[複習] 動径波動関数 (11章)

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

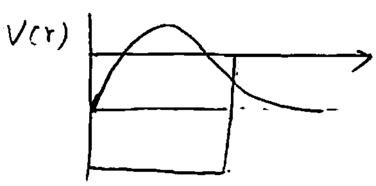
$$\Psi_l(\mathbf{r}) = \frac{u(r)}{r} Y_{lm}(\hat{\mathbf{r}})$$

$\downarrow$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) + \frac{l(l+1)\hbar^2}{2mr^2} - E\right] u_l(r) = 0.$$

$$u_l(r) \sim r^{l+1}$$

(i) $E<0$



spherical Hankel function

$$u_l(r) \propto h_l^{(1)}(i\kappa r) \qquad (r\to\infty)$$

$$h_0^{(1)}(i\kappa r) \sim e^{-\kappa r}$$

$$\kappa = \sqrt{\frac{2m}{\hbar^2}|E|}$$

(ii) $E>0$

$$u_l(r) \to e^{-i(kr-\frac{l\pi}{2})} - \underbrace{S_l}_{e^{2i\delta_l}} e^{i(kr-\frac{l\pi}{2})} \qquad (r\to\infty)$$

$$= -2i\cdot e^{i\delta}\sin\left(kr - \frac{l\pi}{2} + \delta_l\right)$$

位相のずれ

(note 1)　自由粒子 $(V(r)=0)$

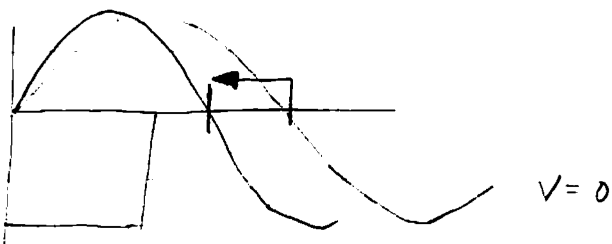
$$u_\ell(r) \propto kr \cdot j_\ell(kr)$$

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

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

(note 2)

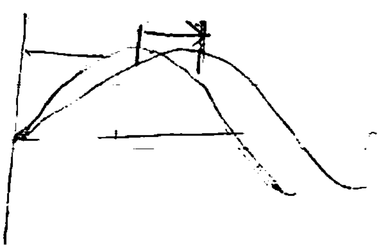
引力ポテンシャル



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

$\sin(\tilde{k} r)$ 　$\to \boxed{\delta_\ell > 0}$

斥力ポテンシャル



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

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

5.3. 部分波解析

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

$\downarrow$ $\quad k \parallel e_z$

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

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

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

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

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 $\quad r\to\infty \quad V(\vec{r})\to\infty$

$\downarrow$

波動関数の漸近形 (asymptotic form):

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

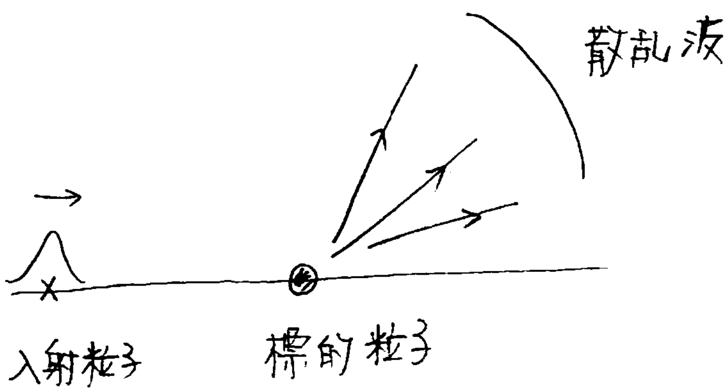
$$-e^{i(kr-\frac{l\pi}{2})} + e^{i(kr-\frac{l\pi}{2})}$$

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

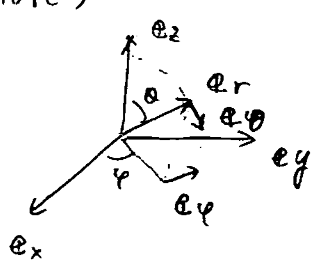
$\frac{\partial r}{\partial x}\partial_r + \frac{\partial\theta}{\partial x}\partial_\theta + \frac{\partial\varphi}{\partial x}\partial_\varphi$

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

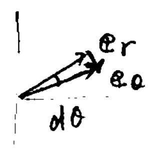
$$\partial_z = \cos\theta\,\partial_r - \frac{\sin\theta}{r}\,\partial_\theta$$

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

(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)

$$\nabla \cdot \mathbb{e}_r = \partial_r$$

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

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

$$\Downarrow$$

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

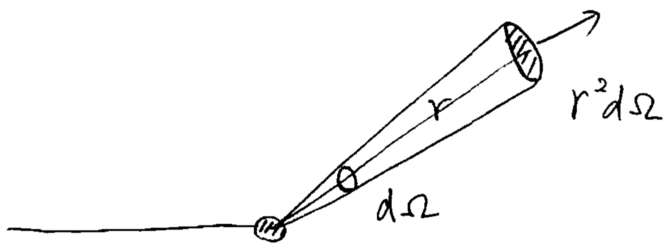
$$\Downarrow$$

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

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

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

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



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：

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

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

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

$$S_\ell = e^{2i\delta_\ell}$$ （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

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

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

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