$$H = \frac{-\hbar^2}{2m} \nabla^2 + V(r)$$

$$\Psi(\vec{r}) = R_l(r)\, Y_{lm}(\hat{r})$$

$$\downarrow \quad -\frac{\hbar^2}{2m}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right) R_l + \left(V(r) + \frac{l(l+1)\hbar^2}{2mr^2} - E\right) R_l = 0$$

$V(r) = 0$ のとき

$$R_l(r) = j_l(kr)$$

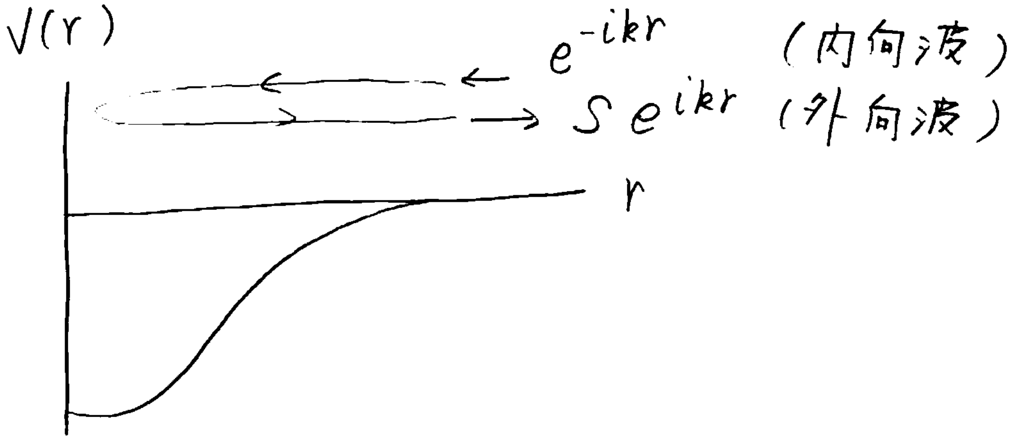
$$\longrightarrow \frac{1}{kr} \sin\left(kr - \frac{l\pi}{2}\right)$$

$$= \frac{-1}{2ikr}\left(e^{-i(kr - \frac{l\pi}{2})} - e^{i(kr - \frac{l\pi}{2})}\right)$$

$V(r) \neq 0$ のとき

$$R_l(r) \longrightarrow -\frac{1}{2ikr}\left(e^{-i(kr - \frac{l\pi}{2})} - \underbrace{S_l}_{e^{2i\delta_l}}\, e^{i(kr - \frac{l\pi}{2})}\right)$$

$$= \frac{e^{i\delta_l}}{kr} \sin\left(kr - \frac{l\pi}{2} + \underbrace{\delta_l}_{\text{位相のずれ}}\right)$$


V(r)
e^{-ikr} (内向波)
S e^{ikr} (外向波)
r

(note 1) 自由粒子 ($V(r)=0$)

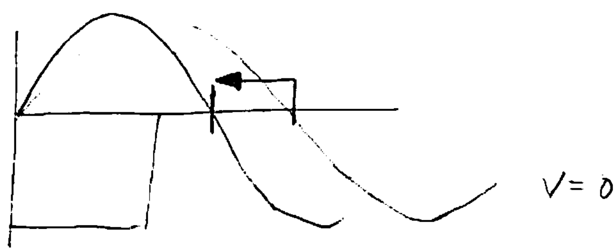
$$u_\ell(r) \propto kr \cdot j_\ell(kr)$$

$$\to \sin\left(kr - \frac{\ell\pi}{2}\right)$$

$\updownarrow$ $\delta_\ell = 0$ $\updownarrow$ $S_\ell = 1$

(note 2)

引力ポテンシャル



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

$$\sin(\tilde{k}r)$$

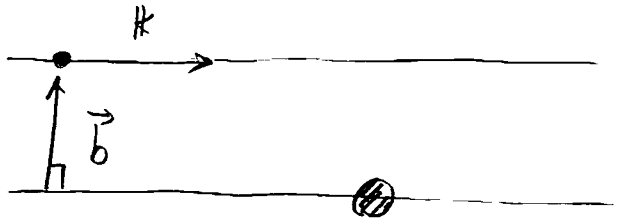
$$\to \boxed{\delta_\ell > 0}$$

斥力ポテンシャル

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

$$\to \boxed{\delta_\ell < 0}$$

◦衝突係数 (impact parameter)



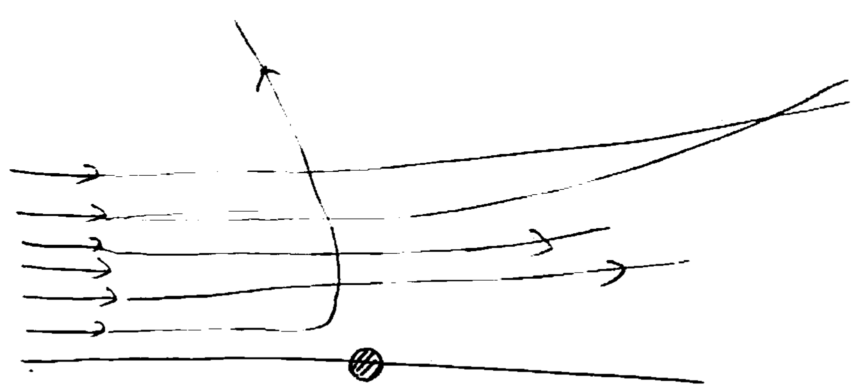
$$\vec{l} = \vec{r} \times \vec{p} \qquad \updownarrow \qquad l = b k \hbar$$

衝突係数

$$e^{i\mathbb{k}\cdot\mathbb{r}} = \sum_{l=0}^{\infty} (2l+1)\, i^{l}\, j_l(kr)\, P_l(\cos\theta)$$

$\updownarrow$

いろいろな衝突係数が合わさっている。



5.3. 部分波解析

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

$\downarrow$ $k \parallel e_z$

$$\psi(r) = e^{ik\cdot r} = e^{ikr\cos\theta}$$

$$= \sum_{l=0}^{\infty}(2l+1)\, i^l\, j_l(kr)\, P_l(\cos\theta)$$

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

$$\to \frac{i}{2k}\sum_{l=0}^{\infty}(2l+1)\, i^l \left[e^{-i(kr-\frac{l\pi}{2})} - e^{i(kr-\frac{l\pi}{2})}\right]\frac{1}{r}\cdot P_l(\cos\theta)$$

ポテンシャルがある場合:

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

AS $r\to\infty$ $V(\vec{r}) \to 0$

$\downarrow$

波動関数の漸近形 (asymptotic form):

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

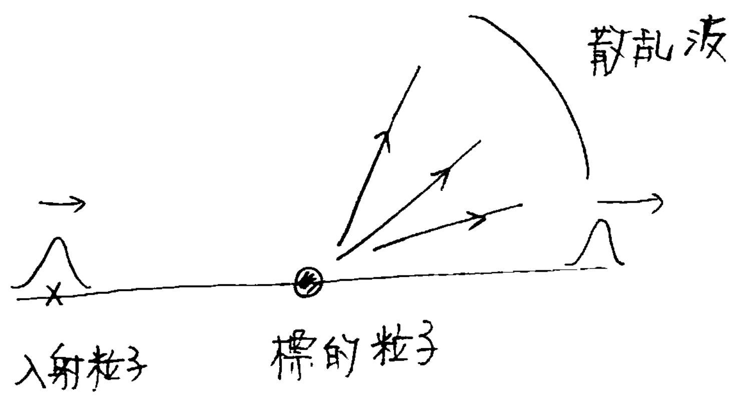
$$-e^{i(kr-\frac{l\pi}{2})} + e^{i(kr-\frac{l\pi}{2})}$$

"S 行列"

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

$$= e^{i\mathbf{k}\cdot\mathbf{r}} + \underbrace{\left[\sum_{\ell}(2\ell+1)\,\frac{S_\ell - 1}{2ik}\,P_\ell(\cos\theta)\right]}_{= f(\theta)}\cdot\frac{e^{ikr}}{r}$$

= (入射波) + (散乱波)



(弾性散乱のみを考える場合)　$|S_\ell| = 1$

散乱波： $\psi_{sc}(\mathbf{r}) \sim f(\theta)\dfrac{e^{ikr}}{r}$ に伴うフラックス：

$$\vec{j} = \frac{\hbar}{2im}\left[\psi_{sc}^{*}\nabla\psi_{sc} - c.c.\right]$$

(note) $\displaystyle \partial_x = \sin\theta\cos\varphi\,\partial_r + \frac{1}{r}\cos\theta\cos\varphi\,\partial_\theta - \frac{\sin\varphi}{r\sin\theta}\,\partial_\varphi$

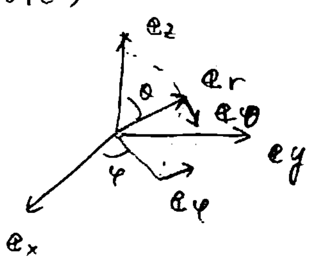
$\displaystyle \frac{\partial r}{\partial x}\partial_r + \frac{\partial\theta}{\partial x}\partial_\theta + \frac{\partial\varphi}{\partial x}\partial_\varphi$

$$\partial_y = \sin\theta\sin\varphi\,\partial_r + \frac{1}{r}\cos\theta\sin\varphi\,\partial_\theta + \frac{\cos\varphi}{r\sin\theta}\,\partial_\varphi$$

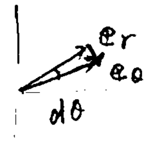
$$\partial_z = \cos\theta\,\partial_r - \frac{\sin\theta}{r}\,\partial_\theta$$

$$\downarrow\quad \nabla = \left[\sin\theta\cos\varphi\,\partial_r + \frac{1}{r}\cos\theta\cos\varphi\,\partial_\theta - \frac{\sin\varphi}{r\sin\theta}\,\partial_\varphi\right]\mathbf{e}_x$$
$$+\left[\sin\theta\sin\varphi\,\partial_r + \frac{1}{r}\cos\theta\sin\varphi\,\partial_\theta + \frac{\cos\varphi}{r\sin\theta}\,\partial_\varphi\right]\mathbf{e}_y$$
$$+\left[\cos\theta\,\partial_r - \frac{\sin\theta}{r}\,\partial_\theta\right]\mathbf{e}_z$$

(note)



$$\mathbf{e}_r = \sin\theta\cos\varphi\,\mathbf{e}_x + \sin\theta\sin\varphi\,\mathbf{e}_y + \cos\theta\,\mathbf{e}_z$$
$$\mathbf{e}_\theta = \cos\theta\cos\varphi\,\mathbf{e}_x + \cos\theta\sin\varphi\,\mathbf{e}_y - \sin\theta\,\mathbf{e}_z$$
$$\mathbf{e}_\varphi = -\sin\varphi\,\mathbf{e}_x + \cos\varphi\,\mathbf{e}_y$$



(note)

$$\nabla \cdot \mathbb{e}_r = \partial r$$

$$\nabla \cdot \mathbb{e}_\theta = \frac{1}{r} \partial \theta$$

$$\nabla \cdot \mathbb{e}_\varphi = \frac{1}{r\sin\theta} \partial \varphi$$

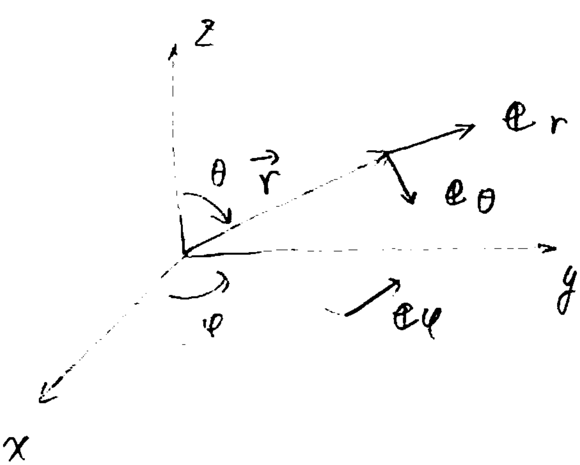
$$\boxed{\nabla = \mathbb{e}_r \, \partial_r + \frac{1}{r} \mathbb{e}_\theta \, \partial_\theta + \frac{1}{r\sin\theta} \mathbb{e}_\varphi \, \partial_\varphi}$$

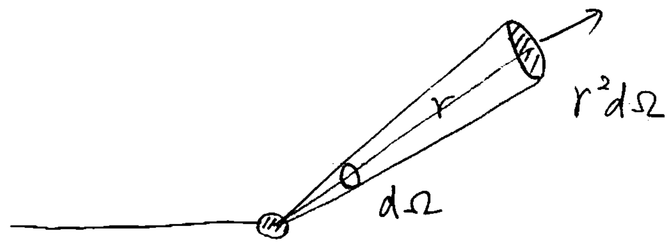
$$\vec{j} = \frac{\hbar}{2im} \left[f^*(\theta) \frac{e^{-ikr}}{r} \left(\mathbb{e}_r \, \partial_r + \mathbb{e}_\theta \cdot \frac{1}{r} \partial_\theta \right) f(\theta) \frac{e^{ikr}}{r} - c.c. \right]$$

$$= \frac{\hbar}{2im} \left[f^*(\theta) \frac{e^{-ikr}}{r} \left\{ f(\theta) \left(\frac{ik}{r} e^{ikr} - \frac{1}{r^2} e^{ikr} \right) \mathbb{e}_r + \frac{e^{ikr}}{r^2} f'(\theta) \cdot \mathbb{e}_\theta \right\} - c.c. \right]$$

$$\sim \frac{\hbar}{2im} \cdot ik \cdot \frac{|f(\theta)|^2}{r^2} \cdot 2 \, \mathbb{e}_r \quad (r \to \infty)$$

$$= \frac{k\hbar}{m} \frac{|f(\theta)|^2}{r^2} \mathbb{e}_r$$





単位時間に
立体角 $d\Omega$ に散乱される粒子の数： $\frac{k\hbar}{m} \frac{|f(\theta)|^2}{\cancel{r^2}} \cdot \cancel{r^2} d\Omega$

散乱断面積：

$$\boxed{\frac{d\sigma}{d\Omega} = \frac{1}{j_{in}} \cdot \frac{k\hbar}{m} |f(\theta)|^2 = |f(\theta)|^2}$$

・全断面積：

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

$$= \sum_{\ell\ell'} (2\ell+1)(2\ell'+1) \frac{S_\ell - 1}{2ik} \frac{S_{\ell'}^* - 1}{-2ik} \underbrace{\int d\Omega\, P_\ell(\cos\theta) P_{\ell'}(\cos\theta)}_{= \frac{4\pi}{2\ell+1} \delta_{\ell\ell'}}$$

$$= \frac{\pi}{k^2} \sum_\ell (2\ell+1) |S_\ell - 1|^2$$

$$S_\ell = e^{2i\delta_\ell}$$ （位相のずれ）

$$\downarrow$$

$$\sigma_{tot} = \frac{\pi}{k^2}\sum_\ell (2\ell+1)\left| e^{2i\delta_\ell} - 1 \right|^2$$

$$= \frac{\pi}{k^2}\sum_\ell (2\ell+1)\left| e^{i\delta_\ell}\frac{e^{i\delta_\ell}-e^{-i\delta_\ell}}{2i}\cdot 2i \right|^2$$

$$= \frac{4\pi}{k^2}\sum_\ell (2\ell+1)\sin^2\delta_\ell .$$

◦ 光学定理．

$$\mathrm{Im}\, f(\theta=0) = \mathrm{Im}\sum_\ell (2\ell+1)\cdot\frac{S_\ell - 1}{2ik}\underbrace{P_\ell(1)}_{=1}$$

$$= \mathrm{Im}\sum_\ell (2\ell+1)\cdot\frac{e^{i\delta_\ell}(e^{i\delta_\ell}-e^{-i\delta_\ell})}{2ik}$$

$$= \frac{1}{k}\sum_\ell (2\ell+1)\sin^2\delta_\ell \quad = \frac{k}{4\pi}\sigma_{tot} .$$

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} + f(\theta)\,\frac{e^{ikr}}{r} \qquad (r\to\infty)$$

$$= e^{ikr\cos\theta} + f(\theta)\,\frac{e^{ikr}}{r}$$

$\downarrow$

$$\nabla\psi = i\mathbf{k}\,e^{i\mathbf{k}\cdot\mathbf{r}} + \mathbf{e}_r f(\theta)\left(\frac{ik}{r} - \frac{1}{r^2}\right)e^{ikr} + \mathbf{e}_\theta\cdot f'(\theta)\,\frac{e^{ikr}}{r^2}$$

$\downarrow$

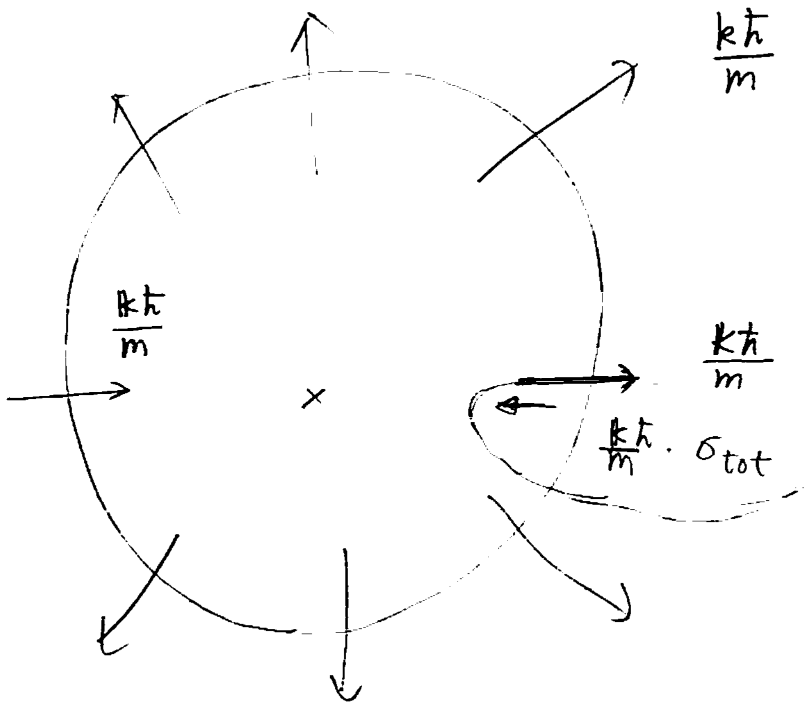
$$\mathbf{j} = \frac{\hbar}{2im}\Big\{\left[e^{-i\mathbf{k}\cdot\mathbf{r}} + f^*(\theta)\frac{e^{-ikr}}{r}\right]\cdot\left[i\mathbf{k}\,e^{i\mathbf{k}\cdot\mathbf{r}} + \mathbf{e}_r f(\theta)\left(\frac{ik}{r} - \frac{1}{r^2}\right)e^{ikr} + \mathbf{e}_\theta f'(\theta)\frac{e^{ikr}}{r^2}\right] - c.c.\Big\}$$

$$= \frac{\hbar}{2im}\Big\{ i\mathbf{k} + \mathbf{e}_r \frac{ik}{r^2}|f|^2 + \mathbf{e}_r\frac{ik}{r} f(\theta)\,e^{-i\mathbf{k}\cdot\mathbf{r}+ikr} + i\mathbf{k}\,f^*(\theta)\,\frac{1}{r}\,e^{i\mathbf{k}\cdot\mathbf{r}-ikr} - c.c.\Big\}$$

$\mathbf{k} \parallel \mathbf{e}_z$

$$\sim \frac{\hbar}{m}\mathbf{k} + \frac{k\hbar}{m}\frac{|f(\theta)|^2}{r^2}\mathbf{e}_r + \frac{k\hbar}{2im}\mathbf{e}_r\left(\frac{if}{r}e^{-ikz+ikr} + \frac{if^*}{r}e^{ikz-ikr}\right) + \frac{\hbar}{2im}\cdot\frac{\mathbf{k}}{r}\left(if^* e^{ikz-ikr} + if e^{-ikz+ikr}\right)$$

$$= \frac{\hbar}{m}\mathbf{k} + \frac{k\hbar}{m}\frac{|f(\theta)|^2}{r^2}\mathbf{e}_r + \frac{k\hbar}{2mr}(\mathbf{e}_r + \mathbf{e}_z)\left(f e^{-ikz+ikr} + f^* e^{ikz-ikr}\right)$$



全入射フラックス： $\frac{k\hbar}{m}$

全放出フラックス： $\frac{k\hbar}{m} + \frac{k\hbar}{m}\sigma_{tot} + \left(\begin{array}{l}j\text{の第3項の}\\\text{積分}\end{array}\right)$

↑

入射波と散乱波の干渉

$\parallel$

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

$\theta=0$ 以外では

$e^{ikr-ikz}=e^{ikr(1-\cos\theta)}$

が激しく振動して打ち消し合う。

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

$$\Rightarrow\quad \boxed{\mathrm{Im}\,f(0) = \frac{k}{4\pi}\sigma_{tot}}$$