・部分波解析

自由粒子： $-\frac{\hbar^2}{2m}\nabla^2\psi = E\psi = \frac{k^2\hbar^2}{2m}\psi$

↓

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} = e^{ikr\cos\theta}$$

$$= \sum_{\ell=0}^{\infty}(2\ell+1)\, i^\ell\, j_\ell(kr)\, P_\ell(\cos\theta)$$

$$j_\ell(kr) \to \frac{1}{kr}\sin\left(kr-\frac{\ell\pi}{2}\right) \qquad (r\to\infty)$$

$$\to \frac{i}{2k}\sum_\ell (2\ell+1)\, i^\ell \left[e^{-i(kr-\frac{\ell\pi}{2})} - e^{+i(kr-\frac{\ell\pi}{2})}\right] \times P_\ell(\cos\theta)\cdot\frac{1}{r}$$

ポテンシャルがある場合：

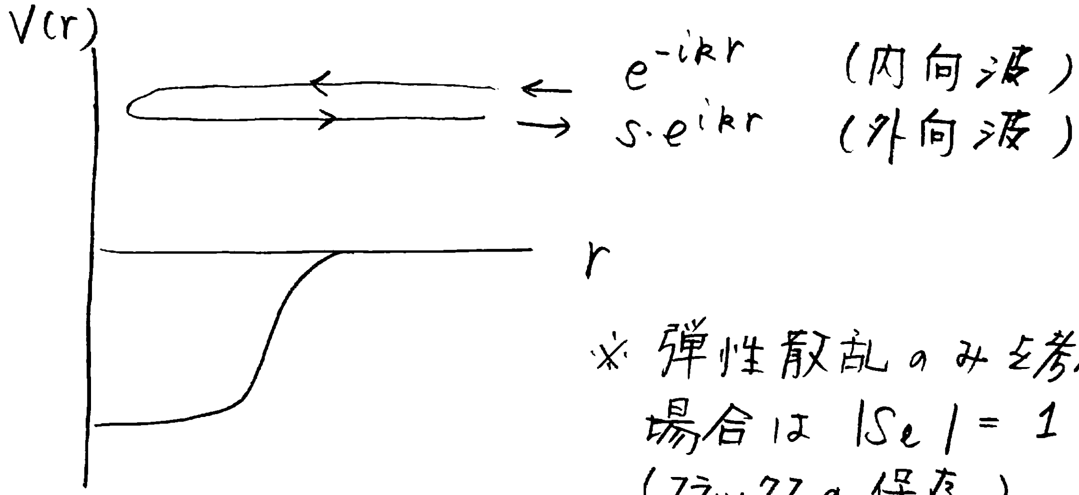
$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r) - E\right]\psi(\mathbf{r}) = 0$$

$$V(r)\to 0 \qquad (r\to\infty)$$

↓

波動関数の漸近形 (asymptotic form) は自由粒子の場合と同様

$$\psi(\mathbf{r}) \to \frac{i}{2kr}\sum_\ell (2\ell+1)\, i^\ell \left[e^{-i(kr-\frac{\ell\pi}{2})} - \underbrace{S_\ell}_{S\text{行列}}\, e^{+i(kr-\frac{\ell\pi}{2})}\right] \times P_\ell(\cos\theta)$$



※弾性散乱のみを考える場合は $|S_l| = 1$
（フラックスの保存）

$$\psi(\mathbf{r}) \to \frac{i}{2kr} \sum_l (2l+1)\, i^l \left[e^{-i(kr-\frac{l\pi}{2})} - e^{+i(kr-\frac{l\pi}{2})} + e^{+i(kr-\frac{l\pi}{2})} - S_l\, e^{+i(kr-\frac{l\pi}{2})} \right] P_l(\cos\theta)$$

$$= e^{i\mathbf{k}\cdot\mathbf{r}} + \underbrace{\left[\sum_l (2l+1) \frac{S_l - 1}{2ik} P_l(\cos\theta) \right]}_{\equiv\, f(\theta)} \cdot \frac{e^{ikr}}{r}$$

$i^l e^{-i\frac{l\pi}{2}} = i^l \cdot (-i)^l = 1$

$$= e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta) \cdot \frac{e^{ikr}}{r}$$

散乱断面積 ： $\frac{d\sigma}{d\Omega} = |f(\theta)|^2$.

全断面積：

$$\sigma_{tot} = \int \frac{d\sigma}{d\Omega} d\Omega = \int |f(\theta)|^2 d\Omega$$

$$= \sum_{l,l'} (2l+1)(2l'+1) \frac{S_l - 1}{2ik} \cdot \frac{S_{l'}^* - 1}{-2ik}$$

$$\times \underbrace{\int d\Omega\, P_l(\cos\theta)\, P_{l'}(\cos\theta)}_{= \frac{4\pi}{2l+1}\delta_{l,l'}}$$

$$\leftarrow \int_{-1}^{1} P_l(x)\, P_{l'}(x)\, dx = \frac{2}{2l+1} \times \delta_{l,l'}$$

$$= \frac{\pi}{k^2} \sum_l (2l+1) |S_l - 1|^2.$$

$S_l = e^{2i\delta_l}$ （位相のずれ）を用いて書き直すと

$$\sigma_{tot} = \frac{\pi}{k^2} \sum_l (2l+1) \left| e^{2i\delta_l} - 1 \right|^2$$

$$= \frac{\pi}{k^2} \sum_l (2l+1) \left| e^{i\delta_l} \frac{e^{i\delta_l} - e^{-i\delta_l}}{2i} \cdot 2i \right|^2$$

$$= \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2 \delta_l$$

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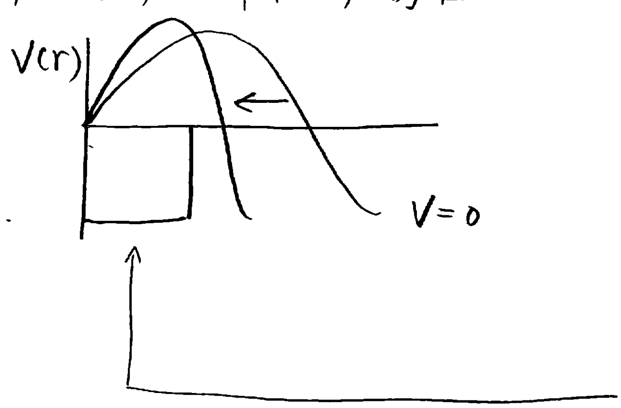
(note) 位相のずれの意味：

$$u_\ell(r) \to e^{-i(kr-\frac{\ell\pi}{2})} - \underbrace{S_\ell}_{= e^{2i\delta_\ell}} e^{+i(kr-\frac{\ell\pi}{2})}$$

$$= e^{i\delta_\ell}\left[e^{-i(kr-\frac{\ell\pi}{2}+\delta_\ell)} - e^{i(kr-\frac{\ell\pi}{2}+\delta_\ell)} \right]$$

$$= -2i\, e^{i\delta_\ell} \cdot \sin\Big(kr-\frac{\ell\pi}{2}\underbrace{+\delta_\ell}_{\text{位相が } \delta_\ell \text{ だけずれる}}\Big)$$

引力ポテンシャルの場合

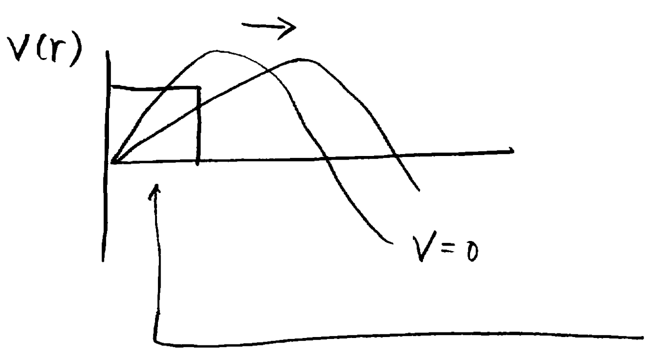


$$\sqrt{\frac{2m}{\hbar^2}(E-V(r))} > \sqrt{\frac{2m}{\hbar^2}E}$$

$$\to \delta_\ell > 0$$

$$\sin(\tilde{k}r) = \sin(kr+\delta)$$

斥力ポテンシャルの場合



$$\sqrt{\frac{2m}{\hbar^2}(E-V(r))} < \sqrt{\frac{2m}{\hbar^2}E}$$

$$\to \delta_\ell < 0$$

$$\sin(\tilde{k}r) = \sin(kr-\delta)$$

四 光学定理

$$\mathrm{Im}\, f(\theta=0) = \mathrm{Im} \sum_l (2l+1)\cdot\frac{S_l-1}{2ik}\underbrace{P_l(1)}_{=1}$$

$$= \mathrm{Im} \sum_l (2l+1)\cdot\frac{\cos(2\delta_l)+i\sin(2\delta_l)-1}{2ik}$$

$$= \sum_l (2l+1)\cdot\frac{1}{\cancel{2}k}\left(\underbrace{1-\cos(2\delta_l)}_{=\cancel{2}\sin^2\delta_l}\right)$$

$$= \frac{k}{4\pi}\cdot\underbrace{\frac{4\pi}{k^2}\sum_l (2l+1)\sin^2\delta_l}_{\sigma_{tot}}$$

◦ 光学定理の意味

$$\psi(\mathbf{r}) \to e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta)\cdot\frac{e^{ikr}}{r}$$ のフラックス

$$\mathbf{j} = \frac{\hbar}{2im}\left(\psi^* \nabla\psi - c.c.\right)$$

$$\sim \frac{\mathbf{k}\hbar}{m} + \frac{k\hbar}{m}\mathbf{e}_r |f(\theta)|^2 \cdot \frac{1}{r^2}$$

$$+ \underbrace{\frac{k\hbar}{2m}\cdot\frac{1}{r}\left(\mathbf{e}_r + \mathbf{e}_k\right)\left(f(\theta)e^{ikr(1-\cos\theta)} + c.c.\right)}_{e^{i\mathbf{k}\cdot\mathbf{r}}\ \text{と}\ f(\theta)\cdot\frac{e^{ikr}}{r}\ \text{の干渉項}}$$

$\int \mathbf{e}_r\cdot\mathbf{j}\ r^2 d\hat{\mathbf{r}}$ に対する第3項からの寄与

$$= \frac{k\hbar}{2m}\cdot\frac{1}{\cancel{r}}\int (1+\cos\theta)\left(f(\theta)e^{ikr(1-\cos\theta)} + c.c.\right) r^{\cancel{2}} d\hat{\mathbf{r}}$$

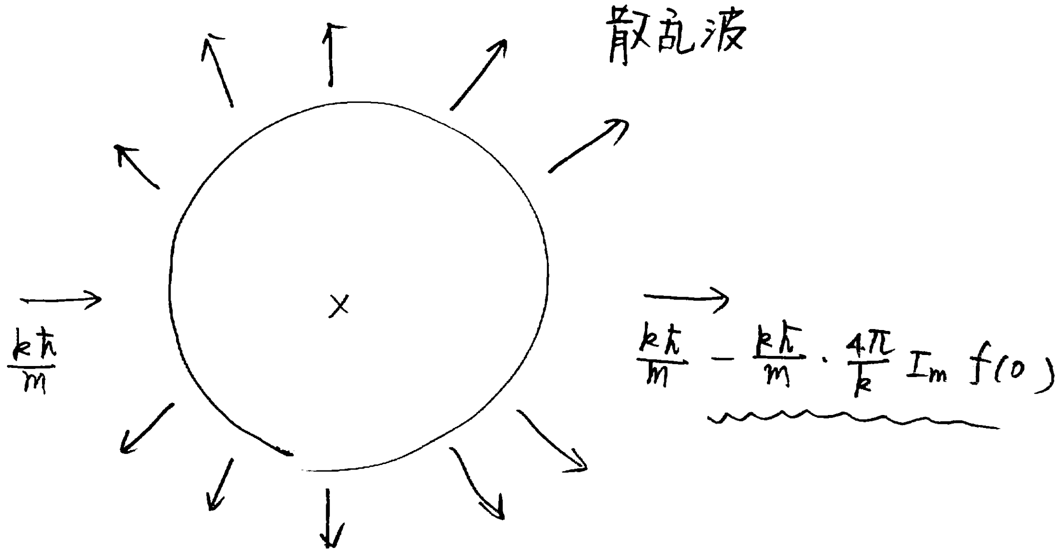
$$= \frac{k\hbar}{2m}\cdot r\cdot 2\pi \int_{-1}^{1} d(\cos\theta)\,(1+\cos\theta)\left(f(\theta)\,e^{ikr(1-\cos\theta)} + c.c.\right)$$

$$= \frac{k\hbar}{2m}\cdot r\cdot 2\pi\left\{ -\frac{1}{ikr} f(\theta)(1+\cos\theta)e^{ikr(1-\cos\theta)}\Big|_{\cos\theta=-1}^{1} \right.$$

$$+ \frac{1}{ikr}\underbrace{\int \left(\frac{d}{d(\cos\theta)} f(\theta)(1+\cos\theta)\right)e^{ikr(1-\cos\theta)}\, d(\cos\theta)}_{O(\frac{1}{r})}$$

$$\left. + c.c. \right\}$$

$$= \frac{k\hbar}{2m}\cdot\cancel{r}\cdot 2\pi\left(-\frac{2}{ik\cancel{r}}f(0) + \frac{2}{ik\cancel{r}}f^*(0)\right) = -\frac{k\hbar}{m}\cdot\frac{4\pi}{k}\,\mathrm{Im}\,f(0)$$



入射フラックスの減少分が散乱フラックスとなる

$$\frac{k\hbar}{m}\cdot\frac{4\pi}{k}\,\mathrm{Im}\,f(0) = \frac{k\hbar}{m}\cdot\sigma_{tot}$$