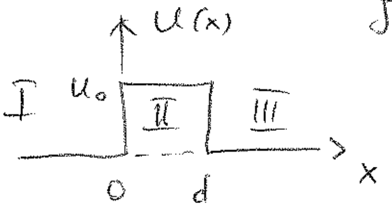
2.04.08

I Symmetric potential barrier

§1. Symmetric barrier: R & L solutions



We consider all states with energies $\varepsilon < \varepsilon_F$. For each energy ε, two solutions exist: one corresponding to transmission to the R from the left (L solution), and one R-solution (R→L). We shall now derive both explicitly.

1.1. L-solution

Three regions:

$$\text{I} \quad x<0; \qquad \text{II} \quad 0<x<d; \qquad \text{III} \quad x>d$$

Schrödinger eq. (a.4):

$$\text{I}: \quad \cancel{\frac{\hbar^2}{2m}} \; -\frac{1}{2}\frac{d^2}{dx^2}\psi = \varepsilon\psi \;\rightarrow\; \psi^L_{\text{I}} = e^{ikx} + r_L\, e^{-ikx}$$

with $\varepsilon = \dfrac{k^2}{2}$, $k = \sqrt{2\varepsilon}$.

$$\text{II}: \left[-\frac{1}{2}\frac{d^2}{dx^2} + U_0\right]\psi = \varepsilon\psi \;\rightarrow\; \psi^L_{\text{II}} = C_L e^{iqx} + D_L e^{-iqx}$$

with $\varepsilon = \frac{1}{2}q^2 + U_0$, $q = \sqrt{2(\varepsilon - U_0)}$

$$\text{III}: \; -\frac{1}{2}\frac{d^2}{dx^2}\psi = \varepsilon\psi \;\rightarrow\; \psi^L_{\text{III}} = t_L e^{ikx}, \qquad \varepsilon = \frac{k^2}{2},\; k = \sqrt{2\varepsilon}$$

Continuity of ψ & $d\psi/dx$ allows determination of coefficients:

$x=0$

$$\begin{cases} 1 + r_L = C_L + D_L \\ k(1 - r_L) = q(C_L - D_L) \end{cases} \quad (1)$$

$x=d$

$$\begin{cases} C_L e^{iqd} + D_L e^{-iqd} = t_L e^{ikd} \\ q\left(C_L e^{iqd} - D_L e^{-iqd}\right) = k t_L e^{ikd} \end{cases} \quad (2)$$

From (2):

$$C_L e^{iqd} + D_L e^{-iqd} = \frac{q}{k}\left(C_L e^{iqd} - D_L e^{-iqd}\right)$$

$$C_L e^{iqd}\left(1 - \frac{q}{k}\right) = -\left(1 + \frac{q}{k}\right) D_L e^{-iqd}$$

$$C_L = -\frac{q+k}{k-q}\, e^{-2iqd} D_L = \frac{q+k}{q-k}\, e^{-2iqd} D_L \equiv \varkappa_L D_L$$

Then, from (1): $r_L = C_L + D_L - 1$ into the 2nd eq. of (1):

$$1 - (C_L + D_L - 1) = \frac{q}{k}(C_L - D_L)$$

$$2 - C_L - D_L = \frac{q}{k} C_L - \frac{q}{k} D_L$$

$$2 - \varkappa_L D_L - D_L = \frac{q}{k}\varkappa_L D_L - \frac{q}{k} D_L$$

$$2 = \left(\frac{q}{k}\varkappa_L - \frac{q}{k} + \varkappa_L + 1\right) D_L \quad , \quad D_L = \frac{2}{1 + \varkappa_L + \frac{q}{k}(\varkappa_L - 1)}$$

where $\varkappa_L = e^{-2iqd}\,\dfrac{q+k}{q-k}$, so that

$$D_L = \frac{2}{1 + \frac{q+k}{q-k} e^{-2iqd} + \frac{q}{k}\left(\frac{q+k}{q-k} e^{-2iqd} - 1\right)}$$

$$= \frac{2}{1 - \frac{q}{k} + \frac{q+k}{q-k} e^{-2iqd}\left(1 + \frac{q}{k}\right)} = \frac{2(q-k)\cdot k}{-(q-k)^2 + (q+k)^2 e^{-2iqd}}$$

$$\boxed{D_L = \frac{-2k(q-k)}{(q-k)^2 - (q+k)^2 e^{-2iqd}}} \qquad \boxed{C_L = \frac{-2k(q+k)\, e^{-2iqd}}{(q-k)^2 - (q+k)^2 e^{-2iqd}}}$$

We now write r_L and t_L:

$$r_L = C_L + D_L - 1 = (\varkappa_L + 1) D_L - 1 = -1 + \frac{-2k(q-k)}{(q-k)^2 - (q+k)^2 e^{-2iqd}} \times$$

$$\times \left[\frac{q+k}{q-k} e^{-2iqd} + 1\right] = -1 + \frac{-2k\cancel{(q-k)}}{(q-k)^2 - (q+k)^2 e^{-2iqd}} \cdot \frac{(q+k)e^{-2iqd} + (q-k)}{\cancel{q-k}}$$

$$= \frac{-(q-k)^2 + (q+k)^2 e^{-2iqd} - 2k(q+k)e^{-2iqd} - 2k(q-k)}{(q-k)^2 - (q+k)^2 e^{-2iqd}}$$

The nominator $= -(q-k)(q-k+2k) + (q+k)e^{-2iqd}(q+k-2k)$

$$= -(q-k)(q+k) + (q+k)(q-k)e^{-2iqd} = (q^2-k^2)(e^{-2iqd} - 1)$$

and

$$\boxed{r_L = \frac{(q^2-k^2)(e^{-2iqd}-1)}{(q-k)^2-(q+k)^2 e^{-2iqd}}}$$

Finally,

$$t_L = \left(C_L e^{iqd} + D_L e^{-iqd}\right)e^{-ikd}$$

$$= e^{-ikd}\left\{ \frac{-2k(q+k)e^{-2iqd}}{\text{denom}} e^{iqd} + \frac{-2k(q-k)}{\text{denom}} e^{-iqd} \right\}$$

$$= e^{-ikd}e^{-iqd}\,\frac{-2k(q+k)-2k(q-k)}{\text{denom}} = \frac{-4kq}{\text{denom}}\,e^{-ikd}e^{-iqd}$$

$$\boxed{t_L = \frac{-4kq\,e^{-i(k+q)d}}{(q-k)^2-(q+k)^2 e^{-2iqd}}}$$

The solution depends on the energy ε versus the barrier:

(i) $\underline{\varepsilon > u_0}$ $\to$ q - real, and we express everything via energy now

$$\cancel{D_L = \frac{-2\sqrt{2\varepsilon}\left(\sqrt{2(\varepsilon-u_0)}-\sqrt{2\varepsilon}\right)}{\left(\sqrt{2(\varepsilon-u_0)}-\sqrt{2\varepsilon}\right)^2-\left(\sqrt{2(\varepsilon-u_0)}+\sqrt{2\varepsilon}\right)^2 e^{-2iqd}}}$$

$$D_L = \frac{-2k(q-k)}{(q^2+k^2)(1-e^{-2iqd})-2qk(1+e^{-2iqd})}$$

$$= \frac{-2k(q-k)\,e^{iqd}}{(q^2+k^2)(e^{iqd}-e^{-iqd})-2qk(e^{iqd}+e^{-iqd})}$$

$$= \frac{-2k(q-k)\,e^{iqd}}{(q^2+k^2)\,2i\sin(qd)-2qk\,2\cos(qd)} = \boxed{\frac{-k(q-k)\,e^{iqd}}{i(q^2+k^2)\sin(qd)-2kq\cos(qd)}}$$

Here $\frac{q^2}{2}+u_0 = \frac{k^2}{2}$, $q^2 = k^2-2u_0$, $q = \sqrt{k^2-2u_0}$ via k.

$$D_L = \frac{-k(\sqrt{k^2-2U_0}-k)\, e^{iqd}}{(2k^2-2U_0)\sin(qd) - 2k\sqrt{k^2-2U_0}\cos(qd)} \rightarrow \text{a function of } k \text{ (or } \varepsilon) \text{ only.}$$

No much simplification, we keep k & q.

$$C_L = \frac{-2k(q+d)\, e^{-iqd}}{(q-k)^2 e^{iqd} - (q+k)^2 e^{-iqd}} = \frac{-2k(q+\cancel{k})\, e^{-iqd}}{(q^2+k^2)(e^{iqd}-e^{-iqd}) - 2kq(e^{iqd}+e^{-iqd})}$$

$$\boxed{C_L = \frac{-k(q+k)\, e^{-iqd}}{i(q^2+k^2)\sin(qd) - 2kq\cos(qd)}}$$

Next,

$$r_L = \frac{(q^2-k^2)(e^{-iqd}-e^{iqd})}{(q-k)^2 e^{iqd} - (q+k)^2 e^{-iqd}} = \boxed{\frac{-i(q^2-k^2)\sin(qd)}{i(q^2+k^2)\sin(qd) - 2kq\cos(qd)}}$$

$$t_L = \frac{-4kq\, e^{-ikd}}{(q-k)^2 e^{iqd} - (q+k)^2 e^{-iqd}} = \boxed{\frac{-2kq\, e^{-ikd}}{i(q^2+k^2)\sin(qd) - 2kq\cos(qd)}}$$

(ii) $0 < \varepsilon < U_0$ Here $q = i\sqrt{2(U_0-\varepsilon)} = i\lambda$ purely imaginary.

$\boxed{\sin(i\lambda x) = i\sinh(\lambda x)}$ and $\boxed{\cos(i\lambda x) = \cosh(\lambda x)}$

$$\left[\begin{aligned} \sin(ix) &= \frac{1}{2i}(e^{i(ix)} - e^{-i(ix)}) = \frac{1}{2i}(e^{-x}-e^{x}) = -\frac{1}{i}\sinh(x) \\ \cos(ix) &= \frac{1}{2}(e^{iix}+e^{-iix}) = \frac{1}{2}(e^{-x}+e^{x}) \equiv \cosh(x) \end{aligned}\right]$$

Using these, we reexpress: sin/cos via sinh/cosh:

$$D_L = \frac{-k(q-k)\, e^{-\lambda d}}{-(q^2+k^2)\sinh(\lambda d) - 2kq\cosh(\lambda d)} = \frac{k(i\lambda-k)\, e^{-\lambda d}}{(k^2-\lambda^2)\sinh(\lambda d) - 2ik\lambda\cosh(\lambda d)}$$

$$C_L = \frac{-k(q+k)\, e^{\lambda d}}{-(q^2+k^2)\sinh(\lambda d) - 2kq\cos(\lambda d)} = \frac{k(k+i\lambda)\, e^{\lambda d}}{(k^2-\lambda^2)\sinh(\lambda d) - 2ki\lambda\cosh(\lambda d)}$$

$$r_L = \frac{(q^2-k^2)\sinh(\lambda d)}{-(q^2+k^2)\sinh(\lambda d) - 2kq\cosh(\lambda d)} \equiv \frac{(\lambda^2+k^2)\sinh(\lambda d)}{(k^2-\lambda^2)\sinh(\lambda d) - 2ki\lambda\cosh(\lambda d)}$$

$$t_L = \frac{-2kq\, e^{-ikd}}{-(q^2+k^2)\sinh(\lambda d) - 2kq\cos(\lambda d)} \equiv \frac{2ki\lambda\, e^{-ikd}}{(k^2-\lambda^2)\sinh(\lambda d) - 2ki\lambda\cosh(\lambda d)}$$

- We now combine all coefficients into this Table:

	$0 < \varepsilon < U_0$	$\varepsilon > U_0$
	$\lambda = \sqrt{-k^2+2U_0} = \sqrt{2(U_0-\varepsilon)}$	$q = \sqrt{k^2-2U_0} = \sqrt{2(\varepsilon-U_0)}$
D_L	$\dfrac{k(i\lambda-k)\, e^{-\lambda d}}{(k^2-\lambda^2)\sinh(\lambda d) - 2ik\lambda\cosh(\lambda d)}$!	$\dfrac{k(k-q)\, e^{iqd}}{i(q^2+k^2)\sin(qd) - 2kq\cos(qd)}$
C_L	$\dfrac{k(k+i\lambda)\, e^{\lambda d}}{(k^2-\lambda^2)\sinh(\lambda d) - 2ik\lambda\cosh(\lambda d)}$	$\dfrac{-k(k+q)\, e^{-iqd}}{i(q^2+k^2)\sin(qd) - 2kq\cos(qd)}$
r_L	$\dfrac{(\lambda^2+k^2)\sinh(\lambda d)}{(k^2-\lambda^2)\sinh(\lambda d) - 2ik\lambda\cosh(\lambda d)}$	$\dfrac{-i(q^2-k^2)\sin(qd)}{i(q^2+k^2)\sin(qd) - 2kq\cos(qd)}$
t_L	$\dfrac{2ik\lambda\, e^{-ikd}}{(k^2-\lambda^2)\sinh(\lambda d) - 2ik\lambda\cosh(\lambda d)}$	$\dfrac{-2kq\, e^{-ikd}}{i(q^2+k^2)\sin(qd) - 2kq\cos(qd)}$

- We can now calculate the current due to this state at energy ε. The current

$$j_{L,\varepsilon} = \langle \psi_\varepsilon^L | \hat{j} | \psi_\varepsilon^L \rangle, \quad \hat{j} = \frac{ie\hbar}{2m}\left[\overleftarrow{\frac{d}{dx}} - \overrightarrow{\frac{d}{dx}}\right]$$

$$j_{L\varepsilon} = \frac{ie\hbar}{2m}\left\{ \frac{d\psi_\varepsilon^{L*}}{dx}\psi_\varepsilon^L - \psi_\varepsilon^{L*}\frac{d\psi_\varepsilon^L}{dx} \right\}$$

In region I, $\psi^L_E = \psi_I = e^{ikx} + r_L e^{-ikx}$

$$j_{LE} = \frac{ie\hbar}{2m}\left\{\left(-ik e^{-ikx} + r_L^* ik e^{ikx}\right)\left(e^{ikx} + r_L e^{-ikx}\right) - \right.$$

$$\left. - \left(e^{-ikx} + r_L^* e^{ikx}\right)\left(ik e^{ikx} - r_L ik e^{-ikx}\right)\right\}$$

$$= \frac{ie\hbar}{2m}\left\{\left(-ik + \cancel{ikr_L^* e^{2ikx}} - \cancel{ikr_L e^{-2ikx}} + |r_L|^2 ik\right) - \right.$$

$$\left. - \left(ik + \cancel{r_L^* ik e^{2ikx}} - \cancel{r_L ik e^{-2ikx}} - ik|r_L|^2\right)\right\}$$

$$= \frac{ie\hbar}{2m}\left\{-2ik + 2|r_L|^2 ik\right\} = \frac{e\hbar k}{m}\left(1 - |r_L|^2\right)$$

The current should not depend on the region. Use ψ_{III} now:

$$j_{LE} = \frac{ie\hbar}{2m}\left\{t_L^*(-ik)e^{-ikx} \cdot t_L e^{ikx} - t_L^* e^{-ikx} \cdot (ik)\, t_L e^{ikx}\right\}$$

$$= \frac{ie\hbar}{2m} |t_L|^2 (-ik2) = \frac{e\hbar k}{m}|t_L|^2$$

so that

$$\boxed{1 - |r_L|^2 = |t_L|^2}$$

This can be checked by an independent calculation, e.g. for $E > U_0$:

$$1 - |r_L|^2 = 1 - \left|\frac{-i(q^2-k^2)\sin(qd)}{i(q^2+k^2)\sin(qd) - 2kq\cos(qd)}\right|^2$$

$$\cancel{= \frac{i(q^2+k^2)S - 2kqC + i(q^2-k^2)S}{i(q^2+k^2)S - 2kqC} = \frac{-2kqC + 2iq^2S}{i(q^2+k^2)S - 2kqC}}$$

$$= 1 - \frac{(q^2-k^2)^2 S^2}{(q^2+k^2)^2 S^2 + (2kq)^2 C^2} = \frac{(q^2+k^2)^2 S^2 + (2kq)^2 C^2 - (q^2-k^2)^2 S^2}{(q^2+k^2)^2 S^2 + (2kq)^2 C^2}$$

where the ~~d~~ nominator

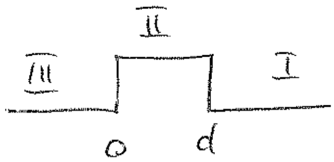
$$=\left((q^2+k^2)^2-(q^2-k^2)^2\right)s^2+(2kq)^2c^2=$$

$$=(\cancel{q^2}+k^2-\cancel{q^2}+k^2)(q^2+\cancel{k^2}+q^2-\cancel{k^2})\,s^2+(2kq)^2c^2$$

$$=4k^2q^2s^2+(2kq)^2c^2=4k^2q^2,$$

and we obtain $\dfrac{4k^2q^2}{\text{denominator}}$, which is exactly $|t_L|^2$.

1.2. R-solution



I: $\quad \psi^R_{I}=e^{-ikx}+r_R\,e^{ikx}, \qquad k=\sqrt{2\varepsilon}$

II: $\quad \psi^R_{II}=C_R\,e^{-iqx}+D_R\,e^{iqx}, \qquad q=\sqrt{2(\varepsilon-U_0)}$

III: $\quad \psi^R_{III}=t_R\,e^{-ikx}$

and the conditions at the boundaries of the regions:

$\underline{x=0}$

$$\begin{cases} t_R=C_R+D_R \\ -k\,t_R=-q\,(C_R-D_R) \end{cases}$$

$\underline{x=d}$

$$\begin{cases} C_R e^{-iqd}+D_R e^{iqd}=e^{-ikd}+r_R e^{ikd} \\ -q\left(C_R e^{-iqd}-D_R e^{iqd}\right)=-k\left(e^{-ikd}-r_R e^{ikd}\right) \end{cases}$$

We can eqs. for $x=d$ into $x=0$ eqs for the L case; e.g. the 1s eq.:

$$C_R\,e^{-iqd}e^{ikd}+D_R\,e^{iqd}e^{ikd}=1+r_R\,e^{2ikd}$$

So after

$$\tilde{C}_R=C_R\,e^{-iqd}e^{ikd}, \quad \tilde{D}_R=D_R\,e^{iqd}e^{ikd}, \quad \tilde{r}_R=r_R\,e^{2ikd}$$

they become:

$$\begin{cases} \tilde{C}_R+\tilde{D}_R=1+\tilde{r}_R \\ q(\tilde{C}_R-\tilde{D}_R)=k(1-\tilde{r}_R) \end{cases}$$

The $x=0$ eqs become:

$$\begin{cases} t_R = \tilde{C}_R e^{iqd} e^{-ikd} + \tilde{D}_R e^{-iqd} e^{-ikd} \\ k t_R = q\left(\tilde{C}_R e^{iqd} e^{-ikd} - \tilde{D}_R e^{-iqd} e^{-ikd}\right) \end{cases}$$

which, ~~after changing~~

$$\cancel{\tilde{t}_R = t_R e^{ikd}} \qquad \tilde{t}_R \equiv t_R$$

become:

$$\begin{cases} \tilde{t}_R e^{ikd} = \tilde{C}_R e^{iqd} + \tilde{D}_R e^{-iqd} \\ k \tilde{t}_R e^{ikd} = q\left(\tilde{C}_R e^{iqd} - \tilde{D}_R e^{-iqd}\right) \end{cases}$$

which are exactly the same as in the L case. Thus, the solutions ~~for $\tilde{C}_R, \tilde{D}_R$~~ are:

$$\tilde{C}_R \equiv C_L, \quad \tilde{D}_R \equiv D_L, \quad \tilde{t}_R \equiv t_L, \quad \tilde{r}_R \equiv r_L \cancel{e^{-ikd}}$$

$$\boxed{\begin{array}{ll} C_R = C_L e^{iqd} e^{-ikd} & t_R = t_L \\ D_R = D_L e^{-iqd} e^{-ikd} & r_R = r_L e^{-2ikd} \end{array}}$$

- The current due to the state ψ_R^ε of energy ε (of k) is then: (we calculate it in region III):

$$j_R^\varepsilon = \frac{ie\hbar}{2m}\left(\frac{d\psi_R^*}{dx}\psi_R - \psi_R^*\frac{d\psi_R}{dx}\right) =$$

$$= \frac{ie\hbar}{2m}\left[t_R^*(ik)e^{ikx}\cdot t_R e^{-ikx} - t_R^* e^{ikx}\cdot t_R(-ik)e^{-ikx}\right]$$

$$= \frac{ie\hbar}{2m}\left(ik|t_R|^2 + ik|t_R|^2\right) = -\frac{e\hbar k}{m}|t_R|^2$$

Since $|t_R|^2 \equiv |t_L|^2$, the $\boxed{j_R^\varepsilon \equiv -j_L^\varepsilon}$, i.e. the total current is indeed zero.