トンネル効果

一次元箱形ポテンシャルによる散乱問題

物理量の期待値の運動方程式

- 物理量の時間変化←波動関数の時間変化

$$\langle A\rangle = \langle\psi|A|\psi\rangle \qquad -\frac{\hbar}{i}\frac{\partial}{\partial t}\psi = \mathcal{H}\psi$$

- 物理量の期待値の運動方程式

$$\frac{d}{dt}\langle A\rangle = \frac{i}{\hbar}\langle[\mathcal{H}, A]\rangle \qquad [\mathcal{H},\, A] = \mathcal{H}A - A\mathcal{H}$$

$\mathcal{H}A = A\mathcal{H} \Rightarrow$ 保存量

- エーレンフェストの定理

$$\begin{cases} \dfrac{d}{dt}\langle\vec{r}\rangle = \dfrac{1}{m}\langle\vec{p}\rangle \\ \dfrac{d}{dt}\langle\vec{p}\rangle = -\langle\nabla V(\vec{r})\rangle \end{cases}$$

物理量の誤差（標準偏差）

$$\Delta A = \sqrt{\langle A^2\rangle - \langle A\rangle^2}$$

- ハイゼンベルグの不確定性関係

$$\Delta p_x \Delta x \geq \hbar \qquad \left(\Delta p_x \Delta x \geq \frac{\hbar}{2}\right)$$

$$\Delta p_y \Delta y \geq \hbar$$

$$\Delta p_z \Delta z \geq \hbar$$

$$\Delta E \Delta t \geq \hbar \qquad \left(\Delta E \Delta t \geq \frac{\hbar}{2}\right)$$

電荷密度と電流

波動関数　$\psi(\vec{r}, t)$

- 粒子の存在確率密度　$|\psi(\vec{r}, t)|^2 = \psi(\vec{r}, t)^*\psi(\vec{r}, t)$
- 電荷密度　$\rho(\vec{r}, t) = e\psi(\vec{r}, t)^*\psi(\vec{r}, t)$

連続の式　$\dfrac{\partial}{\partial t}\rho(\vec{r}, t) + \nabla\vec{j}(\vec{r}, t) = 0$

- 確率密度の流れ

$$\frac{\hbar}{2mi}\left(\psi(\vec{r}, t)^*\nabla\psi(\vec{r}, t) - \psi(\vec{r}, t)\nabla\psi(\vec{r}, t)^*\right)$$

- 電流密度

$$\vec{j}(\vec{r}, t) = \frac{e\hbar}{2mi}\left(\psi(\vec{r}, t)^*\nabla\psi(\vec{r}, t) - \psi(\vec{r}, t)\nabla\psi(\vec{r}, t)^*\right)$$

一次元定ポテンシャル問題

シュレディンガーの**波動**方程式

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi(x) + V\varphi(x) = E\varphi(x)$$

進行波・定在波

$V < E$

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

$$\varphi(x) = C_1 \mathrm{e}^{ikx} + C_2 \mathrm{e}^{-ikx}$$

減衰波

$E < V$

$$\alpha = \frac{\sqrt{2m(V-E)}}{\hbar}$$

$$\varphi(x) = D_1 \mathrm{e}^{\alpha x} + D_2 \mathrm{e}^{-\alpha x}$$

存在確率密度の流れ

確率密度の流れ

$$\vec{j}(\vec{r}, t) = \frac{\hbar}{2mi}\left(\psi(\vec{r}, t)^*\nabla\psi(\vec{r}, t) - \psi(\vec{r}, t)\nabla\psi(\vec{r}, t)^*\right)$$

一次元定常状態⇒

$$j(x) = \frac{\hbar}{2mi}\left(\varphi^*(x)\frac{\partial}{\partial x}\varphi(x) - \varphi(x)\frac{\partial}{\partial x}\varphi^*(x)\right)$$

存在確率密度の流れ

確率密度の流れ

$$j(x)=\frac{\hbar}{2mi}\left(\varphi^*(x)\frac{\partial}{\partial x}\varphi(x)-\varphi(x)\frac{\partial}{\partial x}\varphi^*(x)\right)$$

$\varphi(x)=C\mathrm{e}^{ikx}$

$$\begin{aligned}j(x)&=\frac{\hbar}{2mi}\left(C^*\mathrm{e}^{-ikx}(ik)C\mathrm{e}^{ikx}-C\mathrm{e}^{ikx}(-ik)C^*\mathrm{e}^{-ikx}\right)\\&=\frac{\hbar k}{m}|C|^2\end{aligned}$$

右向き進行波状態の確率密度の流れ

$\varphi(x)=D\mathrm{e}^{-ikx}$

$$\begin{aligned}j(x)&=\frac{\hbar}{2mi}\left(D^*\mathrm{e}^{ikx}(-ik)D\mathrm{e}^{-ikx}-D\mathrm{e}^{-ikx}(ik)D^*\mathrm{e}^{ikx}\right)\\&=-\frac{\hbar k}{m}|D|^2\end{aligned}$$

左向き進行波状態の確率密度の流れ

存在確率密度

波動関数　$\varphi(x)=C\mathrm{e}^{ikx}+D\mathrm{e}^{-ikx}$

$C\neq 0,\ D=0$

$\varphi(x)=C\mathrm{e}^{ikx}$

$$\begin{aligned}|\varphi(x)|^2&=C^*\mathrm{e}^{-ikx}C\mathrm{e}^{ikx}\\&=|C|^2\end{aligned}$$

右向き進行波状態の確率

$C=0,\ D\neq 0$

$\varphi(x)=D\mathrm{e}^{-ikx}$

$$\begin{aligned}|\varphi(x)|^2&=D^*\mathrm{e}^{ikx}D\mathrm{e}^{-ikx}\\&=|D|^2\end{aligned}$$

左向き進行波状態の確率

$C\neq 0,\ D\neq 0$

$$\begin{aligned}|\varphi(x)|^2&=(C^*\mathrm{e}^{-ikx}+D^*\mathrm{e}^{ikx})(C\mathrm{e}^{ikx}+D\mathrm{e}^{-ikx})\\&=|C|^2+|D|^2+CD^*\mathrm{e}^{2ikx}+C^*D\mathrm{e}^{-2ikx}\end{aligned}$$

二つの進行波の干渉効果

存在確率密度の流れ

波動関数　$\varphi(x)=C\mathrm{e}^{ikx}+D\mathrm{e}^{-ikx}$

$$\begin{aligned}j(x)=&\frac{\hbar}{2mi}\Big(\left(C^*\mathrm{e}^{-ik}+D^*\mathrm{e}^{ik}\right)\left(ikC\mathrm{e}^{ik}-ikD\mathrm{e}^{-ik}\right)\\&-\left(C\mathrm{e}^{ik}+D\mathrm{e}^{-ik}\right)\left(-ikC^*\mathrm{e}^{-ik}+ikD^*\mathrm{e}^{ik}\right)\Big)\\=&\frac{\hbar k}{2m}\Big(\left(|C|^2\mathrm{e}^{ik}+D^*C\mathrm{e}^{2ik}-C^*D\mathrm{e}^{-2ik}-|D|^2\right)\\&-\left(-|C|^2-DC^*\mathrm{e}^{-2ik}+CD^*\mathrm{e}^{2ik}+|D|^2\right)\Big)\end{aligned}$$

$$j(x)=\frac{\hbar k}{2m}|C|^2+\left(-\frac{\hbar k}{2m}\right)|D|^2$$

左向き進行波状態の確率

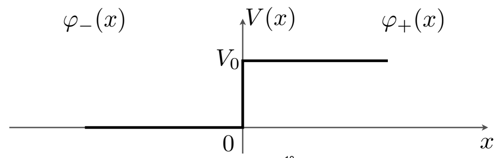
右向き進行波状態の確率

解の接続条件

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi(x)+V(x)\varphi(x)=E\varphi(x)$$

$$V(x)=\begin{cases}0 & (x<0)\\ V_0 & (0\leq x)\end{cases}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi(x)=E\varphi(x)\qquad -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi(x)+V_0\varphi(x)=E\varphi(x)$$

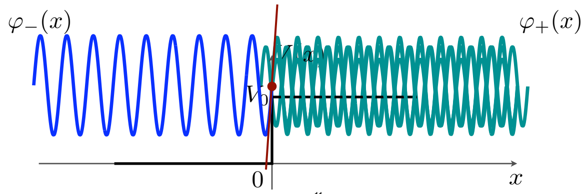


解の接続条件

$$\varphi(x)=\begin{cases}\varphi_-(x) & (x<0)\\ \varphi_+(x) & (0\leq x)\end{cases}$$

$$\varphi_-(-0)=\varphi_+(+0)$$

$$\left.\frac{\partial}{\partial x}\varphi_-(x)\right|_{x=-0}=\left.\frac{\partial}{\partial x}\varphi_+(x)\right|_{x=+0}$$



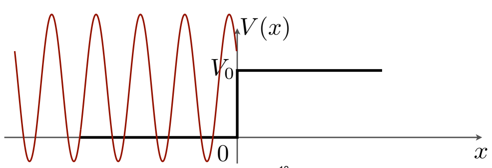
自由電子状態

$x<0$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi(x)=E\varphi(x)\qquad \frac{\partial^2}{\partial x^2}\varphi(x)+k^2\varphi(x)=0$$

$$k=\frac{\sqrt{2mE}}{\hbar}\qquad \varphi_-(x)=A\mathrm{e}^{ikx}+B\mathrm{e}^{-ikx}$$

$$E=\frac{\hbar^2k^2}{2m}\qquad \frac{\partial}{\partial x}\varphi_-(x)=ikA\mathrm{e}^{ikx}-ikB\mathrm{e}^{-ikx}$$



一定ポテンシャル中の状態

$0 \le x \quad E > V_0$

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi(x) + V_0\varphi(x) = E\varphi(x)$$

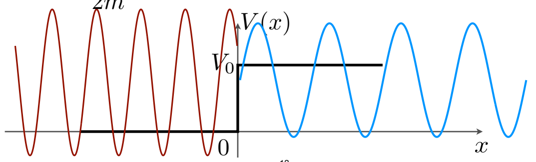
$$E = \frac{\hbar^2 k^2}{2m}$$

$$q = \frac{\sqrt{2m(E-V_0)}}{\hbar}$$

$$E - V_0 = \frac{\hbar^2 q^2}{2m}$$

$$\varphi_+(x) = C\mathrm{e}^{iqx} + D\mathrm{e}^{-iqx}$$

$$\frac{\partial}{\partial x}\varphi_+(x) = iqC\mathrm{e}^{iqx} - iqD\mathrm{e}^{-iqx}$$



ステップによる散乱

$0 \le x \quad E > V_0$

$$\varphi_-(x) = A\mathrm{e}^{ikx} + B\mathrm{e}^{-ikx}$$

$$\varphi_+(x) = C\mathrm{e}^{iqx} + D\mathrm{e}^{-iqx}$$

境界条件

$A = 1$

$D = 0$

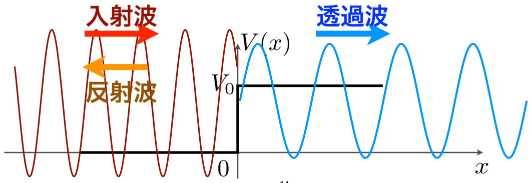
接続条件

$A + B = C + D$

$ikA - ikB = iqC - iqD$

$1 + B = C$

$ik - ikB = iqC$



ステップによる散乱

$1 + B = C$

$ik - ikB = iqC$

$$B = \frac{k-q}{k+q}$$

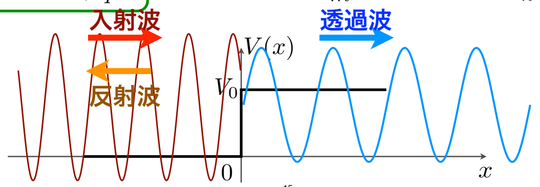
$$C = \frac{2k}{k+q}$$

確率密度の流れ

入射波 $\frac{\hbar k}{m}$

反射波 $-\frac{\hbar k}{m}|B|^2$ 反射率=$|B|^2$

透過波 $\frac{\hbar q}{m}|C|^2$ 透過率=$\frac{q}{k}|C|^2$



ステップによる散乱

$$\varphi_-(x) = \mathrm{e}^{ikx} + B\mathrm{e}^{-ikx}$$

$$\varphi_+(x) = C\mathrm{e}^{iqx}$$

$$k = \frac{\sqrt{2mE}}{\hbar} \qquad q = \frac{\sqrt{2m(E-V_0)}}{\hbar}$$

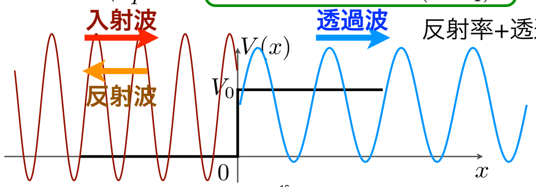
$$B = \frac{k-q}{k+q}$$

$$C = \frac{2k}{k+q}$$

反射率=$|B|^2$=$\frac{(k-q)^2}{(k+q)^2}$

透過率=$\frac{q}{k}|C|^2$=$\frac{4kq}{(k+q)^2}$

反射率+透過率=1



障壁内の波動関数

$0 \le x \quad E < V_0$

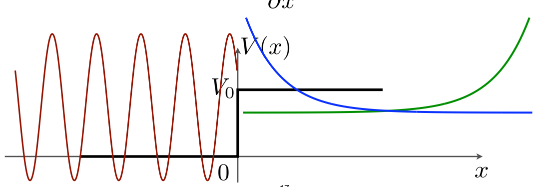
$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\varphi(x) + V_0\varphi(x) = E\varphi(x)$$

$$E = \frac{\hbar^2 k^2}{2m}$$

$$\alpha = \frac{\sqrt{2m(V_0-E)}}{\hbar}$$

$$\varphi_+(x) = C\mathrm{e}^{\alpha x} + D\mathrm{e}^{-\alpha x}$$

$$\frac{\partial}{\partial x}\varphi_+(x) = \alpha C\mathrm{e}^{\alpha x} - \alpha D\mathrm{e}^{-\alpha x}$$



ポテンシャル障壁による反射

$0 \le x \quad E < V_0$

$$\varphi_-(x) = A\mathrm{e}^{ikx} + B\mathrm{e}^{-ikx}$$

$$\varphi_+(x) = C\mathrm{e}^{\alpha x} + D\mathrm{e}^{-\alpha x}$$

境界条件

$A = 1$

$C = 0$

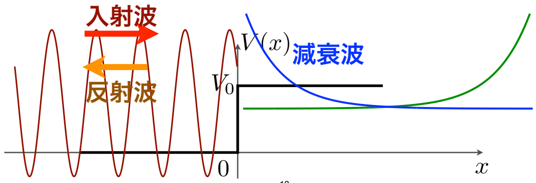
接続条件

$A + B = C + D$

$ikA - ikB = \alpha C - \alpha D$

$1 + B = D$

$ik - ikB = -\alpha D$



ポテンシャル障壁による反射

$1 + B = D$

$ik - ikB = -\alpha D$

$$B = \frac{k - i\alpha}{k + i\alpha}$$
$$D = \frac{2k}{k + i\alpha}$$

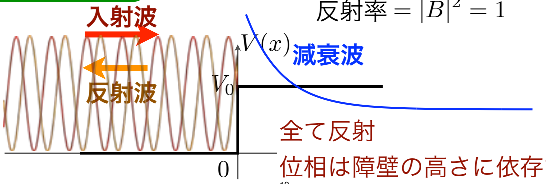
位相のずれ(phase shift)

$$\tan\delta_k = \frac{\alpha}{k} = \sqrt{\frac{V_0 - E}{E}}$$

$$B = \mathrm{e}^{-2i\delta_k}$$

$$D = 1 + \mathrm{e}^{-2i\delta_k}$$

$$反射率 = |B|^2 = 1$$

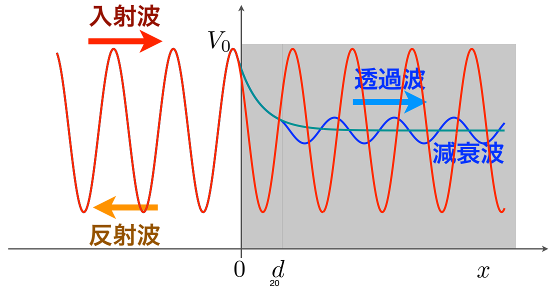


全て反射

位相は障壁の高さに依存する

箱形ポテンシャルによる散乱

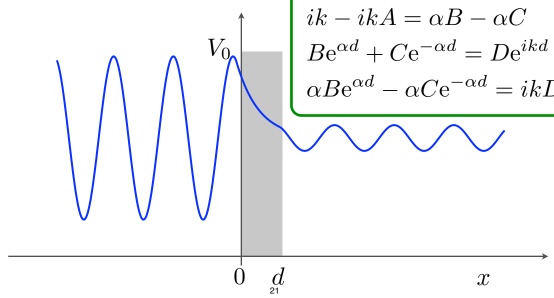
$$\varphi(x) = \mathrm{e}^{ikx} + A\mathrm{e}^{-ikx} \quad (x < 0)$$
$$B\mathrm{e}^{\alpha x} + C\mathrm{e}^{-\alpha x} \quad (0 \le x) < d)$$
$$D\mathrm{e}^{ikx} \quad (d \le x)$$



解の接続条件

$$\varphi(x) = \mathrm{e}^{ikx} + A\mathrm{e}^{-ikx} \quad (x < 0)$$
$$B\mathrm{e}^{\alpha x} + C\mathrm{e}^{-\alpha x} \quad (0 \le x < d)$$
$$D\mathrm{e}^{ikx} \quad (d \le x)$$

$$1 + A = B + C$$
$$ik - ikA = \alpha B - \alpha C$$
$$B\mathrm{e}^{\alpha d} + C\mathrm{e}^{-\alpha d} = D\mathrm{e}^{ikd}$$
$$\alpha B\mathrm{e}^{\alpha d} - \alpha C\mathrm{e}^{-\alpha d} = ikD\mathrm{e}^{ikd}$$

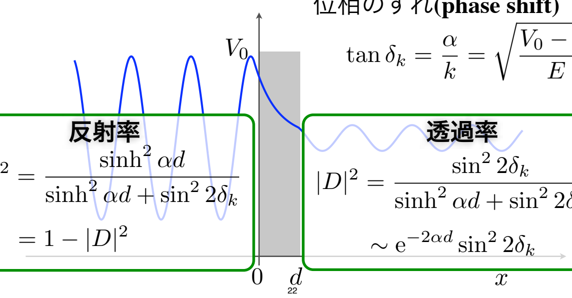


トンネル効果

$$\varphi(x) = \mathrm{e}^{ikx} + A\mathrm{e}^{-ikx} \quad (x < 0)$$
$$B\mathrm{e}^{\alpha x} + C\mathrm{e}^{-\alpha x} \quad (0 \le x < d)$$
$$D\mathrm{e}^{ikx} \quad (d \le x)$$

位相のずれ(phase shift)

$$\tan\delta_k = \frac{\alpha}{k} = \sqrt{\frac{V_0 - E}{E}}$$



反射率

$$|A|^2 = \frac{\sinh^2 \alpha d}{\sinh^2 \alpha d + \sin^2 2\delta_k} = 1 - |D|^2$$

透過率

$$|D|^2 = \frac{\sin^2 2\delta_k}{\sinh^2 \alpha d + \sin^2 2\delta_k} \sim \mathrm{e}^{-2\alpha d} \sin^2 2\delta_k$$

反射率

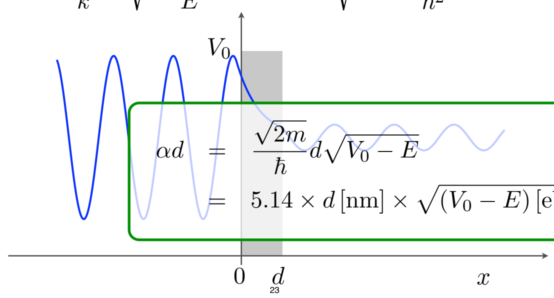
$$|A|^2 = \frac{\sinh^2 \alpha d}{\sinh^2 \alpha d + \sin^2 2\delta_k}$$

透過率

$$|D|^2 = \frac{\sin^2 2\delta_k}{\sinh^2 \alpha d + \sin^2 2\delta_k}$$

支配的因子

$$\tan\delta_k = \frac{\alpha}{k} = \sqrt{\frac{V_0 - E}{E}} \qquad \alpha d = \sqrt{\frac{2m(V_0 - E)d^2}{\hbar^2}}$$



$$\alpha d = \frac{\sqrt{2m}}{\hbar} d\sqrt{V_0 - E}$$
$$= 5.14 \times d\,[\mathrm{nm}] \times \sqrt{(V_0 - E)}\,[\mathrm{eV}]$$