直交破局 (orthogonality catastrophe)

P.W. Anderson [PRL 18, 1049 (1967)]

簡単のため 3次元空間中のSpinless fermion を考える。

$r = 0$にポテンシャル$V\delta(\vec{r})$

ハミルトニアン

$$H_0 = \sum_{\vec{k}} \varepsilon_{\vec{k}} c_{\vec{k}}^\dagger c_{\vec{k}}$$

H_0の基底状態 $|0\rangle$ (filled Fermi sea)

$$H = \sum_{\vec{k}} \varepsilon_{\vec{k}} c_{\vec{k}}^\dagger c_{\vec{k}} + \frac{V}{L^3} \sum_{\vec{k}_1, \vec{k}_2} c_{\vec{k}_1}^\dagger c_{\vec{k}_2}$$

Hの基底状態 $|V\rangle$

重なり積分$\langle 0|V\rangle$を評価したい

Vについて最低次の摂動計算

$$|V\rangle = N\left[|0\rangle + \frac{V}{L^3} \sum_{|\vec{k}_1|>k_F} \sum_{|\vec{k}_2|<k_F} \frac{c_{\vec{k}_1}^\dagger c_{\vec{k}_2}}{\varepsilon_{k_2} - \varepsilon_{k_1}} |0\rangle \right]$$

Nは規格化定数

$N = \langle 0|V\rangle$

$$1=\langle V|V\rangle = N^2\left[1+\left(\frac{V}{L^3}\right)^2 \sum_{|\vec{k}_1|>k_F}\sum_{|\vec{k}_2|<k_F}\frac{1}{\left(\varepsilon_{k_2}-\varepsilon_{k_1}\right)^2}\right]$$

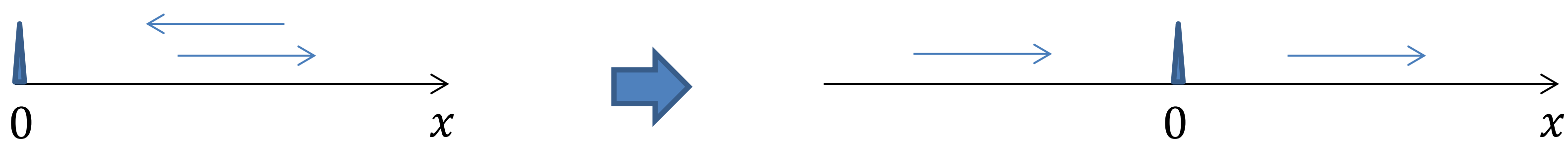
$$\left(\frac{V}{L^3}\right)^2 \sum_{|\vec{k}_1|>k_F}\sum_{|\vec{k}_2|<k_F}\frac{1}{\left(\varepsilon_{k_2}-\varepsilon_{k_1}\right)^2} = V^2 N_F^2 \int_0^D d\varepsilon_1 \int_{-D}^0 d\varepsilon_2 \frac{1}{\left(\varepsilon_2-\varepsilon_1\right)^2} \approx \left(N_F V\right)^2 \int_0^D \frac{d\varepsilon_1}{\varepsilon_1} = \left(N_F V\right)^2 \log\frac{D}{0} = \infty$$

N_F : Fermi面での状態密度　D : band width

一辺の長さ L の箱　　$\varepsilon_L = \frac{v_F}{L}$　　$\left(N_F V\right)^2 \int_{\varepsilon_L}^D \frac{d\varepsilon}{\varepsilon} = \left(N_F V\right)^2 \log\frac{D}{\varepsilon_L} = \left(N_F V\right)^2 \log\frac{DL}{v_F}$

$$N=\left[1+\left(N_F V\right)^2\log\frac{DL}{v_F}\right]^{-1/2} \approx 1-\frac{1}{2}\left(N_F V\right)^2\log\frac{DL}{v_F} \to e^{-\frac{1}{2}\left(N_F V\right)^2\log\frac{DL}{v_F}} = \left(\frac{v_F}{DL}\right)^{\frac{1}{2}\left(N_F V\right)^2}$$

3次元空間におけるS波散乱 → 1次元の問題に帰着



1次元の有効模型

$$H = -iv_F \int_{-\infty}^{\infty} dx \ \psi^\dagger(x)\frac{d}{dx}\psi(x) + v_F N_F :\psi^\dagger(0)\psi(0):$$

bosonization

$$H = \frac{v_F}{4\pi}\int_{-\infty}^{\infty} dx \left(\frac{d\varphi_R}{dx}\right)^2 + v_F N_F V \frac{1}{2\pi}\frac{d\varphi_R(0)}{dx} = \frac{v_F}{4\pi}\int_{-\infty}^{\infty} dx \left(\frac{d\varphi_R}{dx} + N_F V \delta(x)\right)^2 + \mathrm{const}$$

$$H_0 = \frac{v_F}{4\pi}\int_{-\infty}^{\infty} dx \left(\frac{d\varphi_R}{dx}\right)^2$$

$$\left[\varphi_R(x), \varphi_R(y)\right] = i\pi\,\mathrm{sgn}(x-y)$$

$$\left[\varphi_R(x), \partial_y \varphi_R(y)\right] = -2\pi i \delta(x-y)$$

H_0の基底状態　$|0\rangle$　（boson の真空）

$$\frac{\partial}{\partial\alpha} e^{i\alpha\varphi_R(0)} \frac{d\varphi_R(x)}{dx} e^{-i\alpha\varphi_R(0)} = e^{i\alpha\varphi_R(0)}\left[i\varphi_R(0), \frac{d\varphi_R(x)}{dx}\right] e^{-i\alpha\varphi_R(0)} = 2\pi\delta(x)$$

をαで積分して

$$e^{i\alpha\varphi_R(0)} \frac{d\varphi_R(x)}{dx} e^{-i\alpha\varphi_R(0)} = \frac{d\varphi_R(x)}{dx} + 2\pi\alpha\delta(x)$$

$$e^{i\frac{N_F V}{2\pi}\varphi_R(0)} H_0 \ e^{-i\frac{N_F V}{2\pi}\varphi_R(0)} = H + \mathrm{const}$$

H の基底状態　$|V\rangle = e^{i\frac{N_F V}{2\pi}\varphi_R(0)}|0\rangle$　　$\langle V|V\rangle = 1$

$$\langle 0|V\rangle = \langle 0| e^{i\frac{N_F V}{2\pi}\varphi_R(0)} |0\rangle = \langle 0| \exp\left[i\frac{N_F V}{2\pi}\int_0^\infty dk \frac{e^{-\alpha k/2}}{\sqrt{k}}\left(b_k + b_k^\dagger\right)\right]$$

$$= \exp\left[-\frac{1}{2}\left(\frac{N_F V}{2\pi}\right)^2 \int dk \frac{e^{-\alpha k}}{k}\right]$$

$$= \exp\left[-\frac{1}{2}\left(\frac{N_F V}{2\pi}\right)^2 \int_{\varepsilon_L}^{D} \frac{d\varepsilon}{\varepsilon}\right] = \left(\frac{\varepsilon_L}{D}\right)^{\frac{1}{2}\left(\frac{N_F V}{2\pi}\right)^2} \propto L^{-\frac{1}{2}\left(\frac{N_F V}{2\pi}\right)^2} \to 0 \quad (L\to\infty)$$

K.D. Schotte and U. Schotte, Phys. Rev. 182, 479 (1969)

Schrodinger equation

$$\left[-iv_F\frac{d}{dx}+V(x)\right]\psi(x)=E\psi(x) \qquad E=v_Fk$$

$$\psi(x)=\exp\left[ikx-\frac{i}{v_F}\int_{-\infty}^{x}dyV(y)\right] \quad = \begin{cases} e^{ikx} & x<0 \quad \text{入射波} \\ e^{ikx-iN_FV} & x>0 \quad \text{透過波} \end{cases}$$

$$V(x)=v_FN_FV\delta(x)$$

Phase shift δ

$$\frac{1}{r}\sin(kr+\delta)=\frac{1}{2ir}\left(e^{i(kr+\delta)}-e^{-(kr+\delta)}\right)$$

（3次元の場合）

$$\delta=\frac{1}{2}N_FV$$

$$\left|\langle 0|V\rangle\right|^2 \propto L^{-(\delta/\pi)^2}$$

一般に、p波、d波、等の散乱も起こる場合には

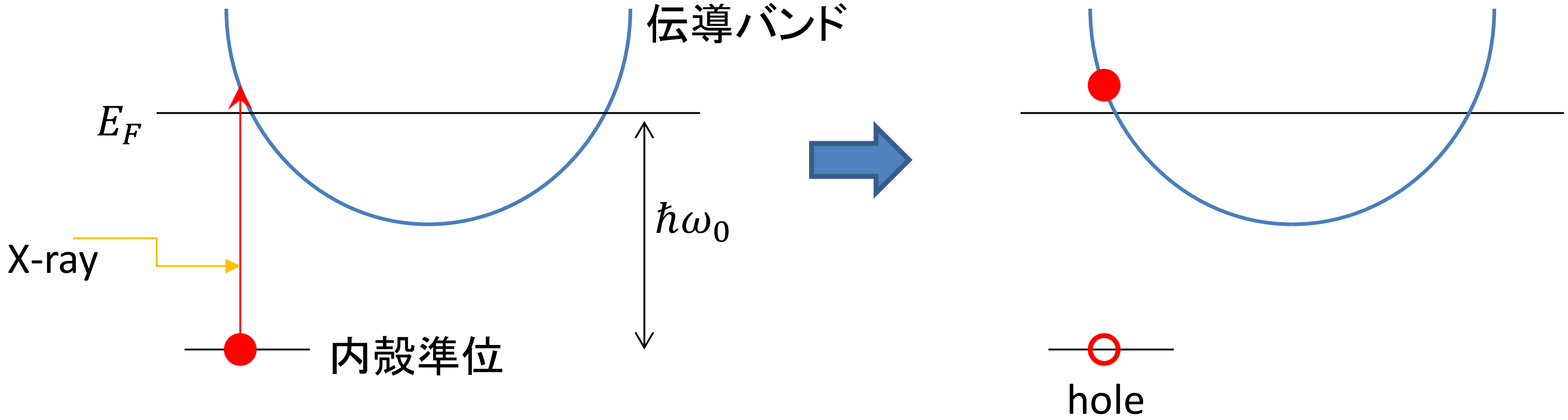
$$\left|\langle 0|V\rangle\right|^2 \propto L^{-\sum_l (2l+1)(\delta_l/\pi)^2}$$

Andersonの直交定理

$l=0$: s-wave scattering, $l=1$: p-wave scattering, …

フェルミ端異常 (Fermi edge singularity)

光を吸収して内殻電子が伝導バンドに遷移するとき、内殻の正孔と伝導電子間の相互作用によって光吸収スペクトルの吸収端付近のエネルギー依存性に異常が生じる



Hamiltonian

$$H = \sum_{\vec{k}} \varepsilon_k c_{\vec{k}}^\dagger c_{\vec{k}} - \frac{V}{L^3} \sum_{\vec{k}_1,\vec{k}_2} c_{\vec{k}_1}^\dagger c_{\vec{k}_2} \left(1 - d^\dagger d\right) + \left(E_F - \hbar\omega_0\right) d^\dagger d$$

伝導電子と正孔間のクーロン引力

$$H' = \frac{\lambda}{L^3} \sum_{\vec{k}} \left(c_{\vec{k}}^\dagger d + d^\dagger c_{\vec{k}}\right) = \lambda\left[\psi^\dagger(0) d + d^\dagger \psi(0)\right]$$

内殻電子と伝導電子の遷移

遷移確率の計算 (Fermi's golden rule)

$$P = \frac{2\pi}{\hbar} \sum_{\varepsilon_f > E_F} \left| \left\langle f \right| \lambda \psi^\dagger(0) d \left| i \right\rangle \right|^2 \delta\left(E_f - E_i - \hbar\omega\right)$$

$$= \frac{\lambda^2}{\hbar^2} \int_{-\infty}^{\infty} dt \left\langle i \right| e^{iHt/\hbar} d^\dagger \psi(0) e^{-iHt/\hbar} \psi^\dagger(0) d \left| i \right\rangle e^{i\omega t}$$

$$= \frac{\lambda^2}{\hbar^2} \int_{-\infty}^{\infty} dt \left\langle \mathrm{FS} \right| e^{iH_i t/\hbar} \psi(0) e^{-iH_f t/\hbar} \psi^\dagger(0) \left| \mathrm{FS} \right\rangle e^{i(\omega-\omega_0)t}$$

$$H_i = \sum_{\vec{k}} \varepsilon_k c_{\vec{k}}^\dagger c_{\vec{k}} \qquad H_f = \sum_{\vec{k}} \varepsilon_k c_{\vec{k}}^\dagger c_{\vec{k}} - V\psi^\dagger(0)\psi(0)$$

相互作用VによるS波散乱問題を1次元系に帰着させる

ボゾン化

$$H_i = \frac{v_F}{4\pi} \int dx \left(\frac{d\varphi}{dx} \right)^2 \qquad H_f = \frac{v_F}{4\pi} \int dx \left(\frac{d\varphi}{dx} \right)^2 - \frac{v_F N_F V}{2\pi} \frac{d\varphi(0)}{dx}$$

$$\psi(0) = \frac{e^{i\varphi(0)}}{\sqrt{2\pi\alpha}} \qquad = \exp\left[-i\frac{\delta}{\pi}\varphi(0) \right] H_i \exp\left[i\frac{\delta}{\pi}\varphi(0) \right] + \mathrm{const}$$

$$P = \frac{\lambda^2}{2\pi\alpha\hbar^2}\int_{-\infty}^{\infty} dt \left\langle \exp\left[i\left(1-\frac{\delta}{\pi}\right)\varphi(0,t)\right]\exp\left[-i\left(1-\frac{\delta}{\pi}\right)\varphi(0,0)\right]\right\rangle e^{i(\omega-\omega_0)t}$$

$$\varphi(x,t) = \int_0^{\infty} dk \frac{e^{-\alpha k/2}}{\sqrt{k}}\left(e^{ik(x-vt)}b_k + e^{-ik(x-vt)}b_k^{\dagger}\right)$$ を用いて相関関数を計算する

$$\left\langle \exp\left[i\left(1-\frac{\delta}{\pi}\right)\varphi(0,t)\right]\exp\left[-i\left(1-\frac{\delta}{\pi}\right)\varphi(0,0)\right]\right\rangle$$

$$= \langle 0|\exp\left[i\left(1-\frac{\delta}{\pi}\right)\int_0^{\infty} dk \frac{e^{-\alpha k/2}}{\sqrt{k}}\left(b_k e^{-ikvt} + b_k^{\dagger} e^{ikvt}\right)\right]\exp\left[-i\left(1-\frac{\delta}{\pi}\right)\int_0^{\infty} dk \frac{e^{-\alpha k/2}}{\sqrt{k}}\left(b_k + b_k^{\dagger}\right)\right]|0\rangle$$

$$= \exp\left[-\left(1-\frac{\delta}{\pi}\right)^2 \int_0^{\infty} dk \frac{e^{-\alpha k}}{k}\left(1-e^{-ikvt}\right)\right] = \left(1+i\frac{vt}{\alpha}\right)^{-\left(1-\frac{\delta}{\pi}\right)^2}$$

$$P \propto \int_{-\infty}^{\infty} dt \left(1+i\frac{v_F t}{\alpha}\right)^{-\left(1-\frac{\delta}{\pi}\right)^2} e^{i(\omega-\omega_0)t} \propto (\omega-\omega_0)^{\mu}\,\theta(\omega-\omega_0)$$

$$\mu = \left(1-\frac{\delta}{\pi}\right)^2 - 1 = -2\frac{\delta}{\pi} + \left(\frac{\delta}{\pi}\right)^2 < 0$$