格林函数，(推迟，超前)

格林函数

物理含义：点源 ——→ 激发

$$G(r, r')$$

r：响应　r'：激发处

$$\psi(\vec{r}) = \overbrace{G(\vec{r}, \vec{r}')}^{\text{响应函数}} S(\vec{r}')$$

$G(\vec{r}, \vec{r}')$：格林函数／传播子

$S(\vec{r}')$：点源激发

① 若点源在一定范围内(r')

$$\psi(\vec{r}) = \int d\vec{r}' \, G(\vec{r}, \vec{r}') \, S(\vec{r}')$$

② 若点源含时　$S(\vec{r}'; t') \to G(\vec{r}, \vec{r}', t, t')$

$$\psi(\vec{r}, t) = \int dt' \, G(\vec{r}, \vec{r}', t, t') \, S(\vec{r}'; t')$$

③ 点源含时<u>且</u>在一定范围内

$$\psi(\vec{r}, t) = \int d\vec{r}' dt' \, G(\vec{r}, \vec{r}', t, t') \, S(\vec{r}'; t')$$

在量子力学中

$$[E-\hat{H}]\underset{\text{响应}}{\psi(r)} = \underset{\text{激发源}}{S(r)}$$

$$\Rightarrow \psi(\vec{r}) = \underbrace{[E-H]^{-1}}\, S(r')$$

通过格林函数定义. $G=[E-H]^{-1}$

例. 1维纳米线中电子 格林函数

$$\hat{H} = -\frac{\hbar^2\nabla^2}{2m} + U_0$$

格林函数满足: $\left(E-U_0+\frac{\hbar^2\nabla^2}{2m}\right)G(r,r') = \delta(r-r')$

作业) 验证: 格林函数的方程确实满足传播子定义:

$$\psi(r) = \int dr' \; G(r-r')\, S(r')$$

$$\Rightarrow \left(E-U_0+\frac{\hbar^2\nabla^2}{2m}\right)\psi(\vec{r}) = \int dr' \underbrace{\left(E-U_0+\frac{\hbar^2\nabla^2}{2m}\right)G(\vec{r}-\vec{r}')}_{\delta(r-r')} S(\vec{r}')$$

$$\Rightarrow \left(E-U_0+\frac{\hbar^2\nabla^2}{2m}\right)\psi(\vec{r}) = S(\vec{r})$$

k空间的格林函数. 一维时 格林函数满足

$$\left(E-U_0+\frac{\hbar^2 d_x^2}{2m}\right)G(r,r') = \delta(r-r')$$

转到k空间:

$$\Rightarrow \left(E-U_0-\frac{\hbar^2k^2}{2m}\right)G(k,E)=1$$

$$\Rightarrow G(k,E)=\frac{1}{E-U_0-\frac{\hbar^2k^2}{2m}}$$

其中
时间相关项可用能量代替.

$$\left(-i\hbar\partial_t-U_0+\frac{\hbar^2\partial_x^2}{2m}\right)G(x,x',t-t')=\delta(x-x')\delta(t-t')$$

$$=\delta(x-x')\int e^{-iE(t-t')}dt$$

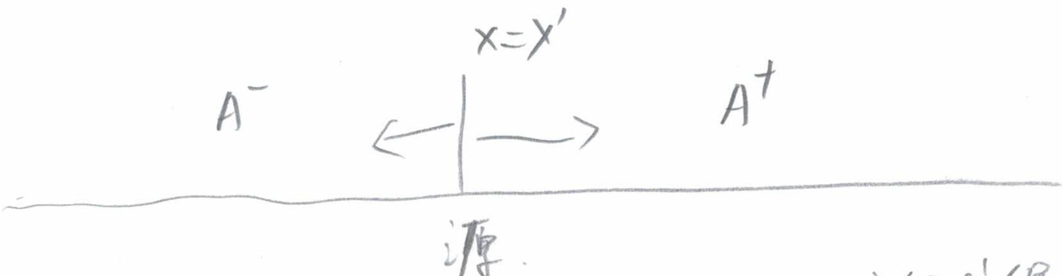
$$=\left(-i\hbar\partial_t-U_0+\frac{\hbar^2\partial_x^2}{2m}\right)\int G(x,x';E)e^{-\frac{iE}{\hbar}(t-t')}dt=\int\delta(x-x')e^{-\frac{iE}{\hbar}(t-t')}dt$$

⇒有

$$\Rightarrow \left(E-U_0+\frac{\hbar^2\partial_x^2}{2m}\right)G(x,x';E)=\delta(x-x')$$

求解格林函数方程.

$$\left(E-U_0+\frac{\hbar^2\partial_x^2}{2m}\right)G(x,x')=\delta(x-x')$$



$$G(x,x')=\begin{cases}A^+e^{ik(x-x')} & x>x'\\ A^-e^{-ik(x-y')} & x<x'\end{cases}$$

代入方程求得

$$k=\frac{\sqrt{2m(E-U_0)}}{\hbar}$$

考察 $x=x'$ 时情况

① $G(x-x')\big|_{x=x_0^+} = G(x-x')\big|_{x=x_0^-}$

② $$\left[\frac{\partial G(x,x')}{\partial x}\Big|_{x=x_0^+} - \frac{\partial G(x,x')}{\partial x}\Big|_{x=x_0^-}\right] = \underbrace{\frac{2m}{\hbar^2}}_{\Downarrow\text{保持}\delta\text{函数归一性}}$$

$$\underbrace{\int_{x_0^-}^{x_0^+}(E-U_0)G(x,x')dx}_{\substack{\shortparallel \\ 0}} + \underbrace{\frac{\hbar^2}{2m}\int_{x_0^-}^{x_0^+}\partial_x^2 G(x,x')dx}_{\frac{\hbar^2}{2m}\underbrace{\left(\frac{\partial G(x,x')}{\partial x}\Big|_{x=x_0^+} - \frac{\partial G(x,x')}{\partial x}\Big|_{x=x_0^-}\right)}_{\frac{2m}{\hbar^2}}} = \underbrace{\int_{x_0^-}^{x_0^+}\delta(x-x')dx}_{\shortparallel\ 1}$$

具体求解

由① $\Rightarrow A^+ = A^-$

由② $\Rightarrow ik(A^+ + A^-) = \frac{2m}{\hbar^2} \Rightarrow A^+ = \frac{2m}{2\hbar^2 ik} = A^-$

也可写为: $A^+ = -\frac{i}{\hbar v}$ $\quad v = \frac{\hbar k}{m}$

$A^- = -\frac{i}{\hbar v}$

$\Rightarrow G(x,x') = -\frac{i}{\hbar v}e^{ik|x-x'|}$ (推迟格林函数

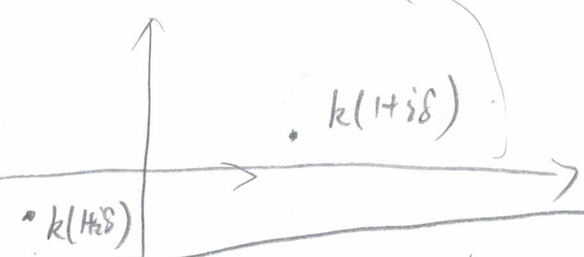
另解:

$G(x,x') = \frac{i}{\hbar v}e^{-ik|x-x'|}$ (超前格林函数)

用 $G(k,t)$ 来做：

$$G^R(x-x') = \int \frac{dk}{2\pi} e^{ik(x-x')} \frac{1}{E - U_0 - \frac{\hbar^2 k^2}{2m} + i\eta} \qquad \eta \to 0^+$$

$$\Rightarrow k = \frac{\pm\sqrt{2m(E-U_0+i\eta)}}{\hbar} \approx \frac{\pm\sqrt{2m(E-U_0)}}{\hbar}\left(1+\frac{i\eta}{2(E-U_0)}\right) = \pm k(1+i\delta)$$



留数定理积分： 作业2

$$G(x-x') = \int \frac{dk}{2\pi} e^{ik(x-x')} \frac{1}{(k-k_0(1+i\delta))(k+k_0(1+i\delta))} \times \left(-\frac{2m}{\hbar^2}\right)$$

$$k_0 = \frac{\sqrt{2m(E-U_0)}}{\hbar}$$

围道选取需保证被积函数不发散

① $x>x'$ 时 $(x-x')>0$ 应取上围道

$$G(x-x') = \frac{1}{2\pi} \cdot 2\pi i \frac{e^{ik_0(1+i\delta)(x-x')}}{2(k_0(1+i\delta))} \times \left(-\frac{2m}{\hbar^2}\right) = -\frac{i2m}{\hbar^2 2k} e^{ik(x-x')} \quad (x>x')$$

② $x<x'$ 时 $(x-x')<0$ 取下围道

$$G(x-x') = \frac{1}{2\pi}(-2\pi i) e^{-ik(x-x')} \frac{1}{-2k} \cdot \left(-\frac{2m}{\hbar^2}\right) = -\frac{im}{\hbar^2 k} e^{-ik(x-x')}$$

$$= -\frac{i}{\hbar v} e^{ik|x-x'|}$$

超前格林函数

$$G^A(x-x') = \int \frac{dk}{2\pi}\, e^{ik(x-x')} \frac{1}{E - i\eta - u_0 - \frac{\hbar^2 k^2}{2m}}$$

线性响应理论

kubo formula for electron conductivity.

$$E(r,t) \propto e^{i\vec{q}\cdot r} e^{-iwt}$$

$$J_\alpha(r,t) = \int dr' \int_{-\infty}^{t} dt\, \tilde{\sigma}_{\alpha\beta}(r-r', t-t') E_\beta(r', t')$$

令 $E_\beta(r',t') = \tilde{E}_\beta\, e^{i\vec{q}\cdot\vec{r} - iwt}$.

$$\Rightarrow J_\alpha(r,t) = \int dr' \int_{-\infty}^{t} dt'\, \tilde{\sigma}_{\alpha\beta}(r-r', t-t')\, \tilde{E}_\beta\, e^{i\vec{q}(r'-r)} e^{-iw(t-t')} \cdot e^{i\vec{q}\cdot r} e^{-iwt}$$

$$= E_\beta(r,t) \int dr' \int_{-\infty}^{t} dt'\, \tilde{\sigma}_{\alpha\beta}(r-r', t-t')\, e^{i\vec{q}(r'-r)} e^{-iw(t-t')}$$

$$= E_\beta(r,t) \int dr' \int_{-\infty}^{\infty} dt'\, \underbrace{\theta(t-t')\tilde{\sigma}_{\alpha\beta}(r-r'; t-t')}_{\sigma_{\alpha\beta}'(r-r', t-t')}\, e^{i\vec{q}(r'-r)} e^{-iw(t-t')}$$

$$E_\beta(r,t) \underline{\int dr' \int dt'\, \sigma_{\alpha\beta}(r-r', t-t')\, e^{-i\vec{q}(r-r')} e^{-iw(t-t')}}$$

$$E_\beta(r,t)\, \sigma_{\alpha\beta}(q, w) \qquad \Rightarrow J(\vec{q}, w) = E(\vec{q}, w)\, \sigma(\vec{q}, w)$$

如何算流(电) $\begin{cases} \text{量子力学} & J_\alpha \\ \text{统计力学} & \rho_\alpha(\text{重}) \end{cases}$

$$J_\alpha(t) = Tr(\rho(t) j_\alpha)$$

$$\frac{d\rho(t)}{dt} = -i[\hat{H}, \rho(t)]$$

$\boxed{\text{作业三.}}$ 算出当存在外加电场时

$$\hat{H} = H_0 + \underset{\uparrow \text{外加电场}}{H'} = H_0 - \underline{\frac{1}{c}\int dr\, j_\alpha A_\alpha(r,t)}$$

解：忽略高次项

$$H = \frac{1}{2m}\sum_i \left(\hat{P}_i - \frac{e}{c}A(r_i)\right)^2$$

$$= \frac{1}{2m}\sum_i \left(\hat{P}_i - \frac{e}{c}A(r_i)\right)\left(\hat{P}_i - \frac{e}{c}A(r_i)\right)$$

$$= \frac{1}{2m}\sum_i \hat{P}_i^2 - \frac{1}{2m}\frac{e}{c}\hat{P}_i \cdot A(r_i) - \frac{1}{2m}\frac{e}{c}A(r_i)\cdot\hat{P}_i$$

$$= H_0 - \left(\sum_i \frac{1}{2m}\frac{e}{c}\left(\hat{P}_{\alpha i} A_\alpha(r_i) + A_\alpha(r_i)\hat{P}_{\alpha i}\right)\right)$$

由 J_α 定义：$j_\alpha = \sum_i \frac{e}{2m}[\hat{P}_j \delta(r-r_j) - \delta(r-r_j)\hat{P}_j]$

$\Rightarrow$ 有：$\int dr\, \hat{j}_\alpha A_\alpha(r,t) = \sum_i \int dr \frac{e}{2m}[\hat{P}_{i\alpha}\delta(r-r_i)A_\alpha(r,t) - \delta(r-r_i)A_\alpha(r,t)\hat{P}_{i\alpha}]$

$$= \sum_i \frac{e}{2m}\left[\hat{P}_{i\alpha} A_\alpha(r_i, t) - A_\alpha(r_i, t)\hat{P}_{i\alpha}\right]$$

即 $$H_0 - \frac{1}{c}\sum_i \frac{e}{2m}\left(\hat{P}_{i\alpha} A_\alpha(r_i) - A_\alpha(r_i)\hat{P}_{i\alpha}\right)$$

$$= H_0 - \frac{1}{c}\int dr\, \hat{j}_\alpha A_\alpha(r, t)$$