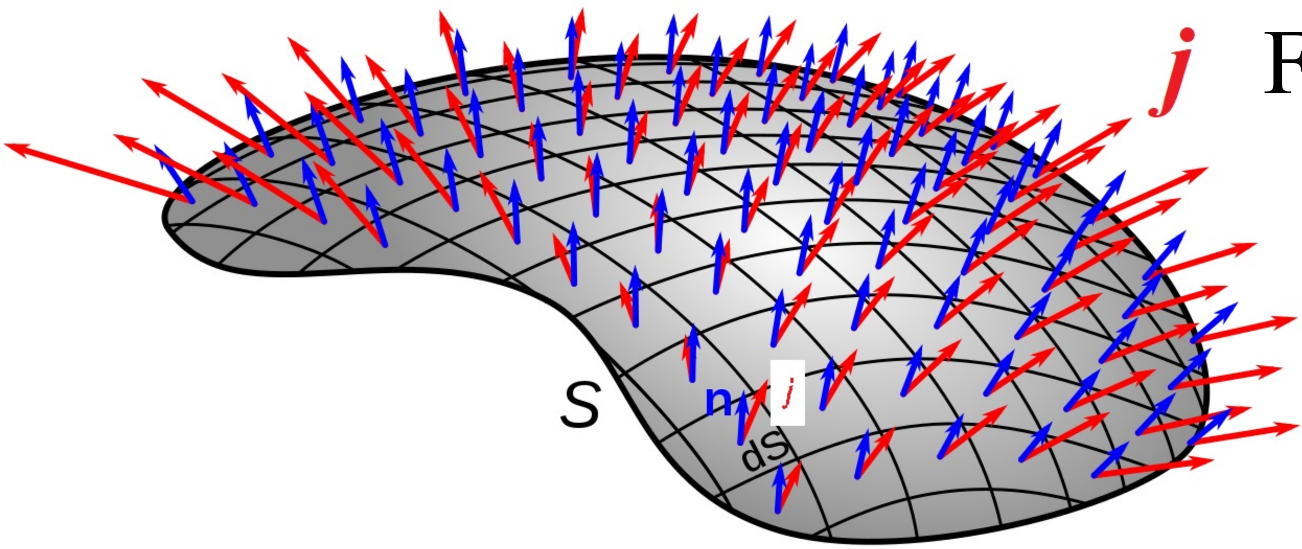
An essential bit about the continuity equation ?

A closed surface of arbitrary shape has N particles inside. Some might be going out and coming in. If particles cannot be created or destroyed, the following must hold.....



$$\text{Flux} \equiv \iint_{\text{surface}} \vec{j}\,.\,\hat{n}\,dS$$

$\hat{n}$ outward normal

$$-\frac{\partial N_{inside}}{\partial t} = \oint\!\!\oint_{\substack{\text{enclosing}\\ \text{surface}}} \vec{j}_{particle}\,.\,\vec{dS} = \int_{\text{volume}} \nabla\,.\,\vec{j}\,d\tau$$

Gauss's theorem

$$N_{inside} \equiv \int_{\text{volume}} \rho\,d\tau \;\Rightarrow\; \int_{\text{volume}} \left(\frac{\partial \rho}{\partial t} + \nabla\,.\,\vec{j}\right) d\tau = 0$$

Consistency of the interpretation of $\Psi^* \Psi$ with continuity theorem

Is our probablilistic interpretation is consistent ?

We can derive a continuity relation for $\rho \equiv \psi^* \psi$

$$\psi^* \left[-\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi \right] = \psi^* \left[i \hbar \frac{\partial \psi}{\partial t} \right] \qquad \dots(1)$$

$$\psi \left[-\frac{\hbar^2}{2m} \nabla^2 \psi + V \psi \right]^* = \psi \left[i \hbar \frac{\partial \psi}{\partial t} \right]^* \qquad \dots(2)$$

Note : $i^* = -i$ and subtract (2) from (1)

$$\Rightarrow \frac{\hbar^2}{2m} \left[\psi \nabla^2 \psi^* - \psi^* \nabla^2 \psi \right] = i \hbar \frac{\partial}{\partial t} \psi^* \psi$$

Simplify LHS using the identity $\nabla . \phi \vec{A} = \nabla \phi . A + \phi \nabla . \vec{A}$

$$\nabla . \left[\psi^* \nabla \psi \right] = \left(\nabla \psi \right)^* . \left(\nabla \psi \right) + \psi^* \nabla^2 \psi$$

$$\nabla . \left[\psi \nabla \psi^* \right] = \left(\nabla \psi \right) . \left(\nabla \psi \right)^* + \psi \nabla^2 \psi^*$$

Consistency of the interpretation of $\Psi^* \Psi$ with continuity theorem

$$\frac{\hbar}{2i\,m}\left[\psi\nabla^2\psi^* - \psi^*\nabla^2\psi\right] = \frac{\partial}{\partial t}|\psi|^2$$

$$-\nabla\cdot\left(\frac{\hbar}{m}\right)\left[\frac{\psi^*\nabla\psi - \psi(\nabla\psi)^*}{2i}\right] = \frac{\partial}{\partial t}|\psi|^2$$

$$\nabla\cdot\left[\Im\frac{\hbar}{m}\psi^*\nabla\psi\right] + \frac{\partial}{\partial t}|\psi|^2 = 0 \;\Rightarrow\; \nabla\vec{j} + \frac{\partial\rho}{\partial t} = 0$$

$$\text{where}\begin{cases}\text{Probability current} & : \vec{j} = \Im\dfrac{\hbar}{m}\psi^*\nabla\psi \\ \text{Probability density} & : \rho = |\psi|^2\end{cases}$$

Notice how the form of the continuity equation emerges naturally from the definition

If $\psi = Ae^{ikx}$ what is $\vec{j}$.......if ψ is real , current MUST be zero!

$$\vec{j} = \frac{\hbar}{m}\Im\left(\psi^* \nabla \psi\right) \qquad \psi = A\, e^{-i\vec{k}.\vec{r}}$$

$$= \frac{\hbar}{m}\Im\left[A^* e^{-i\vec{k}.\vec{r}}(i\vec{k})\, A\, e^{-i\vec{k}.\vec{r}}\right]$$

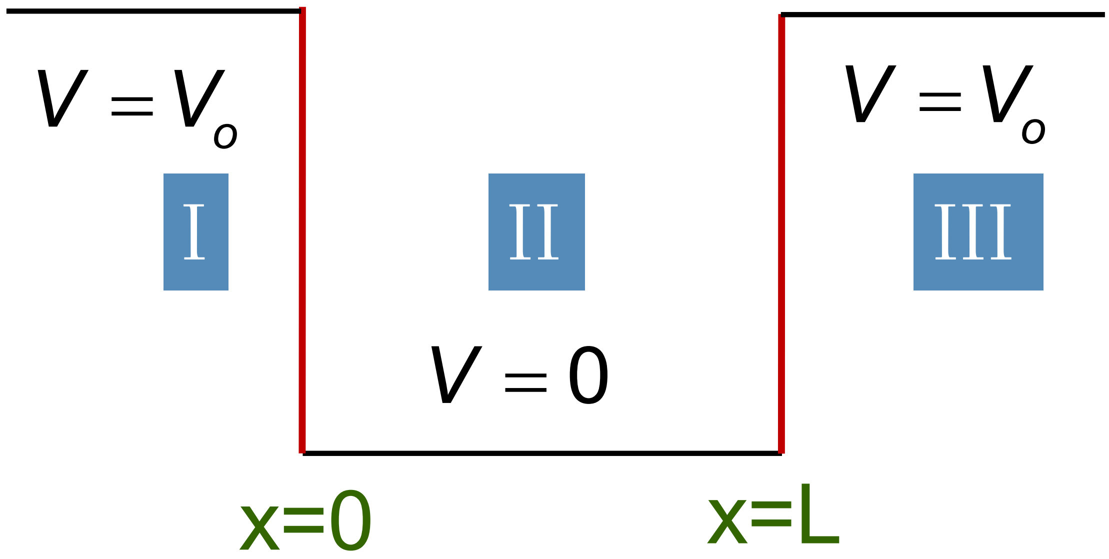
$$= \boxed{|A|^2 \frac{\hbar}{m}\vec{k} = |A|^2 \frac{\vec{p}}{m}}$$

agrees with intuition

If ψ is REAL $\Rightarrow \vec{j} = 0$ always

What if $\psi = A\, e^{i\vec{k}.\vec{r}} + B\, e^{-i\vec{k}.\vec{r}}$?

Problem 3 : a particle in a finite potential well : the first non-trivial one!



We need to know what the wavefunction will do at the boundaries.

The wavefunction MUST be continuous at I-II & II-III

The discontinuity of the potential is *finite* , (in this case), → the derivative of the wavefunction should also be continuous.

We will look for the bound state solutions only. There are of course possible solutions for which the wavefunction does stretch till infinity

Problem 3 : a particle in a finite potential well : the first non-trivial one!

Region I : $-\frac{\hbar^2}{2m}\frac{d^2\psi_I}{dx^2}+V_0\psi_I = E\psi_I \qquad E<V_0$

$$\frac{d^2\psi_I}{dx^2} - \alpha^2\psi_{II} = 0 \qquad \alpha^2=\frac{2m(V_0-E)}{\hbar^2}$$

Wavefn $\psi_I = Ae^{\alpha x}$ finite as $x\to-\infty$

Region II : $-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} + 0\psi_{II} = E\psi_{II} \qquad 0<E<V_0$

$$\frac{d^2\psi_{II}}{dx^2} + k^2\psi_{II} = 0 \qquad k^2=\frac{2mE}{\hbar^2}$$

Wavefn $\psi_{II} = \begin{cases} Ce^{ikx} + De^{-ikx} \\ \text{OR} \\ C\sin kx + D\cos kx \end{cases}$

Region III : $-\frac{\hbar^2}{2m}\frac{d^2\psi_{III}}{dx^2}+V_0\psi_{III} = E\psi_{III} \qquad E<V_0$

Wavefn $\psi_{III} = He^{-\alpha x}$ finite as $x\to\infty$

Problem 3 : finite potential well : Applying the boundary conditions

Using $\psi_{II} = C\sin kx + D\cos kx$ ....

$$\psi_I(0) = \psi_{II}(0) \quad \Rightarrow \quad A = D$$

$$\psi_I'(0) = \psi_{II}'(0) \quad \Rightarrow \quad A\alpha = Ck$$

$$\psi_{II}(L) = \psi_{III}(L) \quad \Rightarrow \quad C\sin kL + D\cos kL = He^{-\alpha L}$$

$$\psi_{II}'(L) = \psi_{III}'(L) \quad \Rightarrow \quad Ck\cos kL - Dk\sin kL = -H\alpha e^{-\alpha L}$$

Use the first two to eliminate C and D......

$$\left.\begin{aligned} \frac{\alpha}{k}\sin kL + \cos kL &= \frac{H}{A}e^{-\alpha L} \\ \alpha\cos kL - k\sin kL &= -\frac{H}{A}\alpha e^{-\alpha L} \end{aligned}\right\} \Rightarrow \tan kL = -\frac{2\alpha k}{\alpha^2 - k^2}$$

Problem 3 : finite potential well : Applying the boundary conditions

$$\tan kL = \frac{2\tan\frac{kL}{2}}{1-\tan^2\frac{kL}{2}} = \frac{2}{k/\alpha - \alpha/k} \Rightarrow \tan\frac{kL}{2} = \begin{cases} \alpha/k \\ -k/\alpha \end{cases}$$

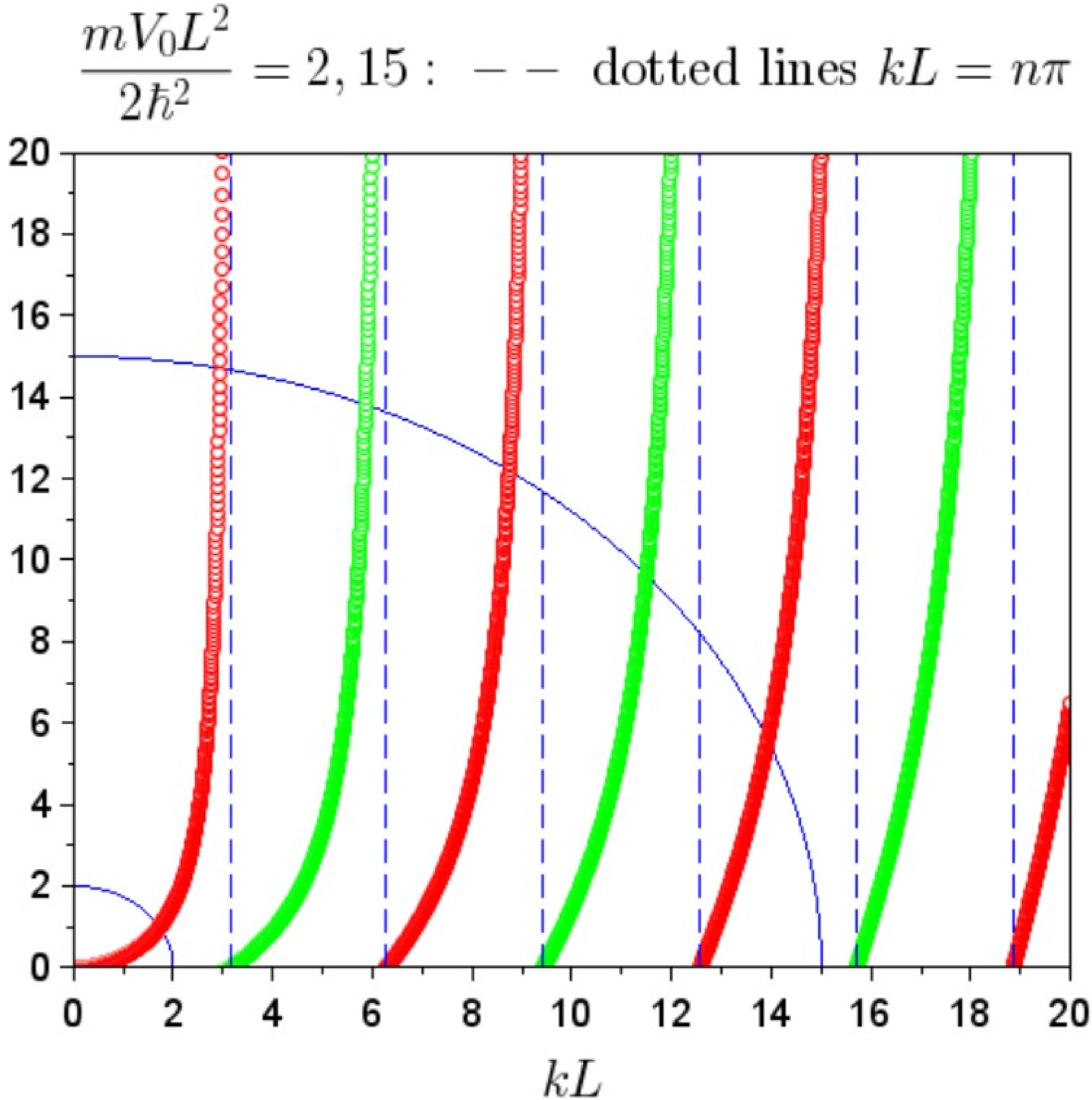
Recall $\alpha^2 = \frac{2m}{\hbar^2}(V_0 - E)$ & $k^2 = \frac{2m}{\hbar^2}E$

The allowed values of k are obtained by solving

$$\frac{kL}{2}\tan\frac{kL}{2} = \sqrt{\frac{mV_0L^2}{2\hbar^2} - \left(\frac{kL}{2}\right)^2}$$

$$-\frac{kL}{2}\cot\frac{kL}{2} = \sqrt{\frac{mV_0L^2}{2\hbar^2} - \left(\frac{kL}{2}\right)^2}$$

Problem 3 : finite potential well : Solving it graphically



Red curve
→ ground state
→ even function

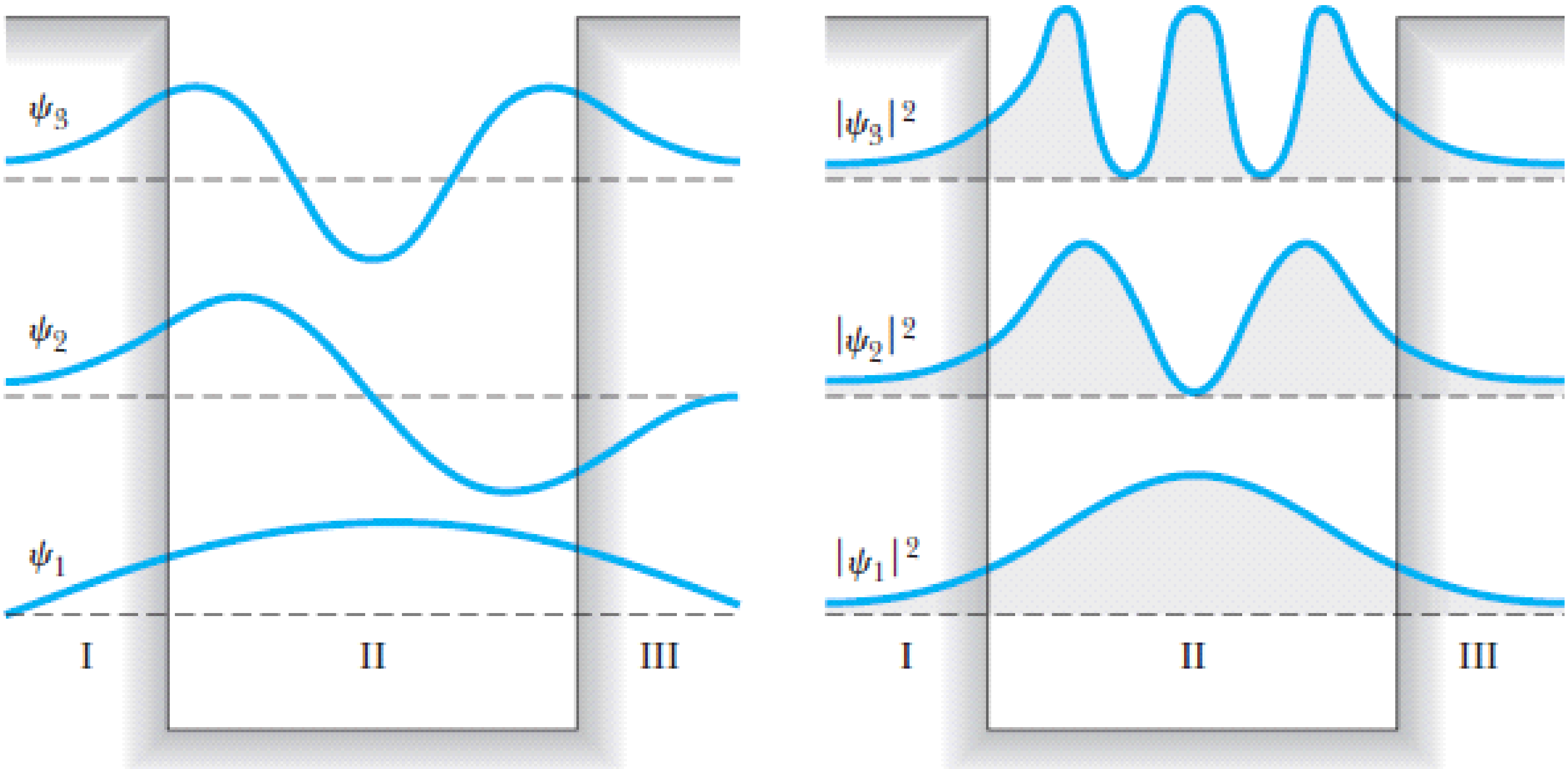
Odd-even (about the center of the potential well) solutions alternate
→ ground state is even

Dotted line
→ infinite well values

At least one solution will always be there.

What is the total number of allowed states ?

Problem 3 : finite potential well : Solving it graphically

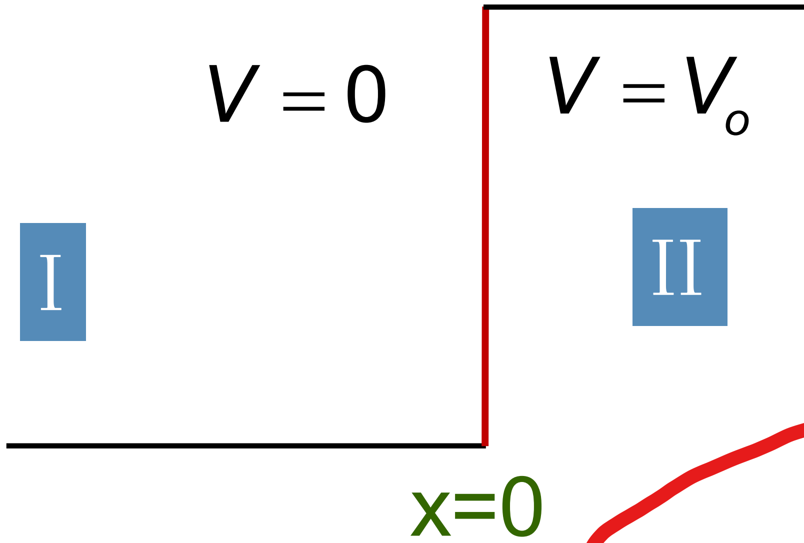


(a) (b)

Notice the that there is a finite probability of locating the particle in "clasically forbidden“ region where E < V and the classical KE < 0. This is a purely quantum phenomena

The lower energy states have lower leakage into the barrier

Problem 4 : The potential step for $E > V_0$



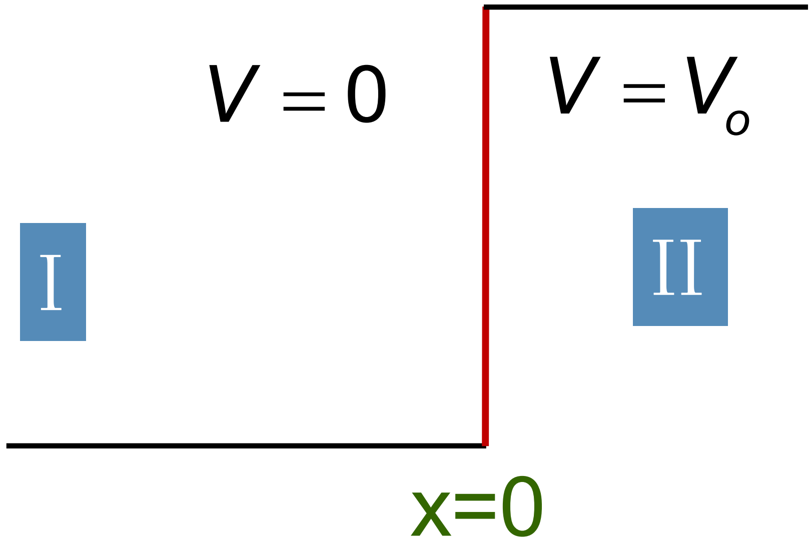
$$k_1^2 = \frac{2mE}{\hbar^2}$$

$$k_2^2 = \frac{2m}{\hbar^2}\left(E - V_0\right)$$

$$E > V_0 \Rightarrow \begin{cases} \psi_I = A e^{i k_1 x} + B e^{-i k_1 x} & \Rightarrow \text{left \& right going waves} \\ \psi_{II} = C e^{i k_2 x} & \Rightarrow \text{only right going waves} \end{cases}$$

$$\left.\begin{array}{lllll} \psi_I(0) = \psi_{II}(0) & \Rightarrow & A + B & = & C \\ \psi_I'(0) = \psi_{II}'(0) & \Rightarrow & ik_1(A - B) & = & i k_2 C \end{array}\right\} \Rightarrow \boxed{\begin{array}{l} \dfrac{B}{A} = \dfrac{k_1 - k_2}{k_1 + k_2} \\[2ex] \dfrac{C}{A} = \dfrac{2k_1}{k_1 + k_2} \end{array}}$$

Problem 4 : The potential step : Is incident current = reflected + transmitted ?



$$j_I = j_{INCIDENT} - j_{REFLECTED}$$
$$j_{II} = j_{TRANSMITTED}$$

$$\psi_I = Ae^{ikx} + Be^{-ikx} \Rightarrow j_I = \Im\left(\frac{\hbar}{m}\psi_I{}^* \frac{d\,\psi_I}{dx}\right) = \frac{\hbar k_1}{m}\left(|A|^2 - |B|^2\right)$$

$$\psi_{II} = Ce^{ikx} \Rightarrow j_{II} = \Im\left(\frac{\hbar}{m}\psi_{II}{}^* \frac{d\,\psi_{II}}{dx}\right) = \frac{\hbar k_2}{m}|C|^2$$

We need to show : $j_{INCIDENT} = j_{REFLECTED} + j_{TRANSMITTED}$

Problem 4 : The potential step : Is incident current = reflected + transmitted ?

$$j_{INCIDENT} = \frac{\hbar}{m} k_1 |A|^2$$

$$j_{REFLECTED} = \frac{\hbar}{m} k_1 |B|^2 = \frac{\hbar}{m} k_1 \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2 |A|^2$$

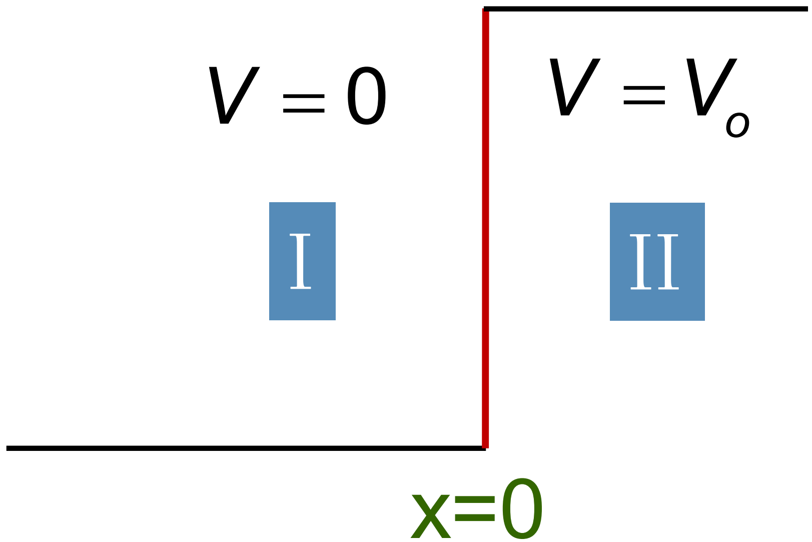
$$j_{TRANSMITTED} = \frac{\hbar}{m} k_2 |C|^2 = \frac{\hbar}{m} k_2 \left(\frac{2k_1}{k_1 + k_2} \right)^2 |A|^2$$

They add up exactly as expected from conservation of current

Notice that even when the energy is high enough to go over the barrier there is a finite probablity of the particle being reflected. This too is a quantum mechanical effect with no classical analogue.

You should be able to convince yourself that if the barrier height exceeds the energy then the particle is completely reflected even though the wavefunction will be present in the barrier (step) region. Can you say this without doing the calculation ?

Problem 4 : The potential step for $E < V_0$



$$k_1^2 = \frac{2mE}{\hbar^2}$$

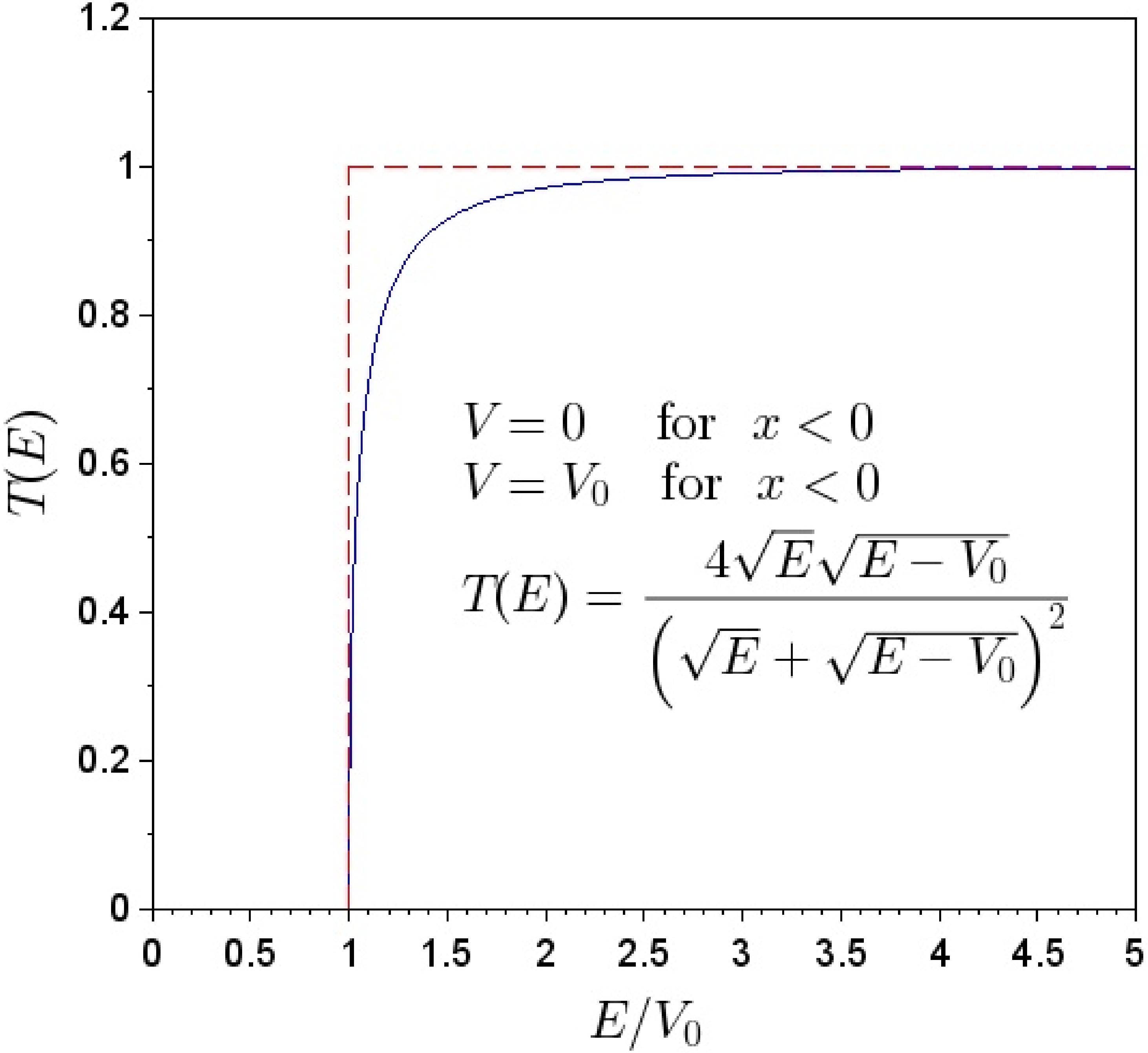
$$k_2^2 = \frac{2m}{\hbar^2}\left(V_0 - E\right)$$

$$E < V_0 \Rightarrow \begin{cases} \psi_I = A e^{i k_1 x} + B e^{-i k_1 x} & \Rightarrow \text{left and right going waves} \\ \psi_{II} = C e^{-k_2 x} & \Rightarrow \text{decaying solution } \psi(\infty) \to 0 \end{cases}$$

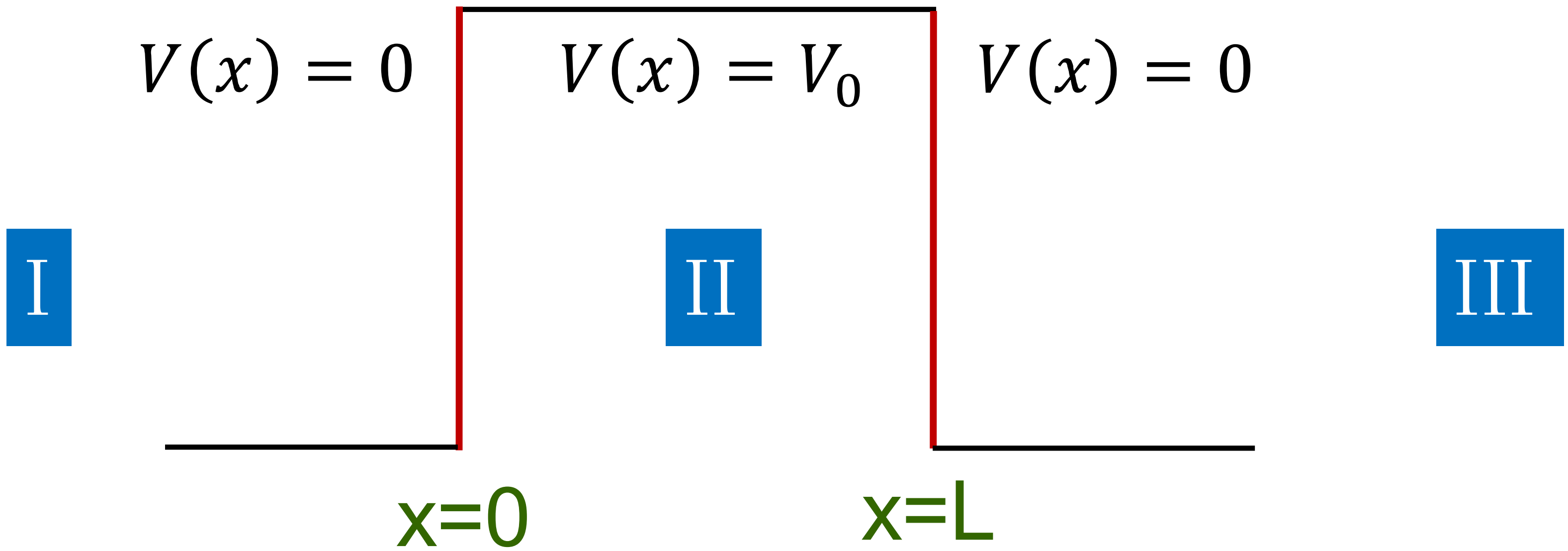
$$\left.\begin{array}{lllll} \psi_I(0) & = \psi_{II}(0) & \Rightarrow & A + B & = C \\ \psi_I{}'(0) & = \psi_{II}{}'(0) & \Rightarrow & ik_1(A - B) & = -k_2 C \end{array}\right\} \Rightarrow \begin{array}{l} \dfrac{B}{A} = -\dfrac{k_2 + ik_1}{k_2 - ik_1} \\ \dfrac{C}{A} = \dfrac{2k_2}{k_2 - ik_1} \end{array}$$

ψ_{II} is real $\Rightarrow j_{TRANSMIITTED} = 0$ which is fully consistent with $|A| = |B|$

Problem 4 : The potential step for $E < V_0$ and $E > V_0$



Problem 5 : The potential barrier for $E > V_0$ or $E < V_0$



$$k_1^2 = \frac{2mE}{\hbar^2} \qquad k_2^2 = \frac{2m}{\hbar^2}(E - V_0) \qquad \alpha^2 = \frac{2m}{\hbar^2}(V_0 - E)$$

$$A e^{ik_1 x} + B e^{-ik_1 x} \qquad \begin{Bmatrix} C e^{ik_2 x} & + & D e^{-ik_2 x} \\ C e^{\alpha x} & + & D e^{-\alpha x} \end{Bmatrix} \qquad G e^{ik_1 x}$$

We need to relate G with A

Problem 5 : The potential barrier for $E > V_0$ or $E < V_0$

$E > V_0$

$$\psi_I(0) = \psi_{II}(0) \quad \Rightarrow \quad A + B = C + D$$

$$\psi_I{}'(0) = \psi_{II}{}'(0) \quad \Rightarrow \quad ik_1(A - B) = ik_2(C - D)$$

$$\psi_{II}(L) = \psi_{III}(L) \quad \Rightarrow \quad C e^{ik_2 L} + D e^{-ik_2 L} = G e^{ik_1 L}$$

$$\psi_{II}{}'(L) = \psi_{III}{}'(L) \quad \Rightarrow \quad ik_2\left(C e^{ik_2 L} - D e^{-ik_2 L}\right) = i k_1 G e^{ik_1 L}$$

$E < V_0$

$$\psi_I(0) = \psi_{II}(0) \quad \Rightarrow \quad A + B = C + D$$

$$\psi_I{}'(0) = \psi_{II}{}'(0) \quad \Rightarrow \quad ik_1(A - B) = \alpha(C - D)$$

$$\psi_{II}(L) = \psi_{III}(L) \quad \Rightarrow \quad C e^{\alpha L} + D e^{-\alpha L} = G e^{ik_1 L}$$

$$\psi_{II}{}'(L) = \psi_{III}{}'(L) \quad \Rightarrow \quad \alpha\left(C e^{\alpha L} - D e^{-\alpha L}\right) = i k_1 G e^{ik_1 L}$$

Problem 5 : The potential barrier for $E > V_0$ or $E < V_0$

Express A & B in terms of C & D using first two eqns

Use the last two equations to write C, D in terms of G

Combine the two sets of expressions to obtain a relation between A,B and G

$$\begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 1 + k_2/k_1 & 1 - k_2/k_1 \\ 1 - k_2/k_1 & 1 + k_2/k_1 \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix}$$

$$\begin{pmatrix} C \\ D \end{pmatrix} = \frac{G}{2} e^{i k_1 L} \begin{pmatrix} \left(1 + k_1/k_2\right) e^{-i k_2 L} \\ \left(1 - k_1/k_2\right) e^{i k_2 L} \end{pmatrix}$$

Problem 5 : The potential barrier for $E > V_0$ or $E < V_0$

$$A = \frac{e^{ik_1L}}{4}\left[\left(2+\frac{k_1}{k_2}+\frac{k_2}{k_1}\right)e^{-ik_2L}+\left(2-\frac{k_1}{k_2}-\frac{k_2}{k_1}\right)e^{ik_2L}\right]G$$

$$|A|^2 = \left[1+\frac{1}{4}\left(\frac{k_1}{k_2}-\frac{k_2}{k_1}\right)^2\sin^2 k_2 L\right]|G|^2$$

$$\frac{|G|^2}{|A|^2} = \frac{1}{1 + \dfrac{V_0^{\,2}}{4E\left(E-V_0\right)}\sin^2 k_2 L} \qquad E > V_0$$

recall : $k_2^{\,2} = \dfrac{2m}{\hbar^2}\left(E - V_0\right)$

There are resonances (complete transmission) for $kL = n\pi$

An integer number of oscillations fit in the barrier

Problem 5 : The potential barrier for $E > V_0$ or $E < V_0$

Express A & B in terms of C & D using first two eqns

Use the last two equations to write C, D in terms of G

Combine the two sets of expressions to obtain a relation between A,B and G

$$\begin{pmatrix} A \\ B \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 - i\alpha/k_1 & 1 + i\alpha/k_1 \\ 1 + i\alpha/k_1 & 1 - i\alpha/k_1 \end{pmatrix}\begin{pmatrix} C \\ D \end{pmatrix}$$

$$\begin{pmatrix} C \\ D \end{pmatrix} = \frac{G}{2} e^{i k_1 L}\begin{pmatrix} \left(1 + ik_1/\alpha\right) e^{-\alpha L} \\ \left(1 - ik_1/\alpha\right) e^{\alpha L} \end{pmatrix}$$

Problem 5 : The potential barrier for $E > V_0$ or $E < V_0$

$$A = \frac{e^{i k_1 L}}{4}\left[\left(2 + i\frac{k_1}{\alpha} - i\frac{\alpha}{k_1}\right)e^{-\alpha L} + \left(2 - i\frac{k_1}{\alpha} - i\frac{\alpha}{k_1}\right)e^{\alpha L}\right]G$$

$$|A|^2 = \left[1 + \frac{1}{4}\left(\frac{k_1}{\alpha} + \frac{\alpha}{k_1}\right)^2 \sinh^2 \alpha L\right]|G|^2$$

$$\frac{|G|^2}{|A|^2} = \frac{1}{1 + \dfrac{V_0^{\;2}}{4E\left(V_0 - E\right)}\sinh^2 \alpha L} \qquad E < V_0$$

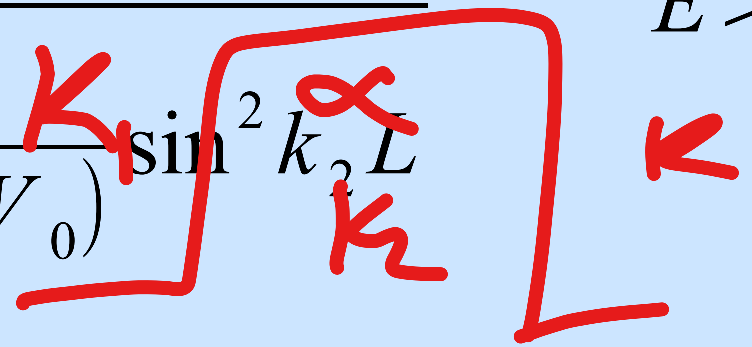
recall : $\alpha^2 = \dfrac{2m}{\hbar^2}\left(V_0 - E\right)$

There are no resonances for $E < V_0$

Problem 5 : The potential barrier for $E > V_0$ or $E < V_0$

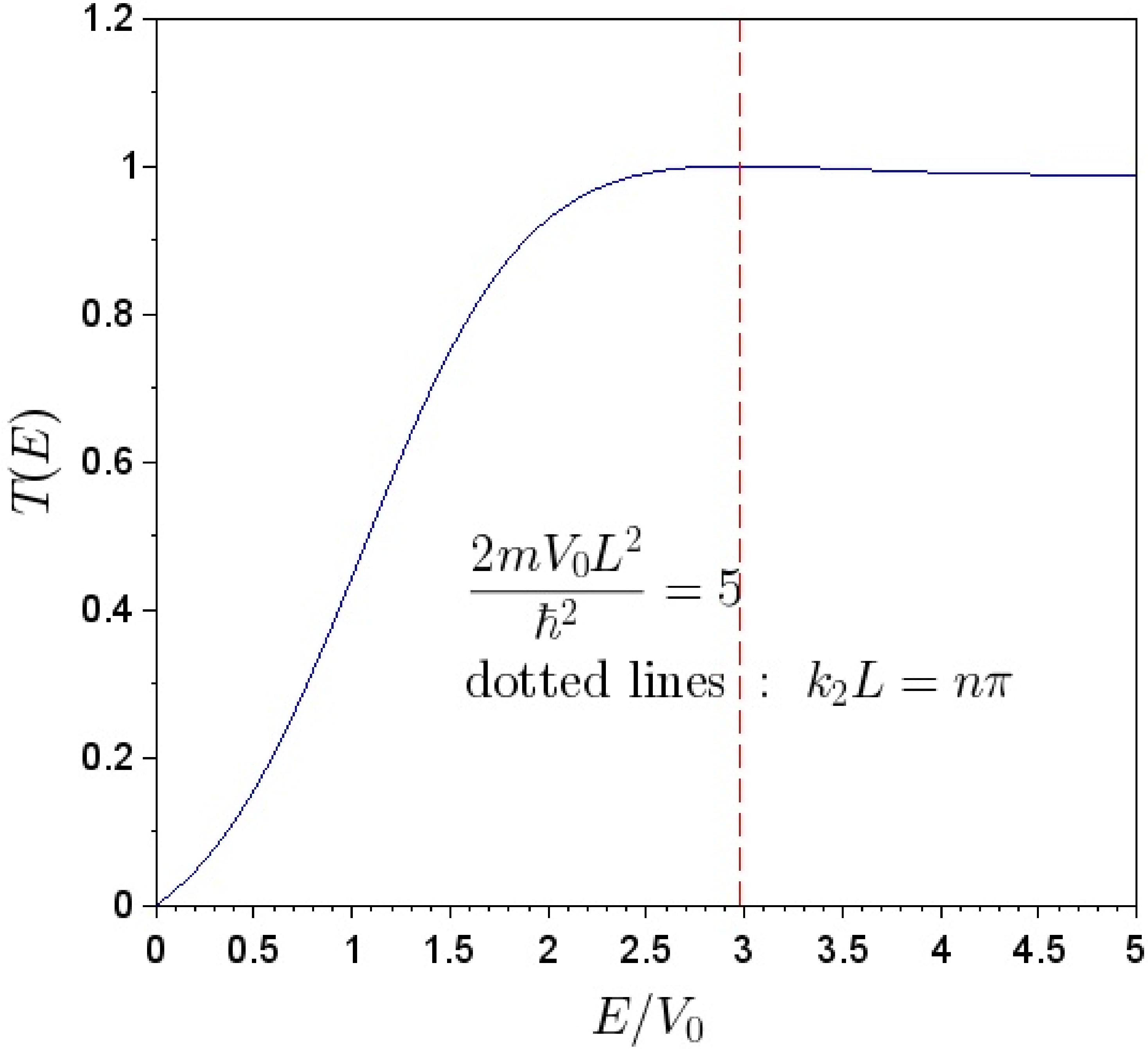
Combining the two results

$$\frac{|G|^2}{|A|^2} = T(E) = \begin{cases} \dfrac{1}{1 + \dfrac{V_0^{\,2}}{4E(V_0 - E)}\sinh^2 \alpha L} & E < V_0 \\[2ex] \dfrac{1}{1 + \dfrac{V_0^{\,2}}{4E(E - V_0)}\sin^2 k_2 L} & E > V_0 \end{cases}$$

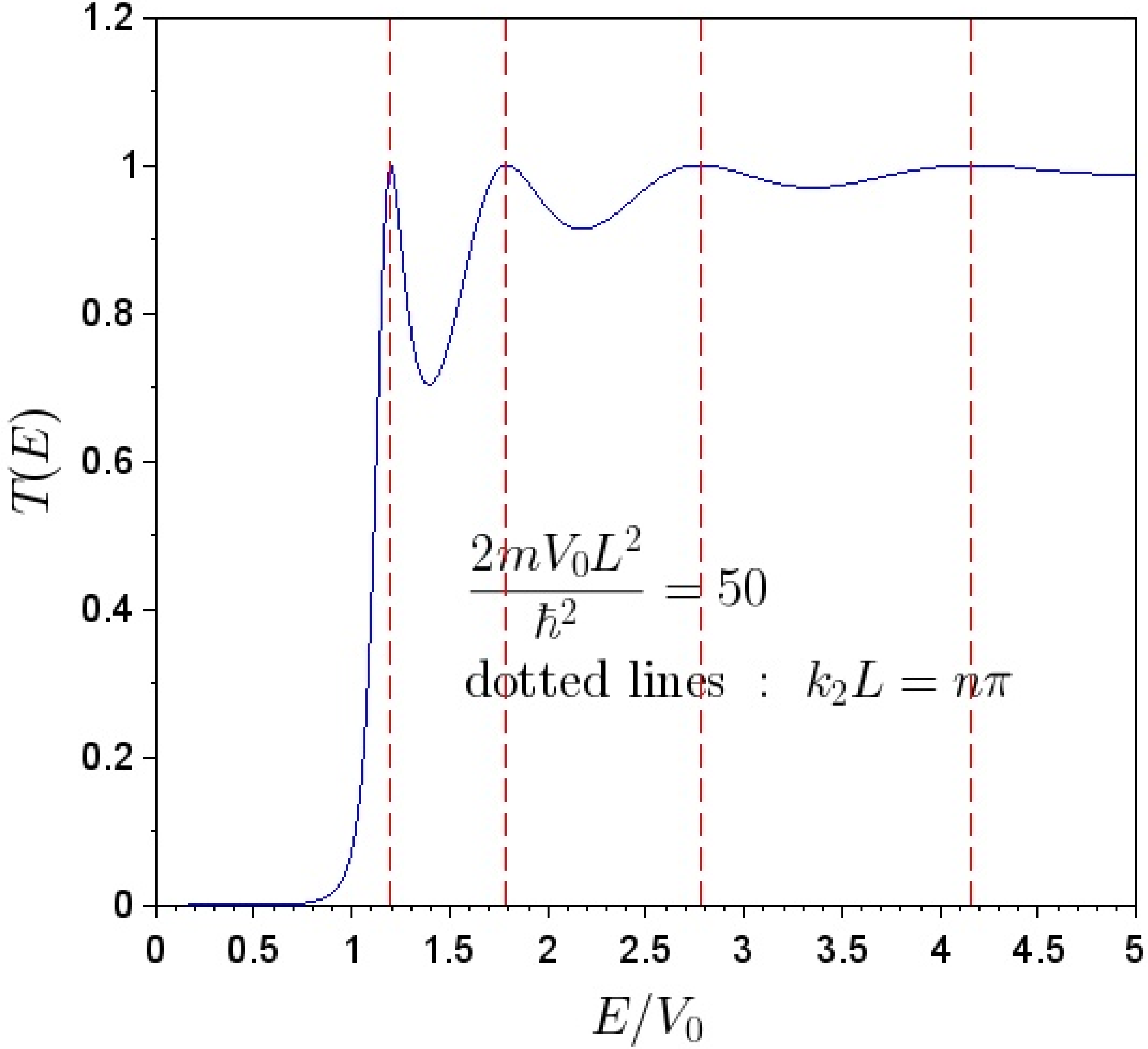


These are the tunnelling/ transmission probabilities

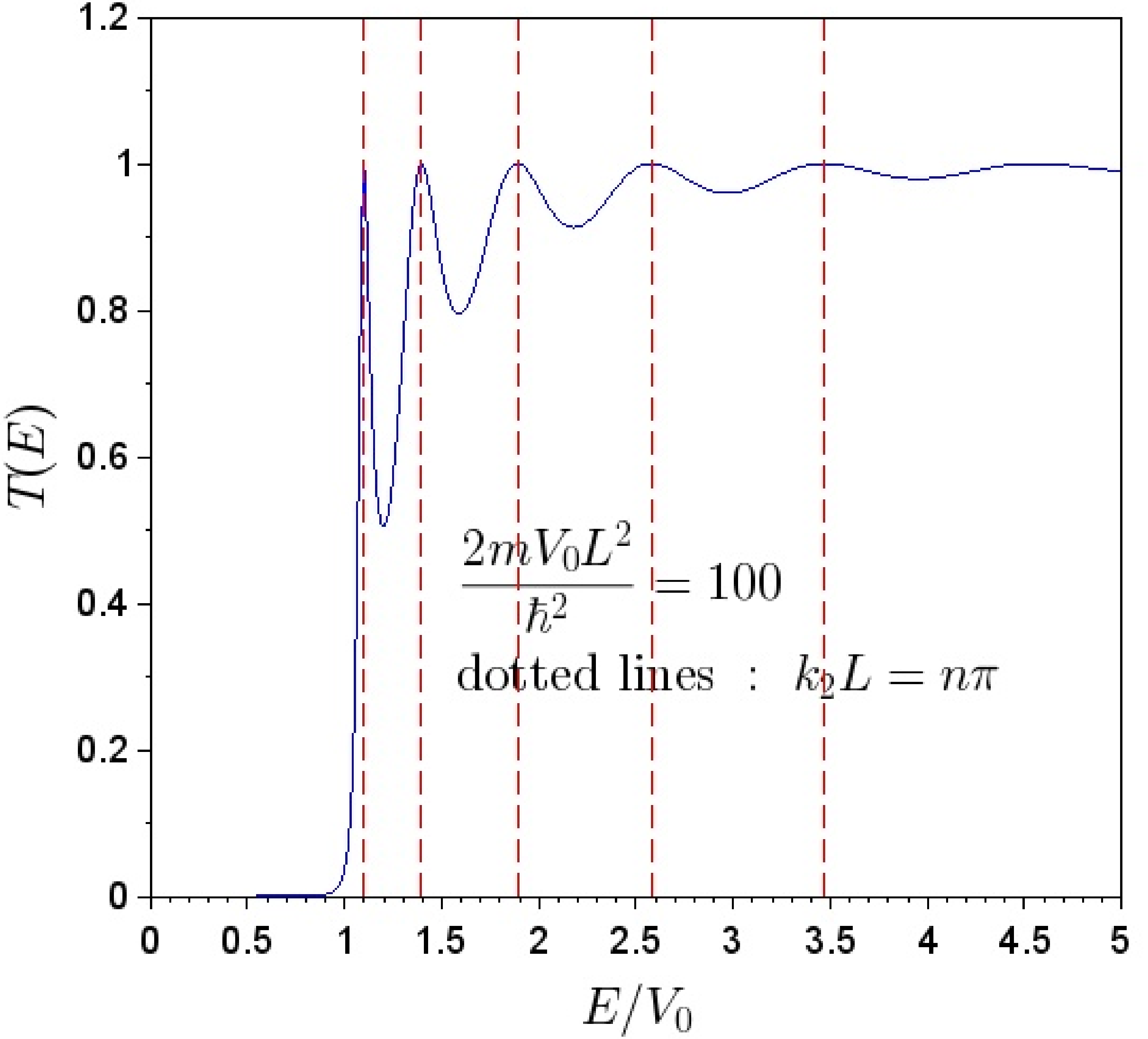
Problem 5 : The potential barrier keep V_0 fixed and increase L



Problem 5 : The potential barrier keep V_0 fixed and increase L



Problem 5 : The potential barrier keep V_0 fixed and increase L



Problem 5 : $T(E)$ for $E \ll V_0$: An useful approximation

$$T(E) = \frac{1}{1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2 \alpha L}$$

$$\approx \frac{E}{E + \frac{V_0}{4} \sinh^2 \alpha L} \qquad (V_0 - E \approx V_0)$$

$E \ll V_0$

$$\approx 16 \frac{E}{V_0} e^{-2\alpha L} \qquad \alpha^2 \approx \frac{2mV_0}{\hbar^2}$$

Low energy tunneling is exponentially suppressed with increasing barrier height .... useful general result