-t_1)} \times e^{iE(-t'+t_2)E} \times e^{i(E-\omega)(t_1-t_2)} \quad e^{it_1E} \, e^{-it_2E} \quad e^{-i\omega(t_1-t_2)}$$

$$\Rightarrow (-i)^3 \sum_q M_q^2 \times \int_R G^{(0)}(p.t-t_1) e^{iE(t-t_1)} dt \int_R G^{(0)}(p.t_2-t') e^{-iE(t_2-t')} dt_2$$

$$\times \int dt_1\, G^{(0)}(p-q.\overset{t_1-t_2}{E-\omega}) e^{i(E-\omega)(t_1-t_2)} \frac{1}{2\pi} \times D^{(0)}(q.\omega) d\omega$$

$$= (-i)^3 \sum_q M_q^2 \left[G^{(0)}(p.E)\right]^2 \underbrace{\int_R G^{(0)}(p-q.E-\omega) \frac{1}{2\pi} D^{(0)}(q.\omega) d\omega}_{\Sigma^{(1)}(p.E)\ q)}$$

We define: ~~Self~~ Self-Energy.

$$\Sigma^{(1)}(p.E) = i\int_R \frac{dw}{2\pi} \sum_q M_q^2 D^{(0)}(q.w) G(p-q. E-w).$$

So that:

$$G(p.E) = G^{(0)}(p.E) + [G^{(0)}(p.E)]^2 \Sigma^{(1)}(p.E).$$

What About the $n=4$ term for electron-phonon interaction?

$$n=4: \; [G^{(0)}(p.E)]^3 [\Sigma^{(1)}(p.E)]^2 + [G^{(0)}(p.E)]^2 [\Sigma^{(2a)}(p.E) + \Sigma^{(2b)}(p.E) + \Sigma^{(2c)}(p.E)]$$

where:

$$\Sigma^{(2a)}(pE) = \int_{R\times R} \frac{dw\,dw'}{(4\pi)^2} \sum_{qq'} M_q^2 M_{q'}^2 D^{(0)}(q.w) D^{(0)}(q.w') G(p+q. E+w)$$

$$G^{(0)}(p+q+q'. E+w+w') G^{(0)}(p+q'. E+w')$$

$$\Sigma^{(2b)}(p.E) = ( \cdots \cdots ) G^{(0)}(p+q. E+w).$$

$$\Sigma^{(2c)}(p.E) = \int \frac{dw}{2\pi} \sum_q M_q^4 D^{(0)}(q.w) G^{(0)}(p+q. E+w) \times \int \frac{dw'}{2\pi} \sum_K G^{(0)}(K.w) G^{(0)}(K+q. w+w')$$

If we Def:

$$\Sigma(p.E) = \sum_j{}^{(j)} \Sigma^{(j)}(p.E) = \Sigma^{(1)}(p.E) + \Sigma^{(2a)}(p.E) + \Sigma^{(2b)}(p.E) + \Sigma^{(2c)}(p.E) + \cdots$$

$$G(p.E) = \frac{G^{(0)}(p.E)}{1 - G^{(0)}(p.E)\Sigma(p.E)} = G^{(0)} + \underbrace{(G^{(0)})^2\Sigma}_{\text{include } (G^{(0)})^2\Sigma^{(1)} + n=4 \text{ part } 2} + \underbrace{(G^{(0)})^3\Sigma^2}_{\text{include } n=4 \text{ part}}$$

$$D(p.w) = \frac{D^{(0)}(p.w)}{1 - D^{(0)}(p.w)\Pi(p.w)}$$

Therefore. Once we calculate self-energy $\Sigma$. we can express $G$ over $G^{(0)}$.

$$G^{(0)}(p.E) = \frac{1}{E-\xi_p+i\delta_p} \qquad G(p.E) = \frac{1}{E-\xi_p+i\delta_p-\Sigma(p.E)}$$

phonons:

$$D^{(0)}(p.\overset{w}{E}) = \frac{2W_q}{w^2-W_q^2+i\delta} \qquad D(p.\overset{w}{E}) = \frac{2W_q}{w^2-W_q^2+i\delta-2W_q\Pi(q.w)}$$

Calculate Self-Energy: electron-electron interaction $V_q = \frac{4\pi e^2}{q^2 V}$

$\Sigma(p.E)$ Like electron-phonon example except the $D^{(0)}$ term.

$\Sigma^{(1)}$ and $\Sigma^{(2a)}, \Sigma^{(2b)}$ consider, that is.

$\boxed{\text{Term I}}$: $\Sigma^{(1)}$, part 1. Unscreened Exchange Energy

$$\frac{i}{2\pi}\int_R dw \int \frac{d^3q}{(2\pi)^3}\frac{4\pi e^2}{Vq^2} G^{(0)}(p+q.\,w+E).$$

First Integrate $w$ (Sum over $q$). $\frac{dx}{x+a}$

$$= \frac{i}{2\pi}\int_R dw \frac{1}{w+E-\xi_{p+q}+i\delta_{p+q}}$$ 部分发散. 不能直接积.

$$= \frac{i}{2\pi}\int_R dw \int_R dt \cdot e^{it(w+E)}\, G^{(0)}(p+q.\,t)$$

Using: $\int_R \frac{dw}{2\pi} e^{itw} = \delta(t)$

$$= iG^{(0)}(p+q.\,t=0) \begin{cases} t\to 0^+ & G^{(0)}(p+q.\,t\to 0^+) = -i[1-n_F(\xi_{p+q})] \\ t\to 0^- & G^{(0)}(p+q.\,t\to 0^-) = i\,n_F(\xi_{p+q}) \end{cases}$$

therefore. we call $\boxed{\text{Term 1}}$

$$\Sigma_x(p) = -\frac{1}{V}\sum_q V_q\, n_F(\xi_{p+q})$$

$\boxed{\text{Term 2}}$ $\Sigma^{(1)}$ part a $q=0$.

Similarly $\displaystyle\int_{R\times R} \frac{-i}{(2\pi)^4}\, dE'\, d^3q\; V_{q=0}\, G^{(0)}(p', E')$. 不一定发散. 正负中和之电中性

$$\Sigma_H = \left(\sum_p\right)\Sigma(p,E) = V_{q=0}\sum_p n_F(\xi_{p'}) = \underbrace{V_{q=0}N}$$ 均匀分布 $q=0$.

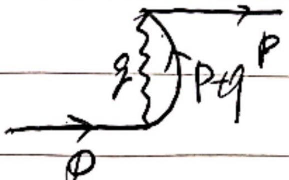
$\boxed{\text{Term 3}}$ $\Sigma^{(2a)}$. (Later calculated)

$$\Sigma(p,E) = \int\frac{dE'}{2\pi}\int\frac{d^3q}{(2\pi)^3}\, V_q^2\, P^{(1)}(q,E)\, G^{(0)}(p+q, E+E')$$

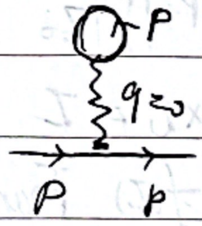
$$P^{(1)}(q,E) = 2\int\frac{dE}{2\pi}\int\frac{d^3p}{(2\pi)^3}\, G^{(0)}(p,E)\, G^{(0)}(p+q, E+\omega)$$

Graphs:

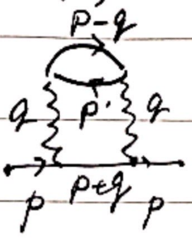
$\boxed{\text{Term 1}}$

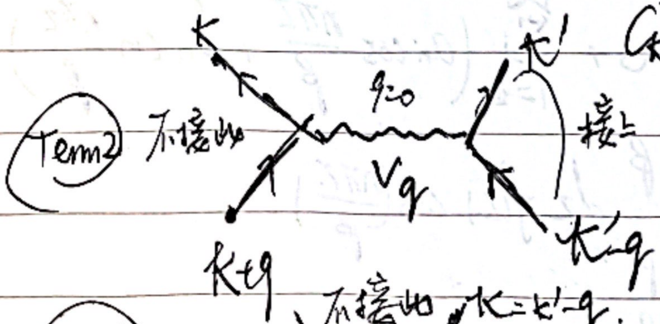



Term 2



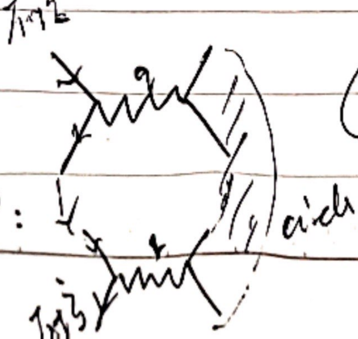

$\boxed{\text{Term 3}}$



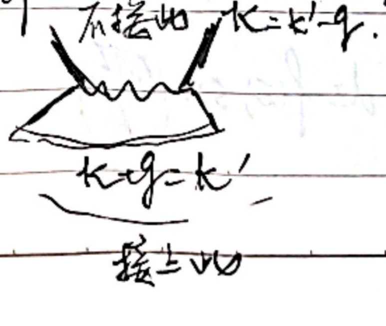




$c^\dagger_{k+q}c^\dagger_{k'-q}c_{k'}c_k$

Term3:



Term1



DATE . . NOTES

Finite temperature calculation:

$$\langle e^{-\beta H} e^{iHt} \rangle \quad H = H_0 + V$$

if only $\langle e^{iHt} \rangle \rightsquigarrow \hat{T} \exp\left(-i\int_0^t dt_1 V(t_1)\right) = U$

if introduce $\langle e^{-\beta H} \rangle$ No more interactive representation.

Hardly can we express $U$ !!

Moreover. $G^{(0)}$. $n_F$ $i$ is with $\omega_n$ 奇点(singlar points Naturally).

$$n_F(\xi_p) = \frac{1}{e^{\beta \xi_p} + 1} = \frac{1}{2} + \frac{1}{\beta} \sum_{n=-\infty}^{\infty} \frac{1}{(2n+1)i\pi/\beta - \xi_p}$$

$$n_B(\omega_q) = \frac{1}{e^{\beta \omega_q} - 1} = -\frac{1}{2} + \frac{1}{\beta} \sum_{-\infty}^{\infty} \frac{1}{2n\pi i/\beta - \omega_q}$$

$e^{\beta \xi_p} + 1$ 极点 $(2n+1)i\pi/\beta$. 留数:

$$\cancel{(2n+1)i\pi}/ \quad \frac{(e^{\beta\xi_p}+1)^{-1}\big|_{z_0}}{(z - z_0)} \quad 1$$

$$z_0 \quad \frac{1}{(e^{\beta \xi_p} + 1)'\big|_{z_0}} = \frac{1}{(e^{\beta \xi_p})'\big|_{z_0}} = \frac{1}{\beta} \quad \text{故为上作.}$$

if replace $i \times t = \tau$

for certain $f(\tau)$ Fourier

$$f(\tau) = \frac{1}{2} a_0 + \sum_{n=1}^{\infty} \left( a_n \cos \frac{n\pi\tau}{\beta} + b_n \sin \frac{n\pi\tau}{\beta} \right)$$

$$a_n = \frac{1}{\beta} \int_{-\beta}^{\beta} d\tau f(\tau) \cos\left(\frac{n\pi\tau}{\beta}\right)$$

$$b_n = \frac{1}{\beta} \int_{-\beta}^{\beta} d\tau f(\tau) \sin\left(\frac{n\pi\tau}{\beta}\right)$$

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Therefore, for Bosons: $\sum_n \frac{1}{i\omega_n - \xi_p}$ is G.D$^{(0)}$

Def: $\omega_n = \frac{2n\pi}{\beta}$ $f(i\omega_n)$ is Green function,

we can define it's fourier transform in Imaginary Space Like it.

·Matsubara Green's Function: $\tau = it$

$$\mathcal{G}(p.\tau-\tau') = -\langle T_\tau C_p(\tau) C_p^+(\tau') \rangle$$

$$= T_r\left(e^{-\beta(H-\mu N-\Omega)} T_\tau e^{\tau(H-\mu N)} C_p e^{-(H-\mu N)(\tau-\tau')} \times C_p^+ e^{-\tau'(H-\mu N)}\right)$$

$$e^{-\beta\Omega} = T_r\left(e^{-\beta(H-\mu N)}\right) \text{ 配分函数}$$

Def: $K = H - \mu N$

Using $Tr(ABC\cdots XYZ) = Tr(ZABC\cdots XY)$.

One reaches: $\mathcal{G}(p.\tau) = -\mathcal{G}(p, \tau+\beta)$ $-\beta<\tau<0$

is at $\beta$ circle. Like what's in Fourier Above

$$\begin{cases} \mathcal{G}(p.i\omega_n) = \int_0^\beta d\tau\, \mathcal{G}(p.\tau)\, e^{i\tau\omega_n} \\ \mathcal{G}(p.\tau) = \frac{1}{\beta} \oint \sum_n e^{-i\omega_n\tau}\, \mathcal{G}(p.i\omega_n). \end{cases}$$

calculate $\mathcal{G}^{(0)}$

$$H = H_0 = \Sigma_p \varepsilon_p C_p^+ C_p$$

$$K_0 = H_0 - \mu N = \Sigma_p \xi_p C_p^+ C_p$$

$$\begin{cases} C_p(\tau) = e^{\tau K_0} C_p e^{-\tau K_0} = e^{-\tau \xi_p} C_p \\ C_p^+(\tau) = \qquad e^{\tau \xi_p} C_p^+ \end{cases}$$

Using: $e^A C e^{-A} = C + [A.C] + \frac{1}{2!}[A.[A.C]] + \cdots\cdots$

Therefore: Start from 0. end at $\tau$ in $[0,\beta]$ circle or $[-\beta.0]$

$$\mathcal{G}^{(0)}(p.\tau) = -\theta(\tau) e^{-\tau\xi_p} \langle C_p C_p^+ \rangle + \theta(-\tau) e^{-\tau\xi_p} \langle C_p^+ C_p \rangle$$

$$\mathcal{G}^{(0)}(p.\tau) = -e^{-\tau\xi_p}[\theta(\tau) - n_F(\xi_p)]$$

$e^{-\beta H}$ 包含于此 $n_F$ 中

where: $n_F(\xi_p) = \dfrac{1}{e^{\beta\xi_p}+1}$

Fourier: $\mathcal{G}^{(0)}(p.i\omega_n) = \int_0^\beta d\tau\, e^{+i\omega_n\tau} \mathcal{G}^{(0)}(p.\tau)$

$$\begin{cases} \omega_n = i(2n+1)\pi/\beta \\ e^{i\beta\omega_n} = -1 \end{cases} \quad = \quad \text{离散 Fourier 结论}$$

$$\Rightarrow \mathcal{G}^{(0)}(p.i\omega_n) = \frac{[1-n_F(\xi_p)](e^{-\beta\xi_p}+1)}{i\omega_n - \xi_p}$$

$$\Rightarrow \mathcal{G}^{(0)}(p,i\omega_n) = \frac{1}{i\omega_n - \xi_p}$$

$$D(q.\tau-\tau') = -\langle T_\tau A(q.\tau) A(-q.\tau') \rangle \quad e^{-\beta(H+\Omega)}\cdots$$

$$A(q.\tau) = e^{\tau H}(a_q + a_{-q}^+) e^{-\tau H}$$ phonons: No chemical potential

$\omega_n = \frac{2\pi n}{\beta}\cdots$

Resutts:

$$\mathcal{G}^{(0)}(p, i\omega_n) = \frac{1}{i\omega_n - \xi_p} \quad \xi_p: \varepsilon_p - \mu. \quad \omega_n: (2n+1)\pi/\beta. \quad \mathcal{G}^{(0)}(\tau) = -\mathcal{G}^{(0)}(\tau+\beta)$$

$$\mathcal{D}^{(0)}(q, i\omega_n) = -\frac{2w_q}{\omega_n^2 + w_q^2} \quad w_q: w_q(\mu=0) \quad \omega_n: 2n\pi/\beta. \quad \mathcal{D}^{(0)}(\tau) = \mathcal{D}^{(0)}(\tau+\beta).$$

Maths:

Fermions $f(\tau) = -f(\tau+\beta)$ Boson: $f(\tau) = f(\tau+\beta)$

$$\begin{cases} f(i\omega_n) = \int_0^\beta d\tau\, f(\tau)\, e^{i\omega_n\tau} \\ f(\tau) = \frac{1}{\beta}\sum_n e^{-i\omega_n\tau} f(i\omega_n) \\ \omega_n = \frac{(2n+1)\pi}{\beta} \text{ Fermion} \quad \frac{2n\pi}{\beta} \text{ Boson} \end{cases}$$

Retarded Green's Function $G(t>t')$

Advanced Green's Function $G(t<t')$.

Spectral function $A(p, \omega) = -2\,\mathrm{Im}\, G_{ret}(p, \omega)$

properties: $\int A(p, \omega)\frac{d\omega}{2\pi} = 1$

$G^{(0)}(p\omega) = \frac{1}{\omega - \xi_p + i\delta} \Rightarrow A(p\omega) = 2\pi\delta(\omega - \xi_p) = -2\,\mathrm{Im}\, G^{0}_{ret}(\omega p)$

Dyson's Equation:

Def: $K = K_0 + V = H_0 - \mu N + V \quad \mathcal{H} = H_0 + V$

$$U(\tau) = e^{\tau K_0} e^{-\tau K}$$

$$U^{-1}(\tau) = e^{\tau K} e^{-\tau K_0}$$

$$\hat{C_p}(\tau) = e^{\tau K_0} C_p e^{-\tau K_0}$$

Then: $(\tau > 0)$ $$\mathcal{G}(p.\tau) = \frac{-Tr[e^{-\beta K_0} U(\beta) U^{-1}(\tau) \hat{C_p}(\tau) U(\tau) \hat{C_p^{\dagger}}(0)]}{Tr[e^{-\beta K_0} U(\beta)]}$$

Also: $$\partial / \partial \tau\, U(\tau) = -e^{\tau K_0} V e^{-\tau K_0} (e^{\tau K_0} e^{-\tau K}) = -\hat{V}(\tau) \hat{U}(\tau)$$

区别之前的式子. 少一个 $i$

$$\Rightarrow U(\tau) = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^{\tau} d\tau_1 \cdots d\tau_n \; T_{\tau}[\hat{V}(\tau_1) \cdots \hat{V}(\tau_n)]$$

$$= T_{\tau} \exp\left[-\int_0^{\tau} d\tau \hat{V}(\tau)\right]$$

Also. $S(a.b)$ share similar definite with $U(\tau)$.

$$S(\tau_1.\tau_2) = T_{\tau} \exp\left[-\int_{\tau_1}^{\tau_2} d\tau \hat{V}(\tau)\right]$$

$$\Rightarrow \mathcal{G}(p.\tau) = \frac{-Tr[e^{-\tau K_0} S(\beta.\tau) \hat{C_p}(\tau) S(\tau) C_p^{\dagger}(0)]}{Tr[e^{-\beta K_0} S(\beta)]}$$

Attention: $Tr[e^{-\beta K_0}(A)]$ 就是 $\langle A \rangle_0$ non-interactive $K_0 = H_0 - \mu N$

$$\Rightarrow \frac{-{}_0\langle T_{\tau}[S(\beta) C_p(\tau) C_p^{\dagger}(0)] \rangle_0}{{}_0\langle S(\beta) \rangle_0}$$

$\beta = \frac{1}{k_B T}$ $T \to 0$ $\beta \to \infty$ 回到之前 Dyson 级数.

Similarly we want to express $\mathcal{G}$ over $\mathcal{G}_0$.

$$ {}_0\langle T_\tau S(\beta) C_p(\tau) C_p^\dagger(0) \rangle_0 = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!} \int_0^\beta d\tau_1 \cdots d\tau_n \, T_\tau[\hat{C_p}(\tau) \hat{V}(\tau_1) \cdots \hat{V}(\tau_n) \hat{C}_p^\dagger(0)] $$

Apply Wick's Theorem:

Adding connected cancelled $\langle S(\beta) \rangle_0$

Adding different cancelled $\frac{1}{n!}$

$$ \Rightarrow \mathcal{G}(p.\tau) = -\sum_{n=0}^{\infty} (-1)^n \int_0^\beta d\tau_1 \cdots d\tau_n \; {}_0\langle T_\tau [\hat{C_p}(\tau) \hat{V}(\tau_1) \cdots V(\tau_n) \hat{C}_p^\dagger(0)] \rangle_0 $$

Also its Fourier transform:

$$ \mathcal{G}(p.ip_n) = \frac{\mathcal{G}^{(0)}(p.ip_n)}{1 - \mathcal{G}^{(0)}(p.ip_n)\Sigma(p.ip_n)} \qquad p_n = \frac{(2n+1)\pi}{\beta} \qquad \mathcal{G}(p.ip_n) = \int_0^\beta e^{ip_n\tau} \mathcal{G}(p.\tau) d\tau $$

$$ \mathcal{D}(q.i\omega_n) = \frac{\mathcal{D}^{(0)}(q.i\omega_n)}{1 - \mathcal{D}^{(0)}(q.i\omega_n)\pi(q.i\omega_n)} \qquad \omega_n = \frac{2n\pi}{\beta} $$

Example: using Matsubara Method solving finite T

$$ \mathcal{H} = H_0 + \frac{1}{\sqrt{V}} \sum_{qk} M_q A_q C_{k+q}^\dagger C_k $$

$n=2$ term:

$$ \frac{1}{V} \sum_{qq'} M_q M_{q'} \int_0^\beta d\tau_1 d\tau_2 \; {}_0\langle T_\tau [\hat{C_p}(\tau) \sum_k C_{k+q}^\dagger(\tau_1) C_k(\tau_1) \sum_{k'} C_{k'+q'}^\dagger(\tau_2) C_{k'}(\tau_2) $$

$$ \hat{C}_p^\dagger(0)] \rangle_0 \times \underbrace{{}_0\langle T_\tau A_q(\tau_1) A_{q'}(\tau_2) \rangle_0}_{} $$

$$ \Downarrow $$

$$ -\delta_{q+q'} \mathcal{D}^{(0)}(q.\tau_1 - \tau_2). $$

only we change $t \to \tau$

if we coside connected, different graph. thee's still one.

$$\mathcal{G}_2(p,\tau) = -\frac{1}{V}\sum_q M_q^2 \int_0^\beta d\tau_1 \int_0^\beta d\tau_2\, D^{(0)}(q,\tau_1-\tau_2)\, \mathcal{G}_0^{(0)}(p,\tau-\tau_1)$$

$$\times\, \mathcal{G}^{(0)}(p+q,\tau_1-\tau_2)\,\mathcal{G}^{(0)}(p,\tau_2)$$

Fourier transform:

$$\mathcal{G}(p,ip_n) = \int_0^\beta d\tau\, \mathcal{G}(p,\tau)\, e^{ip_n\tau}$$

$$\mathcal{G}^{(0)}(p,\tau-\tau_1) = \frac{1}{\beta}\sum_{ip_n'} e^{-ip_n'(\tau-\tau_1)}\mathcal{G}^{(0)}(p,ip_n')$$

$$\Rightarrow \mathcal{G}_2(p,ip_n) = -\frac{1}{V}\sum_q M_q^2 \sum_{n'n''n'''m} D^{(0)}(q,i\omega_m)\,\mathcal{G}^{(0)}(p,ip_n')\,\mathcal{G}^{(0)}(p-q,ip_n'')$$

$$\times\, \mathcal{G}^{(0)}(p,ip_{n'''})\int_0^\beta d\tau d\tau_1 d\tau_2 \exp\Big(ip_n\tau - i\omega_m(\tau_1-\tau_2) - ip_n'(\tau-\tau_1)$$

$$-\, ip_n''(\tau_1-\tau_2) - ip_{n'''}\tau_2\Big)$$

Using $\int_0^\beta d\tau\, e^{i\tau(p_n-p_n')} = 0$ if $n\neq n'$, or $\delta_{p_n,p_n'}$.

$\Rightarrow i\tau(p_n-p_n')$ $\qquad i\tau_2(\omega_m+p_n''-p_n''')$

$i\tau_1(-\omega_m+p_n'-p_n'')$

$\Rightarrow p_n=p_n' \quad p_n'=p_n''+\omega_m \quad p_n = p_n''+p_n'''-p_n'' \quad p_n''+\omega_m = p_n = p_n' = p_n'''$

$\omega_m = p_n''' - p_n'' \quad p_n = p_n'''$

$$\Rightarrow \mathcal{G}_2(p,ip_n) = \mathcal{G}^{(0)}(p,ip_n)\,\Sigma^{(1)}(p,ip_n)$$

$$\Sigma^{(1)}(p,ip_n) = -\frac{1}{\beta V}\sum_q\sum_{i\omega_n} M_q^2\, D^{(0)}(q,i\omega_n)\,\mathcal{G}^{(0)}(p-q,ip_n-i\omega_n),$$

Frequency Summations:

Result:

$$-\frac{1}{\beta}\sum_{i\omega_n} b^{(0)}(q, i\omega_n)\, \mathcal{G}^{(0)}(p, ip_n+i\omega_n) = \frac{N_q + n_F(\xi_p)}{ip_n + \omega_q - \xi_p}$$

$$\frac{1}{\beta}\sum_{ip_n} \mathcal{G}^{(0)}(p, ip_n)\, \mathcal{G}^{(0)}(K, ip_n+i\omega_n) = \frac{n_F(\xi_p)}{i\omega_n + \xi_p - \xi_k}$$

$$-\frac{1}{\beta}\sum_{ip_n} \mathcal{G}^{(0)}(p, ip_n)\, \mathcal{G}^{(0)}(K, i\omega_n - ip_n) = \frac{1 - n_F(\xi_p) - n_F(\xi_k)}{i\omega_n - \xi_p - \xi_k}$$

$$\frac{1}{\beta}\sum_{ip_n} \mathcal{G}^{(0)}(p, ip_n) = n_F(\xi_p)$$

where: $N_q = \frac{1}{e^{\beta\omega_q} - 1}$ $\quad n_F(\xi) = \frac{1}{e^{\beta\xi}+1}$

) consider: $\boxed{\text{对 } i\omega_n \text{ 求和.}}$

$$-\frac{1}{\beta}\sum_{i\omega_n} b^{(0)}(q, i\omega_n)\, \mathcal{G}^{(0)}(p, ip_n+i\omega_n)$$

$$= \frac{1}{\beta}\sum_{n=-\infty}^{\infty} \frac{2\omega_q}{\omega_n^2+\omega_q^2} \times \frac{1}{ip_n + i\omega_n - \xi_p} = -\frac{1}{\beta}\sum_n f(i\omega_n)$$

Seen As Function of $(i\omega_n)$ $f(i\omega_n)$. $z = i\omega_n$

$$f(z) = \frac{2\omega_q}{z^2-\omega_q^2} \times \frac{1}{ip_n + z - \xi_p}$$

$\left(\cancel{f(z)\cot\pi z}\right)$ ~~在f(z)的~~ ~~极点替代求和~~.

Poles: ~~① $z_i = 2n\pi i/\beta \Rightarrow \cot\pi z$~~

① $z_1 = \omega_q$, $R_1 =$

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我们可以先求:

$$\int_{R\to\infty} f(z)\frac{1}{e^{\beta z}-1}\frac{dz}{2\pi i} \text{ Contour} = I$$

when $R\to\infty$ $I\to 0$ 绕一圈 $R\to\infty$ 为 0

① $f(z)\to 0$ ② $\frac{1}{e^{\beta z}-1}\to 0$ ③ $2\pi z / e^{\beta z}-1 \to 0$

Then:

$$\int f(z)\frac{1}{e^{\beta z}-1}\frac{dz}{2\pi i} = \text{Res}:$$

① $z=\frac{2n\pi}{\beta}$ ③ $z=-W_q$

② $z=W_q$ ④ $z=\xi_p-ip_n$

Res ①: $z_0=\frac{2n\pi}{\beta}$

$$\text{Res} = \frac{f(z_0)}{\beta e^{\beta z_0}} = \frac{1}{\beta}\cdot f(i\omega_n)$$

$\frac{2n\pi}{\beta}$

Therefore:

$\text{Res}1 = \frac{1}{\beta}\sum f(i\omega_n)$ 即所求式

$(z^2-W_q^2)'$

Res② $z_0=W_q$ $\left(\frac{1}{e^{\beta z_0}-1}\times\frac{2W_q}{ip_n+W_q-\xi_p}\right)\Big/ 2W_q$

$$= N_q / ip_n+W_q-\xi_p$$

Res③ 同理 $N_q+1 / ip_n-W_q-\xi_p$

$(ip_n+z-\xi_p)'$

Res ④

$$\frac{1}{e^{\beta z_0}-1}\times\left(z_0^2-W_q^2\right)^{-1}\times 2W_q \Big/ \left(\cancel{ip_n-\xi_p}\right) 1$$

$$= \frac{-2W_q\, n_F(\xi_p)}{(ip_n-\xi_p)^2-W_q^2}$$

Therefore: $I=0=\frac{1}{\beta}\sum_{\omega_n} f(i\omega_n) + \text{Res}② + \text{Res}③ + \text{Res}④$

Therefore the summation is:

$$S = \frac{N_q + n_F(\xi_p)}{ip_n - \xi_p + w_q} + \frac{N_q + 1 - n_F(\xi_p)}{ip_n - \xi_p - w_q}.$$

Ⅰ Consider 对 $ip_n$ 求和. 利用. $n_F(z) f(z)$

$$\int f(z) \frac{1}{e^{\beta z}+1} \frac{dz}{2\pi i} \quad z_1 = \frac{(2n+1)\pi}{\beta} \text{ electron } \cancel{\text{Fermion}} \text{ 形式}$$

similar results can be obtained

Ⅲ Consider:

$$\frac{1}{\beta}\sum_{ip_n} g^{(0)}(p, ip_n). \quad g^{(0)}(p,\tau) = \frac{1}{\beta}\sum_{ip_n} e^{-ip_n\tau} g^{(0)}(p, ip_n)$$

$$= -\langle T_\tau \hat{C_p}(\tau) \hat{C_p^\dagger}(0) \rangle$$

We only choose the $\tau \to 0$ limit

If we want to reach $n_F$. we shall choose $\tau \to 0^-$ limit.

$$-\langle T_\tau C_p(\tau) C_p^\dagger(\tau) \rangle_{\tau \to 0^-} = \langle C_p^\dagger C_p \rangle = n_F(\xi_p).$$

DATE . . NOTE

Homework.

1. calculate: $\frac{1}{\beta}\sum_{ip_n} \mathcal{G}^{(0)}(p, ip_n)\,\mathcal{G}^{(0)}(k, ip_n+i\omega_n)$.

2. calculate: $-\frac{1}{\beta}\sum_{ip_n} \mathcal{G}^{(0)}(p, ip_n)\,\mathcal{G}^{(0)}(k, i\omega_n-ip_n)$

3. calculate: $\frac{1}{\beta}\sum_{i\omega_n} D^{(0)}(q, i\omega_n)\,D^{(0)}(k, i\omega_n+iq_n)$

4. calculate: $\frac{1}{\beta}\sum_{iq_n} \mathcal{G}^{(0)}(p, ip_n+iq_n)\,D(q, iq_n)$

1. $\frac{1}{\beta}\sum_{ip_n} \frac{1}{ip_n-\xi_p}\,\frac{1}{ip_n+i\omega_n-\xi_k}$

$\Rightarrow Z_0=\xi_p \quad Z_1=\xi_k-i\omega_n$. $\quad \frac{2n\pi}{\beta}$

$\Rightarrow \quad \frac{n_F(\xi_p)-n_F(\xi_k-i\omega_n)}{i\omega_n+\xi_p-\xi_k} \qquad n_F(i\omega_n)=1$

$\Rightarrow \quad \frac{n_F(\xi_p)-n_F(\xi_k)}{i\omega_n+\xi_p-\xi_k}\times\frac{1}{\beta}$

2. $-\frac{1}{\beta}\sum_{ip_n} \frac{1}{ip_n-\xi_p}\,\frac{1}{i\omega_n-ip_n-\xi_k}$

$\Rightarrow Z_0=\xi_p \quad Z_1=i\omega_n-\xi_k \qquad \frac{1}{e^{-\xi_k}+1}=\frac{e^{\xi_k}}{e^{\xi_k}+1}=1-\frac{1}{e^{\xi_k}+1}=1-n_F(\xi_k)$

$\Rightarrow \quad n_F(\xi_p)-n_F(-\xi_k)$

$= \quad \frac{1-n_F(\xi_p)-n_F(\xi_k)}{i\omega_n-\xi_p-\xi_k}$

3. $\frac{1}{\beta}\sum_{i\omega_n} \frac{-2\omega_q}{\omega_n^2+\omega_q^2} \times \frac{1}{i\omega_n - ip_n - \xi_k}$ $\quad z = i\omega_n \quad -z^2+\omega_q^2$

$\frac{2\omega_q}{z^2-\omega_q^2}$

$\Rightarrow z_1=\omega_q \quad z_2=-\omega_q \quad z_3 = ip_n+\xi_k$

对 $\omega_n$ 求和. 用 $n_B$. $\quad 2z$

$\frac{1}{\beta} n_B(\omega_q)\times\frac{1}{2\omega_q}\times 2\omega_q\times\frac{1}{\omega_q - ip_n-\xi_k}$ $\quad n_B(-x) = \frac{1}{e^{-x}-1} = \frac{e^x}{1-e^x}$

$+\frac{1}{\beta}n_B(-\omega_q)\times\frac{1}{-2\omega_q}\times 2\omega_q\times\frac{1}{-\omega_q-ip_n-\xi_k}$ $\quad = -1+\frac{1}{1-e^x}$

$= -1-\frac{1}{e^x-1}$

$+\frac{1}{\beta}n_B(ip_n+\xi_k)\times\frac{-2\omega_q}{(ip_n+\xi_k)^2+\omega_q^2}$ $\quad n_B(ip_n)=-1$ $\quad = -1-n_B(x).$

$\Rightarrow n_B(-\xi_k) = 1 - n_B(\xi_k)$

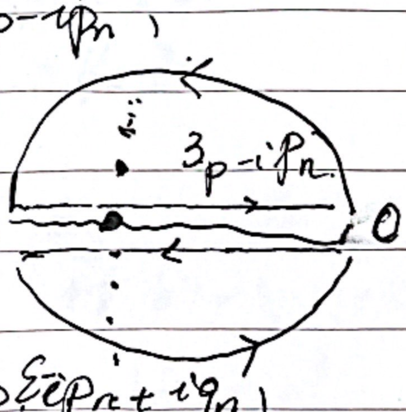
$=\frac{1}{\beta}\left[\frac{n_B(\omega_q)}{\omega_q-ip_n-\xi_k} + \frac{-1-n_B(\omega_q)}{-\omega_q-ip_n-\xi_k} + \frac{(1+n_B(\xi_k))(2\omega_q)}{(ip_n+\xi_k)^2+\omega_q^2}\right]$

$z=iq_n$

4. $\frac{1}{\beta}\sum_{z} \frac{1}{z+ip_n-\xi_p}\times\frac{-2\omega_q}{-z^2+\omega_q^2+2\omega_q P(q,z)}$

Res:

$=\frac{-2\omega_q}{\xi_p - ip_n + \omega_q^2 + 2\omega_q P(q,\xi_p - ip_n)}\, n_F(\xi_p-ip_n)$




得出 $I = \int n_F f(z)\frac{dz}{2\pi i}$

此积分为: $\int_R \frac{d\varepsilon}{2\pi} n_F(\varepsilon) A(p,\varepsilon) G^{(0)}(p,\varepsilon - ip_n + iq_n)$.

$A(p,\varepsilon) = 2i\,\mathrm{Im}\,G_{ret}(p,\varepsilon)$.

$\Rightarrow$ Summation 最简为: $S = \frac{-2\omega_q\, n_F(\xi_p-ip_n)}{\xi_p-ip_n+\omega_q^2+2\omega_q P(q,\xi_p-ip_n)} + \int_R \frac{d\varepsilon}{2\pi} n_F(\varepsilon) A(p,\varepsilon)\, G^{(0)}(p,\varepsilon - ip_n + iq_n)$

Dec. 18th.

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Next part we introduce the Kondo Model:

~~ba~~ The case earlier is a $b^+$ bond state, without considering spin ~~dis~~con tribution, it's nonmagnetic scattering making contribution to resistivity independent of temperature.

However, a magnetic impurity causes a minimum resistance even at $T=0$, resulting from spin-flip scattering

$$\mathcal{H}_0 = \sum_{k\sigma} \epsilon_k C^+_{k\sigma} C_{k\sigma} + E_p \quad p \text{ is localized spin}$$

$$V_{sd} = -\frac{J}{N}\sum_{\substack{kp\\ \alpha\beta}} \exp[iR_j\cdot(k-p)]\, \underbrace{\delta_{\alpha\beta}\cdot S}_{\text{Exchange spin}} \cdot C^+_{k\alpha} C_{p\beta}$$

Now we shall calculate self-energy to $\boxed{3^{rd} \text{ order}}$

$n=$ ~~1 order~~. Using Mastbara Green's Function cancell [exp] term in the $\tau \to \omega$ Fourier Transform.

$$C_{k\sigma}(\tau)C_{k'\sigma'}(\tau') \Rightarrow \mathcal{G} = \langle T_\tau C_{k\sigma}(\tau) C^+_{k'\sigma'}(\tau')\rangle$$

We choose different $(\sigma,\sigma')$ as $\mathcal{G}$ function to express the spin-flip process $\sigma\to\sigma'$, $\underset{\tau}{\sigma} \xrightarrow[k]{} \underset{\tau'}{\sigma'}$ 然而后文会看见$\delta_{\sigma\sigma'}$即$\sigma'=\sigma$费曼图才出现

$$\mathcal{G}(k\sigma\tau, k'\sigma'\tau') = \sum_{n=0}^{\infty}(-J)^n \int_0^\beta \prod_n d\tau_n \langle T_\tau S(\tau_1)\cdots S(\tau_n)\rangle_0$$

$$\times \langle T_\tau C^{(\tau_1)}_{k\alpha} \sigma_{\alpha\beta} C^{(\tau_1)}_{p\beta} \cdots C^{(\tau_n)}_{k\alpha'} \sigma_{\alpha'\beta'} C^{(\tau_n)}_{p'\beta'} C^{(\tau)}_{k\sigma} C_{k'\sigma'}(\tau')\rangle_0$$

$= (\sigma_{\uparrow\downarrow} + \sigma_{\downarrow\uparrow}, \dots)$

• $(\sigma_d^x, \sigma_d^y, \sigma_d^z)$

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More explicit: $S(\tau)\cdot\sigma_{\alpha\beta}$

$S(\tau) = (S^x(\tau), S^y(\tau), S^z(\tau))$ 对于 d $\boxed{S^d}$

$S^x(\tau)$ = pauli Matrix $\sigma_x$

or: 回忆 $\hat{S}$ 算符: $[S^{d(x)}, S^{d(y)}, S^{d(z)}]$

$$\Rightarrow S^{x,y,z}_{(\tau)} = \frac{1}{2}\begin{pmatrix} C^\dagger_\uparrow(\tau) \\ C^\dagger_\downarrow(\tau)\end{pmatrix} \text{pauli}(x,y,z) \begin{pmatrix}C_\uparrow(\tau)\\ C_\downarrow(\tau)\end{pmatrix}$$

而: $\sigma^x_{\alpha\beta} = \langle\alpha|\text{pauli}\,x|\beta\rangle$

比如 $\sigma^x_{\uparrow\downarrow} = \begin{pmatrix}1\\0\end{pmatrix}\begin{pmatrix}1&0\\0&-1\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} \Rightarrow$ a number

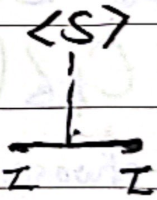
因此: $\underbrace{C^\dagger_{k\alpha}(\tau)\, C_{k\beta}(\tau)}_{\text{electron}}\ \underbrace{S^d(\tau)}_{\text{spin}}\ \sigma_{\alpha\beta}$ 可分离

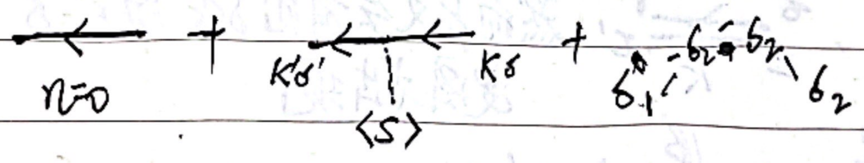
$\langle T_\tau CC\rangle \times \langle T_\tau S^d\rangle \times \langle \text{number}\rangle$

Altogether

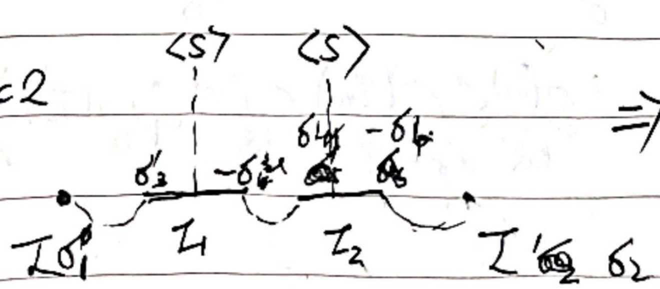
虚线

$\langle C_k^\dagger C_k \times CC \times CC \cdots\rangle \times \langle S^d \cdots S^d\rangle$

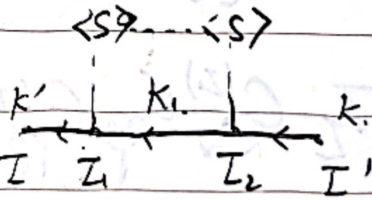
2线, 1个$S^d$　　3线, 2个$S^{(d)}$　　$V =$ 


$n=2$




$\Rightarrow$




$\sigma_1 = \sigma_3,\ -\sigma_4 = \sigma_2 = \sigma_1$

可行!

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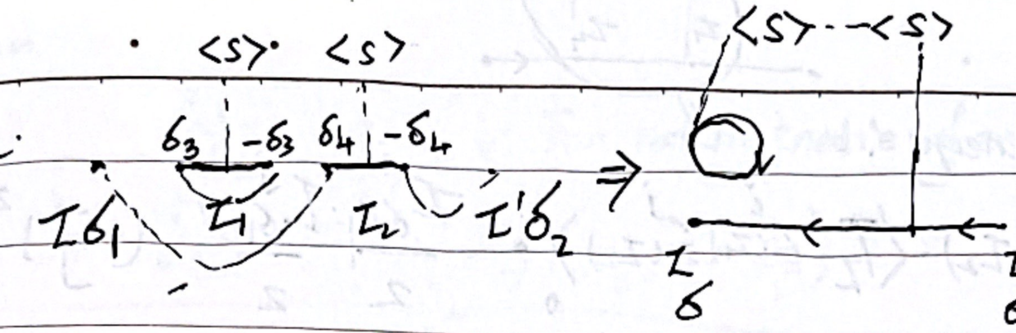
$n=2$.



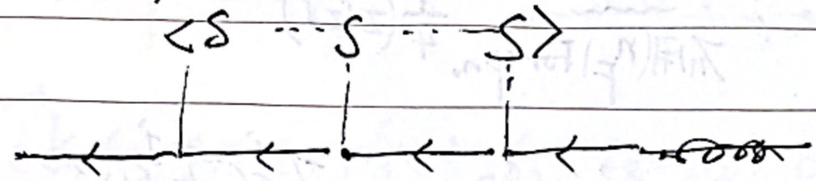

$\boxed{\text{Disconnected}}$

出现一个 $(I_{\sigma\sigma_1} I_{\sigma_1\sigma'})$

现在先不议 $\sigma=\sigma'$ 之后会看见由于 $(I_{\sigma\sigma_1} I_{\sigma_1\sigma'})$ 项. 必有 $\sigma'=\sigma$.

$n=3$. 不看 ~~Feynman Loop 了. 必为 Disconnected Graph.~~

$n=3$




因此, 观察这些费曼图. 对于 $n=1$ 阶:

sum over $(\alpha,\beta)$. $\langle C^{\dagger}_{k\sigma'}(\tau') \cancel{\sigma_{\alpha\beta}} \; C_{k\sigma}(\tau)$ $\delta_{kk'}$

$$\sum_{\sigma\sigma'} I_{\sigma\sigma'} \times \langle c_{k\sigma}(\tau_1) c^{\dagger}_{k\sigma}(\tau)\rangle_0 \langle C^{\dagger}_{k\sigma'}(\tau_1) C_{k\sigma'}(\tau')\rangle_0 \times \langle S^d\rangle_0$$

$$= \sum_{\sigma\sigma'} I_{\sigma\sigma'} \times \langle S^d\rangle_0 \times \mathcal{G}^{(0)}_{\sigma}(k,\tau)^{\tau_1} \mathcal{G}^{(0)}_{\sigma'}(k,\tau_1-\tau') \exp[-i\omega\tau]$$

Fourier

$$\Rightarrow \sum_{\sigma\sigma'} [\mathcal{G}^{(0)}_{\sigma}(k,\omega)_{\sigma'}]^2 \langle I_{\sigma\sigma'} S^d\rangle_0$$

如果 $\sigma'=-\sigma$, 计算: $\sigma^x_{\uparrow\downarrow}=\bar{0}'$ $\sigma^x_{\downarrow\uparrow}=\bar{0}'$ 不算此项

$\sigma'=\sigma$ $\sigma^x_{\uparrow\uparrow}=1$ $\sigma^x_{\downarrow\downarrow}=-1$ cancel 为零.

同理. $\sigma^y$. $\sigma^z$ 皆为零.

$\Leftrightarrow \langle I_{\sigma\sigma} S^d\rangle_{\uparrow,\downarrow,0}$ 由 $\langle S^d_{\uparrow} - S^d_{\downarrow}\rangle_0$

Because we consider system of electron $|\rangle_0$ non-magnetic. this term always zero $\boxed{\Sigma^{(1)}=0}$

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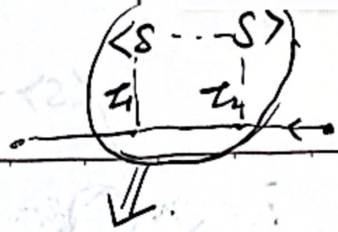



$\boxed{n=2}$. Self-energy

$$\sum_{\substack{K\sigma_1 \\ ij\in(x,y,z)}} g^{(0)}_c(K,\tau_1-\tau_2)_{\sigma_1} \cdot \langle T_\tau \, S^i(\tau_1) S^j(\tau_2)\rangle_0 \cdot \frac{\tau^i_{\sigma\sigma_1}}{2}\frac{\tau^j_{\sigma_1\sigma'}}{2}(-J)^2$$

we use: $\langle S^i_0 S^j\rangle_0 = \frac{1}{8}\,\delta^{ij}\, T_r[\overset{\text{Pauli}}{\tau^i}\tau^j]$

choosing $S^z$: $|\uparrow,\downarrow\rangle$ basis $\quad \underbrace{\frac{1}{2}}_{\text{不用}(n_F)\text{ For spin}}[\langle\uparrow|S^iS^j|\uparrow\rangle + \langle\downarrow|S^iS^j|\downarrow\rangle]$

$\frac{1}{4}(\tau^i\tau^j)$

$\frac{1}{8}T_r[\tau^i\tau^j] = \frac{1}{4}\delta_{ij}$

因此. 原式 $= \sum_{\substack{K\sigma_1 \\ ij\in(x,y,z)}} \delta_{ij}\frac{1}{4}\, g^{(0)}(K\sigma_1,\tau_1-\tau_2)\frac{\tau^i_{\sigma\sigma_1}}{2}\frac{\tau^j_{\sigma_1\sigma'}}{2}(-J)^2$

$= \sum_K \frac{1}{4} g^{(0)}(K\sigma_1,\tau_1-\tau_2)\sum_{\sigma_1 i}\frac{\tau^i_{\sigma\sigma_1}\tau^i_{\sigma_1\sigma'}}{4}(-J)^2$

$\boxed{① \sigma=\sigma'}$ 比如: $\sigma=\uparrow$

而 $\sum_i \tau^i_{\sigma\sigma_1}\tau^i_{\sigma_1\sigma'} = \sum_i \tau^i_{\sigma\sigma_1}\tau^i_{\sigma_1\sigma}$ 查表

$= \underset{\sigma_1=\uparrow}{1} + \underset{\sigma_1=\downarrow}{2} = 3$

$\boxed{表}$

$\tau^x_{\uparrow\uparrow}=0 \quad \tau^x_{\downarrow\downarrow}=0 \quad \tau^x_{\uparrow\downarrow}=1 \quad \tau^x_{\downarrow\uparrow}=1 \quad \begin{pmatrix}0&1\\1&0\end{pmatrix}$

$\tau^y_{\uparrow\uparrow}=0 \quad \tau^x_{\downarrow\downarrow}=0 \quad \tau^y_{\uparrow\downarrow}=i \quad \tau^y_{\downarrow\uparrow}=-i \quad \begin{pmatrix}0&-i\\i&0\end{pmatrix}$

$\tau^z_{\uparrow\uparrow}=1 \quad \tau^z_{\downarrow\downarrow}=-1 \quad \tau^z_{\uparrow\downarrow}=0 \quad \tau^z_{\downarrow\uparrow}=0. \quad \begin{pmatrix}1&0\\0&-1\end{pmatrix}.$

② $\sigma'=-\sigma$ 比如 $\sigma=\uparrow$

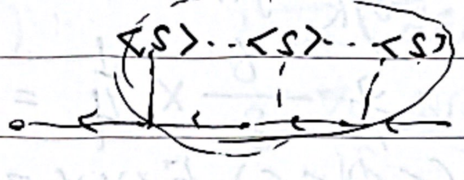
$\sum_{i\sigma_1}\tau^i_{\uparrow\sigma_1}\tau^i_{\sigma_1\downarrow} = 0$

因此：利用 $g_\uparrow = g_\downarrow$ For non-magnetic fermion.

$$\Sigma^{(2)} = \delta_{\sigma\sigma'}\frac{3J^2}{16}\sum_{k_1} g^{(0)}(k_1, \tau_1-\tau_2).$$

$$\boxed{\Sigma^{(2)}(ik_n) = \delta_{\sigma'\sigma}\frac{3J^2}{16}\sum_{k_1}\frac{1}{ik_n-\xi_{k_1}}}$$

$\boxed{n=3}$. self-energy




$$\int_0^\beta \sum_{\substack{k_1k_2\\ \sigma_1\sigma_2}} g^{(0)}(k_1\sigma_1, \tau_1-\tau_3)\, g^{(0)}(k_2\sigma_2, \tau_3-\tau_2)\, d\tau_3 \times (-J)^3$$

$$\times \langle T_\tau\{S^i(\tau_1)S^j(\tau_2)S^k(\tau_3)\rangle_0 \times \frac{1}{8} I^i_{\sigma\sigma_1} I^j_{\sigma_1\sigma_2} I^k_{\sigma_2\sigma'}$$

($T_\tau$) 表明 $\hat{S}$ 有顺序：$[S^i, S^j]$ 并不对易，时序必须考虑.

其中：$I^i_{\sigma\sigma_1} I^j_{\sigma_1\sigma_2} I^k_{\sigma_2\sigma'} = \sum_{\sigma_1\sigma_2}\langle\sigma|I^i|\sigma_1\rangle\langle\sigma_1|I^j|\sigma_2\rangle\langle\sigma_2|I^k|\sigma'\rangle$

$$= \langle\sigma|I^iI^jI^k|\sigma'\rangle$$

① $\sigma = \sigma' \Rightarrow Tr[I^iI^jI^k]$ $\begin{pmatrix} & i\\ -i & \end{pmatrix}\begin{pmatrix} 1 & \\ & -1\end{pmatrix}$

② $\sigma = -\sigma'$ $\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}0&-i\\i&0\end{pmatrix}\begin{pmatrix}1&0\\0&-1\end{pmatrix} = i\langle\sigma|\hat{I}|\sigma\rangle = 0$

eg. $\sigma = \uparrow$ $\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}1&0\\0&-1\end{pmatrix} = \hat{I} \Rightarrow 0$ 同上矩阵. 为零

$(i,j,k) =$

又：$Tr[I^iI^jI^k] = 2i\varepsilon_{ijk}$ 对 $i=j$ 为零

否则求和得到：(即必须 $i \neq j \neq k$) $\sigma = -\sigma'$ 项为零

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同上 $\langle S^i S^j S^k \rangle = -\delta_{ijk} \varepsilon_{ijk}$ 本让 $i \neq j \neq k$.

这样 $\sum_{\sigma_1 \sigma_2 \sigma \sigma'} \tau^i_{\sigma_1 \sigma_1} \tau^j_{\sigma_1 \sigma_2} \tau^k_{\sigma_2 \sigma'}$ 只有 $\sigma = \sigma'$ 非零. $\sigma \neq -\sigma'$ $i \neq j \neq k$

时必须为零. $\sigma = \sigma'$ 此项为 $\varepsilon_{ijk}$

两者相乘: $\sum_{ijk} \varepsilon_{ijk}^2 = 6$

前面系数因此为 $\frac{6}{8} \times \frac{1}{4} = \frac{3}{16}$

现在求和了 $(\sigma\sigma')(\sigma_1\sigma_2)$ 与 $(x\,y\,z)$. 考虑 $(\tau_1 . \tau_2 . \tau_3)$ 时序

令 $\tau_2 = 0$, 时间 $\tau_3 > \tau_1$. $\tau_3 < \tau_1$. 区分. $\tau_2$ 必最小、

$$\theta(\tau_1 - \tau_3) \langle S^i S^j S^k \rangle + \theta(\tau_3 - \tau_1) \langle S^j S^i S^k \rangle = \frac{2i}{8} \operatorname{sgn}(\tau_1 - \tau_3) \underline{\varepsilon_{ijk}}$$

负号占此

因此. 原式 =

$$\sum_{k_1 . k_2} g^{(0)}(k_1 . ik_n) \, g^{(0)}(k_2 . ik_n) \times \frac{3}{16} \times (-J)^3$$

$\Downarrow$

$$\Sigma^{(3)} = \sum_{k_1 k_2} \frac{1}{(ik_n - \xi_{k_1})(ik_n - \xi_{k_2})} \left( \frac{-3J^3}{16} \right)$$ 与 $(k . k')$ 无关

$$\Sigma(k . k', ik_n) \Longleftrightarrow \Sigma(ik_n).$$

如何求和? 对 $\tau_3$ 积分

$$\sum_{k_1 k_2} \int_0^\beta d\tau_3 \, g^{(0)}(k_1 . \sigma_1, \tau_1 - \tau_3) \, g^{(0)}(k_2 \sigma_2 . \tau_3) \underset{\text{时序}}{\underline{\operatorname{sgn}(\tau_1 - \tau_3}}$$

using Fourier Transform. $e^{i(\tau_1 - \tau_3) q_n'} g^{(0)}(k_1 . iq_n)$.

再对 $q_n'$ 求和. 得.

$$\Sigma^{(3)} = \frac{-3}{16}J^3 \cdot \sum_{p,q} \frac{1}{ik_n-\xi_q} \times \left[\frac{1}{ik_n-\xi_p} - \frac{4n_F(p)}{\xi_p-\xi_q}\right]$$

其中.第二项贡献了 $\ln(T)$ 的电阻.

$$\sum_{p,q}\frac{4n_F(p)}{(ik_n-\xi_q)(\xi_p-\xi_q)} \qquad \int \frac{dN}{dk}\cdot\frac{dk}{d\varepsilon}\cdot d\varepsilon\cdot f(\varepsilon)$$

$$\sum_{p,q} f(\varepsilon_p) = \int_{-W}^{B} g(\varepsilon) f(\varepsilon)\, d\varepsilon = \sum_k n(k)\cdot f(\varepsilon)$$

对动量空间中p的求和 可以用态密度 $g(\varepsilon)$ 积分替代 连续谱$[-W,B]$中

$$\sum_{p,q} \to -\frac{3}{16}J^3 \int_{-W}^{B} d\varepsilon_1 \frac{g(\varepsilon_1)}{ik_n-\varepsilon_1}\int_{-W}^{B}\frac{n_F(\varepsilon_2)g(\varepsilon_2)}{\varepsilon_1-\varepsilon_2}d\varepsilon_2.$$ 截断.

求自能虚部

$$\Sigma^{ret}(ik_n\to\omega+i\eta)$$

$$\mathrm{Im}\Sigma^{ret} = \mathrm{Im}\left[\left(-\frac{3}{16}J^3\right)\right]\int_{-W}^{B} d\varepsilon_1 \frac{g(\varepsilon_1)}{\omega-\varepsilon_1+i\eta}\int_{-W}^{B}\frac{n_F(\varepsilon_2)g(\varepsilon_2)}{\varepsilon_1-\varepsilon_2}d\varepsilon_2$$

取虚部,此项变为 $-\pi\delta(\omega-\varepsilon_1)$

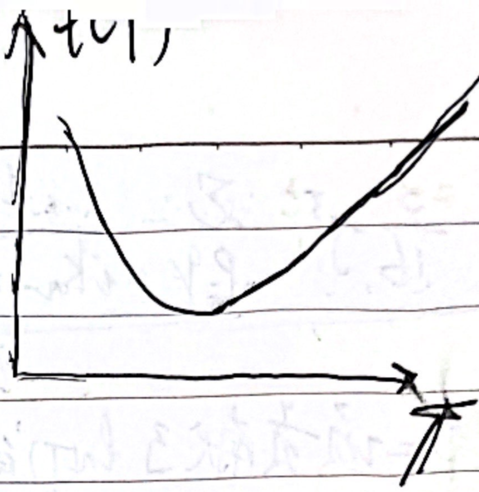
因此.第一个积分 $\int_{-W}^{B}\delta(\omega-\varepsilon_1)g(\varepsilon_1)\,d\varepsilon_1 = g(\omega)$

$$\mathrm{Im}\left[\Sigma^{ret(3)}\right] = \left(-\frac{3}{16}J^3\right)\cdot g(\omega)\cdot\int_{-W}^{B}\frac{n_F(\varepsilon_2)g(\varepsilon_2)}{\omega-\varepsilon_2}d\varepsilon_2.$$

近藤问题属于低温极限 $T\to 0$ $\mu\to 0$ 对 $\varepsilon>0$ 无分布, 对 $\varepsilon<0$
满分布 $n_F(\varepsilon)=1$ for $\varepsilon<0$. 则原式 $= \int_{-W}^{0}\frac{g(\varepsilon_2)}{\omega-\varepsilon_2}d\varepsilon_2$

$$\int_{-W}^{0}\frac{g(\varepsilon_2)}{\omega-\varepsilon_2}d\varepsilon_2 \approx g(\omega)\ln\left|\frac{\omega}{W}\right|$$

由于 $g(\omega)$ 随 $\omega$ smooth 变化. $g(\omega)\to g(0)$



因此·此项贡献自能虚部为：

$$\mathrm{Im}\Sigma(\omega) = \frac{-3\pi}{16} J^3 \cdot g(0) \cdot \ln\left|\frac{\omega}{W}\right|$$

电阻与自能虚部有关 $\omega \to k_B T$

$$\rho(T) = -\frac{3\pi}{16} J^3 g(0) \cdot \ln\left|\frac{k_B T}{W}\right|$$

Bond Sta

$$\rho(T)_{All} = A\ln(T) + BT^5 + C_0\rho(\omega) \quad \nearrow \text{T-independ}$$

(Kondo) e-phonon scatter first-term.

Argument: $\mathrm{Im}\Sigma \Leftrightarrow \rho$

$\rho \propto \frac{1}{G_{电导}}$ ; $G_{电导} \propto$ 流流关联函数 $\propto \mathrm{Im}G \propto \frac{1}{\mathrm{Im}\Sigma}$ $\langle[\ ]\rangle$

$\Rightarrow \rho \propto \mathrm{Im}\Sigma$ Argue: 流流函数约为 $G^{(0)}\times G^{(0)}$

公式：$G = \frac{i\pi}{\omega}\Pi^R(\omega)$ $\Pi^R(\omega) = -i\theta(t-t')\langle[I(t)\ I(t')]\rangle$

取电导实部倒数为电阻，即取 $\boxed{\text{Wick: } G^{(0)}\times G^{(0)}}$

$\mathrm{Im}\left[\frac{\Pi^R(\omega)}{\omega}\right]$ $\Pi^R(\omega)$类似推迟Green's Function

推迟$g^{(0)}$: $ik_n \to \omega - i\eta \to G$

$$= \mathrm{Im}\left[\frac{G^R(\omega)}{\omega}\right] = \mathrm{Im}\left[\frac{1}{\omega}\times\left(\frac{1}{\omega_n - i\eta + \Sigma}\right)^2\right]$$

$$= \frac{1}{\omega}\times \mathrm{Im}\left[\frac{1}{[(\mathrm{Im}\Sigma+\eta)\times i + \omega_n + \mathrm{Re}\Sigma]^2}\right]$$

$$= \frac{1}{\omega}\times\frac{\mathrm{Im}\Sigma\,\omega}{\omega^2A^2 + (\mathrm{Im}\Sigma)^2} \quad \mathrm{Im}\Sigma = \ln\omega \Rightarrow \left(\frac{1}{\omega}\times\omega\right)\times\frac{\ln\omega}{(\ln\omega)^2} = \frac{1}{\ln\omega}$$

$$\Rightarrow G = \frac{1}{\omega}\cancel{\times\frac{\ln\omega}{\ldots}} \Rightarrow \rho = \frac{(\ln\omega)^2}{\omega\ln\omega} \simeq \ln\omega$$

$1/\ln\omega$

The theory above is valid at high temperature, In low-T, spin ↑, spin ↓, for the local spin ceases to share the same energy. In fact. local spin is locked into a collective state with the band spins $|\uparrow_{local}\downarrow_{band}\rangle$, forming a Kondo singlet. Therefore. connecting to different bands. local spin has different energy. Only above kondo tempeatwe can $\Sigma^{(3)}$ theory be valid.

For $(J<0)$, at low temperature, is a singlet. we define the collective state. Def:

$$|\uparrow\rangle_d\ \alpha\ ;\ |\downarrow\rangle_d\ \beta\ ;\ S=\frac{1}{2}\ ;\ J<0\ ;\ |\text{Fermi Sea}\rangle : |F\rangle$$

There's a localized spin effecting to a fermi-sea at low. T. we write out it's wave function: Normal 反对称费米态

$$\psi_1 = \sum_{|k|>k_F} a_k \left[ C^\dagger_{k\downarrow}|\uparrow\rangle\otimes|F\rangle - C^\dagger_{k\uparrow}|\downarrow\rangle\otimes|F\rangle \right] \qquad \underbrace{C^\dagger_{k\downarrow}|\uparrow\rangle}_{\text{singlet}}$$

or

$$\psi_2 = \sum_{|k|<k_F} b_k \left[ C_{k\downarrow}|\uparrow\rangle\otimes|F\rangle + C_{k\uparrow}|\downarrow\rangle\otimes|F\rangle \right] \qquad \underbrace{C_{k}|\uparrow\rangle}_{\text{hole state}}$$

$$|F\rangle = \prod_{|p|<k_F} C^\dagger_{p\uparrow} C^\dagger_{p\downarrow}|\text{empty}\rangle$$

$$\psi_2 \Rightarrow \left[ C_{k\downarrow}|\uparrow\rangle + C_{k\uparrow}|\downarrow\rangle \right] C^\dagger_{k\uparrow} C^\dagger_{k\downarrow}|0\rangle = \psi_1$$

就是 $\psi_1$ 加两个、 出-负号

we form the hole and the particle state for singlet $(\psi_1 - \psi_2)$.

DATE . .

We apply the variational method to calculate $E$ without spin localized

$$\mathcal{H}_0 = \sum_{k\sigma} \varepsilon_k C^\dagger_{k\sigma} C_{k\sigma} \qquad E_G = 2\sum_{|k|<k_F} \varepsilon_k$$

Adding localized spin, one add $V_{sd} \Rightarrow \delta_{\alpha\beta}\, S \cdot C^\dagger_{k\alpha} C_{p\beta} \times (-J)$

$$(\mathcal{H}_0 + V_{sd})\varphi_{1or2} = (E_G + \delta E_{1or2})\,\varphi_{1\,or\,2}$$

$\varphi_{1.2}$ is our trial state we assume $V_{sd}$ make a effect on the singlet state, $\delta E_{1or2}$ is the energy shift. In fact, the $V^{sd}$ can generate states like: $(q=k)$

$$\sum_{pq} C^\dagger_{p\uparrow} C_{q\downarrow} S^{(-)}_d \sum_{|k|>k_F} \delta_{q.k} \cdot a_k \cdot |\uparrow\rangle_d C^\dagger_{k\downarrow}|F\rangle \quad (S^{(-)}|\uparrow\rangle = |\downarrow\rangle)$$

$$= \sum_{|k|>k_F} a_k \sum_{|p|>k_F} |\downarrow\rangle C^\dagger_{p\uparrow}|F\rangle$$

a valid state

But when $q \neq k$. also many states can be generated by $V^{sd}$ but Not $(\varphi_1 . \varphi_2)$. Nevertheless, we apply the approxiamation.

$$\text{Variational } E = \frac{\langle \varphi_{1.2}|\mathcal{H}|\varphi_{1.2}\rangle}{\langle \varphi_{1.2}|\varphi_{1.2}\rangle} = E_G + \delta E$$

$$\langle \varphi_1 |\, \mathcal{H}_0 + V^{sd} - E_G - \delta E \,| \varphi_1 \rangle = 0$$

~~$\langle \varphi_1 | \frac{1}{\sqrt{N}} \sum_{|k|>k_F} E_G + \varepsilon_k$~~

Seperate calculation in parts.

$$|\, \mathcal{H}_0 - E_G - \delta E \,|\varphi_1\rangle \Rightarrow \mathcal{H}_0 [\,|\uparrow\rangle C^\dagger_{k\downarrow} - |\downarrow\rangle C^\dagger_{k\uparrow}]|F\rangle$$

$$= \varepsilon_k + E_G \qquad \varepsilon_k + E_G$$

此项 $\Rightarrow$ $(\varepsilon_k - \delta E)|\varphi_1\rangle = \frac{1}{\sqrt{N}} \sum_{|k|>k_F} a_k (\varepsilon_k - \delta E_a) [\,|\uparrow\rangle C^\dagger_{k\downarrow} - |\downarrow\rangle C^\dagger_{k\uparrow}]\,|F\rangle$

左矢作用：

$$\langle F| \uparrow \cdot c_{k\downarrow} | \sum_{|k|>k_F} \frac{1}{\sqrt{N}} (\varepsilon_k - \delta E_a) |\uparrow\rangle c^{+}_{k\downarrow} - |\downarrow\rangle \cancel{c^{+}_{k\uparrow}} |F\rangle$$

$\delta_{k \cdot k'}$

$$= \frac{1}{\sqrt{N}} a_k (\varepsilon_k - \delta E_a)$$

$-\langle F| \downarrow c_{k\uparrow}|$ 同理为上式之相反数 $\times(-1) \Rightarrow (-1)\times(-1) = 1$

$$\Rightarrow \langle \psi_1 | H_0 - E_G - \delta E_a | \psi_1 \rangle = \frac{2}{\sqrt{N}} a_k (\varepsilon_k - \delta E_a)$$

$k : c_k$

第一部份：分解 $\hat{S} \cdot \sigma_{\alpha\beta} c^{+}_{k\alpha} c_{p\beta}$，Z 方向为：

$$S^{(z)} [c^{+}_{p\uparrow} c_{q\uparrow} - c^{+}_{p\downarrow} c_{q\downarrow}] \sum_{k>|k_F|} a_k |\uparrow\rangle c^{+}_{k\downarrow} |F\rangle$$

$\Rightarrow S^{(z)} |\uparrow\rangle = \frac{1}{2} |\uparrow\rangle$；① $p = q$ $(n_{p\uparrow} - n_{p\downarrow}) c^{+}_{k\downarrow} |F\rangle = -1$

② $q = k$，$\sum_p c^{+}_{p\downarrow} \cdot |\uparrow\rangle \cdot |F\rangle$，其余均 $\langle\ \rangle$ 为 0. 不比上多1个

此两项结果：对 $S^z$ 而言，为：

$$-\frac{1}{2} \sum_{|k|>k_F} a_k |\uparrow\rangle \cdot c^{+}_{k\downarrow} |F\rangle - \frac{1}{2} \Big[\sum_{|k|>k_F} a_k\Big] \Big[\sum_{|p|>k_F} |\uparrow\rangle c^{+}_{p\downarrow} |F\rangle\Big]$$

第一部份，x·y 方向 $S^x \cdot S^y$ 为

$$= |\uparrow| c_{k\downarrow} [c^{+}_{p\uparrow} c_{q\downarrow} - c^{+}_{p\downarrow} c_{q\uparrow}] c^{+}_{k\downarrow} |F\rangle |\uparrow\rangle$$

自旋不守恒，全为零，再忽略 $S^z$ 第一项（比第二项少一个 N）.

总共，$V_{sd} \psi_1 = \frac{3J}{2N^{3/2}} \Big[\sum_{|k|>k_F} a_k\Big] \times$

$$\Big[\sum_{|p|>k_F} a_p [|\uparrow\rangle c^{+}_{p\downarrow} - |\downarrow\rangle c^{+}_{p\uparrow}] |F\rangle$$

We can add $V^{sd}$ and $H_0$ term, our 变分参数是 $\varphi_1$ 中的 $a_k$ 项. 因此, 用 $\langle\varphi|H - E_G - E_2|\varphi\rangle = 0$. 得到 $a_k$ 关系.

$$\varphi_1: \quad a_k = -\frac{3J}{2N}\frac{1}{\varepsilon_k - \delta E_a}\sum_{|p|>k_F} a_p$$

$$\varphi_2: \quad b_k = \frac{3J}{2N}\frac{1}{\varepsilon_k + \delta E_b}\sum_{|p|<k_F} b_p$$

$$\begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix} = -\frac{3J}{2N}\begin{pmatrix} \frac{1}{\varepsilon_1-\delta E_a} & \cdots & \frac{1}{\varepsilon_1-\delta E_a} \\ \frac{1}{\varepsilon_2-\delta E_a} & & \vdots \\ \vdots & & \\ \frac{1}{\varepsilon_N-\delta E_a} & \cdots & \end{pmatrix}\begin{pmatrix} a_1 \\ \vdots \\ a_N \end{pmatrix}$$

Eigenvalue $a_1(\mathrm{Eig}) = 0 \Rightarrow \quad 1 = -\frac{3J}{2}\int_0^B d\varepsilon \, \frac{g(\varepsilon)}{\varepsilon - \delta E_a}$

因此: $\delta E_a$ 就解出了. 同理 $\delta E_b$. 令 $g(\varepsilon) = g$

$$1 = \left(3Jg/2\right)\ln\left|\frac{\delta E_a}{W - \delta E_a}\right| \qquad 1 = \left(3Jg/2\right)\ln\left|\frac{\delta E_b}{W-\delta E_b}\right|$$

$$\Rightarrow \delta E_a = \frac{-W\Lambda}{1+\Lambda} \qquad \delta E_b = -\frac{B\Lambda}{1+\Lambda} \qquad \ln(\Lambda) = \frac{2}{3Jg}$$

$\delta E \ll W, B \Rightarrow \Lambda/_{1+\Lambda} \to 0 \Rightarrow \Lambda < 1 \Rightarrow J < 0$

Only ($J<0$) Antisymmetric case can this singlet be formed.

$$\Lambda = e^{-\frac{2}{3|J|g}}$$

We use variational method; the pertubation method is way too difficult for this case.

Def: Kondo Temperature:

$$k_B T_K = \exp\left(-\frac{1}{2g(0)|J|}\right)\cdot W$$

$$\rho(T) = \rho(0)\left(1+4Jg(0)\ln(k_BT/W)\right).$$

Kondo temperature is defined when ln(T) Kondo Effect can be compared with $\rho(0)$ first term. when it becomes significant.

$1 = 4Jg(0)\ln\frac{k_BT}{W}$ 推得上式

Altogether, for spin S. high temperature:

$$\Sigma_{ret}(\omega) = \frac{cJ}{1-2Jg(\omega)\ln(\omega/W) - i\pi Jg(\omega)S(S+1)}$$

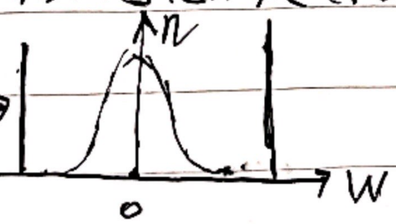
$$Im[\Sigma_{ret}(\omega)] = \frac{\pi cJ^2 g(\omega)S(S+1)}{[1-2Jg(\omega)\ln(\omega/W)]^2 + [\pi Jg(\omega)S(S+1)]^2}$$

总之，系统小于 $T_K$ 时，越来越强的反铁磁性使更多 S-巡游电子与 d 杂质自旋形成近藤单态，形成一个多电子云屏蔽掉局域自旋。结果是形成一个 Kondo 峰，体现为：

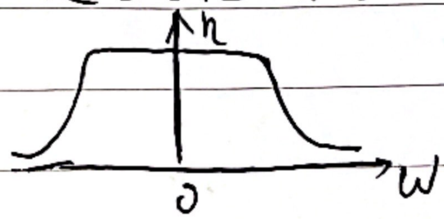
① $T\to 0$ $\rho\to$ const ② $\vec{S}\to 0$ 屏蔽 ③ $\delta$-function 峰

给一种不太准确解释，之前在解释 localized state b 在传导电子中，给出了态密度图(左)，我们又知道电子态密度(T小)

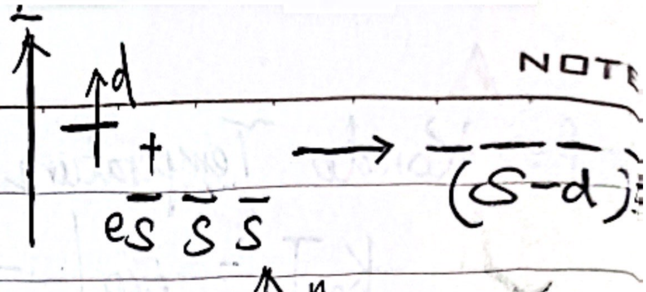
对b (n页前算过)



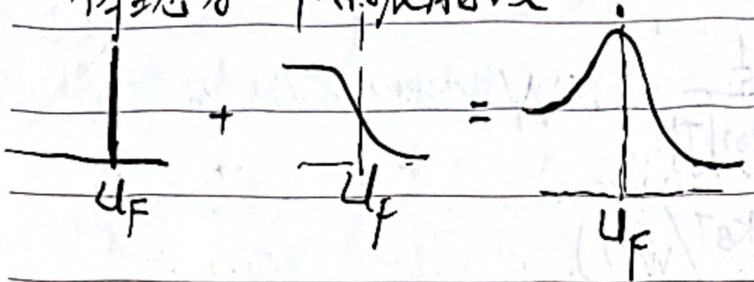
对e



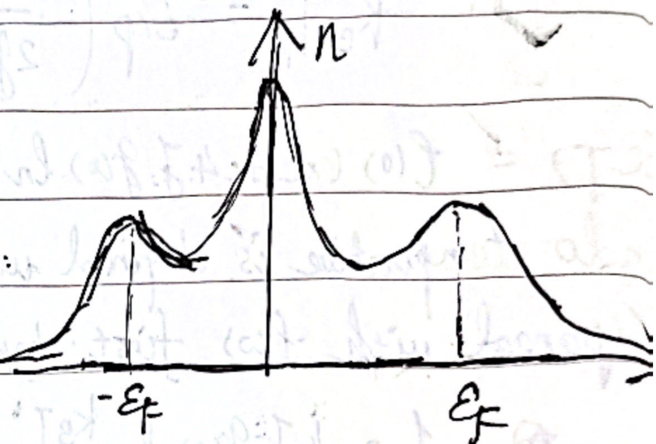
那么左图如何影响右图的？近藤单态的形成，恰好将磁性杂质磁性去除，形成非磁的一大坨，恰类似左图，同时其吸纳了巡游电子，尤其在左、右两个峰(费米面)处；




体现为一个共振能级




at $T<T_K$ 近藤共振越清晰 为:




上文的变分方法基于 Yosida 提出的模型. 给出此单态偏离基态的束缚能 $\delta E$. 我们可以以此定位此激发束缚态的位置. 从而给出 $T_K$ 的近似表述。但此法依然不准确. 基于费米液体理论的准粒子激发图像虽然有多体引入. 但仍激发 $|C_k^+|\text{Fermi Sea}\rangle$

$T<T_K$ 关联长度 $\sim 4000$ Å. 高度关联系统不能以单个准粒子激发来描述.

在 $T>T_K$ 时, 巡游电子通过翻转自旋来隧穿, 在 $T<T_K$ 时, 巡游电子通过与局域自旋形成近藤单态, 把价 $d$ 能量拉下来, 形成在费米面附近的多体态可用于隧穿.

真正严格解决 Kondo Problem 有赖 Wilson (1974) 发展的非微扰数值重整化方法.

Dec. 20

DATE . .

NOTES

Single-Site Anderson Model.

Unlike Kondo Model., which treats impurity as a seperate part from electrons. Anderson Model treats impurity as just another electron. it has $\varepsilon_k$. on-site $U$, coupling with electrons. it's hamiltonian:

$$\mathcal{H}_0 = \sum_{k\sigma} \varepsilon_k C^+_{k\sigma} C_{k\sigma} + \varepsilon_f \sum_{\sigma} n_{\sigma} + U \sum n_{\uparrow} n_{\downarrow}$$

We put it in $\mathcal{H}_0$. too large to pertubate

$$n_\mu = f^+_\mu f_\mu$$

$$V = \frac{1}{\sqrt{N}} \sum_{k\sigma} V_{k\sigma} \left( C^+_{k\sigma} f_{\sigma} + f^+_{\sigma} C_{k\sigma} \right)$$

有 d 自己 on-site, $U$ 项; $\varepsilon_k$ 项; coupling 项。对于翻转自旋作用. $C^+_k f$ 减 $f_\downarrow$ 与 $f^+ C$ 增 $f\uparrow$ 共同作用了翻转过程.

$$(C^+ f + f^+ C)(|\uparrow 0\rangle - |\downarrow 0\rangle) \Rightarrow (|\downarrow 0\rangle - |\uparrow 0\rangle)$$

$U n_{d\downarrow} n_{d\uparrow} \neq 0$ 体现此两过程非独立性.

(下.下.页)

Methods: 
- Non-crossing Approxiamation
- expand S-Matrix
- slave boson.

DATE . . NOTE

Homework for Kondo.

$\boxed{1.}$ Show bound states of Kondo hamiltonian

$$\mathcal{H} = \underbrace{\sum_{k\sigma} \varepsilon_{k\sigma} C^+_{k\sigma} C_{k\sigma}}_{\hat{A}} - \sum_{kk'} \Big[ J_z S^z \big( \underbrace{C^+_{k\uparrow} C_{k'\uparrow}}_{\hat{B}} - \underbrace{C^+_{k\downarrow} C_{k'\downarrow}}_{\hat{C}} \big) + J_\perp \big( \underbrace{C^+_{k\uparrow} C_{k'\downarrow} S^{(-)}}_{\hat{D}} + \underbrace{C^+_{k\downarrow} C_{k'\uparrow} S^{(+)}}_{\hat{E}} \big) \Big]$$

① $\phi_1 = \sum_k a_k C^+_{k\uparrow} |\uparrow\rangle$

$$\hat{A}\phi_1 = \delta_{kk'} \sum_{a_k} \varepsilon_{k\sigma} a_k \underset{(1)}{\underset{=}{n_k}} C^+_{k\uparrow} |\uparrow\rangle =$$

$$\delta_{k \cdot k_2} \begin{cases} S^z |\uparrow\rangle = |\uparrow\rangle \\ S^+ |\downarrow\rangle = |\uparrow\rangle \\ S^- |\uparrow\rangle = |\downarrow\rangle \end{cases}$$

$$\hat{B}\phi_1 = -\sum_{k_1 k_2} C^+_{k_1\uparrow} C_{k_2\uparrow} \sum_k a_k C^+_{k\uparrow} |\uparrow\rangle$$

$$= \Big[\sum_k a_k\Big] \Big[\sum_{k'} C^+_{k'\uparrow} |\uparrow\rangle\Big] \times (-J_z)$$

$\hat{C}\phi_1 = 0$ $\quad \hat{E}\phi_1 = 0 \; (S^{(+)} |\uparrow\rangle = 0)$

$\hat{D}\phi_1 = 0$

$$\Psi = \mathcal{H}\hat{\phi}_1 = \sum_k a_k \varepsilon_{k\uparrow} C^+_{k\uparrow} |\uparrow\rangle + \Big[\sum_k a_k\Big] \Big[\sum_{k'} C^+_{k'\uparrow} |\uparrow\rangle\Big] \times (-J_z)$$

$$\langle \phi_1^* | \Psi \rangle = \Big(\sum_k \varepsilon_{k\uparrow} a_k\Big) + \Big[\sum_k a_k\Big]^* \times (-J_z) \times \sum_k a_k$$

$C_{k\uparrow} |\uparrow|$

$\langle \phi_1 | \delta E_2 | \phi_1 \rangle = \delta E_2 \sum_k a_k^*$ 相减为零

Eigen Equation: $[\varepsilon_{k\uparrow} - \delta E_2] a_k^* = J_z \big[\sum_k a_k\big]$

$$\Rightarrow \frac{J_z}{\varepsilon_{k\uparrow} - \delta E_2} \sum_k a_k = a_k$$

Eigenfunction: $1 = J_z \int_0^B d\varepsilon_\uparrow \frac{g(\varepsilon_\uparrow)}{\varepsilon_\uparrow - \delta E_2}$ Bound State

② $\phi_2 = \sum_k b_k C^+_{k\downarrow}|\Downarrow\rangle$ $S^z|\Downarrow\rangle = -|\Downarrow\rangle$

$A\hat{\phi_2} = \sum_k b_k \varepsilon_{k\downarrow}|\Downarrow\rangle$ $B\hat{\phi_2} = 0$ $C\hat{\phi_2} = -J_z \cdot [\sum_k b_k][\sum_{k'} C^+_{k'\downarrow}|\Downarrow\rangle]$

$D\hat{\phi_2} = 0$ ($S^-|\Downarrow\rangle = 0$) $E\phi_2 = 0$.

同①: $1 = J_z \int_0^B d\varepsilon_\downarrow \frac{g(\varepsilon_\downarrow)}{\varepsilon_\downarrow - \delta E_2}$

③ $\phi_3 = \sum_k d_k [C^+_{k\uparrow}|\Downarrow\rangle - C^+_{k\downarrow}|\Uparrow\rangle] = \phi_{31} - \phi_{32}$.

$A\hat{\phi}_{31} = \sum_k d_k \varepsilon_{k\uparrow}|\Downarrow\rangle$ $B\phi_{31} = +J_z)[\sum_k d_k] \cdot [\sum_{k'} C^+_{k'\uparrow}|\Downarrow\rangle]$

$C\hat{\phi}_{31} = 0$ $\hat{D}\hat{\phi}_{31} = 0$ $E\hat{\phi}_{31} =$

$= \sum_{k_1 k_2} C^+_{k_1\downarrow} C_{k_2\uparrow} S^{(+)} \sum_k d_k C^+_{k\uparrow}|\Downarrow\rangle$ $S^+|\Downarrow\rangle = |\Uparrow\rangle$ $\delta_{k \cdot k_2}$

$= [\sum_k C^+_{k\downarrow}|\Uparrow\rangle][\sum_{k'} d_{k'}] \times (J_\perp)$

$A\hat{\phi}_{32} = \sum_k d_k \varepsilon_{k\downarrow}|\Uparrow\rangle$ $B\phi_{32} = 0$ $C\phi_{32} = J_z[\sum_k d_k][\sum_{k'} C^+_{k'\downarrow}|\Uparrow\rangle]$

$D\hat{\phi}_{32} = J_\perp[\sum_k d_k][\sum_k C^+_{k\uparrow}|\Downarrow\rangle]$ $E\phi_{32} = 0$.

$H\phi = [\sum_k d_k \varepsilon_{k\uparrow} |\Downarrow\rangle - \sum_k d_k \varepsilon_{k\downarrow}|\Uparrow\rangle]$

$+ J_z[\sum_k d_k][\sum_{k'} C^+_{k'\uparrow}|\Downarrow\rangle - \sum_{k'} C^+_{k'\downarrow}|\Uparrow\rangle]$

$+ J_\perp[\sum_k d_k][\sum_{k'} C^+_{k'\downarrow}|\Uparrow\rangle - \sum_{k'} C^+_{k'\uparrow}|\Downarrow\rangle]$ $\longrightarrow (J_z - J_\perp)$

DATE

$\langle c_{k\uparrow}|\downarrow| - c_{k\downarrow}|\uparrow| \Psi$

$$= (\varepsilon_{k\uparrow} - \varepsilon_{k\downarrow}) d_k + (J_z - J_\perp) \sum_k d_k + \delta E \cdot d_k = 0$$

Eigenfunction:

$$1 = \int_0^B \frac{-J_z + J_\perp}{\varepsilon_{k\uparrow} - \varepsilon_{k\downarrow} - \delta E} g(\varepsilon_{\uparrow\downarrow})$$

④ 同理. 为 $J_z + J_\perp$, $\varepsilon_{k\uparrow} + \varepsilon_{k\downarrow}$

$$1 = \int_0^B \frac{g(\varepsilon_{\uparrow\downarrow})}{\varepsilon_{k\uparrow} - \varepsilon_{k\downarrow} - \delta E} \cdot (-J_z - J_\perp)$$

If $\delta E < 0$. singlet ; or $\delta E > 0$ triplet. ($J < 0$)

①②④ are triplet ; ③ is singlet

$\boxed{2}$. Evaluate $\Lambda(\varepsilon)$ for the $g(\varepsilon)$ below: $\rho(\omega) = J^2 g(\omega)$

$$\Lambda(\varepsilon) = \int_{-W}^{0} d\varepsilon' \frac{g(\varepsilon')}{\varepsilon' - \varepsilon}$$

① $g(\varepsilon) = 1/2W$ $\quad g(0) = \frac{1}{2W}$

$$\Lambda = \frac{1}{2W} - \ln (\varepsilon - \varepsilon') \Big|_{-W}^{0} = \boxed{\frac{1}{2W}} \left( - \ln \frac{\varepsilon}{\varepsilon + W} \right)$$

$= \cancel{\frac{1}{2W} \ln}$ proportional to $\rho(\omega)$

$$\Lambda = \int_{-W}^{W} = \frac{1}{2W} \int_{-W}^{W} \frac{1}{\varepsilon} d\varepsilon' = 1$$

$g(\varepsilon)$

DATE NOTES

② $g(\varepsilon) = \frac{2\sqrt{W^2-\varepsilon^2}}{\pi W^2}$ ; $\Lambda = \frac{1\times 2}{\pi W^2}\int_{-W}^{0} \frac{\sqrt{W^2-\varepsilon'^2}}{\varepsilon'-\varepsilon} d\varepsilon'$

$\Rightarrow \int_{-W}^{W} g(\varepsilon) d\varepsilon = \frac{2}{\pi W^2}\int_{-W}^{W} \sqrt{W^2-\varepsilon^2} d\varepsilon$

$= \frac{1}{2} x\sqrt{x^2-W^2} - a^2 \ln|x+\sqrt{x^2-W^2}| \Big|_{-W}^{W} \times \frac{2}{\pi W^2}$

$= 1$

③ $g(\varepsilon) = (W-|\varepsilon|)/W^2$ $\quad g(0) = \frac{1}{W}$

$\int_{-W}^{W} \frac{W-|\varepsilon|}{W^2} d\varepsilon = 2\int_{0}^{W} \frac{W-\varepsilon}{W^2} d\varepsilon = \frac{2\varepsilon^2}{2W^2}\Big|_0^W = 1$

$\frac{1}{W}\int_{-W}^{0} \frac{W-|\varepsilon'|}{\varepsilon'-\varepsilon} d\varepsilon' = \int_{-W}^{0} \frac{W+\varepsilon'}{\varepsilon'-\varepsilon} d\varepsilon' = \int_{-W}^{0} \frac{W}{\varepsilon'-\varepsilon} - 1 + \frac{\varepsilon}{\varepsilon'-\varepsilon} d\varepsilon'$

$= \left[(W+\varepsilon)\left(-\ln\frac{\varepsilon}{\varepsilon+W}\right) - W\right]\frac{1}{W^2}$ $\quad \left[\frac{W+\varepsilon}{W^2}\right] \ln\frac{\varepsilon}{\varepsilon+W}$ $\quad \rho(0) = \frac{1}{W}$

proportional to $\rho(0)$.

Collective states with $S=1$

3. $\mathcal{H} = |e\rangle \otimes |S\rangle$ $\qquad$ $|j\ m\ S_1\ S_2\rangle$ $\quad |\tfrac{3}{2}.\tfrac{1}{2}.1.\tfrac{1}{2}\rangle$

$S=\frac{1}{2}$ $\quad S=1$ $\qquad j=1/2 = \sqrt{\frac{1}{3}}|1\ -\tfrac{1}{2}\rangle + \sqrt{\frac{2}{3}}|0.\tfrac{1}{2}\rangle$

For $j=3/2$ state: $\quad C^{\dagger}_{k\uparrow}|1\rangle$ $\qquad j=3/2$ $\quad |\tfrac{3}{2}.\tfrac{3}{2}.1.\tfrac{1}{2}\rangle$

For $j=1/2$ state: $\qquad = |1.\tfrac{1}{2}\rangle$

$\sqrt{\frac{1}{3}} C^{\dagger}_{k\downarrow}|1\rangle + \sqrt{\frac{2}{3}} C^{\dagger}_{k\uparrow}|0\rangle$

For $J<0$. Antiferromatic.

$C^{\dagger}_{k\uparrow}|1\rangle$ spin the same Direction Not preferred.

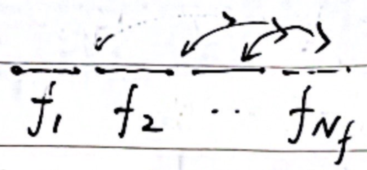
$C^{\dagger}_{k\downarrow}|1\rangle$ spin opposite direction. $j=1/2$ is preferred.

Date. 22~~th~~nd.

重写此 $H_0$ Hamiltonian $\mathcal{H}^{[N]} = |e\rangle_{L N_f} \otimes \overset{f}{|\cancel{d}\rangle}_{N_f}$

$\mathcal{H}_0^f = \varepsilon_f \sum_i n_i + U \sum_{i>j} n_i n_j \qquad \mathcal{H}_0^d = \sum_k \varepsilon_k c_k^\dagger c_k$

注意！single-site 中杂质只一个格点，在此格点原子上，f 轨道上电子称为局域自旋. f 轨道上有 $N_f$ 个电子. 能量为 $H_0^f$:




$H_0 \Rightarrow E_n = n\varepsilon_f + \frac{n(n-1)}{2}U$

这里没有自旋 $n_\uparrow n_\downarrow$ Hubbard 项. 而是 $n_i n_j$ 对于同一个 f 能级的 $(i.j)$ 轨道. 同样. 电子占据 d 轨道, $V[c_k^\dagger f]$ 体现的就是 d.f 轨道之间的杂化. 轨道杂化强度定义为:

$\Delta(\varepsilon) = \frac{\pi}{N}\sum_k V_k \delta(\varepsilon - \varepsilon_k) = V(\varepsilon)^2 \pi \rho(\varepsilon)$

↑ d 连续能带.

$\mathcal{H}_0: n\varepsilon_f + \frac{n(n-1)}{2}U$ 有一个 $\min(H_0)$ at $n = L$

对每个材料不同 $(\varepsilon_f . U)$，$L$ 也不同.

$Ce^{3+}$: $n_f = 1$, $\rightarrow S = \frac{1}{2}$ $\quad L = 3$

$4f^1(5d^1 6s^2)$ $\qquad$ 算出 $(\varepsilon_f . U)$.

轨道自由度是虚的 $p_m^L$. 满足 $E_{min}$ 即可

自旋实的 $S = 1/2$.

$J = |L - S| = 5/2$ 基态简并度 6

然而. 同一个 f 轨道, 由于 splitting. 能量不同, 直接写出广泛简并度. 对于 $E_n$. n 个电子 f 在 $N_f$ 轨中. 有 $Z_n = C_{N_f}^{n}$ 简并.
配分函数为:

$$Z = \sum_{n=0}^{N_f} Z_n e^{-\beta E_n}$$

when $U=0$:

$$Z = \left[1+e^{-\beta\varepsilon_f}\right]^{N_f}$$

对于 Anderson, 直接不管 S-L 耦合. f 能量全同. 因此有 $Z_n$ 极大之简并. 即只关心 (f-d) 耦忽略 f 自身 (S-L) 耦合. 先看 V=0 仅 f 轨之基态. 有 ($\varepsilon_f$. U) 项:

$$g_f(i\omega_n) = -\sum_{i\text{轨}} \int_0^\beta d\tau\, e^{-\omega_m \tau} \left\langle T_\tau f_i(\tau) f_i^\dagger(0)\right\rangle$$

where $|\rangle = |n\rangle$ with n electrons in f-orbit

$$= \frac{1}{Z}\sum_{i,n} Z_n \langle n|f_i|n+1\rangle\langle n+1|f_i^\dagger|n\rangle \frac{e^{-\beta E_n}+e^{-\beta E_{n+1}}}{i\omega_n+E_n-E_{n+1}}$$

对于 $\langle n+1|f_i^\dagger|n\rangle$ 对于 $N_f$ 中已经填入的 n 个轨道, $f_i^\dagger$ 作用加上一个电子, 可以加入任一 ($N_f-n$) 个余下个空轨道中, 有 ($N_f-n$) 选择. $\langle n+1|f_i^\dagger|n\rangle = N_f-n$

$$g_f(i\omega_n) = \frac{1}{Z}\sum_{n=0}^{N_f} Z_n e^{-\beta E_n}\left\{\frac{N_f-n}{i\omega_n+E_n-E_{n+1}} + \frac{n}{i\omega_n+E_{n-1}-E_n}\right\}$$

$i\omega \to i\eta+\omega$

$$A_f(\omega) = 2I_m[G_f(\omega)] = \frac{2\pi}{Z}\sum_{n=0}^{N_f} Z_n e^{-\beta E_n}\Big[(N_f-n)\delta(\omega+E_n-E_{n+1}) + n\delta(\omega+E_{n-1}-E_n)\Big]$$

Using lowest Eigenvalue $\lim E_n = E_L$ ($L \neq 0. N_f$)

$$Z = \sum_{n=0}^{\infty} Z_n e^{-\beta E_n}$$ ($E_{n\,min}$) 最主要. only count $E_L$. $E_{L\pm1}$

$$\Rightarrow Z = \tilde{Z}\cdot Z_L e^{-\beta E_L} \quad \tilde{Z} = 1+\frac{L}{N_f+1-L}e^{-\beta\Delta_-} + \frac{N_f-L}{L+1}e^{-\beta\Delta_+}$$

$$\Delta_\pm = E_{L\pm1}-E_L$$

代入 $A(\omega)$ Four Peaks $\delta(\omega+\Delta_-)$ $\delta(\omega-\Delta_-)$

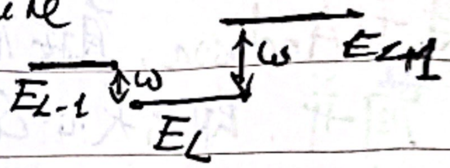
$\delta(\omega+E_{L-2}-E_{L-1})$ $\delta(\omega+E_{L+1}-E_{L+2})$.

Ignore $E_{L-2}$. $E_{L+2}$ Anyway (like $l=1$)

$$A_f(\omega) \approx 2\pi\left[L\,\delta(\omega+\Delta_-)+(N_f-L)\,\delta(\omega-\Delta_+)\right]$$

$\int \frac{A_f(\omega)}{2\pi}d\omega = N_f$ we only have excitations like

we apply this approxiamation




现在,加入杂化引入 $V$: (d-f) 轨间作用.
单粒子 Green's Function 之前讨论过了,两粒 Green's Function,或 关联函数 (e.e)(流.流). 现在为 n个 f 轨道电子之关联 Green's Function

$$H = H_0 + V$$

$$H_0:\ E_n\ (\text{Above})\quad |n\rangle$$

$$H:\ \varepsilon_\alpha\ (\text{unknown}).\quad |\alpha\rangle$$

Basis: $|n\rangle$, which is Eigen for $H_0$.

$$Z = \sum_{n\alpha} Z_n |\langle n|\alpha\rangle|^2 e^{-\beta\varepsilon_\alpha}$$

$$= \sum_{n\alpha} Z_n \int \frac{d\omega}{2\pi} e^{-\beta\omega} A_n(\omega)$$

where: $A_n(\omega) = 2\pi\langle n|\delta(\omega-H)|n\rangle$

$$= 2\pi\sum_\alpha |\langle n|\alpha\rangle|^2\,\delta(\omega-\varepsilon_\alpha)$$

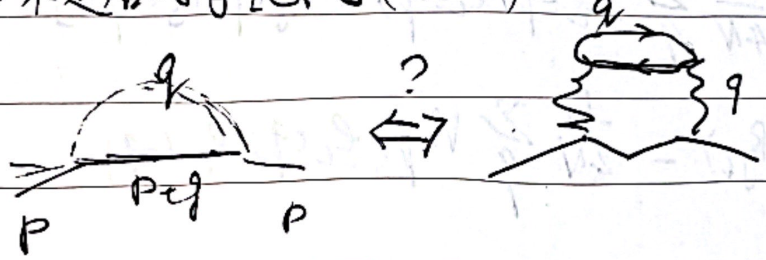
$$G_{n}(\omega) = \frac{1}{\omega - E_n - \Sigma_{(n)}(\omega)}$$

Non-crossing Approximation (NCA).

$$\begin{cases} \Sigma_n(\omega) = n S'_{n-1}(\omega) + (N_f - n)\, S_{n+1}(\omega) \\ S_{n+1}(\omega) = \frac{1}{N} \Sigma_k V_k^2 n_k G_{n+1}(\omega + \varepsilon_k) \\ S'_{n-1}(\omega) = \frac{1}{N} \Sigma_k V_k^2 (1 - n_k) G_{n-1}(\omega - \varepsilon_k) \end{cases}$$

(why?)

期末作业是否为 $[G^{(0)}]^2(\Sigma')$ 此项




是否能以一个声子q过程等价？

何处近似？

DATE

Hubbard Model : (extended)

$$H_H = -t \sum_{\langle ij \rangle} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$H_{XH} = H_H + \frac{1}{2} \sum_{\substack{j \neq l \\ \sigma\sigma'}} n_{j\sigma} n_{l\sigma'} V(R_j - R_l)$$

$$V(R) = e^2/R$$

Seperate SPin. Charge freedom :

$$\rho_{q\sigma} = \sum c^\dagger_{k+q,\sigma} c_{k\sigma} \qquad \rho_{cq} = \rho_{q\uparrow} + \rho_{q\downarrow} \qquad \rho_{sq} = \rho_\uparrow(q) - \rho_{\downarrow q}$$

$$\Rightarrow U \sum_j n_{j\uparrow} n_{j\downarrow} = \frac{U}{4N} \sum_q [\rho_c(q)\rho_c(-q) - \rho_s(q)\rho_s(-q)]$$

$$\frac{1}{2} \sum_{\substack{j \neq l \\ \sigma\sigma'}} n_{j\sigma} n_{l\sigma'} V(R_{jl}) = \frac{1}{2N} \sum_q V(q) \rho_c(q) \rho_c(-q)$$

We can set the two terms in spin. charge dimension

$$U + V = V_c + V_s$$

$$V_c = \frac{1}{2N} \sum_q \left(V_q + \frac{1}{2} U\right) \rho_c(q) \rho_c(-q) \qquad \begin{cases} \rho_{cq} : (\rho_{q\,All}) & \text{CDW} \\ \rho_{sq} (n_\uparrow - n_\downarrow) & \text{SDW} \end{cases}$$

$$V_s = -\frac{U}{2N} \sum_q \rho_s(q) \rho_s(-q)$$

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NOTES

Def: $\underset{\text{正}}{C^{+}_{i\sigma}} = d_{i\sigma}(-1)^{i}$ $\quad d^{+}_{i\sigma} d_{i\sigma} = m_{i\sigma}$

$$\mathcal{H} = \sum_{\langle ij\rangle\sigma} (t)\, d^{+}_{j\sigma} d_{i\sigma} + U \sum_{i} (1 - m_{i\uparrow} - m_{i\downarrow} + m_{i\uparrow} m_{i\downarrow})$$

$$= \sum_{\langle ji\rangle\sigma} t\, d^{+}_{j\sigma} d_{i\sigma} + U \sum_{j} m_{j\uparrow} m_{j\downarrow} + U \underbrace{N}_{\text{格点数}} - U \underbrace{N_e}_{\text{电子数}}$$

加1个 electron $C^{+}$ ⟺ 加一个 hole $d$

$\mathcal{H}_{(d)}$ 定义在满带上 $|\uparrow\downarrow\rangle_i \otimes$ Full. $\mathcal{H}_{(c)}$ 定义在 $|0\rangle$ 空态上.

$\mathcal{H}_{(d)}, \mathcal{H}_{(c)}$ 形式一致 (差了常数. No problem. $t$ 反号) 表明

$\mathcal{H}_{(d)}$ Basis 与 $\mathcal{H}_{(c)}$ Basis 同. $n$ 个电子与 $2N-n$ 电子对于

Hubbard Model 相同. 电子-空穴对称性.

At half-filling: $\mu = U/2$ $\quad \mathcal{H}_{(c)} = \mathcal{H}_{(d)}$

如果 Def: Hubbard Model as:

$$\mathcal{H}_2 = \mathcal{H}_0 + U \sum \cancel{(n_{i\uparrow})(n_{i\downarrow})} (n_{i\uparrow} - 1/2)(n_{i\downarrow} - 1/2)$$

$$= \mathcal{H}_0 + U \sum (\underbrace{1 - m_{i\uparrow}}_{-1/2})(\underbrace{1 - m_{i\downarrow}}_{-1/2}) \quad \text{在 (Half-filling)}$$

$$= \mathcal{H}_0 + U \sum (m_{i\uparrow} - 1/2)(m_{i\downarrow} - 1/2)$$

说明 $\mathcal{H}_2$ 也满足 $\mathcal{H}_{(c)} = \mathcal{H}_{(d)}$, 即在 Half-filling 下.

$\mathcal{H}_2 = \mathcal{H}_{\text{Hubbard}} \Rightarrow \sum_i -1/2\, n_{\text{All}}\, U\, N = 1/4\, U N$ ✓

也表明: $\mathcal{H} = (\mathcal{H}_0' + U) + \underline{(-1/2\, U) \times \sum n_i} + \text{const}$

$(-\mu) \sum n_i \Rightarrow \mu = U/2$

DATE . .

We Apply MF to Hubbard Model first . parameter for $\mathcal{H}$

$$\langle n_{i\uparrow}\rangle ; \langle n_{i\downarrow}\rangle ; \langle C^+_{i\uparrow} C_{i\downarrow}\rangle ; \langle C^+_{i\downarrow} C_{i\uparrow}\rangle$$

We can extra terms:

$$\sum_i -4 S_i\langle S_i\rangle - \frac{1}{2}\langle n_i\rangle^2 - 2\langle S_i\rangle^2 + n_i\langle n_i\rangle$$

We can do it self-consistently:

(CDW) for $\langle n_{i\uparrow}\rangle + \langle n_{i\downarrow}\rangle$ order-parameter. $\langle \rho_q\rangle = \sum_q C^+_{k-q}$

(SDW) for $\langle n_{i\uparrow}\rangle - \langle n_{i\downarrow}\rangle$ order parameter $\langle \rho_s q\rangle = \sum_{q\,k} \langle C^+_{k+q\uparrow} C_{k\uparrow}\rangle - \langle C^+_{k}$

Furthermore. also we can Apply $\boxed{\text{DMFT}}$ (Dynamic MF)

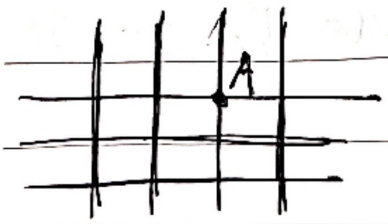
We assume self-energy is localized

$$\Sigma_{(ij\sigma)}(Z) = [\Sigma(Z)](\delta_{ij})$$

$$G_{K\sigma}(Z) = \frac{1}{Z+\mu-\varepsilon_K-\Sigma_\sigma(Z)}$$

$$G_{ii}(Z) = \sum_K \frac{1}{N}\frac{1}{Z+\mu-\varepsilon_K-\Sigma_\sigma(Z)}$$

Consider lattice: $\boxed{\text{DMFT Assume}}$




当我考虑A点时,忽略环境的相互作用,只有环境与A相互作

Actually, 就是一个 Anderson impurity model.

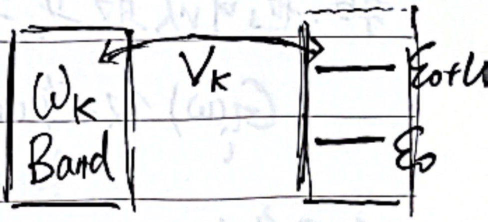
DATE . .　　　　　　　　　　　　　　　　　　NOTES

$\mathcal{H}_{Hubbard} \rightarrow H_{Anderson}$ band impurity. dispersion.

$$H_{A\text{-point}} = [\mathcal{H}_k] + \sum_k [V_k a^{+}_{k\sigma} c_\sigma + c^{+}_\sigma a_{k\sigma}]$$

impurity.

$$+ \varepsilon_0 (n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow$$




if $U=0$. 即连续能带中有一离散能级(见前几页).

$$G(\omega) = \frac{1}{\omega - \varepsilon_0 - \sum_k \frac{V_k^2}{\omega - \omega_k}} \quad V_K: \text{hybridization.}$$

$$\Delta(\omega) = \sum_k \frac{V_k^2}{\omega - \omega_k} \quad \omega \to i\omega + \eta \to I_m \to \sum_k \delta(\omega - \omega_k) |V_k|^2 \to \Sigma(\varepsilon)$$

hybridization function

Then add $U$ for petubation. there exists $\Sigma$ self-energy.

$$G_{ii}(\omega) = \frac{1}{\omega - \varepsilon_0 - \Delta(\omega) - \Sigma_i(\omega)}$$

Also we writes out $G(\omega)$ for original Hubbard Model 对A点(i)来说:

$$G_{H_k}(\omega) = \frac{1}{\omega - \varepsilon_k - \Sigma_k(\omega)} \qquad G_{ii}(\omega) = \sum_k G_{H(k)}(\omega) \times \frac{1}{N}$$

自能没有k依赖. localized 如同 Anderson Ma

$\boxed{\text{Idea of DMFT}}$: Self energy is the same for Anderson and Hubbard Model. $\Sigma(\omega) = \Sigma_k(\omega)$. , 又已知两 Green's function 相同

$$\frac{1}{N} \sum_k \frac{1}{\omega - \varepsilon_k - \Sigma_k(\omega)} = \frac{1}{\omega - \varepsilon_0 - \Delta(\omega) - \Sigma_i(\omega)}$$

Self-consistent solving

① 取一个自能 $\Sigma(\omega)$, 计算 $G_{ii}(\omega)$

② 求解 $\Delta(\omega)$ 得到 $V_K$ (参数皆已知 再做一整套 $\Sigma(\omega)$)

③ Anderson $V_K$ 已知. 求解 Anderson model, 再得到 $\Sigma(\omega)$)

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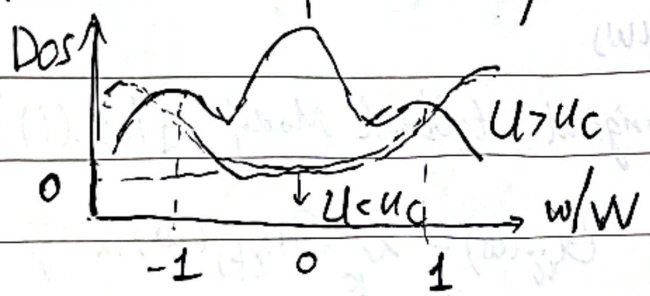
相互作用项仅于impurity上，相对于直接求解 Hubbard Model 的自能，大大简略了。但原则上，要应用一个 $\sum_K$ 无穷大环境求和，也可以取若干K近似

$G_i(\omega)$ 仅一个impurity 不会有 k-space 信息

应用多个impurity 也可知 $G(k.\omega)$ 和 k-space 信息，利用此 E

if there exists long-range correlation. single-site impurity approxiamation also fails.

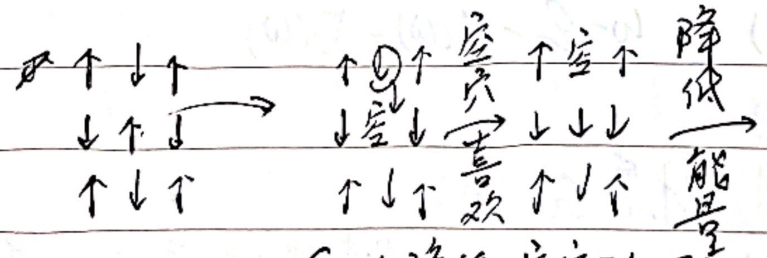
Hubbard Model at half-filling exists Mott-metal transition but at 1-D. for little U. it opens Gap., at higher De, phase transition point $U_c$ by $\boxed{\text{DMFT}}$




[1-D, Squaare lattice] 无 $U_c$. ($\Delta$. ⬡) exists $U_c$

1-D Gapless spin excitation.

GS for Hubbard., ~~Add~~ Dope One Hole: 空穴喜欢铁磁.

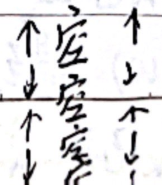



① two hole hopes toge

② $\boxed{\text{条纹相}}$ 基态

$\varepsilon_k$ (降低.空穴动了).

⇐ U 升能(空穴喜欢)



DATE　　　　　　　　本来 ↑↑↓ 应该↓. 现在右边为↑. 破坏AF连续性，有一掺入空穴.　　NOTES

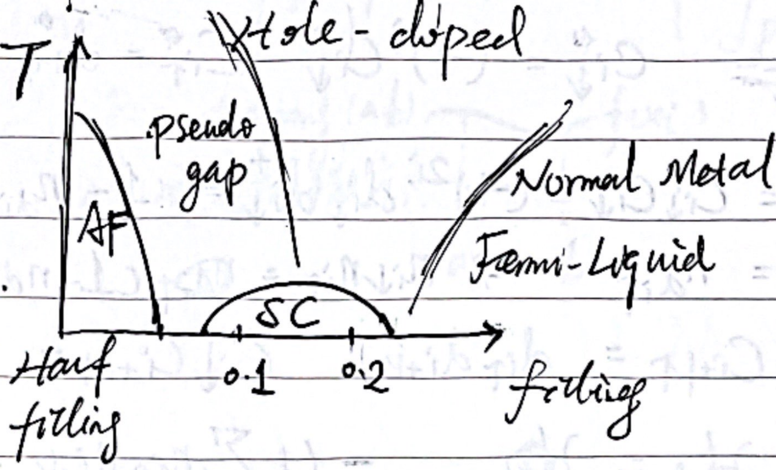
条纹相

↑↓↑↓ ---- ↑↓ 空 ↑↓ ---- ↑↓ 空 ↑

AF　　　　AF

空穴

⇒ pseudogap




If we introduce $t'$

次近邻 $t' C_i^{\dagger} C_{i+\delta_2 \sigma}$ .

Break particle-hole symmetry.

Different Phase for electron and hole dopping.

$t'$ is sensitive to filling. 2-D calculation difficult.

DATE :

# Homework 12.

1. particle-hole transformation for Hubbard Model on a square lattice with spin $\uparrow \downarrow$

$\cancel{d_{i\downarrow} =}$ $c_{i\downarrow}^{\dagger} = (-1)^i d_{i\downarrow}^{+}$ $\quad c_{i\uparrow} = d_{i\uparrow}$ No change

$n_{i\downarrow} = c_{i\downarrow}^{+} c_{i\downarrow} = (-1)^{2i} d_{i\downarrow} d_{i\downarrow}^{+} = 1 - n_{di\downarrow}$

$n_{i\uparrow} = n_{di\uparrow} \Rightarrow n_{i\downarrow} n_{i\uparrow} = (1 - n_{di\downarrow}) n_{di\uparrow}$ $\quad \overset{N_e}{\Uparrow}$

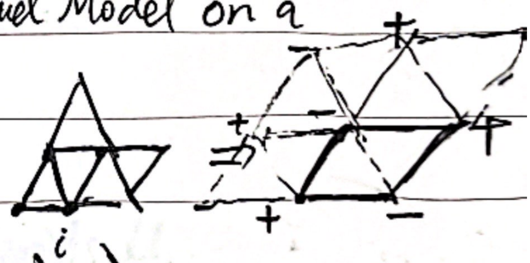
$c_{i\uparrow}^{+} c_{i+1\uparrow} = d_{i\uparrow}^{+} d_{i+1\uparrow} \quad c_{i\downarrow}^{+} c_{i+1\downarrow} = t\, d_{i+1}^{+} d_i + 1 \cdot \mu$

$\Rightarrow H_d = H_e - U \sum n_{i\uparrow} n_{i\downarrow} + U \sum n_{i\uparrow}$

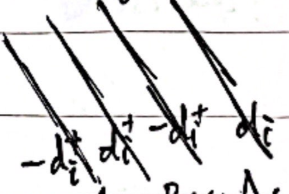
$+ t \sum_{\sigma_\downarrow} c_{i\sigma} c_{j\sigma} - t \sum_{\sigma_\uparrow} c_{i\sigma} c_{j\sigma} + h.c.$

2. particle-hole transformation for Hubbard Model on a spinless triangle lattile

平均下来. 3个 + 3个 -




$-t \sum_{\langle ij \rangle} c_{i\sigma}^{+} c_{j\sigma}$ i对有6个j Line

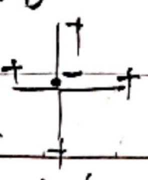
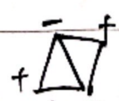



$= -t \sum_{\substack{\langle AA \rangle \\ \langle BB \rangle}} d_{i\sigma}^{+} d_{j\sigma} + t \sum_{\langle AB \rangle} d_{i\sigma}^{+} d_{j\sigma}$

$c_i = -d_i^{+}$ for A

$+ U \sum_{A \text{ and } B} n_{d_\uparrow} n_{d_\downarrow} + UN - UN_e$

$c_i = (-1)^2 d_i^{+}$ for B

因为方格上  正负必成对，而三角上  有负负一对

故要按(A.B)讨论.

Dec. 27th.

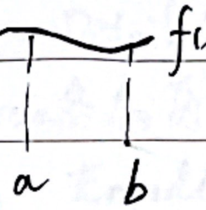
Quantum Monte Carlo.

Integral by MC.

$$\int_a^b f(x)\,dx = (b-a)\cdot\int_a^b \frac{f(x)}{b-a}\,dx \Leftrightarrow \int_a^b f(x)p(x)\,dx \quad \text{where} \begin{cases} p(x) \geq 0 \\ \int p(x) = 1 \end{cases}$$

$$= \frac{b-a}{N}\sum_{i=1}^{N} f(x_i)$$ $P$=const among $(a,b)$

$(a,b)$间随机撒点.




where $\delta(I) \propto \frac{1}{\sqrt{N}}$

Also. 梯形法则:

$$\int_a^b f(x)\,dx = \frac{\Delta x}{2}\cdot\left[f(x_0) + 2f(x_1) + \cdots f(x_{n-1}) + f(x_N)\right] \quad \Delta x = \frac{b-a}{N}$$

$$\delta(I) \propto \frac{1}{N}$$

But at Higher Dimension: $\delta(I)_{MC} \propto \frac{1}{\sqrt{N}}$ efficient!

$\delta(I)_{梯} \propto N^{1/d}$

Important Sampling:

We can chose any $w(x) \geq 0$ $\int w(x) = c$ as probability. $c \to p(x) = \frac{w(x)}{c}$

$$\int_a^b f(x)\,dx = \int_a^b p(x)\left[\frac{f(x)}{p(x)}\right]dx = \int_a^b p(x)g(x)\,dx$$

$$= \frac{1}{N}\sum_{n=1}^{N} \frac{f(x_i)}{p(x_i)}$$

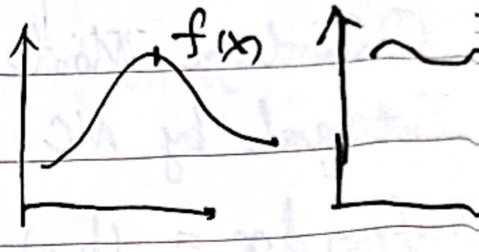
where $\delta^2(I) = \frac{1}{N^2}\cdot\left[\langle (f/p)^2\rangle - \langle f/p\rangle^2\right]$

~~① $p = f$ ; but we should already know $\int w(x) = c$~~

$\delta = 0$

So we should carefully choose ~~的~~ $p(x)$. similar to $f(x)$

we want for large $f(x)$; $p(x)$ also large to eliminate flux.




What about $f(x)<0$, should we choose $p(x)<0$ ?

Ising Model Classical.

$$\mathcal{H} = -J \cdot \sum_{\langle ij \rangle} S_i S_j \qquad S_i = \pm 1$$

partition function at $T = 1/\beta$. $Z = \sum_{2^N} e^{-\beta E(\text{构型})}$

observables: $\langle A \rangle = \frac{1}{Z} \sum_{2^N} e^{-\beta E(\text{构型})} \cdot A(\text{构型})$

取概率 $P(\text{构型}) = \frac{1}{Z} e^{-\beta E(\text{构型})}$ $\quad P>0$

$$\langle A \rangle = \sum_{2^N} P(\text{构型}) A(\text{构型}) \qquad \sum p = 1$$

$\langle A \rangle = \frac{1}{2^N} \cdot \sum_i A(\text{构型}_i)$ 构型出现概率为 P. 投针

Metropolis algorithm: 如何投针?

马尔可夫链: 我希望从出发开始一套操作生成各种构型满足分布 P

比如从 $t_0$ 1 -1 1 出发

$t_1 \downarrow$ ?

$t_2 \downarrow$ ?

构型 $t_2 = f[\text{构型} t_1]$ 仅与 t 前一个有关.

$$\boxed{P_A T(A\to B) A(A\to B) = P_B T(B\to A) A(B\to A)}$$

$$W = T\cdot A$$

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Transition value

$$\frac{dP_A(t)}{dt} = \sum_{\substack{A\neq B\\B}} \left[ P_B(t) W(B\to A) - P_A(t) W(A\to B) \right]$$

从A走，从B来，即A之变化

where $W(A\to B) \geq 0$ $\sum_B W(A\to B) = 1$

at $\dot{P}_A = 0$ $P_A(t) \sum_{\substack{A\neq B\\B}} W(A\to B) = \sum_{\substack{A\neq B\\B}} P_B(t) W(B\to A)$ 细致平衡条件 Detailed Balance.

充分条件 $\Rightarrow$ $P_A T(A\to B) A(A\to B) = P_B T(B\to A) A(B\to A)$ 各态历经条件 Ergodicity.

$P_A = \dfrac{e^{-\beta E(\text{构型})}}{Z}$ $P_A/P_B = e^{-\beta(E_A - E_B)}$.

令 $T(A\to B) = T(B\to A) = \frac{1}{N}$ 每格构句选取申请概率

$$\frac{A(B\to A)}{A(A\to B)} = \underbrace{e^{-\beta(E_A - E_B)}}_{\text{接收概率}}$$

取 $A_{meet}(A\to B) = \min[1, 接收概率^*]$

若 $E_B < E_A$. $A = 1$; 否则为接收概率$^*$ $= e^{-\beta(E_B - E_A)}$

如： A: $\uparrow \downarrow \boxed{\uparrow}$ $\uparrow \cdots$ B: $\uparrow \downarrow \boxed{\downarrow}$ $\uparrow \cdots$

以此定义，若 $E_B > E_A$ : $\dfrac{A(B\to A)}{A(A\to B)} = \dfrac{1}{e^{-\beta(E_B - E_A)}} = e^{-\beta(E_A - E_B)}$

新的构型若降低能量，一定接收，否则概率接收。

产生一个 rand(0.1). 落在 $[0, e^{-\beta(E_B - E_A)}]$ 接收，否则不接收.

We can solve $\langle A \rangle$. but can't solve $Z$.

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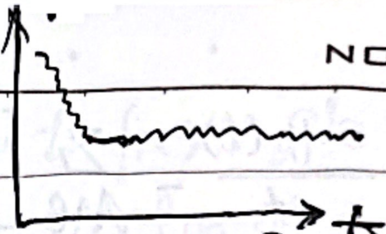


## Metropolis Algorithm

① initialize all spin randomly

② perform $N = L^D$ random trial moves. until balance $\frac{dP_A(t)}{dt} = 0$

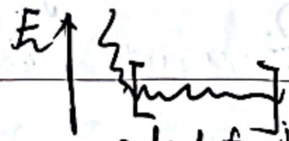
(a) randomly choose a site

(b) turn spin. get $E_B$. $\Delta E = E_B - E_A$

(c) generate random number $a = \mathrm{rand}(0,1)$ uniform.

if $a \in [0, e^{-\beta \Delta E}]$, Do FLIP THE SPIN

③ calculate observables. when approaching 热平衡.



$e^{-\beta E(c)}$ calculate 此段平均即满足期望的时间平均, 即 $\langle A \rangle$.

[~] 并非 $E(c)$; [~~] 是 $E(c)$ A

## Quantum Monte Carlo (Auxilary Field)

$$|\hat{\Phi}\rangle = \hat{\Phi}_i^+ \cdots \hat{\Phi}_M^+ |0\rangle \quad \Phi_m^+ = \sum_i^N C_i^+ \varphi_{im}$$

N site. M electrons. Slater determinant (Gaussian state)

$$|\varphi\rangle = \det \begin{pmatrix} \varphi_{11} & \cdots & \varphi_{1M} \\ \vdots & & \vdots \\ \varphi_{N1} & \cdots & \varphi_{NM} \end{pmatrix}$$

$\varphi_{1M} \cdots \varphi_{NM}$ → Single particle state; (M×N), (N×M)

where $\langle \Phi | \phi \rangle = \det(\varphi^+ \phi)$

数学I

Def: $B = \exp[\sum_{ij} C_i^+ u_{ij} c_j] = (C_1^+ \cdots C_N^+) e^{\begin{pmatrix} u_{11} & \cdots & u_{1N} \\ \vdots & & \\ u_{M1} & \cdots & u_{MN} \end{pmatrix}} \begin{pmatrix} C_1 \\ \vdots \\ C_N \end{pmatrix}$

where $B|\varphi\rangle = |\varphi'\rangle$; $\varphi' = \exp[u] \cdot \varphi$

数学II

$$\mathrm{Tr}[e^{c^+ T_1 c} e^{c^+ T_2 c} \cdots e^{c^+ T_n c}] = \det[1 + e^{T_1} e^{T_2} \cdots e^{T_n}]$$

数学IV 不同 Slater 行列式或对应同一个 $|\Phi\rangle$

$|\Phi\rangle = \det[A]$ $A = QR$ $\det[QR] \to R$

unitary 上三角

$\det[A] = \underbrace{\det[R]}_{\text{差一个系数}} \cdot |Q_{real}\rangle$ slater.

$QR: \left( Q_1 R_1 .\ Q_1 R_{12} + Q_2 R_{22} \ldots .\ Q_1 R_{1M} + Q_2 R_{2M} + \cdots + Q_M R_{MM} \right)$

Q 的: $\varphi_j^+ = \sum_i Q_{ij} c_i$ 若以 Q 作为 $|\Phi\rangle$ 而非 U

$QR: \left( R_1 \varphi_1^+ ( R_{12} \varphi_1^+ + R_{22} \varphi_2^+ ) \ldots\ldots R_{1M} \varphi_1^+ + R_{2M} \varphi_2^+ \cdots + R_{MM} \varphi_M^+ \right) |0\rangle.$

$= (R_{11} R_{22} \cdots R_{MM}) |\hat{\Phi}\rangle$

即: $|\hat{\Phi}\rangle \Leftrightarrow \prod_i R_{ii} |\hat{\Phi}\rangle$ 一个 $|\Phi\rangle$ 有多种表示.

Math V One-body reduced density matrix.

$$G_{ij} = \frac{\langle \varphi | c_i^+ c_j | \phi \rangle}{\langle \varphi | \phi \rangle} = \left[ \phi (\varphi^+ \phi)^{-1} \varphi^+ \right]_{ji}$$

Two-body

$$\frac{\langle \varphi | c_i^+ c_j^+ c_k c_l | \phi \rangle}{\langle \varphi | \phi \rangle} = G_{jk} G_{il} - G_{ik} G_{jl}.$$

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How to calculate GS Energy?

$$\mathcal{H} = -t\sum_{\langle ij\rangle\sigma} c_{i\sigma}^{+} c_{j\sigma} + U\sum_i n_{i\uparrow} n_{i\downarrow}.$$

Imaginary time Revolution. $it = \beta$

$|\psi_g\rangle = e^{-\beta H}|\psi_0\rangle = \sum_i C_i e^{-\beta E_i}|i\rangle$ 基态衰减最慢 $e^{-\beta E_0}$

when $\beta \to \infty$ at $t(\infty)$, only GS survives.

Trotter-Suzuki decomposition:

$$e^{-\beta H} = [e^{-\delta H}]^M \quad \delta = \frac{\beta}{M}$$

when $\delta \to 0$, though $[H_0, V] \neq 0$.

$$e^{-\delta H} = e^{-\delta H_0} e^{-\delta V} + o(\delta^2)$$

Hubbard-Stratonovich transformation: (HS)

$$e^{-\lambda V^2/2} = \int_R dx \cdot \frac{e^{-1/2 x^2}}{\sqrt{2\pi}} \cdot e^{x\sqrt{-\lambda} V}$$

for $V^2$ four fermion, decompose of $V$ 2 fermion operator.

自旋分解 $$e^{-\Delta\tau \cdot U n_\uparrow n_\downarrow} = e^{-\Delta\tau U(n_\uparrow + n_\downarrow)/2} \cdot \sum_{x=\pm 1} \frac{1}{2} e^{rx(n_\uparrow - n_\downarrow)}$$

introduce auxilary $\vec{x} = \pm 1$ like classical spin to seperate $V$ term. where $\cosh r = e^{(\Delta\tau U/2)}$

or charge 分解 $$e^{-\Delta\tau U n_\uparrow n_\downarrow} = e^{-\Delta\tau U(n_\uparrow + n_\downarrow - 1)/2} \sum_{x=\pm 1} \frac{1}{2} e^{rx(n_\uparrow + n_\downarrow - 1)}$$

$$\cosh r = \exp(-\Delta\tau U/2)$$

~~for H~~ 0.

Also we can Do Hubbard Model

$$\mathcal{H}_V = \sum_{ijkl} V_{ijkl}\, c_i^+ c_j^+ c_k c_l$$

$$= -\frac{1}{2}\sum_r \lambda_r \{\rho_r, \rho_r^+\} + \rho_0.$$

$\rho_r = \sum_{ij} R_{ij,r}\, c_i^+ c_j$ use $[CC]^2$ separate CCCC

$\Rightarrow \mathcal{H}([\sqrt{V}]^2)$ use HS tranformation $\Rightarrow$ $\mathcal{H} = \int \sqrt{V}\, dx_{auxilary}$

+ Auxilary Field

Observables

① $$\frac{\langle \Psi_g | O | \Psi_g \rangle}{\langle \Psi_g | \Psi_g \rangle} = \frac{\langle \Psi_0 | e^{-\beta H} O e^{-\beta H} | \Psi_0 \rangle}{\langle \Psi_0 | e^{-2\beta H} | \Psi_0 \rangle} = \frac{\langle \Psi_0 | e^{-\delta H} \cdots e^{-\delta H} O e^{-\delta H} \cdots e^{-\delta H} | \Psi_0 \rangle}{\langle \Psi_0 | e^{-\delta H} \cdots e^{-\delta H} | \Psi_0 \rangle}$$

② $$e^{-\delta H} = e^{-\delta H_0} \prod_i e^{-\delta U n_{i\uparrow} n_{i\downarrow}}$$

$$= e^{-\delta H_0} \sum_{\{x_i\}} \prod_i \left[ \frac{1}{2} e^{-\delta U (n_\uparrow + n_\downarrow)/2} \frac{1}{2} e^{\Gamma x_i (n_\uparrow - n_\downarrow)} \right]$$

③ $$\langle O \rangle_{GS} \overset{\beta \to \infty}{=} \sum_{\{x^\tau, y^\tau\}} \frac{\langle \Psi_0 | \prod e^{P_i^\tau (x_i^\tau)}\, O \prod e^{Q_i^\tau (y_i^\tau)} | \Psi_0 \rangle}{\langle \Psi_0 | \prod e^{P_i^\tau (x_i^\tau)} \prod e^{Q_i^\tau (y_i^\tau)} | \Psi_0 \rangle}$$

④ 1-D Hubbard. 每个i有$x_i$辅助场

giving Auxilary Field

$(\tau_1, x_i = \uparrow)$ $x_i = \downarrow$ $x_i = \uparrow$ $x_i = \uparrow$ → 格点

$(\tau_2, x_i) \downarrow$ ↓ 虚时

$(\tau_3, x_i) \downarrow$

$(\tau, x_i)$ 系数中

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⑤ calculate $|\varphi_0\rangle$ : slater.

$\langle \varphi_0 | \prod$单体 $\cdot \hat{O} \cdot \prod$单体$|$slater$\rangle$

= slater 行列式求和 for give $(x_i, \tau_j)$ 系数

$$= \frac{\sum P(x, y)\, O(x, y)}{\sum p(x, y)}$$

按照经典方法给出辅助场 $(x, y)$ 或 $(x_i, \tau_i)$ 再按照上法做蒙卡即可.

Jan. 3rd

Def:

$$\mathcal{Z} = T_r\left[e^{-\beta(H-\mu N)}\right] = T_r\left[\left(e^{-\tau H_V}\, e^{-\tau H_t}\right)^m\right] + O(\tau^2)$$

$$\frac{T_r\left[e^{-\beta H}\hat{O}\right]}{T_r\left[e^{-\beta H}\right]} = \sum_S P_S \langle O \rangle_S + O(\tau^2)$$

$$P_S = \frac{\det\left[\hat{I} + B_S(\beta, 0)\right]}{\sum_S \det\left(1 + B_S(\beta, 0)\right)}$$

$$\langle O \rangle_S = \frac{T_r\left[U_S(\beta, \tau)\, O\, U_S(\tau, 0)\right]}{T_r\left[U_S(\beta, 0)\right]}$$

$$U_S(\tau_2, \tau_1) = \prod_{n=n_1+1}^{n_2} e^{c^\dagger V(S_n) c}\, e^{-\tau c^\dagger T c}$$

$$B_S(\tau_2, \tau_1) = \prod_{n=n_1+1}^{n_2} e^{V(S_n)}\, e^{-\tau T}$$

$$H_t = \sum_{xy} C_x^\dagger T_{xy} C_y = c^\dagger T c \quad \text{certain Matrix}$$

我们有Hs变换后的 $C^+VC$ 与 $c^+TC$

利用 $\boxed{数学Ⅲ}$:

$Tr[e^{-\beta H}\hat{O}] = \det(I + \cdots 忆)$ $V(S_n)$ 依赖辅助场

总之 $\langle O \rangle$ 可求出. 利用 $P_S$ 辅助场概率.

## Sign Problem. 符号问题 $P_S < 0$ ? 负概率.

能否以 $|P_S|$ 作为概率? Actually. $P_S$ 本身大 ±1 逆 而均值甚小 → 0.

→ (+1 +1 ⋯) 不可. 因涨落大而均值小, $|P_S|$ 消去涨落无法 sample 原函数.

Half-filling Hubbard Model: 仅作单个自旋的变换

$$\begin{cases} C_{i\uparrow}^+ = d_{i\uparrow}^+ \\ C_{i\downarrow} = (-1)^i d_{i\downarrow} \end{cases} \qquad n_{i\uparrow} + n_{i\downarrow} = 1$$

$\Rightarrow U n_{i\uparrow} n_{i\downarrow} = -U n_{(di)\uparrow} n_{(di)\downarrow} + U n_{(di)\uparrow}$ at Half-filling

此时皆以 $U_{(di)\uparrow}$ 替代 $U_{(i)}$ Particle ⤳ Hole.

$$e^{-\mathcal{I}V} \to e^{-\mathcal{I}(-U n_\uparrow n_\downarrow + U n_\uparrow)}$$

作Hs变换 $[e^{-\frac{\mathcal{I}(-U)/2}{>0}}] = \cos(h\gamma) \Rightarrow \gamma \in \mathbb{R}$

$P(x,y) = e^{\gamma(\cdots)} \cdot e^{\gamma(\cdots)} > 0$ 在Hole-Hubbard 无符号问题

If there's certain propetics that arrives $P_S > 0$ that works for QMC !

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World-Line QMC., suitble for spin system.

XXZ: $H_{1d} = J_x \sum_i \left(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y\right) + J_z \sum_i S_i^z S_{i+1}^z$

$S = 1/2$ ···o—o—o—o··· $S_i$ $S_{i+1}$

$\begin{cases} S_{i+L} = S_i \quad \text{PBC.} \\ S^{x.y.z} = \text{Pauli}^{xyz} \\ \text{Basis}(S^z) \end{cases}$

用绝对值不可.

$$\langle \hat{O} \rangle = \frac{\sum_x P(x)\, \hat{O}(x)}{\sum_x P(x)}$$

Def: $\mathrm{sgn}(P(x)) = \dfrac{P(x)}{|P(x)|}$

$$\langle \hat{O} \rangle = \frac{\langle \mathrm{sgn}(x) O(x) \rangle}{\langle \mathrm{sgn}(x) \rangle} \qquad \langle A(x) \rangle = \sum_x \frac{|P(x)|\, f(x)}{\sum_x |P(x)|} = \sum_x \tilde{P}(x)\, f(x).$$

可以证明

$\langle \mathrm{sgn}(x) \rangle = (+1, -1 \cdots) = e^{-\beta N c}$ $(N\uparrow, T\downarrow)$ 几不可 sample 无穷小

因其要比无穷小还小

又有: $\langle \mathrm{sgn}^2(x) \rangle = 1$，则误差过大 variance 发散.

利用 XXZ Model: 2 sites. $H(1.2)$.

We can find eigenvalues.

$H$: $\frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$ $\left(-\frac{J_z}{4} - \frac{J_x}{2}\right)$

$\frac{1}{\sqrt{2}}\left(|\downarrow\uparrow\rangle + |\uparrow\downarrow\rangle\right)$ $\left(-\frac{J_z}{4} + \frac{J_x}{2}\right)$

$|\uparrow\uparrow\rangle$ $J_z/4$

$|\downarrow\downarrow\rangle$ $J_z/4$

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Now we have $N$ sites.

seperate the hamiltonian via odd/even site numbers.

$$\mathcal{H} = \sum_n H^{(2n+1)} + H^{(2n)}$$

$$\mathcal{H}_1 = \sum H^1 + H^3 + \cdots$$

$$\mathcal{H}_2 = H^2 + H^4 + \cdots$$

$[\mathcal{H}^1, H^3]=0$ $H_1$与$H_2$中每一项在XX Model中对易

Trotter-Suzuki decomposition:

$$T_r[e^{-\beta H}] = T_r[(e^{-\Delta\tau H})^m] \quad \mathcal{H} = \mathcal{H}_1 + \mathcal{H}_2$$

$\mathcal{H}_1 \cdot \mathcal{H}_2$内部对易

$$= T_r[e^{-\Delta\tau(H_1+H_2)} e^{-\Delta\tau(H_1+H_2)} \cdots\cdots e^{-\Delta\tau(H_1+H_2)}]$$

$[\mathcal{H}_1, H_2]$本身不对易

$$= T_r[e^{-\Delta\tau H_1} e^{-\Delta\tau H_2} e^{-\Delta\tau H_1} e^{-\Delta\tau H_2} \cdots e^{-\Delta\tau H_1} e^{-\Delta\tau H_2}] + O(\tau^2)$$

At $S^z$ basis $|\sigma_1\rangle\langle\sigma_1|$ $\quad Tr(\ ) = \sum_\sigma \langle\sigma|\ \ |\sigma\rangle$

$$= \sum_\sigma \sum_{\sigma_1 \cdots \sigma_{2m-1}} \langle\sigma|e^{-\Delta\tau H_1}|\sigma_1\rangle\langle\sigma_1|e^{-\Delta\tau H_2}|\sigma_2\rangle \cdots \langle\sigma_{2m-2}|e^{-\Delta\tau H_1}|\sigma_{2m-1}\rangle$$

$$\otimes \langle\sigma_{2m-1}|e^{-\Delta\tau H_2}|\sigma_1\rangle$$

$$= \sum_{2m\text{求和}} \Omega(w)$$

$|\sigma_i\rangle$ is the many body $S^z$ Basis $|\sigma_{1,i}\, \sigma_{2,i} \cdots \sigma_{j,i} \cdots \sigma_{N,i}\rangle$

$\mathcal{H}_2 = H_{i=2} + H_{i=4} + \cdots$ $\quad \underline{H_{i=2} = H(2,3)}$ $\quad H_{i=4} = H(4,5)$

只与2.3 site相关

以此构建 $\langle\sigma_i|e^{-\Delta\tau H_2}|\sigma_{i+1}\rangle$

$$= \langle\sigma_{3,i}\,\sigma_{2,i}|e^{-\Delta\tau H_{i=2}}|\sigma_{3,i}\,\sigma_{2,i}\rangle \langle\sigma_{4,i}\,\sigma_{5,i}|e^{-\Delta\tau H_{i=4}}|\sigma_{4,i}\,\sigma_{5,i}\rangle$$

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$$= \prod_i \langle \sigma_{2i,\tau+1}, \sigma_{2i+1,\tau+1} | e^{-\Delta\tau H^{2i}} | \sigma_{2i,\tau+1}\, \sigma_{2i+1,\tau+1} \rangle$$

而$H^{2i}$在2格点例子中已经算出来了，因此每部分皆可知.

We calculate: (已知 $H^{2\text{-site}}$ eigenvalue. eigenvector)

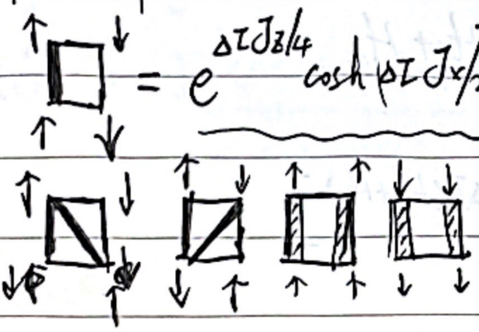
$$\langle \uparrow\downarrow | e^{-\Delta\tau H^{2\text{-site}}} | \uparrow\downarrow \rangle = e^{-\Delta\tau J_z/4} \sinh\left(\frac{\Delta\tau J_x}{2}\right)$$

$\langle\uparrow\uparrow|$ $\langle\downarrow\downarrow|$ $\langle\downarrow\uparrow|$ Basis the similar calculation.

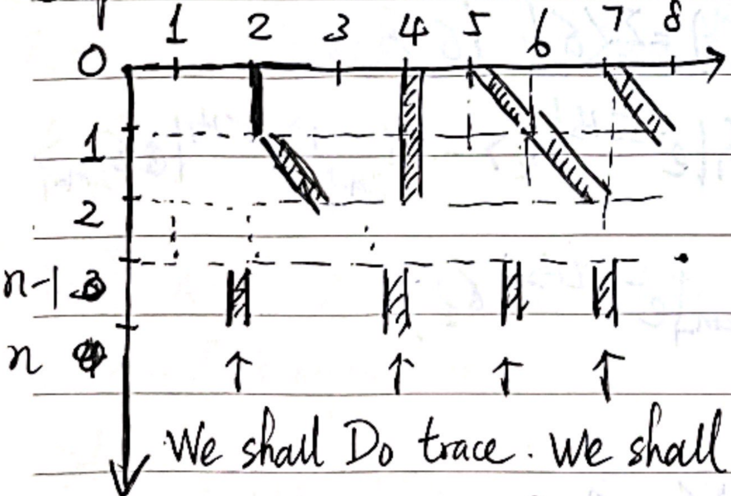
$C_4^2 = 6$ terms.

Graph Expression. $\boxed{\text{Sigh Problem}}$

$= e^{\Delta\tau J_z/4} \cosh(\Delta\tau J_x/2)$ If. $(J_x<0)$ we can't solve by PG (



Graph




We shall Do trace. We shall connect these world lines.

is one of $\Omega(w)$

$$Z = \sum_w \Omega(w)$$

Every Graph has a weight $P(w) = \frac{\Omega(w)}{\sum_w \Omega(w)}$, we sum all of these Graphs to calculate MC.