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NOTES

Chapter 3. 线性响应理论. 费米黄金规则. 电导 (Bruus).

When system equilibrium ~~with~~ an $\langle A \rangle$, Now give pertubation. eg: $\vec{E}$, system reacts with eg: I. Liner response theory when react is in proportion with the pertubation, ie: $I = AE$ so that we can define A, ie: production (电导). Normally A is defined by proporties of the equilibrium state, ~~what~~'s ~~more~~ ie: number of states affects reaction so that fermion Golden rule is to be considered defining A (productivity).

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

certain physical quantity

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

Now: $H(t) = H_0 + H'(t) \cdot \theta(t - t_0)$ (happens after t_0)

微扰

so that
$$\langle A \rangle = \begin{cases} A_0 & t < t_0 \\ \frac{1}{Z_0} \cdot \sum_n \langle n(t) | A | n(t) \rangle e^{-\beta E_n} & t > t_0 \end{cases}$$

含时微扰在相互作用绘景可解:

$$|\hat{\varphi}(t)\rangle = e^{-iH_0 t/\hbar} |\varphi(t)\rangle = e^{-iH_0 t/\hbar} U(t, t_0) |\varphi(t_0)\rangle$$

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

线性 Liner: $U(t, t_0) = \int_{t_0}^{t} \delta \tilde{H}(t') U(t', t_0) dt'$ 对 $U(t', t_0)$ 展开

$\Rightarrow$ 作图 $U(t, t_0) = \underbrace{\; t \uparrow t_0 \; + \; t \uparrow t' V(t') \uparrow t_0 \;}$ $+ \; t \uparrow t'' V(t'') \uparrow t' V(t') \uparrow t_0 + \cdots$

Liner 保留前两项.

$$U(t, t_0) = 1 - i \int_{t_0}^{t} dt' \, \delta \tilde{H}(t')$$

so that: $\frac{1}{Z_0} \sum_n \left[e^{-iH_0 t/\hbar} \left[1 - i \int_{t_0}^{t} dt' \, \delta \tilde{H}(t') \right] \right]^{\dagger} A(t) \left[e^{-iH_0 t/\hbar} \left[1 - i \int_{t_0}^{t} dt' \, \delta \tilde{H}(t') \right] \right] | n(t) \rangle$

~~略去~~ $\langle \delta H | A | \delta H \rangle$ $\langle n(t) |$ 小量后. $\times e^{-\beta E_n}$

$\langle n(t_0)| A_{(t)} |n(t_0)\rangle$ $\quad \langle n(t_0)| \sim |n(t_0)\rangle$

we get:

$$\langle A\rangle(t) = \langle A\rangle_0 - i\int_{t_0}^{t} dt' \langle [\tilde{A}(t), \delta \tilde{H}(t')] \rangle_0$$

we define: retarded response function:

$$\delta\langle A\rangle(t) = \langle A(t)\rangle - \langle A\rangle_0 = \int_{t_0}^{\infty} dt'\, C^R_{A\delta H}(t-t')$$

$$C^R_{A\delta H}(t-t') = -i\theta(t-t')\langle [\tilde{A}(t), \delta\tilde{H}(t')]\rangle_0$$

Kubo formula

$$= \int_{t_0}^{t} \sim dt' + \int_{t}^{\infty} \sim dt'$$

已发生: $t' \in (t_0, t)$ $t-t'>0$ $\theta=1$ 未响应: $t'>t$ $t-t'<0$ $\theta=0$

In frequency domain:

when: $\delta H(t) = \hat{B} f(t)$; 响应积累只与时间差有关 (仅例:开放系统算符.)

$f(t)$: 函数 $\hat{B}$: 时间无关算符.

eg: $\hat{E}(t) = \tilde{E}_0 \sin(\omega t+\phi)$ $\quad \langle f(t)\rangle = f(t)$

$$C^R_{A\delta H}(t-t') \Rightarrow \langle A(t) B(t')\rangle = e^{iH_0 t} A e^{-iH_0 t} e^{iH_0 t'} B e^{-iH_0 t'} f(t')$$

$$= e^{iH_0(t-t')} A e^{-iH(t-t')} B f(t')$$

$$\Rightarrow C^R_{AB}(t-t')$$

$$\Rightarrow C^R_{A\delta H} = C^R_{AB}(t-t') f(t')$$

$$= -i\theta(t-t')\langle [\tilde{A}(t-t'), B]\rangle_0 f(t')$$

我们期望、微扰时间平均当 $t\to\infty$, 应不计. 即

$C^R(t-t')$ $t'-t\to\infty$ $C^R = 0$

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We have: $\delta\langle A\rangle(t) = \int_{t_0}^{\infty} dt' \, C^R_{AB}(t-t') f(t')$

我们只考虑非平衡: Let: $t_0 \to -\infty$ 这只是差一个积分常数, st.

变化只在过程中考虑而与初平衡态无关.

$\boxed{\text{Fourier}}$ $\delta\langle A\rangle(\omega) = C^R_{AB}(\omega) f(\omega)$. 卷积定理

比如: $B = \sum_\alpha \int dr \, B^\alpha(r) f^\alpha(r,t)$, Now.

$$\delta\langle A\rangle(\omega) = \sum_\alpha \int dr \, C^R_{AB^\alpha(r)}(\omega) f^\alpha(r,\omega)$$

Conductivity:

A system with charged electrons subjected to magenetic fields has current at: (r,t). which depends on the ~~current~~ field at: (r',t') that is:

$$\vec{J} = \sigma \vec{E}$$

考虑推迟: $J^\alpha(r,t) = \int dt' dr' \sum_\beta \vec{\sigma}^{\alpha\beta}(r,r',t'-t) E^\beta(r',t')$

tensor: (σ) 张量, β方向电场 α方向电流密度. 由$r'\to r$ 产生$t'-t$推迟

eg: $J_y = (\sigma_{yz} E_z + \sigma_{yy} E_y + \sigma_{yx} E_x) \iint (t,r)$

卷积定理 in frequency domain.

$$J^\alpha(r,\omega) = \int dr' \sum_\beta \sigma^{\alpha\beta}(r,r',\omega) E^\beta(r',\omega)$$

所谓响应. 即J对E的响应, 通过σ, 称电导. (conductivity)

此外, 微扰 Hamiltonian: 取规范 st: $(\phi=0)$...

$$T = -\frac{\hbar^2}{2m} \int dr \, \psi^+ \nabla^2 \psi$$

引入微扰: T(由于电磁场E): $\frac{1}{2m} \int dr \, \psi^+ \left(\frac{\hbar}{i}\nabla_r - qA\right)^2 \psi$

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由 Chapter1 (electrodynamics 例子) 知.

T微扰 = δH 即为: $-q\int dr\, \vec{J}\cdot\vec{A}$ 其中 J 有 J^A 与 J^e 两项组成.

考察: J^A 项: $\frac{q^2 A}{r}\psi^\dagger\psi = \frac{q^2 A}{r}\rho(r)$

J^e 项: $\frac{q}{2mi}(\psi^\dagger\nabla\psi - \psi\nabla\psi^\dagger)$

$J = J^e + \frac{q^2}{r}A\rho(r)$.

A 影响 ψ, 故影响 J^e. 终 Both 影响 J^e, $J^A(A)$ 响应在 J 上.
一部分 $q^2/r\, A\rho(r)$ 项自然为对 A 响应, 另外 J^e 用上文响应理论写出 A 项, 假设无外场下无电流. $\langle J^e\rangle_0 = 0$.

$\langle J^e\rangle = \langle J^e\rangle_0 - (\quad)$ 类比

δH 中只有 $J^e(r)$ 无 $J^A(r)$

$\delta H = \hat{B} = \sum_\alpha\int dr\, B^\alpha(r) f^\alpha(r,t)$

Liner A
$\delta H = -q\int dr\, \hat{J}(r)\cdot A(r,t)$

Liner A^2 $\left(\frac{q^2}{m}A^2\rho(r)\right)$ 不微扰

对 J 一阶有作用. 对 δH 则无了. (二阶)

$\delta\langle A\rangle(w) = \sum_\alpha\int dr'\, C^R_{AB}(w) f(w,r')$

$\delta\langle J\rangle(t) = \langle J\rangle(t)$ $(\langle J\rangle_0 = 0)$

so that:

$$\langle J_{total}(r)\rangle(w) = \sum_\beta -e^2\int dr'\, C^R_{J^{e\alpha}(r) J^{e\beta}(r')}(w)\, A^\beta_{外加}(r',w) - \frac{e^2}{m}A_{外加}(r,w)\langle\rho(r)\rangle$$

同时由电导之定义且代入 $\phi = 0$ 时: $E(r,t) = -\partial_t A(r,t)$ 规范st.

$\Rightarrow E = iwA$

$$J = \sum_\beta -e^2\int dr'\frac{1}{iw} C^R_{J^\alpha(r)J^\beta(r')}(w)\, E^\beta(r',w) - \frac{e^2}{iwm}E_{外加}\langle\rho(r)\rangle。$$

又 $\overset{定义}{\equiv}\int dr'\sum_\beta \sigma^{\alpha\beta}(r,r',w)\, E(r',w)$.

最终，得到了推迟电导的含时微扰线性下的形式：

定义 $n(r)=\langle\rho(r)\rangle$。 $\Pi^R = C^R_{J_0J_0}$ (顺磁) 流-流关联函数

$$\Pi^R_{\alpha\beta}(r,r',t'-t) = C^R_{J_0^\alpha(r)J_0^\beta(r')}(t-t') = -i\theta(t-t')\langle[\tilde{J}_0^\alpha(r,t),\tilde{J}_0^\beta(r',t')]\rangle$$

$$\Rightarrow \text{电导: } \sigma^{\alpha\beta}(r,r',\omega) = \frac{ie^2}{\omega}\Pi^R_{\alpha\beta}(r,r',\omega) + \frac{ie^2 n(r)}{\omega m}\delta(r-r')\delta_{\alpha\beta}.$$

此式表明：$|J| = |\sigma_{\alpha\beta}||E|$ 中 $\sigma_{\alpha\beta}$ 推迟项由：$\tilde{J}^\alpha(r,t)$，α方向处于r处电流密度对 $J^\beta(r',t')$，β方向处于r'电流密度在t>t'正推迟，作为剪切作用，以及数密度直接项组成.

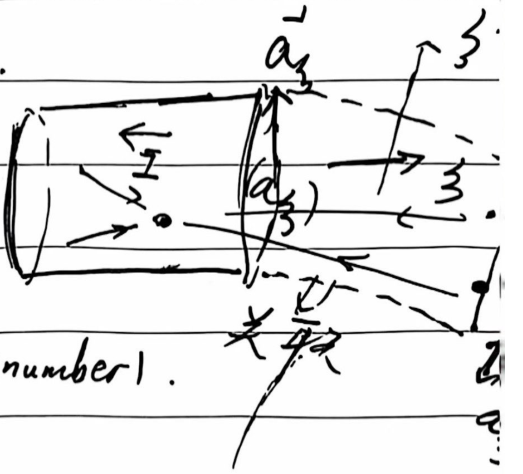
(conductance) 电导表现在电路中称 conductance，定义为 G：

$$G = I/V \quad (\text{电导率}).$$

$$\sigma = J/E \quad (\text{conductivity})$$

$$G = (W/L)\sigma \quad L: \text{length}. \quad W: \text{cross-section wi}$$

这就涉及 (α,β) 方向在电路中的定义了.



比如直流电源中一段 wire $I = \int J(\xi)\, da_\xi$

$$= \int da_\xi \int \underbrace{d\mathbf{r}'}_{dV}\ \hat{\xi}\cdot\sigma(r,r',\omega=0)\cdot\hat{\xi}'\cdot E(\xi') \ (\text{number}).$$

$$dV \to ds\cdot dx = d\xi'\cdot da_{\xi'}$$

$$= \int da_\xi\, da_{\xi'}\, d\xi'\ \hat{\xi}\cdot\sigma(\xi,a_\xi,\xi',a_{\xi'},\omega=0)_{Matrix}\cdot\hat{\xi}'\, E(\xi')$$

又 $I = GV = \int G E(\xi')\, d\xi'$ 类比 + 近似 (取实部).

$$G = \lim_{\omega \to 0} \left[\mathrm{Re} \frac{ie^2}{\omega} C^R_{I(3)I(3')}(\omega) \right] \text{ where } C^R_{I(3)I(3)}(t-t') = -i\theta(t-t')\langle[I(t), I(t')]\rangle$$

which means:

[Minor Importance]. dielectric function.

Now if we consider $\phi = \phi_{inner} + \phi_{outer\ field}$ with Possion Equation $\nabla^2\phi = -\frac{1}{\varepsilon_0}\rho$. normally $\rho_{outer} + \rho_{in}$ 来源于自由+束缚导电子 that discribed by $\vec{D}$. where $\phi_{all} = \varepsilon^{-1}\phi_{out}$ ε(介质极化).

generally: $\phi_{all} = \int dr'dt' \, \varepsilon^{-1}(rt, r't')\phi_{out}(r', t')$

微扰 Hamiltonian $\delta H = q\phi_{all} = \int dv_r \, \rho_e(r)\phi_{out}(r)$

ϕ_{out} 对应 δH. ϕ_{inner} 为非微扰(原本 columb).

类比上文，则: $\rho^{induced}_{\cancel{out}} = \rho_{All} - \rho_{\cancel{inner}\,0}$ ($\rho_{out} \Leftrightarrow \delta\varphi$ 微扰项)

$$\rho^{\cancel{out}}_{induced} = \iint_{t_0}^{\infty} C^R_{\rho(r)\rho(r')}(t, t')\phi(r', t')\,dr'dt'$$

where $C^R_{\rho_{All}(r)\rho_{All}(r')} = -i\theta(t-t')\langle[\rho_{All}(r,t)\ \rho_{All}(r', t')]\rangle_0$

何为 "C" $\rho_{induced} = C\phi d = CE$ 本身 $\rho = \chi E$ $\therefore C = \chi^R_e(rt, r't')$ 本质

$\phi_{inner} = \int \rho_{induced}\, dv\, V_c$ 代入上式

$\therefore \phi_{All} = \phi_{out} + \phi_{inner}$ 代入上式，再代入 Dielectric funct

$\therefore \varepsilon^{-1}(rt, r't') = \delta(r-r')\delta(t-t') + \int dr''\, \underline{V(r-r'')}\, \chi^R_e(r''t'', r't')$

Columb Potention

$\therefore$ 动切电常数由极化势能给出

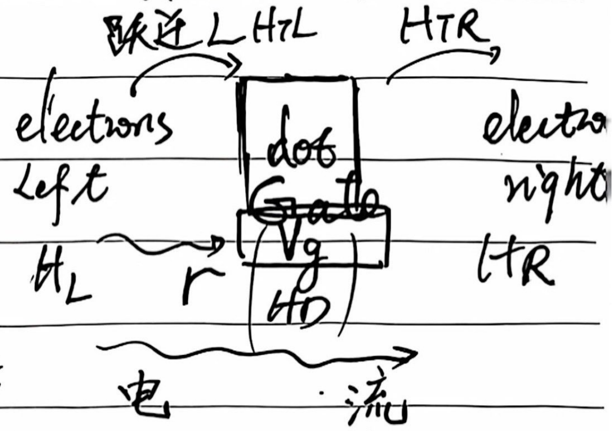
利用连续性方程. $-i\omega\rho_{All}(q, \omega) + iq J_e(q, \omega) = 0 \Rightarrow \varepsilon^{-1} = 1 - i\frac{q^2}{\omega}V_c$

$\chi\phi \quad \leftrightarrow \quad \delta E = \delta q\phi$

在格点系统中电子输运(transport)行为:

有这样一类系统(如图)、左.右传导电子间都是 Non-Interacting. 在量子点 dot (H_D) 间与 H_D 有 interacting.

∴ $H = H_{Left}$(自能动) $+ H_{right} + H_D + H_{TLeft} + H_{Tright}$ (见上文 Anderson Model), 现实中 Nanoelectric device 对应这类系统 (~~MOS~~管 ?(MOS)



Anderson:

$$H_{TL} = \sum_{\nu_L \nu_D} \left(t_{L,\nu_L \nu_D} c^\dagger_{\nu_L} c_D + t^* c^\dagger_{\nu_D} c_L \right)$$

H能表跃迁系.

$$t_{LD} = \int \langle \psi_L^\dagger H_{LD} | \psi_D \rangle dr \neq 0$$ 中间 bracket

即跃迁振幅,后 H_{TL} 即 Second Quantization transport.

自能 自互作用能 (columb in dot).

$$H_D = H_{D0} + H_{int} = \sum_D \varepsilon_D c_D^\dagger c_D + \sum_{1234} \frac{1}{2} V_{1234} c_1^\dagger c_2^\dagger c_3 c_4$$

($U n_{d\uparrow} n_{d\downarrow}$).

在连续跃迁中 (~~Fermion~~ Golden Rule).

beginning state i, at time t. probability at state f is

$|\langle f | i(t)\rangle|^2$ = 相互作用绘景线性响应, 微扰 $V(t) = V e^{\eta t}$

$$\left| \langle f | e^{-i\hat{H}_0 t} \left(1 + \frac{1}{i}\int_{t_0}^{t} e^{iH_0 t'} [V e^{\eta t'}] e^{-iH_0 t'} dt' \right) e^{iH_0 t} | i \rangle \right|$$

$$= \left| \langle f|V|i\rangle e^{i(E_i - E_f)t} \frac{1}{i} \int_{-\infty}^{t} e^{i(E_f - E_i - i\eta)t'} dt' \right|^2$$

$$P(t) = |\ \ |^2 = |\langle f|V|i\rangle|^2 \frac{e^{2\eta t}}{(E_f-E_i)^2+\eta^2}$$

$\frac{dP(t)}{dt}$ = 称为跃迁(连续) $\Rightarrow \Gamma_{fi} = |\langle f|V|i\rangle|^2 \cdot \frac{2\eta e^{2\eta t}}{(E_f-E_i)^2+\eta^2}$ (per unit time)

更进一步: 类比 $\int_R \delta(x) = 1$ 若 st: $\int_R \frac{e^{2\eta t}\cdots}{(\Delta E)^2+\eta^2} d\Delta E \cdot \frac{1}{c} = \cdots$

则要求: η为小量. when $\Delta E \neq 0 \rightsquigarrow 0$ $\quad \Delta E = 0 \to \infty$

积出 $\Rightarrow \frac{1}{\eta}\arctan\frac{\Delta E}{\eta}\Big|_0^{+\infty} \times 2 = 2\pi \quad \therefore$ 系数 $c = \frac{1}{2\pi} \Rightarrow \frac{1}{c} = 2\pi$

⇒ 后 ☆ Fermi Golden Rule $\quad \eta \to 0$ 时: V 少变:

△ $\Gamma_{fi} = 2\pi |\langle f|V|i\rangle|^2 \delta(E_f - E_i)$

总跃迁为 $i \to f$ 与 $f \to i$ 之和. 定态时为0

$$0 = \frac{\partial P(\alpha)}{\partial t} = \underbrace{-\sum_\beta \Gamma_{\beta\alpha}}_{\text{Tunnel out of } \alpha} P(\alpha) + \underbrace{\sum_\beta \Gamma_{\alpha\beta} P(\beta)}_{\text{Tunnel in to } \alpha}$$

库仑阻塞效应:

$$H_D = \sum \varepsilon_D c^+ c^- + \underbrace{U n_\uparrow n_\downarrow}_{E(N)}$$

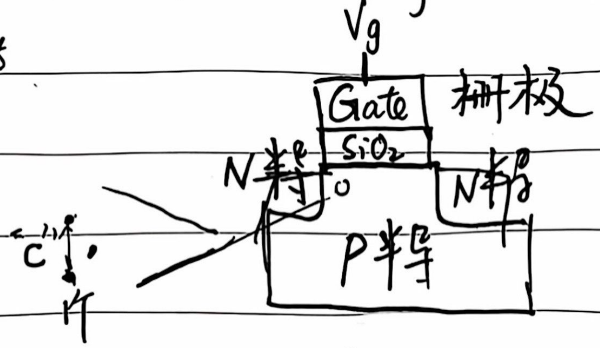
Gate电势

$$= E_C N^2 \quad E_C = e^2/2C + eV_g N$$

如图 N_{Left} cross P to N_{Left} at the help of V_g, $H_D = H_{P结} =$

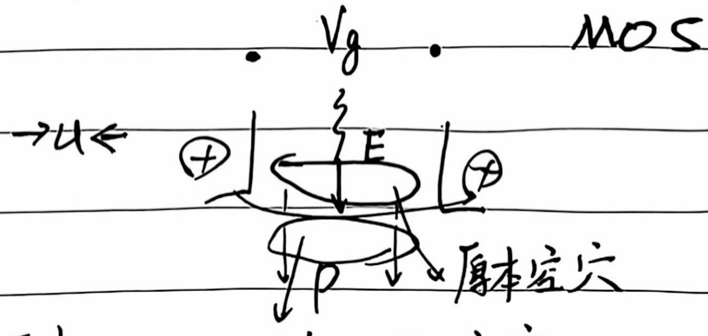
$E_{p\,itself} + E_{outer\,V_g}$

$= E_C N^2 - eV_g N \quad E_C = e^2/2C$



Tunnelling: 跃迁: 左→中 一个电子

左加1, 中加1 $c_d^+ c_{Left}$



$\Rightarrow \sum_{LD}$

$$\Gamma^L_{N+1,N} = 2\pi \sum_{iN} |\langle \alpha_N | c_d^+ c_L H_{TL} | iN\rangle|^2 \delta(E_{N'} - E)$$

Now: E下空穴

空穴被V_g压下 左右⊕载流 在U下得以穿越

$\langle f| = \langle c_d^+ c_L i|$
$= \langle i| c_L^+ c_d$

(中、右中每个i态电子都空间可能发生此跃迁

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$= 2\pi \left|\langle i_N | c_d^+ c_L^+ H_{TL} | e_N\rangle\right|^2 \cdot W_{i_N} \cdot \delta\left(E(N+1)-E(N)+\varepsilon_d-\varepsilon_L\right)$

$\Rightarrow \sum_{\nu_L \nu_D} \sum_{i_N} \rightarrow$ 每个能级. 末: Middle: $E(N+1)+\varepsilon_d$ Left: 0 初: Left: ε_L. Middle: $E(N)$

每个点中格点. $W_{i_N} = W_{i_{N_D}} \times W_{i_L}$ } 3能级5简 ⇝ 4能 3简并. $W = 5\times 3$

代入 $H_T = t\, c_d^+ c_L$

where: $|i_{Left}\rangle \otimes |i_{middle}\rangle = |i_N\rangle$, 直积展开

$\cancel{\langle i_N | c_d^+ c_L c_d H_{TL} | i_N\rangle} = \langle i_{N_d}| \otimes \langle i_{L}| \cdot c_L^+ c_d\, c_D^+ c_L | i_L\rangle \otimes |i_{Nd}\rangle$

$= \langle i_L | c_L^+ c_L | i_L\rangle \cdot \langle i_{Nd} | c_d^+ c_d | i_{Nd}\rangle$ (d中 $n\to n+1$ L中 1个)

观察式: $\sum W_{i_L} \langle i_L | c_L^+ c_L | i_L\rangle \Rightarrow =1$ 只余 W_{iL} 费米子L级简并

满足 n_F: Fermi-Dirac 分布 此项为 $n_F(\varepsilon_L - \mu_L) \rightarrow$ 化学势.

观察式: $\sum_{i_{N_D}} W_{i_{N_D}} \langle i_{N_D} | c_d^+ c_d | i_{N_D}\rangle \quad \frac{1}{\exp(\ )+1}$ why?

Dot中本应 N const 正则系综, Now: 费米面甚大, 粒子 $= (1-n_F)$ ($c_d c_d^+$ 交换 $c_L^+ c_L$)

而跃迁齐对 ν_L, ν_D 是 t, 对其求和 数扰动少, 同与电子库相连 巨正则 系综描述即可

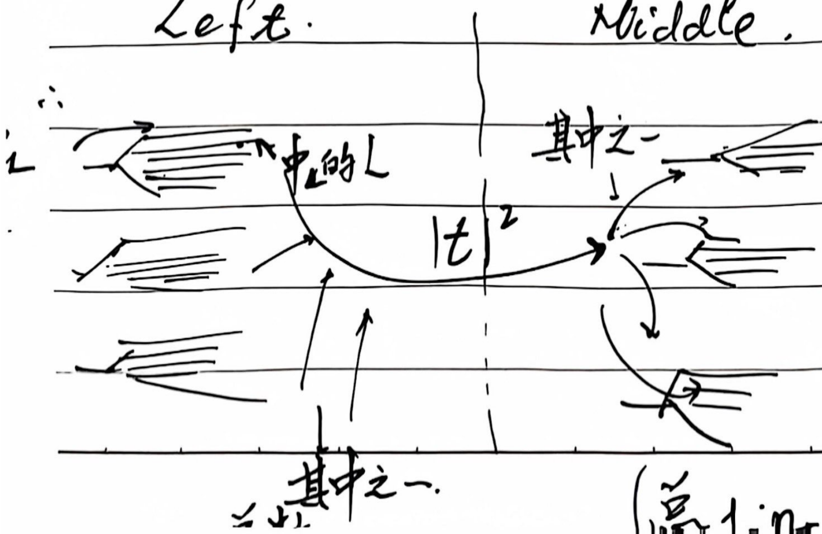
$\sum_{L,\nu_D \nu_{T_L}} |t_{L,\nu_D,\nu}|^2 \cdot 2\pi = \int_R t^2 \cdot \rho(t) \cdot d\varepsilon_L d\varepsilon_D$

assume:

$\Downarrow$ $d_D d_L$ 就是体积元. 在 $d_D d_L$ 小区间 t 为定

$\gamma \triangleq |t_L|^2 d_D d_L$

$= \gamma^{Left} \int_R d\varepsilon_L d\varepsilon_D$



✡

$\therefore \Gamma^{Left}_{N+1,N} = \gamma^{Left} \int_R d\varepsilon_L d\varepsilon_D \cdot n_F(\varepsilon$

$\cdot [1-n_F(\varepsilon_D - \mu_D)] \cdot \delta[E(N+$

$- E(N) + \varepsilon_D - \varepsilon_L]$

(赢 1-n_F)

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(可证.已验) $n_F(\varepsilon_1)(1-n_F(\varepsilon_2)) = n_{Boson}(\varepsilon_1-\varepsilon_2)\cdot[n_F(\varepsilon_2)-n_F(\varepsilon_1)]$

(以及) $\int_R d\varepsilon \cdot [n_F(\varepsilon)-n_F(\varepsilon+w)] = w$

得到:

$$\Gamma_{N+1,N}^{\text{Left or Right}} = \nu^{\text{Left or Right}} \int_R d\varepsilon_L d\varepsilon_D \cdot n_B(\varepsilon_L-\varepsilon_D+\mu_D-\mu_L)\cdot$$

$\delta(x-a)$

$$[n_F(\varepsilon_L-\mu_L)-n_F(\varepsilon_D-\mu_D)]\,\delta(A+\varepsilon_D-\varepsilon_L)$$

$$=\nu^\alpha \cdot \int d\varepsilon_L \quad n_B(\varepsilon_L-(\varepsilon_L-A)+\mu_D-\mu_L)[n_F(\varepsilon_L-\mu_L)-n_F(\varepsilon_L-A$$

$$=\nu^\alpha \int d\varepsilon_L \cdot n_B(A+\mu_D-\mu_L)\cdot\{n_F(\varepsilon_L-\mu_L)-n_F[\varepsilon_L-(A+\mu_D)]\}$$

与ε_L无关 $\qquad w = \mu_L-\mu_D-A$

$$=\nu^\alpha n_B(A+\mu_D-\mu_L)\cdot(\mu_L-\mu_D-A)$$

$$=\nu^\alpha \cdot \frac{E(N+1)-E(N)+\mu_D-\mu_\alpha}{\exp[\frac{1}{KT}(E(N+1)-E(N)+\mu_D-\mu_\alpha)]-1}$$

$$\therefore \Gamma_{N+1,N}^\alpha = f(E(N+1)-E(N)+\mu_D-\mu_\alpha)\cdot\nu^\alpha \qquad f(E)=\frac{E}{e^{\beta E}-1}.$$

同理:

$$\Gamma_{N-1,N}^{\alpha\ \text{dot和1}} = f(E(N-1)-E(N)-\mu_D+\mu_\alpha)\cdot\nu^\alpha$$

因此,总跃迁率为: 平衡时:

$$\frac{d}{dt}P(N) = -(\Gamma_{N+1,N}+\Gamma_{N-1,N})P(N)+\Gamma_{N,N+1}\,(P(N+1))+\Gamma_{N,N-1}P(N-1) =$$

dot上

dot上有N个? ⇒ ~~左右电极~~ ~~dot上电~~ 意为N个 另

dot上+1 变为N个 $I_{N+1,N}P(N)$ } 从此态离开 为负
dot上-1 变为N-1,从N个 $I_{N-1,N}P(N)$ 走

dot上-1 变为N个. 增:为 $P(N+1)$ 态 × 此跃迁概率 } 变为N的 为+
dot上+1 变为N个,从N-1个为 $P(N-1)$ 态 × 此跃迁概率

解之: $I_{N+1,N}=I_{N,N+1}$ obviously.

$I_{N-1,N}P(N)=I_{N,N-1}P(N-1)$ 为迭代关系(数列).

因此,流的定义为:向左.

$$I=(-e)\sum_N\left[I^{Left}_{N+1,N}-I^{Left}_{N-1,N}\right]P(N)$$

金属库仑阻塞. $V=E_cN^2-eV_gN$ V_{min}: $N=\frac{eV_g}{2E_c}$

对于不同金属外加电压 V_g. N就是st.能最低最优粒子数.

此时,经典 $\phi_{栅}>\phi_{源}$, 两板静电能 $Q^2/2C$.
单子电转移 $(Q-q)^2/2C$ 需能

∴ $Q^2/2C>(Q-q)^2/2C$ $Q>q/2$, 若 $Q<q/2$ 转移不了. 库仑阻塞.

Now: 栅漏极之间有一量子点(金属点)

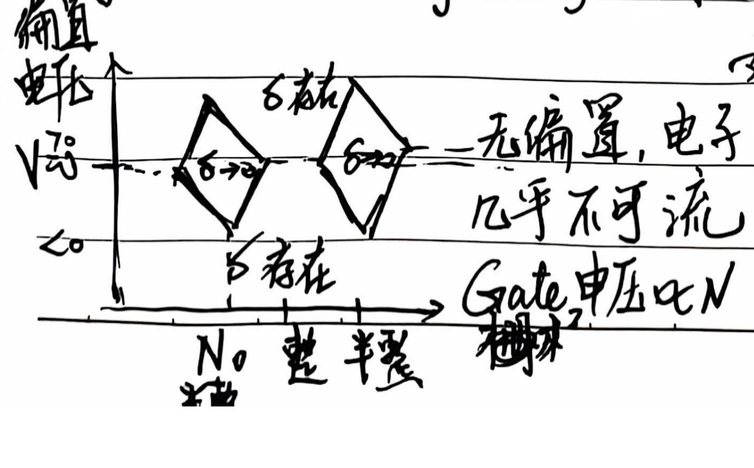
求解P(N)发现 $N_{dot}\in N^*$, P(N), P(N+1) 1个为1, 1为0.

说明dot上有确切占据数. dot与Lead有能差,库仑阻塞

N half-integer. P(N), P(N+1) 简并: ~~0与1~~ 占态. 电子可跃迁,

电导 when: N half-integer 有值. $\in N^*$, 为零 $(T\to 0)$

如图所示.



库仑阻塞(dot甚小)无统计意义 Fermi-Dirac，需每粒子讨论.

这次 I 为：$2\pi \sum_{\gamma_L} |\langle \beta_{D,N+1}| \sum_{\gamma_D} t^*_{L\gamma_D\gamma_L} C^+_{\gamma_D} |\alpha_{D,N}\rangle|^2 n_F(\varepsilon_L-\mu_L)\delta(E_{\beta N+1}-E_{\alpha N}-\varepsilon_{\gamma_L})$

$= \gamma^L |\langle \beta_{D,N+1}| \sum_{\gamma_D} C^+_{\gamma_D} |\alpha_{D,N}\rangle|^2 n_F(E_{\beta N+1}-E_{\alpha N}-\mu_L)$

例子：考虑仅一个量子点，此dot上只可能4情况：$P(0), P(\uparrow), P(\downarrow), P(\uparrow\downarrow)$

由主方程：① $-(I_{\uparrow 0}+I_{\downarrow 0})P(0)+(I_{0\uparrow}+I_{0\downarrow})P(1)=\frac{d}{dt}P(0)=0$.

② $-(I_{\uparrow\downarrow\uparrow}+I_{\uparrow\downarrow\downarrow}+I_{0\uparrow}+I_{0\downarrow})P(1)+(I_{\uparrow\uparrow\downarrow}+I_{\downarrow\uparrow\downarrow})P(2)$

$+(I_{\uparrow 0}+I_{\downarrow 0})P(0)=\frac{d}{dt}P(1)=0$

对称考虑(③) $-(I_{\uparrow\uparrow\downarrow}+I_{\downarrow\uparrow\downarrow})P(2)+(I_{\uparrow\downarrow\uparrow}+I_{\uparrow\downarrow\downarrow})P(1)=0$

由于 $I_{\uparrow\uparrow\downarrow}=I_{\downarrow\uparrow\downarrow}$ $I_{\uparrow(\cdot)}=I_{\downarrow(\cdot)}$ 则：上文 $P(\uparrow)=P(\downarrow)$ 就是 $P(1)$.

$$\begin{cases} -I_{\uparrow 0}P(0)+I_{0\uparrow}P(1)=0 \\ -(I_{\uparrow\downarrow\uparrow}+2I_{0\uparrow})P(\uparrow)+I_{\uparrow\uparrow\downarrow}P(2)+I_{\uparrow 0}P(0)=0 \\ -I_{\uparrow\uparrow\downarrow}P(2)+I_{\uparrow\downarrow 0}P(1)=0 \end{cases}$$

suppose U: large: Kondo situation: $P(2)=0$. Then:

And $P(0)+P(1)+P(2)=1$

$P(0)=1-2P(\uparrow)$

$\Rightarrow P(0)=\frac{I_{01}}{I_{01}+2I_{10}}$; $P(\uparrow)=P(\downarrow)=\frac{I_{10}}{I_{01}+2I_{10}}$

Now. there's a magnetic field: $P(\uparrow)$余:

$P(0)=\frac{I_{0\uparrow}}{I_{0\uparrow}+I_{\uparrow 0}}$; $P(\uparrow)=\frac{I_{\uparrow 0}}{I_{0\uparrow}+I_{\uparrow 0}}$.

the current:

$I=$ 上文公式: $-e\left(\frac{I^R_{0\uparrow}I^L_{\uparrow 0}-I^L_{0\uparrow}I^R_{\uparrow 0}}{I_{0\uparrow}+I_{\uparrow 0}}\right)$

上文公式: $I^{x}_{\uparrow 0} = I^{x}\cdot n_F\cdot(\varepsilon-\mu_x)\cdot|\langle\uparrow|C^{+}_{\uparrow}|0\rangle|^2 \to 1$

$= I^{x}\cdot n_F(\varepsilon-\mu_x)$　反对易-T.

$I^{x}_{0\uparrow} = I^{x}\cdot n_F\cdot[1-n_F(\varepsilon-\mu_x)]\cdot|\langle 0|C_{\uparrow}|\uparrow\rangle|^2 \to 1$

$= I^{x}[1-n_F(\varepsilon-\mu_x)]$

代入:

$$I = e\left[n_F(\varepsilon-\mu_{right}) - n_F(\varepsilon-\mu_{left})\right]\cdot\frac{I^R I^L}{I^R+I^L}$$

电导: $G = I/V$　令: $\mu_L = \mu - eV/2$　$\mu_R = \mu + eV/2$

即: 偏压V为如此时, 计算I得电导.

(下文续上. 反面)

由上: $G = I/V$. 多体中电导如何求?

之前 T_{fi}, $f\to i$, 也可以 $f\to i\to f\to i$ 等高阶项. or $f\ i \leftrightarrows j$

这些也要算之G中. 高阶 process 称 cotunelling.

高阶 Fermi-Golden Rule 也要修正.

$f\to i$　$|i\rangle = \frac{1}{i}\int_{t_0}^{t} dt_1 \hat{V}(t_1) + \frac{1}{i^2}\int_{t_0}^{t} dt_1 \hat{V}(t_1)\int_{t_0}^{t_1}\hat{V}(t_2)\,dt_2 + \cdots\cdots$

$\therefore \langle f|i(t)\rangle = \sum_n \frac{1}{i^n}\langle f|\int_{-\infty}^{t,t',t''}(dt_1 dt_2\cdots)\hat{V}(t_1)\hat{V}(t_2)\cdots\hat{V}(t_n)e^{\eta t_n}|i\rangle$

由上文方法 相互作用绘景 $\hat{V} = e^{-\hat{H}t} V e^{\hat{H}t}$ 积出.

令: T-Matrix: $T = V + V\frac{1}{E_i-H_0+i\eta}V + V\frac{1}{E_i-H_0+i\eta}V\frac{1}{E_i-H_0+i\eta}V + \cdots$

or $T = V + \frac{1}{E_i-H_0+i\eta}T$. we have.

△

$$I_{fi} = 2\pi|\langle f|T|i\rangle|^2\delta(E_f-E_i)$$

$|\langle f|i(t)\rangle| = \left|\frac{e^{\eta t}}{E_i-E_f+i\eta}\langle f|T|i\rangle\right|$

Second Quantization 中，相互作用为跃迁项 H_T，

$$\therefore \hat{T} = \hat{H}_T + \hat{H}_T \frac{1}{E_i - H_0 + i\eta} \hat{T}$$

$$\Gamma^{(2)}_{\beta\alpha} \text{ 第二阶类比上文：} 2\pi \sum_{\alpha\beta} \left| \langle f_\beta | \underbrace{\hat{H}_T}_{\text{类比 } \hat{V}(t_1)} \frac{1}{E_i - H_0} \underbrace{\hat{H}_T}_{\text{类比 } \hat{V}(t_2)} | i_\alpha \rangle \right|^2 W_{i\alpha} \, \delta(E_{f\beta} - E_{i\alpha})$$

当 $\hat{V}(t_1) = \hat{V}(t_2)$ 即如此，但讨论电子从左经 dot 至右，有2可能性

① 左 → dot 随后 dot → 右. $H_{T\,Right} \cdot \frac{1}{E_i - H_0} H_{T\,Left}$

② dot → 右 ~~···~~ 随后 左 → dot $H_{T\,Left} \cdot \frac{1}{E_i - H_0} H_{T\,right}$

f → i

virtual intermediate state

Kondo 表明 dot 能量可被改变了，也可不变。

金属 Quantum dot 中：富于电子 → 交换散射此不一定等，故带一个(′)，对应 ε_D'

Now: $|f\rangle = C_R^\dagger C_L C_D^\dagger C_{D'} |i\rangle$ 对情况1

D → D′

不厌其烦地计算.

$$\Gamma^{(2)}_{R.L} = 2\pi \sum_{f_\beta i_\alpha} \left| \langle f_\beta | H_{TR} \frac{1}{E_{i\alpha} - H_0} H_{TL} + H_{TL} \frac{1}{E_{i\alpha} - H_0} H_{TR} | i_\alpha \rangle \right|^2$$

$$\times W_{i\alpha} \cdot \delta(E_{f\beta} - E_{i\alpha})$$

$$[C_{D'}^\dagger C_D C_L^\dagger C_R] \times t [C_R^\dagger C_{D'} C_D^\dagger C_L + C_D^\dagger C_L C_R^\dagger C_{D'}] \frac{1}{E_{i\alpha} - H_0}$$

$$\times W_{i\alpha} \cdot \delta(E_{f\beta} - E_{i\alpha}).$$

$|f_\beta\rangle = |i_L\rangle \times |i_R\rangle \times |d_N\rangle$，同上. $\sum$ 时. calculate:

$$\sum W_{Left} C_L^\dagger C_L \times \sum W_{right} C_R C_R^\dagger = n_F(\varepsilon_L - \mu_L)[1 - n_F(\varepsilon_R - \mu_R)]$$

以及：作用对象都不同，对易！ $|i_D\rangle \otimes |i_{D'}\rangle$

$$\sum W_D \cdot C_{D'}^\dagger C_D [C_{D'} C_D^\dagger + C_D^\dagger C_{D'}] = \sum W_D' C_{D'}^\dagger C_{D'} \cdot \sum W_D C_D C_D^\dagger$$

$$= n_F(\varepsilon_{D'} - \mu_D)[1 - n_F(\varepsilon_D - \mu_D)]$$

以及余下：$H_{TR} \cdot H_{TL}$ 中 $t_{D.Left} \cdot t_{D.Right}$ 项 $\Leftrightarrow$ $\gamma^R \gamma^L$ 项

原式中 $\dfrac{1}{E_{i2}-H_0}$ Fermi Golden Rule 中 $\langle f|i\rangle$ 皆一次穿，本为2次穿，但仍然，H_0 为一次穿后的 H_0 而非2次穿后的 $E_{fB}-E_{i2}$

∴此项为 $\dfrac{1}{E_{i2}-E_{方1H_0}} + \dfrac{1}{E_{i2}-E_{方2H_0}}$

$$= [E(N)-E(N+1)+\varepsilon_L-\varepsilon_D]^{-1} + [E(N)-E(N-1)-\varepsilon_R+\varepsilon_D']^{-1}.$$

$$I^{(2)}_{R.L.D}(N) = \frac{\gamma^L\gamma^R}{2\pi}\int_R d\varepsilon_L d\varepsilon_R d\varepsilon_D d\varepsilon_D' \, n_F(\varepsilon_L-\mu_L)\, n_F(\varepsilon_D'-\mu_D)[1-n_F(\varepsilon_R-\mu_R)]$$

$$\cdot [1-n_F(\varepsilon_D-\mu_D)]\left\{(E(N)-E(N+1)+\varepsilon_L-\varepsilon_D)^{-1} + [E(N)-E(N-1)-\varepsilon_R+\varepsilon_D']^{-1}\right\}^2 \cdot \delta(\varepsilon_R-\varepsilon_L+\varepsilon_D$$

积出：(略)

Quantum Dot 中：离散能级下 极大可能在相同dot上产生、湮灭粒子，那么 $C_R^+ C_D^+ C_D C_L \Leftrightarrow C_R^+ C_L$ $|f\rangle = C_R^+ C_L |i\rangle$

$I^{(2)}_{R.L.}$ 对于一个初始空dot来说，上式第二项不会发生，则：

$$I^{(2)}_{R.L}(0) = \frac{I^L I^R}{2\pi}\int d\varepsilon_L d\varepsilon_R \cdot \delta(\varepsilon_R-\varepsilon_L) \cdot \left(\frac{1}{\varepsilon_L-\varepsilon_d}\right)^2 \times n_F(\varepsilon_L-\mu_L)[1-n_F(\varepsilon_R-\mu_R)]$$

$I^\alpha = 2\pi |t_\alpha|^2 d_\alpha$ 令 $\mu_L = eV/2$ $\mu_R = -eV/2$. assume: $\begin{cases} \varepsilon_d \gg eV \\ T\to 0 \end{cases}$

积出：$\int d\varepsilon_L d\varepsilon_R \, \delta(\varepsilon_R-\varepsilon_L) \, n_F(\varepsilon_L-\mu_L)[1-n_F(\varepsilon_R-\mu_R)]$

$$= n_B(eV)\times eV \overset{T\to 0}{=} eV\,\Theta(V).$$

$$\therefore I^{(2)}_{R.L}(0) = \Theta(V)\cdot\frac{eV}{\varepsilon_d^2}\cdot\frac{I^L I^R}{2\pi}$$

~~计算电导~~. Chapter 4. Green Function (电导 Part 2).

For Schodinger Equation Hamiltonian $H_0(r)$ with pertubation $V(r)$, i.e.

$$[H_0(r) + V(r)]\psi_E = E\psi_E$$

(量2)中玻恩近似应利用 Green function 写出积分形式: i.e:

$$H_0(r)\psi_0 = E_0\psi_0$$

$$[E - H_0(r)]G_0(r, r', E) = \delta(r - r')$$

$$\Psi_E(r) = \psi_0(r) + \int dr' G_0(r', r, E)V(r')\Psi_E(r')$$

V: pertubation $\Psi_E(r') \approx \psi_0(r') + V \rightarrow O(V^2)$.

$$\Rightarrow \Psi_E(r) = \psi_0(r) + \int dr' G_0(r', r, E)V(r')\psi_0(r') + O(V^2).$$

similarly. 含时情况下: $[i\partial_t - H_0 - V(r)]\Psi(rt) = 0$

$$[i\partial_t - H_0(r)]G_0(rt, r't') = \delta(r - r')\delta(t - t')$$

or $[i\partial_t - H_0(r) - V(r)]G(rt, r't') = \delta(r - r')\delta(t - t')$

$$\Psi(rt) = \Psi_0(rt) + \int dr'dt' G_0(rt, r't')V(r')\Psi(r't')$$

or $\Psi(rt) = \Psi_0(rt) + \int dr'dt' G(r, r' t, t')V(r')\Psi_0(r't')$

$\therefore$ static case: $\psi = \psi_0 + \int G_0 V\psi_0 + \int G_0 V \int G_0 V \psi^0 + \cdots$

$$= \psi_0 + \left(\int G_0 + \int G_0 V \int G_0 + \int G_0 V \int G_0 V \int G_0\right) V$$

又: 含时 case: $\psi = \psi_0 + \int G V \psi_0$

类比

$$\int G V \psi_0 = \left(\int G_0 + \int G_0 V \int G_0 + \cdots\right) V\psi_0$$

去掉积分, 去掉 $V\psi_0$

$$G = G_0 + G_0 V\left[\int G_0 + \int G V \int G_0 + \cdots\right]$$

Dyson Equation: $G(rt, r't') = G_0(rt, r't') + G_0(rt, r_1 t_1)V(r_1)G(r_1 t_1, r't')$

$$\begin{cases} [i\partial_t - H_0(r) - V(r)]\, G(rt, r't') = \delta(r-r')\delta(t-t') \\ \int G\, \psi(rt)\, dr = \psi(rt') \end{cases}$$ 代入 Schodinger Equation:

$$\Rightarrow \int [i\partial_t - H_0(r) - V(r)]\, \delta[G\, \psi(rt')]\, dr'dt' = 0$$

$$= \int \{[i\partial_t - H_0(r) - V(r)] G\} \psi\, dr\, dt + \int G \cdot i\partial_t - H_0(r) - V(r)\, \psi(r't')\, dr'dt'$$

$$\Downarrow$$

$\psi(r, t)\,\delta(t-t')$ $t \neq t'$（先后发生）为0

$$\therefore \psi(rt) = \int G(rt, r't')\, dr'\, \psi(r't')$$

这说明了：某 t' 时刻体积分 dr' 所有 r' 处 ψ 在 $t-t'$ 时间内这些 $\psi(r'$

恰在 t 时抵达 r 处 G 描述此传播振幅

同时 Sakurai 上关于传播子定义为：

$$\psi(x'', t) = \int d^3x'\, K(x'', t, x', t_0)\, \psi(x', t_0)$$

此式是从时间演化角度来看的，以及 $K(x'', t, x', t_0) = \langle x'' | e^{-\frac{iH(t-t_0)}{\hbar}} | x' \rangle$

因此 Green function 又可写作 → 为 satisfy 传播子 Schodinger Equation (Sakurai

$$\underset{\text{Retard}}{G(rt, r't')} = -i\theta(t-t')\langle r | e^{-iH(t-t')} | r' \rangle$$

（因果律）⇒ 算电导必为推迟场

$$\underset{\text{Advanced}}{G(rt, r't')} = i\theta(t'-t)\langle r | e^{-iH(t-t')} | r' \rangle$$

上文为 single-particle Green function. Now apply this to many-body

先写出 Green-function in Second Quantization. Remind $\langle A \rangle = \frac{Tr[\rho A]}{Tr[\rho]}$

Remind 流-流关联也是传播. 凡含时演化必不离相互绘景下的

表示式. 即 $\langle [A, B] \rangle$. 即. Green function 为 ψ_A^+ 与 ψ_B 两场算符

（波函数）之关联. ie:

$$G^R(r\sigma t, r'\sigma' t') = -i\theta(t-t')\left\langle \left[\hat{\Psi}_\sigma^\dagger(rt), \hat{\Psi}_{\sigma'}(r't')\right]_{\text{Boson}} \right\rangle$$

$\{\ \}_{\text{Femion}}$

DATE · $\psi^+\psi^{-1}$ Boson · Fermion

定义：$G^{>} = -i\langle \psi \psi^+ \rangle$ $G^{<} = -i(\pm)\langle \psi^+\psi\rangle$. st.

St: $\begin{cases} G^R = \theta(t-t')(G^{>} - G^{<}) \\ G^A = \theta(t'-t)(G^{<} - G^{>}) \end{cases}$

例：自由电子的格林函数. $\hat{H} = \sum_{k\sigma} \varepsilon_{k\sigma} C^+_{k\sigma} C_{k\sigma}$

$G(r\sigma t) \to G(k\sigma t)$ 作表象变换

$[\psi^+ . \psi] \Rightarrow \sum_{kk'} [\langle r|k\rangle][C^+_k . C_k]$ 前项积分为1 $\Rightarrow [C^+_k . C_k]$

Therefore: 自由电子无势传播距离 $(t-t')$ 仅与时间差 $(t-t')$ 有关

$G_0^{>}(k\sigma, t-t') = -i\langle C_{k\sigma}(t) C^+_{k\sigma}(t')\rangle$

相互作用绘景算符

由于 $\frac{\partial}{\partial t} a^+_\gamma(t) = i[H . a^+_\gamma(t)] = i e^{-iHt}[H . a_\gamma] e^{iHt}$ $\hat{H} = a^+_\gamma a_\gamma \varepsilon_\gamma + \cdots$

$\Rightarrow a^+_\gamma(t) = e^{-i\varepsilon_\gamma t} a^+_\gamma$

$\Rightarrow$ ~~$G_0^{>}(k\sigma . t-t') = -i\langle C_{k\sigma} C^+_{k\sigma}\rangle e^{-i\varepsilon_k(t-t')}$~~

$\langle C_{k\sigma} C^+_{k\sigma}\rangle = 1 - \langle n\rangle = 1 - n_{Fermi-Dirac}$

Therefore: $G_0^{>}(k\sigma . t-t') = -i[1 - n_F(\varepsilon_k)] e^{-i\varepsilon_k(t-t')}$.

$G_0^{<}(k\sigma . t-t') = i\, n_F(\varepsilon_k)\, e^{-i\varepsilon_k(t-t')}$.

比如 $G(k . k' t'-t) = -i\langle C^+_k \text{Ground State} | e^{-iH(t-t')} | C^+_{k'} \text{Ground}\rangle$
$[T=0$ (基态)$]$. $\times e^{iE_0(t-t')}$.

clearly depicts: 态1: k处多1电子基态 态2: k处多1电子基态
在 $t-t'$ 时间中从态1 能 至态2的传播.

Fourier Transform: (不是对 t 做. 对 $t-t'$ 做. 在时间差对应一些
之后换回坐标空间 k 代表 $r \to$ 距离差 $|r-r'|$ ie:

~~$G_0^{>}(r-r', \omega) = -(2\pi i) \cdot [\text{Density 3D}](\omega) \cdot [1-n_F(\omega)] \frac{\sin k_\omega |r-r'|}{|r-r'| k_\omega}$ 其中 $k_\omega^2 = 2m$~~

Lehmann Representation: spectral function (谱函数)

引入谱函数: 对 fermions: $\mathrm{Tr}[\rho A]$.

$$G^{>} = -i\langle c_{k\sigma}(t) c^{\dagger}_{k\sigma}(t')\rangle = -i\frac{1}{Z}\sum_{n}\langle n|e^{-\beta H} c_{\gamma}(t) c^{\dagger}_{\gamma}(t')|n\rangle$$

$$(t-t') = -i\frac{1}{Z}\sum_{nn'} e^{-\beta E_n}\langle n|c_{\gamma}|n'\rangle\langle n'|c^{\dagger}_{\gamma}(t)|n\rangle e^{i(E_n-E_n')(t-t')}$$

$$\langle n|e^{-iHt}c^{\dagger}_{\gamma}e^{iHt}|n'\rangle = e^{i(E_n-E_n')t}c^{\dagger}_{\gamma}$$

Fourier

$$G^{>}(\gamma,\omega) = -\frac{2\pi i}{Z}\sum_{nn'} e^{-\beta E_n}\langle n|c_{\gamma}|n'\rangle\langle n'|c^{\dagger}_{\gamma}|n\rangle\, \delta(E_n-E_n'+\omega)$$

$$G^{<}(\gamma,\omega) = \frac{2\pi i}{Z}\sum_{nn'} e^{-\beta E_n}\langle n|c_{\gamma}|n'\rangle\langle n'|c^{\dagger}_{\gamma}|n\rangle\,\delta(E_n-E_n'-\omega)$$

$$= 2\pi i/Z\sum_{nn'} e^{-\beta(E_n+\omega)}\langle n|c_{\gamma}|n'\rangle\langle n'|c^{\dagger}_{\gamma}|n\rangle\,\delta(E_n'-E_n-\omega)$$

$\therefore G^{<}(\gamma,\omega) = -G^{>}(\gamma,\omega)e^{-\beta\omega}$ (令 $E_n\to E_n'$ $E_n'\to E_n$).

Therefore:

$G^{R}(\gamma,\omega)$ (补充): when $G^{R}(t-t') = -i\theta(t-t')\langle[A(t),B(t')]\rangle$

如何对 $t-t'$ 做 Fourier Transform? when it only depends on $t-t'$ one variable? For Retarded functions: Normally:

$$G(\omega) = \int_{\mathbb{R}} e^{-i\omega t}G(t) \quad t\Leftrightarrow t-t'$$

$t<0$ 由 $\theta(t-t')$ 为0 $\therefore G = \int_{\mathbb{R}^+} e^{-i\omega t}G(t)\,dt$ 衰减

Remind: Kramers-Kronig 公式. 除了定义 δ 函数外, 引入衰项 $e^{-\eta t}$ 也是解决 Fourier 处不 decay 的方法. 比如 $\delta(\omega+1)-\delta(\omega-1) = \int e^{-i\omega x}\sin x\,dx$

也可以 $e^{-i\omega x}e^{-\eta x}\sin x\,dx = \int_{\mathbb{R}} e^{-i\omega x-\eta x}e^{ix}\,dx$ $(-i\omega-\eta+1) = \frac{1}{\omega-\varepsilon+i\eta}$

利用复平面上围道积分. Anyway. Now we define: Retarded Function:

$$G(\omega) = \underset{(\eta\to 0)}{G(\omega)}\int_{\mathbb{R}} e^{-i\omega t}e^{-\eta t}G(t)\,dt \qquad \omega' = \omega+i\eta \text{ 复化频率.}$$

$$G(t) = \frac{1}{2\pi}\int_{\mathbb{R}} e^{i\omega t}G(\omega)\,d\omega$$

做围道积分, $\eta\to 0$.

G_{advanced}: $\omega' = \omega - i\eta$

例子: Fourier Tranform . $f^R(t) = -i\theta(t)\exp(-i\varepsilon t)$ $\quad e^{-\eta t}$ decay

$$-i\int \exp^{(-i\varepsilon + i\omega - \eta)t} dt = \frac{1}{\omega - \varepsilon + i\eta}\exp(i(\varepsilon-\omega))\cdot\exp(-\eta t)\Big|_0^{+\infty} = 1$$

$$\boxed{F[-i\theta(t)\exp(-i\varepsilon t)] = \frac{1}{\omega - \varepsilon + i\eta}}$$ 之后的重要结论

Inverse Fourier Transform

$$\frac{1}{2\pi}\int \frac{1}{\omega-\varepsilon+i\eta}e^{-i\omega t}d\omega$$ 奇点 $\omega = \varepsilon - i\eta$ 处 下围道

$$\int_{C_R} \overset{\text{Contor theron}}{=} 0 \quad \therefore \int_R = 2\pi i \operatorname{Res}_{\omega=\varepsilon-i\eta} \frac{e^{-i\omega t}}{\omega-\varepsilon+i\eta}\cdot\frac{1}{2\pi} = \left(\frac{1}{2\pi}\cdot 2\pi\right)i\,\frac{e^{-i\omega(\varepsilon-i\eta)}}{1}$$

$$= ie^{-i\varepsilon}\cdot e^{\omega\eta} \quad \eta\to 0 = \exp(-i\varepsilon t)(-i)$$
转反了!

Now: we apply this to G^R, we have

$$G^R(\gamma,\omega) = \int dt\, e^{i(\omega+i\eta)t}\frac{1}{Z}\left(\langle n|C_\gamma|n'\rangle\langle n'|C_\gamma^+|n\rangle e^{i(E_n-E_{n'})t} + \langle n|C_\gamma^+|n'\rangle\langle n'|\ldots|n\rangle e^{i(E_n-E_{n'})t}\right)$$ 积出:

$$= \frac{1}{Z}\sum_{nn'}[\langle n|C_\gamma|n'\rangle\langle n'|C_\gamma^+|n\rangle]\times\frac{1}{\omega+E_n-E_{n'}+i\eta}\times(e^{-\beta E_n}+e^{-\beta E_{n'}})$$

$(\omega+i\eta)^{-1} = f(\frac{1}{\omega}) + -i\pi\delta(\omega)$ 取第二项, 则虚部为:

$$2I_m G^R(\gamma,\omega) = -\frac{2\pi}{Z}\sum_{nn'}\frac{\langle n|C_\gamma|n'\rangle\langle n'|C_\gamma^+|n\rangle}{\omega+E_n-E_{n'}+i\eta}(e^{-\beta E_n}+e^{-\beta E_{n'}})\delta(\omega+E_n-E_{n'})$$

$$= -\frac{2\pi}{Z}\sum_{nn'}\langle n|C_\gamma|n'\rangle\langle n'|C_\gamma^+|n\rangle e^{-\beta E_n}(1+e^{-\beta\omega})\delta(\omega+E_n-E_{n'})$$

$$= -i(1+e^{-\beta\omega})G^>(\gamma,\omega)$$

这即是著名涨落-耗散定理. 对涨落: $G^>$: 从 $n\to n'$ 态跳跃. 则热
程度越高, 其带来耗散: $I_m G^R$ 为耗散项: 如: 电极化, 越大
比如谐振子能级↑: $\Delta G^>\uparrow$: $G^R\uparrow$.

DATE . . NOTES

我们定义谱函数为: $A(\gamma,\omega) = -2 I_m G^R(\gamma,\omega)$.

性质: ① $iG^>(\gamma,\omega) = A(\gamma,\omega)[1-n_F(\omega)]$

② $-iG^<(\gamma,\omega) = A(\gamma,\omega)\, n_F(\omega)$

③ $G^R(\gamma,\omega) = \int d\omega' \frac{1}{2\pi} A(\gamma,\omega') \cdot \frac{1}{\omega-\omega'+i\eta}$

pf. ③. $I_m G^R(\gamma,\omega) = \sum_{nn'} (\quad) \cdot (\delta)$

$\int I_m G \cdot \frac{1}{\omega-\omega'+i\eta} d\omega' = \sum_{nn'} (\quad) \cdot \frac{1}{\omega-\omega'+i\eta} \delta(\omega'+E_n-E_{n'}) d\omega'$

$\therefore \omega' = E_{n'}-E_n$

$= \sum_{nn'} \frac{(\quad)}{\omega+E_{n'}-E_n+i\eta}$ 正是 G^R 形式:

similarly: $G^A(\gamma,\omega) = [G^R]^* = \int \frac{d\omega}{2\pi} \cdot \frac{A(\gamma,\omega')}{\omega-\omega'-i\eta}$

④ 自由电子 $A_0(k\sigma,\omega) = 2\pi\delta(\omega-\varepsilon_k)$

$G_0^R(k\sigma,\omega) \overset{代入G}{=} (\omega-\varepsilon_k+i\eta)^{-1}$

⑤ 恒正 (尽管 mostly 为 0).

⑥ 归一 $\int d\omega \frac{1}{2\pi} A(\gamma,\omega) = 1$.

pf. ⑥: $\int d\omega\, \delta(\omega+E_n-E_{n'}) \sum_{nn'} \langle n|C_\gamma|n'\rangle\langle n'|C_\gamma^+|n\rangle (\exp(-\beta E_n) + \exp(-\beta E_{n'}))$

$1 \cdot (\langle C_\gamma C_\gamma^+\rangle + \langle C_\gamma^+ C_\gamma\rangle) = \langle C_\gamma^+ C_\gamma + C_\gamma C_\gamma^+\rangle = \langle 1\rangle = 1$

⑦ γ 态平均占据数:

$\bar{n}_\gamma = \langle C_\gamma^+ C_\gamma\rangle = -iG^<(\gamma,\Delta t=0) = i\int d\omega \frac{1}{2\pi} e^{-i\omega t} G^<(\gamma,\omega)\Big|_{t=0}$

$= \int_R \frac{d\omega}{2\pi} A(\gamma,\omega)\, n_F(\omega)$

类比 $\psi(rt') = \int_R G(rt', rt)\psi(rt)$ A作用将不同能级ω的粒子投

$\bar{n}_\gamma = \int_R A(\gamma,\omega)\, n_F(\omega)$ 影至能级γ上. $A(\gamma,\omega)$ 代表了这些能量的关联. 对自由电子, 代入④. $\bar{n}_\gamma = \int \delta_{(\omega-\varepsilon_k)} n_F(\omega) = n_F(\varepsilon_\gamma)$ 是 Fermi-Dirac Distribution, 系: 谱函数仅 $\omega=\varepsilon_k$ 有尖峰. 无相互作用时代表 填入一个ω能量, 100% 是通过引入 $\omega=\varepsilon_k$ 的电子. 而

不是利用相互作用。100% 是 $\omega=\varepsilon_k$ 的电子贡献 n_γ。其它相互作用时，
$A(\gamma,\omega)$ 就代表一种概率密度（性质：归一），$n_\gamma=\int n_F(\omega)A(\gamma,\omega)\,d\omega$
代表 ω_0 的粒子 $n_F(\omega)$ 有百分之 $A(\gamma,\omega_0)\%$ 变为 n_γ. $\omega_1\ldots$ $A(\gamma,\omega)\%$ 不同初态粒子对末态粒子数的贡献权重。比如 $T\to 0$ 时，$e^{-\beta E_n}$ 项 $\beta\to\infty$
仅基态 $E_0=0$ 此项非零，余下项尽是向基态跃迁 $\sum_{n'}|\langle n'|c_\gamma^\dagger|0\rangle|^2\delta(\omega-E_{n'})$
要产生一个 $|\gamma\rangle$ 可通过不同态 $|n'\rangle$ 跃迁，那么转移能量 $\omega=E_{n'}$ 以 $\delta\neq 0$ 必然。跃迁概率由 $\langle n'|c_\gamma^\dagger|0\rangle$ 决定。谱有展宽（$T\neq 0$，相互）
Actually 代表谱不能用 δ 表示，即 Green function 不再 $\propto e^{i(t-t')}$，亦存衰减项 $e^{-\gamma t}$，比如：$G=-i\theta(t)e^{-i\varepsilon_\gamma t}e^{-t/\tau}\Rightarrow A(\gamma,\omega)=\frac{2}{\tau}\cdot\frac{1}{(\omega-\varepsilon_\gamma)^2+(1/\tau)^2}$
说明多体相互作用下单体 Green function 描述能力欠缺，相当后面再议。

接下来又回到隧穿了，我们利用 Green function 写出电流 ~~写出~~
电子数改变定义为电流。$\langle e\rangle N_1$ 先就 Quantum Dot 为真空(绝缘体)讨论

$$\therefore \hat{I}=i[H,N_{\text{left}}]\qquad H=H_T$$
$$=i\sum_{\gamma\mu}\left[c_{L\gamma}^\dagger c_{R\mu}T_{\gamma\mu}-c_{R\mu}^\dagger c_{L\gamma}T_{\gamma\mu}^*\right]=-i(\hat{L}-\hat{L}^\dagger)$$

更进一步，相互绘景中 $\langle I\rangle$ 用 Kubo Formula 关联函数写出

$$\langle \hat{I}\rangle_{(t)}=\int_R dt'\,C^R_{IH_T}(t,t')$$
$$C^R_{IH_T}(t,t')=-i\theta(t-t')\langle[\hat{I}(t),\hat{H}_T(t')]\rangle_0$$
$$(\hat{L}-\hat{L}^\dagger),\ (\hat{L}+\hat{L}^\dagger)$$

关 $\hat{L}\cdot\hat{L}$ 项，不可能自发地 Left 少2个电子，Right 多2个电子。对每个 subsystem，electron 守恒（extra：超导）。仅余下了

$$(L^\dagger L+LL^\dagger)=L^\dagger L+(L^\dagger L)^*=2\,\mathrm{Re}(L^\dagger L)$$

原式 $=\langle I_p(t)\rangle=2\,\mathrm{Re}\int_R dt'\,\theta(t-t')\sum_{\gamma\mu}\sum_{\gamma'\mu'}T^*_{\gamma\mu}T_{\gamma'\mu'}\langle[c^\dagger_{R\mu}(t)c_{L\gamma}(t),\ c^\dagger_{L\gamma'}(t')c_{R\mu'}(t')]\rangle$

$$\langle\,|\,\rangle\Rightarrow|\,\rangle_L\otimes|\,\rangle_R$$

$\langle\ \rangle_0 = \langle \hat{C}_{L\nu}(t) \hat{C}^{+}_{L\nu'}(t) \rangle_0 \langle C^{+}_{R\mu}(t) C_{R\mu'}(t') \rangle_0 - \langle \hat{C}^{+}_{L\nu}(t) \hat{C}_{L\nu'}(t) \rangle_0 \langle \hat{C}_{R\mu}(t) \hat{C}^{+}_{R\mu'}(t') \rangle$

NOTES

Left与Right不同之处在化学势不同，体现为电压 $V_{Left} > V_{right}$ 宏观上电流右走，相位 $e^{-i(-eV)t}$ $V=V_L, V_R$ 除去相位因子后 μ 相同。那么L.R可用单粒子Green function表述，即 $C^{+}_{L}(t) = e^{-i(-eV_L)t} \tilde{C}^{+}_{L}(t)$，而 $\langle \tilde{C}^{+}_{L\nu}(t)\ \tilde{C}_{L\nu'}(t') \rangle$ 上文为 $G^{>}_{L}(\nu t, \nu t')$，并且 H不显含时 $G(\nu,\nu,t'-t)$ 仅与时间差有关；并且，我们并不取叠加态 $\langle\ \rangle_0$，对0阶Hamiltonian本征态 $|n\rangle$ 仅 $\nu=\nu'$ 才非零，即对角，综上 we have：$\boxed{\text{令变换 } t'-t=t'}$

$$\langle I_p(t) \rangle = 2Re \int_{-\infty}^{0} dt' \sum_{\nu\mu} |T_{\nu\mu}|^2 e^{i(-e)(V_{Left}-V_{right})t'} [G^{>}_{L}(\nu,-t') G^{<}_{R}(\mu,t')$$

$$- G^{<}_{L}(\nu,-t') G^{>}_{R}(\mu,t')]$$

作Fourier变换，对前一半 $G^{>}_1 G^{<}_R$ $\quad V=V_1-V_2$

$$2Re = \frac{1}{4\pi^2} \int d\omega d\omega' \sum_{\nu\mu} |T_{\nu\mu}|^2 G^{>}_1(\omega) G^{<}_2(\omega') \int_{-\infty}^{0} dt' \exp[i(-e(V_1-V_2)+\omega-\omega')]t'$$

而 $2Re\int_{-\infty}^{0} dt' \exp[\ ]t'$ 同样先取 $e^{\eta t}$ 再 $\eta\to 0$ 以先收敛，毕竟 $\int_R$ 才为 δ function，而 $\int_{-\infty}^{0}$ 是否尚需验证。

$$2Re\int_{-\infty}^{0} dt' \exp[\ ]t' e^{\eta t} = Re \frac{1\times 2}{\eta + i(-eV+\omega-\omega')} = \frac{\eta}{\eta^2 + [(-eV)+\omega-\omega']^2}$$

$\eta \to 0$. ie: $\pi\delta(-eV+\omega-\omega')$ (arctan原函数出一个π)

把这个 $\delta(-e(V_1-V_2)+\omega-\omega')$ 代入 $d\omega d\omega'$ 积分 去掉 $d\omega'$，则合并两项。

$$I_p(t) = \frac{1}{2\pi} \int d\omega \sum_{\nu\mu} |T_{\nu\mu}|^2 G^{>}_{L}(\nu,\omega) G^{<}_{R}(\mu,\omega-eV) - G^{<}_{L}(\nu,\omega) G^{>}_{R}(\mu,\omega-eV)$$

用Spectral function 替代 $G^{>}$ $G^{<}$，终得到：

$$\Delta\quad I_p = \int_R \frac{d\omega}{2\pi} \sum_{\nu\mu} |T_{\nu\mu}|^2 \underbrace{A_1(\nu,\omega)}_{\text{表强弱}} A_2(\mu,\omega-eV) [\underbrace{n_F(\omega-eV) - n_F(\omega)}_{\omega-eV\sim\omega\ \text{化学势差推动隧穿}}]$$

W是 sum K $\frac{w'}{dw}$ $w'(E_k)$

对谱函数求K和是什么，比如自由电子.

$$\sum_{k\sigma} A_0(k\sigma,w) = \sum_{k\sigma} 2\pi\delta(w-\varepsilon_k)$$

$$= 2\int\frac{Vdk}{(2\pi)^3}[2\pi\delta(w-\varepsilon_k)] = 2\frac{4\pi V}{(2\pi)^3}\int_{R^+} dk\, k^2[2\pi\delta(w-\varepsilon_k)]$$

$$E_k = \frac{p^2}{2m} = \frac{k^2}{2m}$$

$$= \frac{2\,4\pi V}{(2\pi)^3}\int_{R^+}\left[\frac{(kdk)}{dE_k}\cdot\frac{\sqrt{E_k}}{k}\right] \Leftrightarrow \frac{2(4\pi V)}{(2\pi)^3}\int dE_k \underbrace{\sqrt{\frac{2mE_k}{\hbar^2}}\frac{m}{\hbar^2}}_{g(w)} 2\pi[\delta(w-E_k)]$$

$$= 2\pi g(w)$$ g正是 3-D $\boxed{\text{态密度}}$: $k^2dk = g(w)dw$.

对上面隧穿例子，态密度即：

$$\sum_{\mu}|T_{\nu\mu}|^2 A_R(\mu,w-eV)$$

上述理解：$|T|^2\int A(n_{F1}-n_{F2})$ 即 $(n_{\nu左}-n_{\mu右})|T|^2$ 为可利用电子number与电子跃迁振幅(possibility)表概率，即单位t可用电子振幅：电流.

实验上. 电导 $\propto \sum A_L \sum A_R$ 直接测某材料态密度困难，我们测电导把Right材料全金属(态密度变化迟慢). 在 Left~Right~Dot 体系测电导之尖峰即某材料态密度峰值所在。

双粒子关联函数 极化率.

我们之前看到所有⟨[,]⟩，都是两单体算符间作用. 体现了量子系统对多个粒子之响应eg:[current-current correlation]，中有4个产生.湮灭算符之乘积，是两体Green function.

在Chapter3中，Dielectric function 解极化率给出公式：

$$\mathrm{Re}\,\delta(q,\omega) = -\omega e^2/q\ \chi^R(q,\omega).$$

以及极化反映为电荷-电荷关联 $\langle[\hat{\rho}_1, \hat{\rho}_2]\rangle$，具体计算：

把chapter 3中 $\rho(r,t)$ 先 Fourier 变为 $\rho(k,t)$，得到：令 $r-r' \leftrightarrow k$

$$\chi^R(k,t-t') = -i\theta(t-t')\frac{1}{V}\langle[\rho(k,t),\rho(-k,t')]\rangle$$

ρ 为电荷密度：$\rho = \hat{\psi}_\sigma^+\psi_\sigma = \int a_k e^{ikr}\int a_{k'} e^{ik'r}$ k' 令 $k'=k+q$

$$\rho_{(q)} = \sum_k a_{k\sigma}^+ a_{k+q\sigma}$$

海森堡绘景中：$\rho(q,t) = \sum_{k\sigma} C_{k\sigma}^+ C_{k+q\sigma} e^{i(\varepsilon_k - \varepsilon_{k+q})t}$ 代入

$$\chi^R(q,t-t') = -i\theta(t-t')\frac{1}{V}\sum_{k\sigma}[n_F(\varepsilon_k) - n_F(\varepsilon_{k+q})]e^{i(\varepsilon_k-\varepsilon_{q+k})(t-t')}.$$

Fourier $t-t' \leftrightarrow \omega + i\eta$ Retard

$$\chi^R(q,\omega) = \frac{1}{V}\sum_{k\sigma}\frac{n_F(\varepsilon_k) - n_F(\varepsilon_{k+q})}{\varepsilon_k - \varepsilon_{k+q} + \omega + i\eta}$$ Lindhard函数

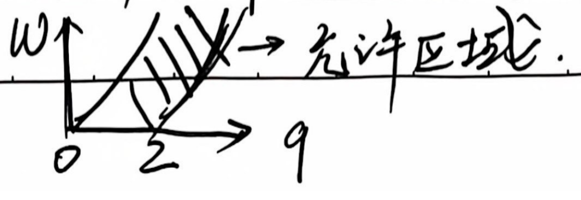
电子-空穴配对激发：

耗散 $W = -\int\frac{d\omega}{2\pi}\frac{1}{V}\sum_q |E(q,\omega)|^2\frac{\omega e^2}{q^2}\,\mathrm{Im}\,\chi^R(q,\omega).$

可见，极化率虚部/电导实部致能损失。

$\mathrm{Im}\,\chi = \delta(\varepsilon_{k+q} - \varepsilon_k + \omega) * (n)$ $\quad \omega = \varepsilon_{k+q} - \varepsilon_k = \frac{1}{2m}(q^2 - k\cdot q)$

那么作 $\omega\sim q$ 图对不同的k，其义为 q, ω k的光子打入k的电子中，激发k至k'散射出而原体系失能 ε_k.（ε_{k+q} 逸出而配对部只能一些 ω 能激发，对于 k：$T\to 0$ 时 $k<k_F$ 才来浮而 $k+q>k_F$ 才散射出：故 $\omega \in [\frac{1}{2m}q^2 - v_F q, \frac{1}{2m}q^2 + v_F q]$ $v_F' \in (-v_F, v_F)$ 变化的k，作图如下，比如 $(\omega, q) = (1, q)$ impossible ω 怎么也打不出Fermi海中q动量的变化



Exercises:

①. 求电导: 1-D电子气 $\hat{H}=\frac{1}{L}\sum_k\left(\frac{k^2}{2m}-\mu\right)C_k^+C_k$

回忆起 chapter 3 求 conductance 对直流电，只要 $C_{II}\to\Pi_{II}$ 就可代表含时演化了. $G=(ie^2/\omega)\cdot\Pi^R(\omega)$

$$\Pi^R(\underbrace{x-x'}_{\text{稍后会知}},t-t')=-i\theta(t-t')\langle[I_p(xt),I_p(x't')]\rangle$$

1. 写出 $I_p(x)$ 这就是单纯的 current. 也不是上文隧穿电流，故直接代入 $I=i[\hat{N},\hat{H}]\Rightarrow\frac{\partial\rho}{\partial t}+\nabla\cdot J=0\quad\frac{\partial\rho}{\partial t}=\frac{i}{\hbar}[\rho,H]$

$\Rightarrow\rho=\Psi^+\Psi=\sum e^{ikq}a_k^+a_{k+q}\Rightarrow\frac{i}{\hbar}[\rho,H]=\sum_{kq\sigma}e^{iqx}q(k+\frac{q}{2})a_k^+a_{k+q}$

仅 $k'=k\quad k=k+q$ 不对易

$\Rightarrow\nabla\cdot J(r)=\frac{d}{dx}J(x)=\sum_{kq\sigma}e^{iqx}(k+\frac{q}{2})q\,a_k^+a_{k+q}$

$\Rightarrow J(x)=\left(\int dx\,e^{iqx}\right)w=\frac{1}{q}\cdot q\cdot(k+\frac{q}{2})=k+\frac{q}{2}$

1-D

$\Rightarrow J(x)=I(x)\Rightarrow I(x)=\sum_{kq\sigma}e^{iqx}(k+\frac{q}{2})a_k^+a_{k+q}\cdot\frac{\hbar}{mL}$

2. 求解 Π.

$=-i\theta(t-t')\left(\frac{\hbar}{mL}\right)^2\langle[\sum_{kq\sigma}(k+\frac{q}{2})C_{k\sigma}^+C_{k+q\sigma}e^{iqx},\sum_{k'q'\sigma'}(k'+\frac{q'}{2})C_{k'\sigma}^+C_{k'+q'\sigma}e^{iq'x'}]\rangle$

对易非零

① $\overset{\sigma=\sigma'}{k=k'}\Rightarrow0$ ② $k'=k+q$ 它与 $k=k'+q$ 两项相消

③ $k'=k+q$ 以及 $k=k'+q'$，则原式 $=$

$$\langle[C_k^+C_{k'}e^{i(k'-k)x}(k+\frac{k'-k}{2})(t),$$
$$C_{k'}^+C_k e^{i(k-k')x'}(k'+\frac{k-k'}{2})(t')]\rangle$$

$= \langle [C_{k'}^{+}C_k - C_k^{+}C_{k'}] \times (\frac{k+k'}{2})^2 \ (t)(t') \rangle$ 令 $k' = k+q$

① $\Rightarrow \langle (t)(t') \rangle - \langle n | (t)(t') | n \rangle = C_{k+q}(t)|n\rangle : \exp i\varepsilon_{k+q} t$

$C_k(t)|n\rangle : \exp i\varepsilon_k t'$

②: $\Rightarrow \langle (t)(t') \rangle$ Altogether: $\exp[i(\varepsilon_k - \varepsilon_{k+q})(t'-t)]$

$\Rightarrow \exp[i(k'-k)x]$: $\Rightarrow \exp(iqx)$

$\Rightarrow [(k'+k)/2]^2 = (k+\frac{q}{2})^2$

$\Rightarrow \langle C_k^{+}C_k \rangle = \langle n_{F_k} \rangle \quad \langle C_{k+q}^{+}C_{k+q} \rangle = n_F(\varepsilon_{k+q})$

∴ 原式 $= \Pi^R(x-x', t-t') = -i\theta(t-t')(\frac{\hbar}{mL})^2 \sum_{kq\sigma} (n_F(\varepsilon_k) - n_F(\varepsilon_{k+q})) \times$

$(k+\frac{q}{2})^2 \exp[i(\varepsilon_k - \varepsilon_{k+q})(t-t')] \exp[iq(x-x')]$

3. set $x'=x$ 情况: $[\ J_{(r)} = \int \delta(r \cdot r', \omega) \vec{E}\, dr' \ ]$

$x=x'$ Π space invariant. 同时 $\omega \to 0$, 代表直流极限 situation.

ie. $\Pi(0,\omega) = (\ldots) \int_0^\infty \exp i(\varepsilon_k - \varepsilon_{k+q})(\underbrace{t-t'}_{\Delta t})\, e^{-\eta \Delta t} e^{i\omega \Delta t}\, d\Delta t$

$(\varepsilon_k - \varepsilon_{k+q} + i\eta + \omega)^{-1}$

虚部 $((-i)\theta(t-t')\ldots)$

$= \sum_{kq\sigma} (\ldots) \times \frac{\omega + \varepsilon_k - \varepsilon_{k+q}}{(\omega+\varepsilon_k - \varepsilon_{k+q})^2 + \eta^2} [n_F(\varepsilon_k) - n_F(\varepsilon_{k+q})]$

$\omega \to 0$, $\eta \to 0$: $\frac{n_F(\varepsilon_k) - n_F(\varepsilon_{k+q})}{(\omega+\varepsilon_k-\varepsilon_{k+q})^2+\eta^2}$ 在 $\omega + \varepsilon_k = \varepsilon_{k+q}$ 才非零 $\quad n_F(\varepsilon_{k+q}) - n_F(\varepsilon_k)$

$= \frac{\partial n_F(\varepsilon_k)}{\partial \varepsilon_k} \cdot \omega$

$\Rightarrow \frac{\pi}{\omega+\varepsilon_k-\varepsilon_{k+q}} \omega \frac{\partial n_F(\varepsilon_k)}{\partial \varepsilon_k} \cdot \delta(\omega + \varepsilon_k - \varepsilon_{k+q})$. $\quad (\frac{f(x+\Delta x) - f(x)}{\Delta x} = f'(x))$

$(\frac{x}{x+a})$ $\lim_{x\to 0} = 1 - (1+\frac{x}{a})^{-1} = \frac{x}{a} = \frac{\omega}{\varepsilon_k - \varepsilon_{k+q}}$

$\Rightarrow$ 原式 $= \lim_{\omega \to 0} I_m \Pi^R(\omega) = -\hbar\omega\pi (\frac{\hbar}{mL})^2 \sum_{kq\sigma} -\frac{\partial n_F(\varepsilon_k)}{\partial \varepsilon_k} \delta(\varepsilon_k - \varepsilon_{k+q})(k+\frac{q}{2})^2$

令: $\frac{\hbar^2(k+q)^2}{2m} = u$. 原式 =

$\frac{1}{L}\int dq \cdot L\,(k+\frac{q}{2})^2\, 2\pi\, \delta\left(\frac{\hbar k^2}{2m} - u\right)$

$= \frac{1}{L}\int du \frac{1}{|k+q|} (k+\frac{q}{2})^2\, 2\pi\, \delta(\frac{\hbar k^2}{2m} - u) = \frac{1}{L}\int du\, f(u)\, \delta(A-u) \cdot L \cdot 2$

$= 2\pi\, f(A) = 2\pi \left.\frac{(k+\frac{q}{2})^2}{k+q}\right|_{q=0} = 2\pi\frac{k^2}{|k|}$

$\Rightarrow$ 在: Fourier Transition 中 ω, 又 $\sum_q$ 连续 Integral, 则:

$\lim_{\omega\to 0} \mathrm{Im}\, \Pi^R(\omega) = \hbar\omega\pi(\frac{\hbar}{m})^2(\frac{m}{\hbar^2})^2 \frac{1}{2\pi L}\sum_{k\sigma}[-\frac{\partial}{\partial\epsilon_k} n_F(\epsilon_k)]\frac{k^2}{|k|}$

Then: Intergral over k

$\int_R dk -\frac{\partial}{\partial\epsilon_k} n_F(\epsilon_k)\frac{k^2}{|k|} = 2\int_{R^+} d\epsilon_k \cdot \frac{1}{k}\cdot k - \frac{\partial}{\partial\epsilon_k} n_F(\epsilon_k) = 2[n_F(\infty) - \underbrace{n_F(0)}_{n_F(u)}]$ $\quad n_F(\infty)=0$

$\therefore$ 原式 $= \frac{\omega}{\hbar\pi}\frac{1}{e^{-\beta u}+1}$

Take the limit: $u \gg kT$ (大量粒子) 1 particle: $\sim kT$., Then..

$G = \frac{ie^2}{\omega}\mathrm{Im}\,\Pi^R(\omega) \Rightarrow$ 取 Im. $= \frac{ie^2}{\omega}\frac{\omega}{\hbar\pi}\frac{1}{e^{-\beta u}+1}$ $\quad \hbar = (2\pi)^{-1} h$

$\therefore \quad G_{1\text{-}D} = \frac{2e^2}{h}$ 近似: ① 大量粒子 ② 直流平衡

Green Function Equation of Motion:

已知 Green Function 关联形式由上文:

单粒子 $G^R(rt, r't') = -i\theta(t-t')\langle[\Psi(rt), \Psi^\dagger(r't')]\rangle_{B.F}$

对 G^R 作 t (非 t') 偏导, 不加证明得到:

$$[i\partial_t + \nabla_r^2 \cdot \frac{1}{2m}]G^R(rt, r't') = \delta(r-r')\delta(t-t') + D^R(rt, r't')$$

$$D^R(rt, r't') = -i\theta(t-t')\langle[-[V_{interact}, \Psi(r)]_{(t)}, \Psi^\dagger(r't')]\rangle_{B.F}$$

同理, 另一表象中

$$D^R(\nu t, \nu' t') = -i\theta(t-t')\langle[a_\nu(t), a_{\nu'}(t')]\rangle$$

$$\sum_{\nu''}(\delta_{\nu\nu''}\partial_t - t_{\nu\nu''})G^R(\nu'' t, \nu' t') = \delta(t-t')\delta_{\nu\nu'} + D^R(\nu t, \nu' t')$$

$$D^R(\nu t, \nu' t') = -i\theta(t-t')\langle[[-V_{int}, a_\nu]_{(t)}, a^\dagger_{\nu'}(t')]_{B.F}\rangle$$

is the equation of motion (ODE) of G^R, so when we perform fourier transformation for retared equation, we have $\partial_t \rightsquigarrow (i\omega) \rightsquigarrow (\omega + i\eta)$, ie:

$$\sum_{\nu''}[\delta_{\nu\nu''}(\omega+i\eta) - t_{\nu\nu''}]G^R(\nu'', \nu', \omega) = \delta_{\nu\nu'} + D^R(\nu, \nu', \omega)$$

$$D^R(\nu, \nu', \omega) = -i\int_R dt\, \exp[i(\omega+i\eta)(t-t')]\,\theta(t-t')\langle[[-V_{int}, a_\nu](t), a^\dagger_{\nu'}(t')]\rangle$$

so that we can solve G

例: Equation of Motion solving G of Anderson Model, using the Mean-Field Approximation.

$$\hat{H} = \sum_{k\sigma}(\varepsilon_k - \mu)c^\dagger_{k\sigma}c_{k\sigma} + \sum_\sigma(\varepsilon_d - \mu)c^\dagger_{d\sigma}c_{d\sigma} + U n_{d\uparrow}n_{d\downarrow} + \sum_{k\sigma} t_k c^\dagger_{d\sigma}c_{k\sigma} + h.c$$

We need to find the change in the dot: d via time.

$$G(d\sigma, t'-t).$$

$$G(d\sigma, t'-t) = -i\theta(t'-t)\langle\{c_{d\sigma}(t), c^\dagger_{d\sigma}(t')\}\rangle$$

Fermion

why: G: $\sim \langle\{\ \}\rangle_{B.F}$

$\chi, \varepsilon, \Pi \sim \langle[\ ]\rangle$.

把 $t=\varepsilon_d-\mu$ 代入上式 $G(\nu''\nu'\omega)$ 公式, we have:

① $\nu''=k,\ \nu'=d$ ② $\nu''=d\ \nu'=k$

①: $(\omega+i\eta-\varepsilon_d+\mu)G^R(d\sigma,\omega)-\sum_k t_k G^R(k\sigma\, d\sigma\, \omega)=1+UD^R(d\sigma,\omega)$

② $(\omega+i\eta-\varepsilon_k+\mu)G^R(k\sigma,d\sigma,\omega)-t_k^{\dagger}G^R(d\sigma,\omega)=0$

where $D^R(d\uparrow,t-t')=-i\theta(t-t')\langle\{n_{d\downarrow}(t)c_{d\uparrow}(t),c_{d\uparrow}^{\dagger}(t')\}\rangle$ ③

MF: $n_{d\uparrow}n_{d\downarrow}=\langle n_{d\uparrow}\rangle n_{d\downarrow}+\langle n_{d\downarrow}\rangle n_{d\uparrow}$ 代入: ①.③

$D^R(d\uparrow,t-t')=\langle n_{d\downarrow}\rangle G^R(d\uparrow,t-t')$

连立①.②. we have: $G^R(d\uparrow,\omega)=[\omega-\varepsilon_d-\mu+U\langle n_{d\downarrow}\rangle-\Sigma^R(\omega$

$\Sigma^R(\omega)=\sum_k|t_k|^2\times(\omega-\varepsilon_k+\mu+i\eta)^{-1}$

一通近似: spectral function

$A(d\uparrow,\omega)=\dfrac{I}{(\omega-\tilde{\varepsilon}+\mu-U\langle n_{d\downarrow}\rangle)^2+(I/2)^2}$ 由 $\langle n(d\uparrow)\rangle=\int A\, n_F(\omega)$

$\langle n_{d\uparrow}\rangle=f(\langle n_{d\downarrow}\rangle)$ 关系给出.称自洽平均场方程.

例: 极化率: $\chi^R(rt,r't')=-i\theta(t-t')\langle[\rho(rt),\rho(r't')]\rangle$

随机相位近似(RPA)

体系: $q\neq 0$ 自由电子气 $q=0$ 与阳离子均匀抵消

from $r\to k$ 表象 $\rho=\sum c_k^{\dagger}c_{k+q}$ (e^{iqr} 项与等号左相消)

$\chi^R(q,t-t')=-i\theta(t-t')\frac{1}{V}\langle[\rho(q,t),\rho(-q,t')]\rangle$ $k'=k+q$

求导 ∂_t: Equation of Motion: 求导 (两项) $k=k'+q'$

$i\partial_t\chi^R(q,t-t')=\sum_k[\delta(t-t')\frac{1}{V}\langle\rho(q,t),\rho(-q,t')\rangle$ $\rho=\sum_k c_k^{\dagger}c_{k-q}$

$-i\theta(t-t')\langle[-[H,c_k^{\dagger}c_{k+q}],\rho(-q,t')]\rangle$

$$\hat{H}=\sum_k \varepsilon_k c_k^+ c_k + \frac{1}{2V}\sum_{kk'q\neq 0} V(q)\, c_{k+q}^+ c_{k'-q}^+ c_{k'} c_k = H_0 + V_{int}$$

$[[-H, c_k^+ c_{k+q}], \rho(-q, t')]$

$\boxed{①}$ $[H_0, c_k^+ c_{k+q}] = [\sum_{k'} \varepsilon_{k'} c_{k'}^+ c_{k'}, c_k^+ c_{k+q}]$

$k'=k+q$ or $-\varepsilon_{k+q} c_k^+ c_{k+q} + \overset{(k'=k)}{} \varepsilon_k c_k^+ c_{k+q}$

$\boxed{②}$ $[V(q) c_{k+q}^+ c_{k'-q}^+ c_{k'} c_k, c_{k''}^+ c_{k''+q'}] =$

① $k''=k'$ ② $k''=k$ ③ $k''+q'=k+q$ ④ $k''+q'=k'-q$

Attention: 试图 $(c_{k''}^+)^2=0$ $k''=k+q$，又 $k''=k'$ 是①特殊，

相当于 (k'', q, q') 替代 $(k, k', q\, q')$ 少一参数，不遍历。

原式 $= \frac{1}{2V}\sum_{\text{4个}} V(q')\,[c_{k+q'}^+ c_{k'-q'}^+ c_{k'} c_{k+q} + c_{k'+q'}^+ c_{k-q'}^+ c_{k+q} c_k$

$\quad - c_{k+q'}^+ c_k^+ c_{k+q+q'} c_{k'} - c_k^+ c_{k'-q'}^+ c_{k'} c_{k+q-q'}]$

用HF近似（chapter 1，4推8）

Hartree

$\cancel{c_{k+q'} c_{k'-q'} \langle c_{k'} c_{k+q}\rangle + c_{k+q} c_{k+q}}$

$c_{k+q'}^+ c_{k+q} \langle c_{k'-q'}^+ c_{k'}\rangle + \langle c_{k+q'}^+ c_{k+q}\rangle c_{k'-q'}^+ c_{k'}$ 第一项推3.

以及：$\langle\ \ \rangle\langle\ \ \rangle$

第一项 $\langle\ \rangle\neq 0$ 要求 $q'=0$ 而 $q\neq 0$ $\therefore$ 必0

二项 $q'=q \Rightarrow \sum_{k'} c_{k'-q}^+ c_{k'} \langle n_{k+q}\rangle$

三项 $\langle\ \rangle\times\langle\ \rangle$ 必0.

综上：Hartree项：

$$[V_{int}, c_k^+ c_{k+q}] = \frac{V(q)}{V}[\langle n_{k+q}\rangle - \langle n_k\rangle]\sum_{k'} c_{k'-q}^+ c_{k'}$$

$\boxed{③}$ $[c_k^+ c_{k+q}, \rho(-q)] = \sum_{k'}[c_k^+ c_{k+q}, c_{k'}^+ c_{k'-q}] = n_k - n_{k+q}$. $\propto$

综上：$[[H_0+V_{int}, c_k^+ c_{k+q}], \hat{\rho}(-q)]$

$= [n_k - n_{k+q}, \hat{\rho}(-q)] + \frac{V(q)}{V}\left(\langle n_{k+q}\rangle - \langle n_k\rangle\right)[\sum_{k'} c_{k'-q}^+ c_{k'}, \hat{\rho}(-q)]$

$k''=k'-q$ $\quad [\rho(q), \rho(-q)]$

$n_k - n_{k-q}$

$$\Rightarrow \left(\sum_{K'} \frac{V(q)}{V} \chi_{K'} + 1\right)\left[\langle n_{K+q}\rangle - \langle n_K\rangle\right] = i\partial_t \chi$$

Fourier transform:

$$(\omega + i\eta + \varepsilon_K - \varepsilon_{K+q})\chi$$

Therefore:

$$\chi^R(q.\omega) = \frac{1}{V}\sum_K \frac{\langle n_K\rangle - \langle n_{K+q}\rangle}{\omega + \varepsilon_K - \varepsilon_{K+q} + i\eta}\left[1 + V(q)\chi^R(q.\omega)\right]$$

$$\Rightarrow \chi^R(q.\omega) = \frac{\chi_0^R(q.\omega)}{1 - V(q)\chi_0^R(q.\omega)}$$

$\chi_0^R(q.\omega)$ 为三页前仅考虑 Free particle 的 χ_0. Now 亦考虑了 V_{int}. 并作 Hartree-Fock 近似 其中 $\langle n_K\rangle. \langle n_{K+q}\rangle = n_{Fermi-Dirac}$. 前文 Free-particle 之 $\chi \to \varepsilon$ 也导仅电子-自旋配对激发. Now 通过 Equation of Motion, 同上激发考虑 $I_m\chi$. 写 χ^R δ函数取 I_m部. 得: $1 - V(q)\chi_0^R(q.\omega) = 0$ 有激发, 即等离激元 (后文

之前考虑了空(绝缘体)为中间介质左~右隧穿, 现在继续求 Anderson impurity model 的 conductance 之前的进展给出了 $I_{N.N+1}$ 的形式, 利用 Fermi Golden Rule, Now 引入 Green function 关联, 可最终求出 G, 我们延续之前 $I = \dot{N}$ 的定义, 不过更换为了 $I_L. I_R$. 并且 $I = \alpha I_L + (1-\alpha) I_R$ 有这么 N 粒子左→右 N_1 回来. N_2透过 N_2 代表 I. $N_1 = RN$ 代表 I_L R: 反射率 隧穿 $= \frac{|t_R|^2}{|t_R|^2 + |t_L|^2} = 2$

$L: \frac{|t_L|^2}{|t_R|^2 + |t_L|^2}$, 原因:

① 讨论稳(直流态) $\langle I\rangle = \langle I_L\rangle = \langle I_R\rangle$ α可任选.

② $I = (L^+ - L)$ 奇偶性有异, Left + Right 加不了,
$H_T = (L^+ + L)$ 需通过线性变换纠正之.

定义此线性变换：

$$H_{T L or R} = \sum_{\gamma\delta} [t_{L or R} C^+_{\gamma L or R \delta} C_{d\delta} + t^*_L C^+_{d\delta} C_{L or R \delta}]$$

简融合R.L $\begin{pmatrix} C_{\gamma e\delta} \\ C_{\gamma o\delta} \end{pmatrix} = \frac{1}{\sqrt{|t_L|^2+|t_R|^2}} \begin{pmatrix} t_L^* & t_R^* \\ -t_R & t_L \end{pmatrix} \begin{pmatrix} C_{\gamma L\delta} \\ C_{\gamma R\delta} \end{pmatrix}$, s.t. $C_{\gamma e}$ 偶算符 $C_{\gamma o}$ 奇算符

$$H_T = \sqrt{|t_L|^2+|t_R|^2} [C^+_{\gamma e\delta} C_{d\delta} + C^+_{d\delta} C_{\gamma e\delta}] \quad L^+ + L$$

$$I_{L or R} = i \sum_{\gamma\delta} [t_{L or R} t_{\gamma L or R} C_{d\delta} - t^*_{L or R} C^+_{d\delta} t_{\gamma L or R}]$$

$$I = \alpha I_L + (1-\alpha) I_R \quad \alpha = |t_R|^2 / |t_L|^2+|t_R|^2 .$$

$$\therefore I = \frac{-i}{\sqrt{|t_L|^2+|t_R|^2}} \sum_{\gamma_o\delta} [t_L t_R C^+_{\gamma o\delta} C_{d\delta} + t_L t_R C^+_{d\delta} C_{\gamma o\delta}] \quad L - L^+$$

现在计算 G，须先计算：$C^R_{II}(t) = i\theta(t) \langle [I(t), I(0)] \rangle$

$I(t\ or\ 0) = L(t\ or\ 0) - L^+(t\ or\ 0)$

$\therefore \langle [I(t), I(0)] \rangle \Rightarrow \langle L(t) L^+(0) \rangle = d$ 加2个 L 少2个 impossible 粒子直流不守恒了，similarly $\langle L(t) L(0) \rangle = 0$, therefore.

$$\langle [L(t), L^+(0)] \rangle \text{余下} = \frac{|t_L|^2|t_R|^2}{|t_L|^2+|t_R|^2} \sum_{\gamma_o \gamma_o' \delta\delta'} [\langle C^+_{\gamma o\delta}(t) C_{d\delta}(t) C^+_{d\delta'} C_{\gamma_o'\delta'} \rangle - \langle C^+_{d\delta'} C_{\gamma_o'\delta'} C^+_{\gamma o\delta}(t) C_{d\delta}(t) \rangle]$$

而 $\langle | \rangle = |d\rangle \otimes |0\rangle$ 则可拆子空间

$$= \langle C^+_{\gamma o\delta}(t) C_{\gamma_o'\delta'} \rangle \langle C_{d\delta}(t) C^+_{d\delta'} \rangle - \langle C^+_{d\delta'} C_{d\delta}(t) \rangle \langle C_{\gamma_o'\delta'} C^+_{\gamma_o\delta}(t) \rangle$$

= 取本征态基 $\langle\ \rangle$ 对角 $\gamma_o' = \gamma_o$ $\delta' = \delta$ 而 $G^> = -i\langle\ \rangle$，则：

$$\text{原式} = \sum_{\gamma_o\delta} \frac{|t_L|^2|t_R|^2}{|t_L|^2+|t_R|^2} G^<(\gamma_o\delta, -t) G^>(cd\delta, t) - G^>(\gamma_o\delta, -t) G^<(d\delta, t)$$

$(t'=0\ t=t)$ $\quad t'=0\ t=t$ $\quad (C_\gamma(t) C^+_\gamma)^* = (C^+_\gamma)^T (C_\gamma)^T = C_\gamma C^+_\gamma(t)$

$C^R_{II}(\omega) = \int_R C^R_{II}(t) e^{i\omega t} dt$ 有4项．．$\langle C_\gamma C^+_\gamma(t) \rangle^T \rangle$

$= -i \int_{R^+} (4\text{项}) e^{i\omega t} dt$.

conductance 为 $C(\omega)$ 虚部 那么 $[G^>(d\delta, t)]^{*}_{\gamma\delta} = (-i \langle C_\gamma(t) C^+_\gamma \rangle)^*$

$= i \langle C_\gamma(t) C^+_\gamma \rangle^* = i \langle C_\gamma C^+_\gamma(t) \rangle = -G^>(\gamma, -t)$

∴ $G = -i \times \text{Real} \Rightarrow G \times G \in R$ 取虚部为:

$$\int dt\, e^{i\omega t} f(t) g(-t) = \int \frac{d\omega'}{2\pi} g(\omega') f(\omega+\omega')$$

利用 $\int h(r-s) g(s)\, ds = F_{\text{fourier}}[h(k) g(k)]$ 卷积定理 ⟸ ①

$$= \mathrm{Im}\, C^R_{II}(\omega) = \frac{i}{2}\int_R \frac{d\omega'}{2\pi}\cdot\frac{|t_L|^2|t_R|^2}{|t_L|^2+|t_R|^2} G^>(d\sigma,\omega')\left[G^<(\nu_0\sigma,\omega'+\omega) - G^<(\nu_0\sigma,\omega'-\omega)\right] - G^<(d\sigma,\omega')\left[G^>(\nu_0\sigma,\omega'+\omega)-G^>(\nu_0\sigma,\omega'-\omega)\right]$$

引入 spectral function: A (上文) 同上文方法直流 $\omega\to 0$

写作偏导形式，对于 $A(\nu_0\sigma,\omega)$ $\omega\to 0$ 时: 引入左.右 Lead 电库

总是无相互作用 即 $A(\nu_0\sigma,\omega) = 2\pi\delta(\omega-\varepsilon_{\nu_0})$ $\omega\to 0$. Therefore.

$$\int A(\nu_0\sigma,\omega) = \int \delta(\omega-\varepsilon_{\nu_0}) \times n_F \ (\text{一维})$$

得到:

$$\cancel{\mathrm{Im}}\ G = \lim_{\omega\to 0} \mathrm{Re}\left[\frac{ie^2}{\omega} C^R_{II}(\omega)\right]$$

$$= e^2 \sum_{\nu_0\sigma} \frac{|t_L|^2|t_R|^2}{|t_L|^2+|t_R|^2} A(d\sigma,\varepsilon_{\nu_0})\left[-\frac{\partial n_F(\varepsilon_{\nu_0})}{\partial \varepsilon_{\nu_0}}\right]$$

回想起 $\nu^\alpha \int |t_\alpha|^2 d_\alpha d_L$ 为求 $\Gamma_{N+1,N}$ 时前系数，代表能级宽度

令 Γ^R, Γ^L 即 ν^α 由于 $\sum_{\nu_0\sigma} = \int d\varepsilon_0 \cdot d(\varepsilon_0)$ 则: $\frac{|t_L|^2|t_R|^2}{|t_L|^2+|t_R|^2}\cdot d$

$= \Gamma^R\Gamma^L / \Gamma^R+\Gamma^L$

$$\therefore G = e^2 \sum_\sigma \int \frac{d\varepsilon}{2\pi} \frac{\Gamma^L\Gamma^R}{\Gamma^L+\Gamma^R} A(d\sigma,\varepsilon) \left[-\frac{\partial n_F(\varepsilon)}{\partial \varepsilon}\right]$$

分析这个电导，近似: ①直流平衡 ② 自由电子 Lead ③ Γ^L, Γ^R 在小范围能带中隧穿振幅 t 恒定 ④ 左.右导线同权

G 与 $(\Gamma^{(0)}, \Gamma^{(2)}, \ldots)$ 包含一切类型隧穿，稍后把 $\Gamma^{(0)}, \Gamma^{(2)}$ 分别对应一部分 G 讨论以验证中间态隧穿之影响

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NOTES

之前讨论了金属库仑阻塞，说 $E(P(N+1))$ 与 $E(P(N))$ 之差，当跃迁後迁能量反而大时，不可跃迁，电导为零。Now apply it to the Anderson Impurity Model 格点上仅 $(d\uparrow, d\downarrow)$ 电子对。

之前说屏蔽与应与格点占据数有关。Now 求 $A(d\sigma, \varepsilon)$ 可知。

上文利用 Equation of Motion 求 A。同样用此方法：

定义 $D^R(d\uparrow, t-t') = -i\theta(t-t')\langle\{n_{d\downarrow}(t)c_{d\uparrow}(t), c_{d\uparrow}^{+}(t')\}\rangle$.

我们有：$D^R(d\uparrow, t-t') = \langle n_{d\downarrow}\rangle G^R(d\uparrow, t-t')$

对：$G^R(d\sigma, t) = -i\theta(t)\langle\{c_{d\sigma}, c^{+}_{d\sigma}\}\rangle$

求 D：

$i\partial_t D^R(d\uparrow, t)\Big|_{\substack{t=t\\ t'=0}}$

$= \delta(t)\langle\{n_{d\downarrow}c_{d\uparrow}(t), c^{+}_{d\uparrow}(0)\}\rangle - i\theta(t)\langle\{[H, n_{d\downarrow}(t)c_{d\uparrow}(t)], c^{+}_{d\uparrow}(0)\}\rangle$

不厌其烦地再重复求 X 利用 Equation of Motion 时的过程

$H = H_D + H_T \quad H_D = \sum_{\sigma} c^{+}_{d\sigma}c_{d\sigma}\varepsilon_d + U n_{d\uparrow}n_{d\downarrow} \quad H_T = \sum_{re}\sqrt{|t_L|^2+|t_R|^2}\,[c^{+}_{re\sigma}c_{d\sigma} + c^{+}_{d\sigma}c_{re\sigma}]$

Therefore: $\quad H_D' = \sum_{re} c^{+}_{re}c_{re}\varepsilon_{re}$

① $[H_D, n_{d\downarrow}(t)c_{d\uparrow}(t)] = (-\varepsilon_{d\uparrow} - U)n_{d\downarrow}c_{d\uparrow}$

② $[H_T, n_{d\downarrow}(t)c_{d\uparrow}(t)] = \tilde{t}\sum_{re}[[c^{+}_{re\sigma}c_{d\sigma} + c^{+}_{d\sigma}c_{re\sigma}], n_{d\downarrow}(t)c_{d\uparrow}(t)]$

验证过了

$-n_{d\downarrow}\sum_{re}\tilde{t}\,c_{re\uparrow} + \sum_{re}\tilde{t}(c^{+}_{re\downarrow}c_{d\downarrow} - c^{+}_{d\downarrow}c_{re\downarrow})c_{d\uparrow}. \quad \tilde{t} = [|t_R|^2+|t_L|^2]$

③ 代入：$\{(-\varepsilon_{d\uparrow} - U)n_{d\downarrow}c_{d\uparrow}, c^{+}_{d\uparrow}\} = D^R(d\uparrow, t)\cdot(-\varepsilon_d - U)$.

定义 $F^R(r\uparrow, t) = -i\theta(t)\langle\{(n_{d\downarrow}c_{re\uparrow})(t), c^{+}_{d\uparrow}\}\rangle$

代入：$\{c^{+}_{re\downarrow}c_{d\downarrow}c_{d\uparrow}, c^{+}_{d\uparrow}\} = \langle c^{+}_{re\downarrow}c_{d\downarrow}\rangle$

☆ 此项，为更高阶项，消灭 $d\downarrow$，产生 $c_{re\downarrow}$ 消灭 $c_{d\uparrow}$，产生 $c_{d\uparrow}$ Kondon 效应，此不议，下文议 Kondo 再议，代表自旋反转，直接丢掉

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对 Equation of Motion 全用上文 F.D 反代·有:

$$\begin{cases} (i\partial_t - \varepsilon_{d\uparrow} - U) D^R(d\uparrow, t) = \delta(t)\langle n_{d\downarrow}\rangle + \sum_\nu \hat{t}\, F^R(\nu\uparrow, t) \\ (i\partial_t - \varepsilon_{\nu\uparrow})\, F^R(\nu\uparrow, t) = \hat{t}\, D^R(d\uparrow, t) \end{cases}$$

Fourier transform:

$$(i(i\omega) - \varepsilon_d - U) D^R(d\uparrow, \omega) = \langle n_{d\downarrow}\rangle + \sum_\nu \hat{t}\, F^R(\nu\uparrow, \omega)$$

$$(i(i\omega) - \varepsilon_{\nu\uparrow})\, F^R(\nu\uparrow, \omega) = \hat{t}\, D^R(d\uparrow, \omega)$$

Therefore:

$$[\omega - \varepsilon_{d\uparrow} - U - \Sigma^R(\omega)]\, D^R(d\uparrow, \omega) = \langle n_{d\downarrow}\rangle$$

代入 G~D 关系中，上式为 Mean-Field G~D 关系，更上文给出:

$$[\omega - \varepsilon_{d\uparrow} - \Sigma^R(\omega)]\, G^R(d\uparrow, \omega) = 1 + U D^R(d\uparrow, \omega)$$

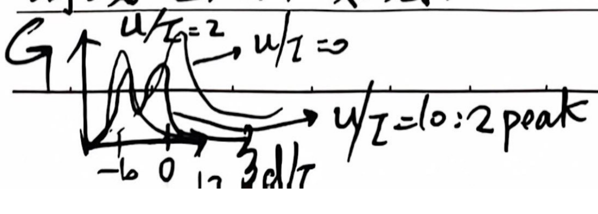
Therefore: 代入 $\Sigma^R(\omega) = \sum_\nu \frac{|\hat{t}|^2}{\omega - \varepsilon_\nu + i\eta} = \int \frac{d\varepsilon}{2\pi} \frac{\Gamma}{\omega - \varepsilon + i\eta}$, we have:

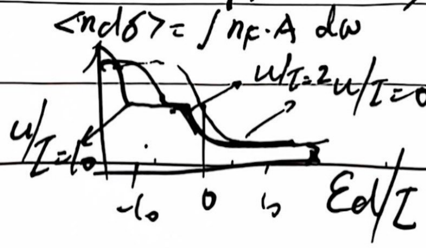
$$G^R(d\uparrow, \omega) = \frac{1 - \langle n_{d\downarrow}\rangle}{\omega - \varepsilon_{d\uparrow} - \Sigma^R(\omega)} + \frac{\langle n_{d\downarrow}\rangle}{\omega - \varepsilon_{d\uparrow} - U - \Sigma^R(\omega)}$$

$$A(d\uparrow, \omega) = -2 I_m G^R$$

$$= \frac{[1 - \langle n_{d\downarrow}\rangle]\Gamma}{(\omega - \varepsilon_{d\uparrow})^2 + (\Gamma/2)^2} + \frac{\langle n_{d\downarrow}\rangle \Gamma}{(\omega - \varepsilon_{d\uparrow} - U)^2 + (\Gamma/2)^2}$$ 再 $\lim \omega \to 0$

这样一来：电导 conductance $G(\langle n_d\rangle, (\Gamma_R \Gamma_L), \varepsilon_d, U)$ 关系已知。第一项：即 $D^R \propto \langle n_d\rangle = 0$ dot 为空时向 dot 上添一电子的态密度；第二项：已经增了一个电子"1"再增一电子的态密度，因此第二个电子还要考虑与第一个电子的 Koloumb 作用 $Un_{d\downarrow}$ 即 U 项，仅当 $\Gamma \gg U$ 时，跃迁不被库仑场影响可认为作平均场近似，如图:





Kondo Model, 电导:

由上文"一般的隧穿"所描述:电子多阶隧穿均贡献 I, ie:

$$\hat{T} = H_S^{(2)} + H_S^{(2)} \frac{1}{E_i - (E_D + H_{LR}) + i\eta} \hat{T}$$

$$I_{RL} = 2\pi \sum_i \frac{1}{2} P_i \sum | t^{(1)} + t^{(2)} + \cdots |^2 \delta(\xi_{\gamma_L} - \xi_{\gamma_R})$$

$$t^{(1)} = \langle f_{\gamma_R \sigma \gamma_L \sigma'} | H_S^{(2)} | i \rangle$$

$$t^{(2)} = \langle f_{\gamma_R \sigma \gamma_L \sigma'} | H_S^{(2)} \frac{1}{E_i - (E_D + H_{LR}) + i\eta} H_S^{(2)} | i \rangle$$

$$H_S^{(2)} = \sum_{\gamma_L \gamma_R} J_{LR} S_d \cdot S_{\gamma_L \gamma_R} + \sum_{\gamma_\alpha \gamma_\beta \sigma} W_{LR} C^+_{\gamma_L \sigma} C_{\gamma_R \sigma}$$

$$J_{LR} = \frac{2U t_L t_R^*}{(\varepsilon_d + U)(-\varepsilon_d)} \qquad W_{LR} = \frac{(2\varepsilon_d + U) t_L t_R^*}{2(\varepsilon_d + U)(-\varepsilon_d)}$$

下面我们不厌其烦地集前所有之大成, step1: 计算 $t^{(1)}$ 贡献.

$$t^{(1)}_{\gamma_L \gamma_R \sigma \sigma'} = \langle f_{\gamma_R \gamma_L \sigma \sigma'} | \sum_{\gamma_L \gamma_R} J_{LR} S_d \cdot S_{\gamma_L \gamma_R} + \sum_{\gamma_L \gamma_R \sigma} W_{LR} C^+_{\gamma_R \sigma} C_{\gamma_L \sigma} | i \rangle$$

考虑 W 贡献: 势能散射自旋不变 $\sigma_f = \sigma_i$, ie: $|f\rangle = C^+_{\gamma_R \sigma} C_{\gamma_L \sigma} |i\rangle$

$$= \sum_{\gamma_L \gamma_R \sigma} \delta_{\sigma_f \sigma_i} \langle i | C^+_{\gamma_L \sigma} C_{\gamma_R \sigma_f} C^+_{\gamma_R \sigma_f} C_{\gamma_L \sigma_i} | i \rangle W_{RL}$$

$$= \sum \delta_{\sigma_f \sigma_i} \, n_{\gamma_L \sigma_i} (1 - n_{\gamma_R \sigma_f}) W_{RL}$$

单粒子态直接用

↑ 自旋可表

dot空间 Lead空间

考虑 J 贡献, 交换散射自旋改变, ie: $| \rangle = |\sigma\rangle \otimes |i\rangle$

$$= \sum_{\gamma_L' \gamma_R'} J_{LR} \langle i | C^+_{\gamma_L \sigma'} C_{\gamma_R \sigma} \frac{1}{2} \sum_{\sigma_1 \sigma_1'} C^+_{\gamma_R' \sigma_1} T^j_{\sigma_1 \sigma_1'} C_{\gamma_L' \sigma_1'} | i \rangle$$

提出 ($\sigma_1 \sigma_1' \to \sigma \sigma'$)

$$\times \langle \sigma_f | \frac{1}{2} \sum_{\sigma \sigma'} C^+_{d\sigma} T^j_{\sigma \sigma'} C_{d\sigma'} | \sigma_i \rangle$$ 然后对 $j: (x, y, z)$ 求和

$\sigma_1 = \sigma'$ 必然 [otherwise $|\Uparrow\rangle$ or $|\Downarrow\rangle$ 只能为 σ' because $\sigma' \neq \sigma$, 此项却加0

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$= \frac{1}{2} J_{LR} \sum_j \langle \delta_f | I(w) | \delta_i \rangle \times I_{\delta\delta'} \, n_{\gamma_L \delta'} (1 - n_{\gamma_R \delta})$

而 $\Rightarrow \langle \delta_f | \frac{1}{2} \sum_{\delta\delta'} c^\dagger_{d\delta} I^j_{\delta\delta'} c_{d\delta'} | \delta_i \rangle \overset{\delta=\delta_f}{\underset{\delta'=\delta_i}{=}} \quad \langle \delta_f | c^\dagger_{d\delta_f} = \langle 0 |$

$\Rightarrow \langle 0 | 0 \rangle I^j_{\delta_f \delta_i} \qquad c_{d\delta_i} | \delta_i \rangle = | 0 \rangle$

$= \frac{1}{2} J_{LR} \left(\sum_j I^j_{\delta_f \delta_i} I^j_{\delta\delta'} \right) n_{\gamma_L \delta'} (1 - n_{\gamma_R \delta})$

求 $|t^{(1)}_{\gamma_L \gamma_R \delta\delta'}|^2$

$\boxed{W} = (n_{\gamma_L \delta})^2 (1 - n_{\gamma_R \delta'})^2 \cdot |W_{RL}|^2 \cdot \langle \delta_f | \delta_i \rangle \cdot \delta_{f i} \; \delta_{\delta_f \delta_i}$

$= (n_{\gamma_L \delta})^2 (1 - n_{\gamma_R \delta'})^2 |W_{RL}|^2 \sum_{\substack{\delta=\delta' \\ \delta_f, \delta \\ \delta_f = \delta_i}} 1$ $\quad$ δ_f 有2个, δ 有2个 : $4 \times 1 = 4$

$= (n_{\gamma_L \delta})^2 (1 - n_{\gamma_R \delta})^2 \, 4 |W_{RL}|^2.$

$\boxed{J} = \frac{1}{16} |J_{LR}|^2 \left[\sum_{jK} I^j_{\delta_f \delta_i} I^j_{\delta\delta'} \left(I^K_{\delta_f \delta_i} I^K_{\delta\delta'} \right) \right] (n_{\gamma_L \delta'})^2 (1 - n_{\gamma_R \delta})^2$ ☆

$= \frac{1}{16} |J_{LR}|^2 \cdot (n_{\gamma_L \delta'})^2 (1 - n_{\gamma_R \delta})^2 \sum_{jK} \underline{I^j_{\delta_f \delta_i} I^j_{\delta\delta'} I^K_{\delta_i \delta_f} I^k_{\delta'\delta}}$

$I^j_{\delta_f \delta_i} = \langle \delta_f | I^j | \delta_i \rangle$ $\qquad$ Pauli Martrix

$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ eg $\Rightarrow$ number $= \sum_{jK} \left(I^j_{\delta_f \delta_i} I^k_{\delta_i \delta_f} \right) \times \left(I^j_{\delta\delta'} I^k_{\delta\delta'} \right)$

Two Pauli 相乘 $(1\;0) \begin{pmatrix} 1 \\ 0 \end{pmatrix} I^j \boxed{\begin{pmatrix} 0 \\ 1 \end{pmatrix} (0\;1)} I^k \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ $\quad \underset{1}{\shortparallel}$

$= \langle \delta_f | I^j I^k | \delta_f \rangle$

Two Pauli 相乘矩阵只对角非零 $\sum_{jK} \left(Tr[I^j I^K] \right)^2$

$\langle \delta | A | \delta \rangle = Tr(A)$ $\qquad$ only $j = K$ $Tr \neq 0$, ie.

$(Tr[I^x I^x + I^y I^y + I^z I^z])^2 = 4 \times 3 = 12$

$I^2 = 1$

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$\therefore \boxed{J} = \frac{1}{16}|J_{LR}|^2 \times 12 = \frac{3}{4}|J_{LR}|^2 (n_{\gamma_L\sigma})^2 (1-n_{\gamma_R\sigma'})^2$

$2\times\boxed{J}\times\boxed{W} = (W)\times\sum_{\sigma\sigma'\sigma_i\sigma_f} \delta_{\sigma\sigma'}\delta_{\sigma_i\sigma_f} I^j_{\sigma_i\sigma_i} I^j_{\sigma\sigma}$ $\begin{pmatrix}1&0\\0&-1\end{pmatrix}\begin{pmatrix}0&-i\\i&0\end{pmatrix}$ $\begin{pmatrix}0&1\\-1&0\end{pmatrix}$ $Tr=0$

而 $\sum_{\sigma\sigma_i} I^j_{\sigma\sigma} I^j_{\sigma_i\sigma_i} = \sum_\sigma I^j_{\sigma\sigma} \times \sum_{\sigma_i} I^j_{\sigma_i\sigma_i} = Tr[I]\times Tr[I] = 0\times 0 = 0$

综上所述：$|t|^2 = |W_{RL}\delta_{\sigma\sigma'}\delta_{\sigma_i\sigma_f} + \frac{J_{RL}}{4}\sum_j I^j_{\sigma_f\sigma_i} I_{\sigma\sigma'}|^2 (n_{\gamma_L\sigma})^2(1-n_{\gamma_R\sigma'})^2$

$= 4|W_{RL}|^2 (n_{\gamma_L\sigma})^2 (1-n_{\gamma_R\sigma})^2 + \frac{3}{4}|J_{LR}|^2 (n_{\gamma_L\sigma})^2 (1-n_{\gamma_R\sigma'})^2$

因此：$I^{(2)}_{RL} = 2\pi\sum_i \frac{1}{2}P_i \sum_{\gamma_L\gamma_R\sigma\sigma'}\sum_{\sigma_i\sigma_f} |t^{(1)}_{\gamma_L\gamma_R\sigma\sigma'}|^2 \delta(\varepsilon_{\gamma_L}-\varepsilon_{\gamma_R})$

$\Rightarrow P_i$（初态电子分布函数，同上文 W_i 简并量）.

$n^2, (1-n)^2$ 非零即一，就是 n $\sum W_i n_i = n_{Fermi-Dirac}$. 那么：

$\sum_{\gamma_R} = \int d\varepsilon_R \cdot d$ $\sum_{\gamma_L} = \int d\varepsilon_L \cdot d$，原式 $=$

$= (4|W_{RL}|^2 + \frac{3}{4}|J_{LR}|^2) \times \int_R d\varepsilon_R d\varepsilon_L \underset{=}{d^2} \cdot 2\pi \cdot n_F(\varepsilon_{\gamma_L}-\mu_L) [1-n_F(\varepsilon_{\gamma_R}-\mu_R)] \delta(\varepsilon_{\gamma_L}-\varepsilon_{\gamma_R})$

δ 函数积出：$\varepsilon_{\gamma_R}=\varepsilon_{\gamma_L}$ 态密度单位 ε_R 中 γ_R 个数

$= \frac{1}{2}\cdot 2\pi d_0^2 \int d\varepsilon\, n_F(\varepsilon-\mu_L)(1-n_F(\varepsilon-\mu_R))(\ n\ )$

$\therefore I^{(2)}_{RL} \approx 2\pi d_0^2 \int d\varepsilon\, n_F(\varepsilon-\mu_L)[1-n_F(\varepsilon-\mu_R)] (W_{RL}^2 + \frac{3}{8}J_{RL}^2)$

这就是 $t^{(1)}$ 贡献了. 可积出

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Step 2：计算 $t^{(2)}$ 贡献：为 $t^{(1)} t^{(2)}$ 耦合项 $|t^{(1)}+t^{(2)}|$ ...

$$I^{(3)}_{RL} = \boxed{4\pi} \sum_{\gamma_R \gamma_L \sigma\sigma' \sigma_i \sigma_f i} \frac{1}{2} P_i \mathrm{Re}\{[t^{(1)}]^* t^{(2)}\} \delta(\gamma_R - \gamma_L)$$

$$t^{(2)}_{\gamma_R \gamma_L \sigma\sigma'} = \langle f | \langle \sigma_f | H_S^{(2)} \frac{1}{E_i - H_{LR} + i\eta} H_S^{(2)} | \sigma_i \rangle | i \rangle$$

$$H^{(2)}_{S\alpha\beta} = \sum_{\gamma_\alpha \gamma_\beta} \sum_{LR} \left[J_{\alpha\beta} \cdot \frac{1}{2} \sum_{\sigma\sigma'} c^+_{\alpha\sigma} \tau_{\sigma\sigma'} c_{\beta\sigma'} \cdot S_d + W_{\alpha\beta} \delta_{\sigma\sigma'} c^+_{\alpha\sigma} c_{\beta\sigma'} \right]$$

定义 $L_{\alpha\beta\sigma\sigma'} = \sum_{\gamma_\alpha \gamma_\beta \sigma\sigma'} W_{\alpha\beta} \delta_{\sigma\sigma'} + \frac{J_{\alpha\beta}}{2} \sum_j S^j_d \tau^j_{\sigma\sigma'}$

$$H^{(2)}_{S\alpha\beta} = \sum_{\gamma_\alpha \gamma_\beta \sigma\sigma'} c^+_{\gamma_\alpha\sigma} c_{\gamma_\beta\sigma'} L_{\alpha\beta\sigma\sigma'} \qquad H_S^{(2)} = \sum_{\alpha\beta} H^{(2)}_{S\alpha\beta}$$

$$|\sigma_f\rangle|f\rangle = c^+_{\gamma_R\sigma} c_{\gamma_L\sigma'} |i\rangle |\sigma_i\rangle$$

全部代入 t 中，不厌其烦地再计算之：

[重要说明] ☆☆☆，以下公式：

$$H_S^{(2)} = f(J_{LL}) + f(J_{LR}) + f(J_{RR}) + f(J_{RL}) + f(W)$$

$H_S^{(2)}(m) H_S^{(2)}$ 十六项了，如何选择非零？$\langle h.t \rangle$

方1：粒子守恒，比如：$J_{LR} J_{LR} = c_L^+ c_R^+ c_L c_R \quad \langle f | J_{LR} J_{LR} | i \rangle$

$= c_R c_L^+ c_L^+ c_R^+ c_L c_R$ 相当于左加1，右减1，不守恒，必零。

比如：$J_{RR} J_{LR} = c_R^+ c_R c_R^+ c_L \quad \langle f | J_{RR} J_{LR} | i \rangle$

$= c_R c_L^+ c_R^+ c_R c_R^+ c_L$ 不加不减，非零

方2：我们要理解何为更高阶的跃迁，Fermi-Golden Rule 更高阶
究竟为何，哪些项能提供电导？

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回忆：$\langle f | i(t)\rangle = \sum_n \int^t \int^{t_n}_{t_{n-1}} V(t_1)V(t_2)\cdots\cdots dt_1 \cdots dt_n e^{\eta t_n}$

Fermi-Golden Rule 一阶：$V(t_1) \rightsquigarrow H^{(2)} = H(t_1)$ 表从0到t只在$V_{(t_1)}$的作用下跃迁，此时左→右仅J_{LR}可行；二阶 $V(t_1)V(t_2) = V(t_1)\frac{1}{E-H+i\eta}V($ 表从0到t先由t_1作用再由t_2作用，跃迁分为两个阶段，那么想从左到右有电导只有$J_{LL}J_{LR}$ 左原地→(左→右) 与$J_{LR}J_{RR}$可行，比如$J_{LR}J_{LR}$ 左→右→左又回来了，零电导。J_{LR}代表反转d使得左→右跃迁，J_{RR}代表反转d 右→中→右跃迁，类似，三阶有三阶段，理应$J_{LL}J_{LR}J_{RR}$，$J_{LL}J_{LL}J_{LR}$，$J_{LR}J_{RR}J_{RR}$，$J_{LR}J_{RL}J_{LR}$ 非零有电导。因此我们可以把t 简化至以下两项（仅讨论一半，×2即可）同样类之前讨论：$J_{LR}J_{RR}$代表先左→右再右→右。or $J_{RR}J_{LR}$，先右边自旋再左→右一个

对于$t^{(2),R}$，情况为：$t^{R(2)}_{\gamma_R\gamma_L\sigma\sigma'} =$

$$\langle i|\sigma_f|\cdot \varsigma_R C^+_{\gamma}\Big(\sum_{\gamma_R'\gamma_L'} C^+_{\gamma_L'\sigma} C_{\gamma_R'\sigma}\Big) L_{LR\sigma\sigma'}\frac{1}{E_{初}-H_{LR}+i\eta}\Big(\sum_{\gamma_R''\gamma_L''} C^+_{\gamma_R''} C^+_{\gamma_R''\sigma} L_{RR\sigma\sigma'}|\sigma_i\rangle|i$$

$$\cancel{\Big(\sim\sim \sum_{\gamma_R\gamma_R'} C^+_{\gamma_R'} C^+_{\gamma_R''\sigma} L_{RR\sigma\sigma'}\Big)\Big(\sim\sim \sum_{\gamma_R''\gamma_L''} C^+_{\gamma_R''} C^+_{\gamma_R\sigma'} L_{LR\sigma\sigma'}\Big) \sim}$$

① $\cancel{\gamma_R''=\gamma_R'=\gamma_R}$ $\gamma_L''=\gamma_L'=\gamma_L$，$\cancel{(\sigma')''=(\sigma')'=\sigma'}$，$(\sigma)''=(\sigma)'=\sigma$ 才非零，记

③ $\langle i|C^+_{\gamma_L}C_{\gamma_L}|i\rangle = n^i_{\gamma_L}$， $(\gamma_1\gamma_2\gamma_3)$皆为(R)的$\gamma$

$$= n_{\gamma_L}\cdot \sum_{\sigma_1\sigma_2\sigma_3\gamma_1\gamma_2\gamma_3} \langle i_R| C_{\gamma_R\sigma} C^+_{\gamma_1\sigma_1} \frac{\langle \sigma_f | L_{RL\sigma_1\sigma'} L_{RR\sigma_2\sigma_3}|\sigma_i\rangle}{E_i - H_{LR}+i\eta} C^+_{\gamma_2\sigma_2}C_{\gamma_3\sigma_3}|i_R\rangle$$

$$+\langle i_R| C_{\gamma_R\sigma} C^+_{\gamma_2\sigma_2} C_{\gamma_3\sigma_3}\frac{\langle \sigma_f | L_{RR\sigma_2\sigma_3} L_{R_1\sigma_1\sigma'}|\sigma_i\rangle}{E_i - H_{LR}+i\eta} C^+_{\gamma_1\sigma_1}|i_R\rangle$$

⟹ σ_2,σ_3 自旋能级随意是要累加的 $\sigma\sigma_1$是t_σ的一部分了。

问：是$\gamma_R\sigma=\gamma_1\sigma_1$ 还是 $\gamma_R\sigma=\gamma_2\sigma_2$，都不是就0了。

而$\sigma_2 \neq \sigma_3$（反转！）故只能$\gamma_R\sigma=\gamma_2\sigma_2$了。

$\gamma_1\sigma_1=\gamma_3\sigma_3$

并且：$(E_i - H_{RR} + i\eta)^{-1}$ 由于之后 $\delta(\xi_R-\xi_L)$ 项，$\xi_R=\xi_L$ 必然。右

第一项：step1 是右自旋，故此 step $E_i - H_0 + i\eta = \underbrace{E_3 - E_2}_{H_{RR}} + i\eta$，$E_i$ 有 E_0 有 E_1 变化多一个 E_3 右少一个 E_2 右：$E_3 - E_2 + i\eta$，E_2 就：$\gamma_R\sigma = \gamma_2\sigma'$ $E_2 = E_R$；$E_3 = E_1 \Rightarrow \xi_1 - \xi_R + i\eta$；第二项：step1 是左→右：

$E_i - H_0 = \xi_L - \xi_R$ （E_i 初态 E，H_0 一次跃迁之后 E），因此：

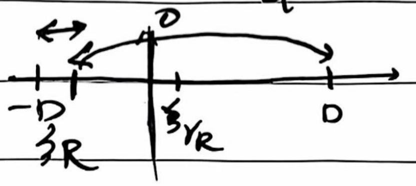
$$t^{(2)R}_{\gamma_R\gamma_L\sigma\sigma'} = -n_{\gamma_L}[1-n_{\gamma_R}]\sum_{\gamma_1\sigma_1}\frac{\langle\sigma_f|L_{RL\sigma_1\sigma'}L_{RR\sigma\sigma_1}|\sigma_i\rangle}{\xi_{\gamma_1}-\xi_{\gamma_R}+i\eta}n_{\gamma_1\sigma_1} + \frac{\langle\sigma_f|L_{RR\sigma\sigma_1}L_{RL\sigma_1\sigma'}|\sigma_i\rangle}{\xi_{\gamma_1}-\xi_{\gamma_R}-i\eta}[1-n_{\gamma_1\sigma_1}]$$

？第一项右→右→右 classical energy-conserving。第二项好像右→右的时候预言了左→右的发生，极不寻常虚拟过程，但仍有振幅提供。

而提出第2项"1"：$\sum_{\sigma_1\gamma_1} = d_0\int_{-D}^{D} d\varepsilon_{\gamma_1}(\cdots)$ 对2D中态密度 d_0 守恒：

$$=\int_{-D}^{D}\frac{1}{\varepsilon_1-\varepsilon_{\gamma_R}}\langle\sigma_f|L_{RR}L_{RL}|\sigma_i\rangle d\varepsilon_1 \propto \ln(\varepsilon_1-\varepsilon_{\gamma_R})\Big|_{-D}^{D}$$

$$\propto \ln\frac{D-\varepsilon_R}{D+\varepsilon_{\gamma_R}}$$



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原式：

$$t^{(2)R}_{\gamma_R\gamma_L\sigma\sigma'} = -n_{\gamma_L}(1-n_{\gamma_R})\sum_{\sigma_1\gamma_1}\frac{\langle\sigma_f|[L_{RL\sigma_1\sigma'}, L_{RR\sigma\sigma_1}]|\sigma_i\rangle}{\varepsilon_1-\varepsilon_R+i\eta}n_{\gamma_1\sigma_1}$$

因此，计算：

$$\langle[L_{RL\sigma_1\sigma'}, L_{RR\sigma\sigma_1}]\rangle$$

即可。

此式为：$\left[\left(W_{RL}\delta_{\sigma,\sigma'}+\frac{J_{RL}}{2}\sum_j S_d^j I^j_{\sigma,\sigma'}\right),\left(W_{RR}\delta_{\sigma\sigma_1}+\frac{J_{RR}}{2}\sum_j S_d^j I^j_{\sigma\sigma_1}\right)\right]$

~~$\Rightarrow W_{RL}W_{RR}$, $W_{RL}J_{RR}$ $W_{RR}J_{RL}$ 都对易，(非算符，所以就不存在一般~~

的散射在 $t^{(2)}$ 中了，必反转自治 δ_2 + δ_3 的讨论

$$=\frac{J_{RL}J_{RR}}{4}\sum_{jK}\langle\sigma_f|[S_d^j,S_d^k]|\sigma_i\rangle\sum_{\sigma_1}I^K_{\sigma\sigma_1}I^j_{\sigma_1\sigma}$$

再次利用Pauli矩阵的性质.　　搜 $I^{(3)}$ 的项.

$$I^{(3)}\propto \mathrm{Re}\left[(t^{(1)})^*t^{(2)}\right]\text{，有项：}$$

$$t^{(1)}=W_{RL}\delta_{\sigma\sigma'}\delta_{\sigma_i\sigma_f}+\frac{J_{RL}}{4}\sum_j I^j_{\sigma_f\sigma_i}I^j_{\sigma\sigma'}$$

$$\sum_{\sigma\sigma'\sigma_i\sigma_f}\delta_{\sigma\sigma'}\delta_{\sigma_i\sigma_f}\cdot\sum_{jK}\langle\sigma_f|[S_d^j,S_d^k]|\sigma_i\rangle\sum_{\sigma_1}I^k_{\sigma\sigma_1}I^j_{\sigma_1\sigma'}$$

代：$\sigma=\sigma'$　$\sigma_i=\sigma_f$

$$=\sum_{\sigma\sigma_i}\sum_{jK}\langle\sigma_i|[S_d^j,S_d^k]|\sigma_i\rangle\sum_{\sigma_1}I^k_{\sigma\sigma_1}I^j_{\sigma_1\sigma}$$

又

$$=S_d^i=\sum_{\sigma\sigma'}c^\dagger_{d\sigma}I^i_{\sigma\sigma'}c_{d\sigma'}\frac{1}{2}=\sum_{\sigma\sigma'}c^\dagger_{d\sigma}\langle\sigma|I|\sigma'\rangle c_{d\sigma'}\frac{1}{2}=\langle 0|I^i|0\rangle$$

$\Rightarrow S_d^i\Leftrightarrow I^i/2$ 代入、　Pauli性质：$I^jI^k=\delta_{jk}+i\sum_l\varepsilon_{jkl}I$

$$\langle\sigma_i|[I^j,I^k]|\sigma_i\rangle=\langle\sigma_i|i\sum_L I^L[\varepsilon_{jkL}-\underbrace{\varepsilon_{kjk}}_{\text{Levi-Civita}}]|\sigma_i\rangle$$

$$=\sum_L(\varepsilon_{jkL}-\varepsilon_{kjL})\langle\sigma_i|i\cancel{\textstyle\sum_L}I^L|\sigma_i\rangle$$

$$=\sum_L(\sim)\,\mathrm{Tr}(I^L)=\sum_L(\sim)\times 0=0$$

此项为零

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另一项：

$$\sum_{L\sigma\sigma'\sigma_i\sigma_f} \langle\sigma_i|S_d^L|\sigma_f\rangle \tau^L_{\sigma'\sigma} \sum_{jk} \langle\sigma_f|[S_d^j, S_d^k]|\sigma_i\rangle \sum_{\sigma_1} \tau^k_{\sigma\sigma_1}\tau^j_{\sigma_1\sigma'}$$

$S_d^i = \tau^i/2$ ① $\langle\sigma_i|S_d^L|\sigma_f\rangle\langle\sigma_f|[S_d^j, S_d^k|\sigma_i\rangle$ 对 σ_f 求和

$$= \langle\sigma_i|S_d^L\cdot[S_d^j, S_d^k]|\sigma_i\rangle = Tr(S_d^L, [S_d^j, S_d^k]) = \frac{1}{8}Tr(\tau^L, [\tau^j, \tau$$

② $\tau^L_{\sigma'\sigma}\tau^k_{\sigma\sigma_1}\tau^j_{\sigma_1\sigma'} = \langle\sigma'|\tau^L|\sigma\rangle\langle\sigma|\tau^k|\sigma_1\rangle\langle\sigma_1|\tau^j|\sigma'\rangle$ 对 σ_1, σ 求和

$$= Tr(\tau^L\tau^k\tau^j)$$

$$\therefore \text{原式} = \sum_{ijk}\frac{1}{8}Tr(\tau^L, [\tau^j, \tau^k])\,Tr(\tau^L\tau^k\tau^j)$$

$$= \sum_{ijk}\frac{1}{4}Tr(\tau^L\tau^j\tau^k)\,Tr(\tau^k\tau^L\tau^j)$$

利用：$\tau^L\tau^j = \delta_{Lj} + i\sum_l \varepsilon_{jkl}\tau^l \Rightarrow Tr(\tau^L\tau^j\tau^k) = Tr((i\sum_k \varepsilon_{Ljk}\tau^k)\tau^k)$

$\Rightarrow \sum_{ijk}\varepsilon_{ijki}$

$$\Rightarrow = \sum_{ijk}(-1)\varepsilon_{Ljk}\varepsilon_{kLj} = -\sum_{jkl}\varepsilon_{Ljk}^2 = \boxed{-6}$$

Therefore:

$$\tau^{(3)}_{RL} = 4\pi\sum_i \frac{1}{2}P_i\,Re\left\{-n_{\gamma L}[1-n_{\gamma R}]\sum_{\sigma_1\gamma_1}\left(\frac{1}{4}\frac{J_{RL}J_{RR}}{\xi_{\gamma_1}-\xi_R+i\eta}\right)\times(-6)\times n_{\gamma_1\sigma_1}\right.$$

$$\delta(\gamma_R-\gamma_L)\cdot\underbrace{J_{RL}}_{t^{(1)}}$$

t^R 项，t^L 项为：

$J_{RL}J_{LL}$ 不变余下

① $\sum_i n_F(\varepsilon_L)(1-n_F(\varepsilon_R))$ 变积分. suppose d_0 态密度不变

② $\gamma_R=\gamma_L$ delta function 积分结果代入

③ $\sum_{\gamma_1} = d_0\int_{-D}^{D} n_F(\gamma_1)\frac{1}{\varepsilon_1-\varepsilon_R+i\eta}$ 代入. $\eta\to 0$

$$\therefore I_{RL}^{(3)} = -\frac{3\pi}{2}(d_0 J_{RL})^2\int d\varepsilon\, n_F(\varepsilon-\mu_L)[1-n_F(\varepsilon-\mu_R)]$$

$$\times(J_{LL}+J_{RR})d_0\int_{-D}^{D}d\varepsilon_1\frac{n_F(\varepsilon_1)}{\varepsilon_1-\varepsilon}$$

Step 3:

我们求 I 与 G:

甚早之前给出 I 与 G 的公式.

$$I=(-e)\sum_N[I_{N+1.N}^{Left}-I_{N-1.N}^{Left}]P(N)$$ (向左) 这里对 t_{RL} 为总的.

$I=\frac{e}{\hbar}\left(I_{RL}^{(3)}+I_{RL}^{(2)}-I_{LR}^{(3)}-I_{LR}^{(2)}\right)$ 代入 $I^{(3)}, I^{(2)}$ 形式:

区别在 $n_F(\varepsilon-\mu_L)[1-n_F(\varepsilon-\mu_R)]-n_F(\varepsilon-\mu_R)[1-n_F(\varepsilon-\mu_L)]$

$=[n_F(\varepsilon-\mu_L)-n_F(\varepsilon-\mu_R)]$ 本质还是化学势驱动电流

另外: 亦给出过 G 的形式:

$$G=e^2\sum_\sigma\int\frac{d\varepsilon}{2\pi}\frac{\Gamma^L\Gamma^R}{\Gamma^L+\Gamma^R}A(d\sigma,\varepsilon)\,\frac{-\partial n_F(\xi)}{\partial\xi}.$$

当: $I=e\sum_\sigma\int\frac{d\xi}{2\pi}\frac{\Gamma^L\Gamma^R}{\Gamma^L+\Gamma^R}A(d\sigma,\varepsilon)\left(n_F(\varepsilon-\mu_L)-n_F(\varepsilon-\mu_R)\right)$ 时

可见:

把 I 中 (n_F-n_F) 改为 $\frac{-\partial n_F}{\partial\xi}$ ~~出~~ 令 $\mu_L=\mu_R=0$ 即可:

$G=I/V\to$ 除掉了 chemical potential.

终于. we arrive:

$$I=\frac{e}{h}\int d\varepsilon\,[n_F(\varepsilon-\mu_L)-n_F(\varepsilon-\mu_R)]\,T(\varepsilon).$$

$$G=\frac{e^2}{h}\int d\varepsilon\,-\frac{\partial n_F(\varepsilon)}{\partial\varepsilon}\,T_{\mu_L=\mu_R=0}(\varepsilon)$$

$$T(\varepsilon)=4\pi^2(W_{RL}\,d_0)^2+\frac{3}{2}\pi^2(J_{RL}\,d_0)^2\left(1-2(J_{LL}+J_{RR})\,d_0\,P\int_{-D}^{D}d\varepsilon_1\frac{n_F(\varepsilon_1)}{\varepsilon_1-\varepsilon}\right)$$

从中还可知道 $A(d_0,\varepsilon)$ 毕竟 $T^L=(t^L)\,d_0^2$ 而 t^L, t^R 可有 $J_{LL}\ J_{RR}$ 的关联.

电子-~~自旋~~空穴 对称点?

若令: $W_{RL}=0$, 积分: $P\int_{-D}^{+D}d\varepsilon_1\frac{n_F(\varepsilon_1)}{\varepsilon_1-\varepsilon}$.

$$\Rightarrow\int d\varepsilon\int_{-D}^{D}d\varepsilon_1\,-\frac{\partial n_F(\varepsilon)}{\partial\varepsilon}\left(\frac{n_F(\varepsilon_1)}{\varepsilon_1-\varepsilon}\right)$$

$$=\int_{d\varepsilon}\frac{1}{T}\exp(\varepsilon/T)\cdot\frac{-1}{(e^{\varepsilon/T}+1)^2}\cdot\int_{\boxed{0}}^{D}d\varepsilon_1\times\frac{n_F(\varepsilon_1)}{\varepsilon_1-\varepsilon}+\frac{1-n_F(\varepsilon_1)}{-\varepsilon_1-\varepsilon}\,d\varepsilon_1$$

$$=\int d\varepsilon\int_0^D d\varepsilon_1\,\underbrace{\frac{1}{T}\exp\left(\frac{\varepsilon}{T}\right)\cdot\frac{-1}{(e^{\varepsilon/T}+1)^2}}\cdot\left(\frac{2\varepsilon\,n_F(\varepsilon_1)}{-\varepsilon_1^2+\varepsilon^2}+\frac{1}{\varepsilon+\varepsilon_1}\right)$$

(偶) 此项: $(e^{\varepsilon/T}+2+e^{-\varepsilon/T})$ 此项: (奇) 对 ε 积分为0.

余下: $$\int d\varepsilon\int_0^D d\varepsilon_1\,\frac{1}{T}\frac{-\exp(\varepsilon/T)}{(e^{\varepsilon/T}+1)^2}\,\frac{1}{\varepsilon+\varepsilon_1}$$

$$=\int d\varepsilon\,\ln\frac{D+\varepsilon}{\varepsilon}\cdot\frac{1}{T}\frac{\exp(\varepsilon/T)}{(e^{\varepsilon/T}+1)^2}$$ 令 $x=\varepsilon/kT$

$$=\int_R dx\cdot\frac{e^x}{(e^x+1)^2}\cdot\left(\cancel{\ln\frac{x}{kT}-\ln x}\right)\ \ln\left(\frac{D}{kTx}+1\right)$$

$(\cancel{D/\varepsilon\gg1})$

总之和出大差不差：$G = \frac{3\pi^2 e^2}{2h} \cdot (J_{RL} d_0)^2 \left(1 + 2(J_{LL} + J_{RR}) f(D/T)\right)$

$f(x) = \ln(x) + 0.568 \cdots \simeq \ln(x)$ for $x: D/kT \ll 1$

anyway, $T \to 0$, $f(x) \to \infty$, $G \to \infty$. why?

we use pertubation theory, Fermi Golden Rule valid when:

$\delta(E_i - E_j)$：态密度 $|t|^2 d_0$ 在 ΔE 间不变，然 $T \to 0$ $(E_i, E_j) \sim E_{V_F}$,

距 V_F 一段距离 $(E_i, E_j) \sim n$ 态密度骤变，不适用。

when $T_K = D\exp(-1/2(J_{LL} + J_{RR}))$. $f(D/T)\, 2(J_{LL} + J_{RR})$

$= \ln \exp[1/2(J_{LL} + J_{RR}) D]\, 2(J_{LL} + J_{RR}) = 1 - 1 = 0$

∴ 定义 Kondo Temperature when $G = 0$,

$$T_K = D \exp\left[-\frac{1}{2(J_{LL} + J_{RR})}\right]$$

一张图：

$\mathcal{I}^{(3)}, t^{(2)}$ 中的2个过程可以描述为 $J_{RR}J_{RL}$: $L\to R$ $R\to R$, 反转两次自旋, 用算符即为 $\hat{S}^-\hat{S}^+ C^\dagger_{R\uparrow}C_{R\downarrow}C^\dagger_{R\downarrow}C_{L\uparrow} + S^+S^- C^\dagger_{R\downarrow}C_{L\uparrow}C^\dagger_{R\uparrow}C_{R\downarrow}$

~~Step I~~

其中第一项 $S^-S^+C^\dagger_{R\uparrow}C_{R\downarrow}C^\dagger_{R\downarrow}C_{L\uparrow}$ S: 自旋算符. $S^- = S_x - iS_y$

$s^-s^+ = C^\dagger_{s-}C_{s-}C^\dagger_{s+}C_{s+}$ 两消两生两反转过程.

spin: localized, lead 作用为 $s\cdot S = s^-\cdot S^+ + s^+\cdot S^- + s_z\cdot S_z$.

$t^{(2)} \propto J_{RR}J_{RL}\sum_\gamma \left(\frac{s^-s^+(1-n_\gamma)}{-\xi_\gamma}\right.$ 后四项 $\left. - \frac{s^+s^-n_\gamma}{\xi_\gamma}\right)$

由于 $[S^+, S^-] = S_z \neq 0$. 求和 $t^{(2)} \propto S_z \int \frac{1}{\xi_\gamma} d\xi_\gamma$

以 ln 发散, 体现大量 ξ_γ 中间态叠加之多体效应.

Kondo Model 下文还会反复议多次.

上文方法用T矩阵n阶直接解同样可得到.