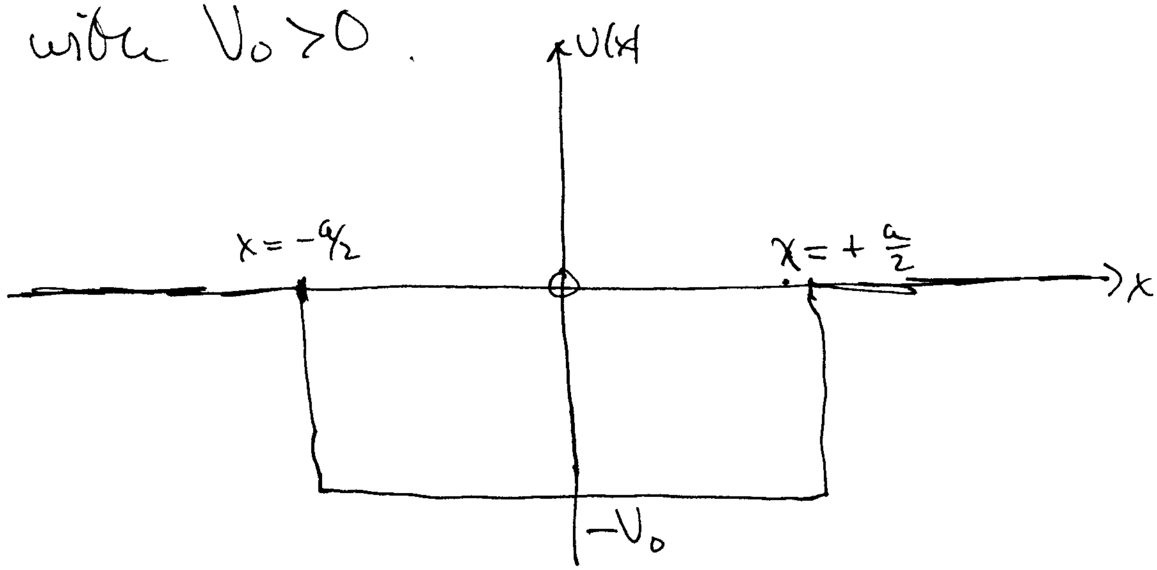
II D) Finite Square Well: another case of both bound and scattering state.

$$V(x) = \begin{cases} 0, & \text{if } |x| > \frac{a}{2} \\ -V_0, & \text{if } |x| \le a/2 \end{cases}$$

with $V_0 > 0$.



The Schrödinger equation is given by

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\,\psi(x) \quad , \text{ for } |x| > \frac{a}{2}$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) - V_0\psi(x) = E\,\psi(x) \quad , \text{ for } |x| \le \frac{a}{2}.$$

Bound States: $\underline{E<0}$ (but $|E|<V_0$).

II b) As usual Define

$$E = -\frac{\hbar^2 \chi^2}{2m} \quad , \text{that is} \quad \chi \equiv \sqrt{\frac{2m(-E)}{\hbar^2}} > 0$$

$$q \equiv \sqrt{\frac{2m(E+V_0)}{\hbar^2}} > 0 \quad \text{since } V_0 > |E| .$$

The Schrödinger equation becomes

$$\frac{d^2\psi}{dx^2} - \chi^2 \psi = 0 \quad , \text{for } |x| > \frac{a}{2}$$

$$\frac{d^2\psi}{dx^2} + q^2 \psi = 0 \quad , \text{for } |x| \leq \frac{a}{2}$$

The general solution to this DE is:

$$\psi(x) = \begin{cases} A_< e^{\chi x} + B_< e^{-\chi x} & , \text{for } x < -\frac{a}{2} \\ A e^{iqx} + B e^{-iqx} & , \text{for } -\frac{a}{2} \leq x \leq \frac{a}{2} \\ A_> e^{\chi x} + B_> e^{-\chi x} & , \text{for } x > \frac{a}{2} \end{cases}$$

The BC on ψ and ψ' will further determine the solution:

II D) 1) ψ is finite everywhere

For $x \to -\infty \Rightarrow$ $\boxed{B_< = 0}$

For $x \to +\infty \Rightarrow$ $\boxed{A_> = 0}$

2) Continuity of ψ and $\frac{d\psi}{dx}$ at $x = -\frac{a}{2}$

a) $\psi(x = -\tfrac{1}{2}a^-) = \psi(x = -\tfrac{1}{2}a^+) \Rightarrow$

$$A_< e^{-\kappa \frac{a}{2}} = A e^{-iq\frac{a}{2}} + B e^{+iq\frac{a}{2}}$$

b) $\psi'(x = -\tfrac{1}{2}a^-) = \psi'(x = -\tfrac{1}{2}a^+) \Rightarrow$

$$\kappa A_< e^{-\kappa \frac{a}{2}} = iq\left(A e^{-iq\frac{a}{2}} - B e^{+iq\frac{a}{2}}\right)$$

Combining these for A & B we have

$$\boxed{\begin{aligned} A &= \tfrac{1}{2}\left(1 + \frac{\kappa}{iq}\right) e^{(iq-\kappa)\frac{a}{2}} A_< \\ B &= \tfrac{1}{2}\left(1 - \frac{\kappa}{iq}\right) e^{(-iq-\kappa)\frac{a}{2}} A_< \end{aligned}}$$

II D)

3) Continuity of ψ and $\frac{d\psi}{dx}$ at $x = +\frac{a}{2}$

a) $\psi(x = \frac{1}{2}a^-) = \psi(x = \frac{1}{2}a^+) \Rightarrow$

$$B_> e^{-\kappa \frac{a}{2}} = A e^{iq\frac{a}{2}} + B e^{-iq\frac{a}{2}}$$

b) $\psi'(x = \frac{1}{2}a^-) = \psi'(x = \frac{1}{2}a^+) \Rightarrow$

$$-\kappa B_> e^{-\kappa \frac{a}{2}} = iq\left(A e^{iq\frac{a}{2}} - B e^{-iq\frac{a}{2}}\right)$$

Now substituting for A & B from case 2 above ~~and~~ find 2 expressions for the same $\underline{B_>}$

$$\boxed{\begin{aligned} &a)\quad B_> = \left[\tfrac{1}{2} e^{iqa}\left(1 + \frac{\kappa}{iq}\right) + \tfrac{1}{2} e^{-iqa}\left(1 - \frac{\kappa}{iq}\right)\right] A_< \\ &b)\quad B_> = \frac{-iq}{\kappa}\left[\tfrac{1}{2} e^{iqa}\left(1 + \frac{\kappa}{iq}\right) - \tfrac{1}{2} e^{-iqa}\left(1 - \frac{\kappa}{iq}\right)\right] A_< \end{aligned}}$$

II D) For a non-trivial ψ to exist, Both expressions for $B_>$ must be equal

$\Rightarrow$

$$\tfrac{1}{2}\left[e^{iqa}\left(1+\frac{\kappa}{iq}\right)+e^{-iqa}\left(1-\frac{\kappa}{iq}\right)\right]$$
$$=-\frac{iq}{2\kappa}\left[e^{iqa}\left(1+\frac{\kappa}{iq}\right)-e^{-iqa}\left(1-\frac{\kappa}{iq}\right)\right]$$

$\Rightarrow$

$$e^{iqa}\left(1+\frac{\kappa}{iq}\right)\left[1+\frac{iq}{\kappa}\right]$$
$$=e^{-iqa}\left(1-\frac{\kappa}{iq}\right)\left[\frac{iq}{\kappa}-1\right]$$

$\Rightarrow$

$$e^{2iqa}\frac{1}{iq\kappa}(\kappa+iq)(\kappa+iq)$$
$$=\frac{1}{\kappa iq}(iq-\kappa)(iq-\kappa)$$

$\Rightarrow$

$$\boxed{e^{2iqa}=\left(\frac{\kappa-iq}{\kappa+iq}\right)^2}$$

II D) Since κ and q depend on E, this equation will lead to discrete allowed values for the bound state energies E. Since the RHS is a square, there are 2 cases

Case 1)
$$-e^{+iqa} = \frac{\kappa - iq}{\kappa + iq}$$

Case 2)
$$+e^{+iqa} = \frac{\kappa - iq}{\kappa + iq}.$$

Case 1)
$$-e^{+iqa} = \frac{\kappa - iq}{\kappa + iq} = \frac{-i(q + i\kappa)}{+i(q - i\kappa)}$$

$\Rightarrow$

$$e^{+iqa} = \frac{q + i\kappa}{q - i\kappa}$$

but $q + i\kappa = \rho e^{i\theta}$

with $\rho = \sqrt{q^2 + \kappa^2}$, $\tan\theta = \frac{\kappa}{q}$

$\Rightarrow \quad q - i\kappa = \rho e^{-i\theta}$

II D) Case 1) So

$$e^{iqa} = e^{2i\theta}$$

$$\Rightarrow \quad \frac{qa}{2} = \theta$$

$$\Rightarrow \quad \tan\theta = \tan\frac{qa}{2}$$

$$\tan\theta = \frac{\kappa}{q}$$

Hence Case 1) $\boxed{\frac{\kappa}{q} = \tan\frac{qa}{2}}$

Since $\kappa > 0, q > 0 \Rightarrow \boxed{\tan\frac{qa}{2} > 0}$

Now Define

$$q_0 \equiv \sqrt{q^2+\kappa^2} = \sqrt{\frac{2mV_0}{\hbar^2}}$$

Hence we have

$$\frac{\kappa^2}{q^2} = \tan^2\frac{qa}{2} = \sec^2\frac{qa}{2} - 1$$

or

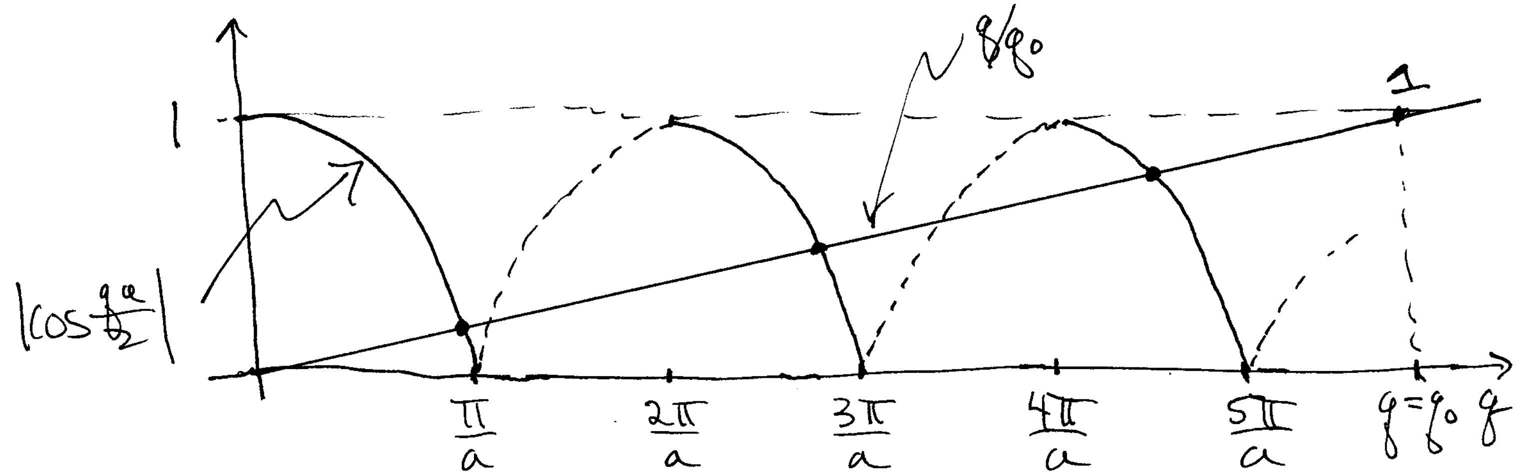
$$\kappa^2 + q^2 = q^2 \frac{1}{\cos^2\frac{qa}{2}}$$

$$\Rightarrow \quad \cos^2\frac{qa}{2} = \frac{q^2}{q_0^2}$$

II D) case 1) Since $q > 0$ this becomes

$$\boxed{\left|\cos\frac{qa}{2}\right| = \frac{q}{q_0}}$$

We have also $\boxed{\tan\frac{qa}{2} > 0}$. We can solve the above transcendental equation by graphing $\frac{q}{q_0}$ and $\left|\cos\frac{qa}{2}\right|$ and finding the points of intersection



The solid $\left|\cos\frac{qa}{2}\right|$ curve lines also have $\tan\frac{qa}{2} > 0$; The dashed lines correspond to $\tan\frac{qa}{2} < 0$, and are excluded in case 1 solutions. The intersection of q/q_0 with $\left|\cos\frac{qa}{2}\right|$, indicated by dots, are the allowed solutions q to the transcendental equation. In the case drawn here, we have, for the q_0 indicated, 3 allowed bound states in case 1.

$\Rightarrow$ D) Case 2)

$$+e^{iqa} = \frac{\kappa - iq}{\kappa + iq} = -\frac{(q+i\kappa)}{(q-i\kappa)}$$

Now let $q + i\kappa = \rho e^{i\theta}$ again $\Rightarrow$

$$e^{iqa} = -e^{2i\theta} = e^{i\pi} e^{2i\theta}$$

$$= e^{i(2\theta+\pi)}$$

$\Rightarrow$

$$qa = 2\theta + \pi$$

$$\Rightarrow \quad \frac{qa}{2} = \theta + \frac{\pi}{2}$$

$$\Rightarrow \quad \boxed{\tan\frac{qa}{2} = \tan\left(\theta + \frac{\pi}{2}\right) = -\cot\theta = -\frac{q}{\kappa}}$$

Since $q > 0, \kappa > 0 \Rightarrow \boxed{\tan\frac{qa}{2} < 0}$

Using $q_0 = \sqrt{q^2+\kappa^2} = \sqrt{\frac{2mV_0}{\hbar^2}}$ again, this becomes

II D) (Case 2) $\frac{q^2}{\kappa^2} = \tan^2\frac{qa}{2} = \sec^2\frac{qa}{2} - 1$

$$\Rightarrow \quad \kappa^2 + q^2 = \kappa^2 \sec^2\frac{qa}{2} = \frac{\kappa^2}{\cos^2\frac{qa}{2}}$$

$$\Rightarrow \quad \cos^2\frac{qa}{2} = \frac{\kappa^2}{q^2+\kappa^2}$$

$$\cos^2\frac{qa}{2} = 1 - \sin^2\frac{qa}{2}$$

$$\Rightarrow \quad \boxed{\sin^2\frac{qa}{2} = 1 - \frac{\kappa^2}{q^2+\kappa^2} = \frac{q^2}{q_0^2}} = \frac{q^2+\kappa^2-\kappa^2}{q^2+\kappa^2}$$

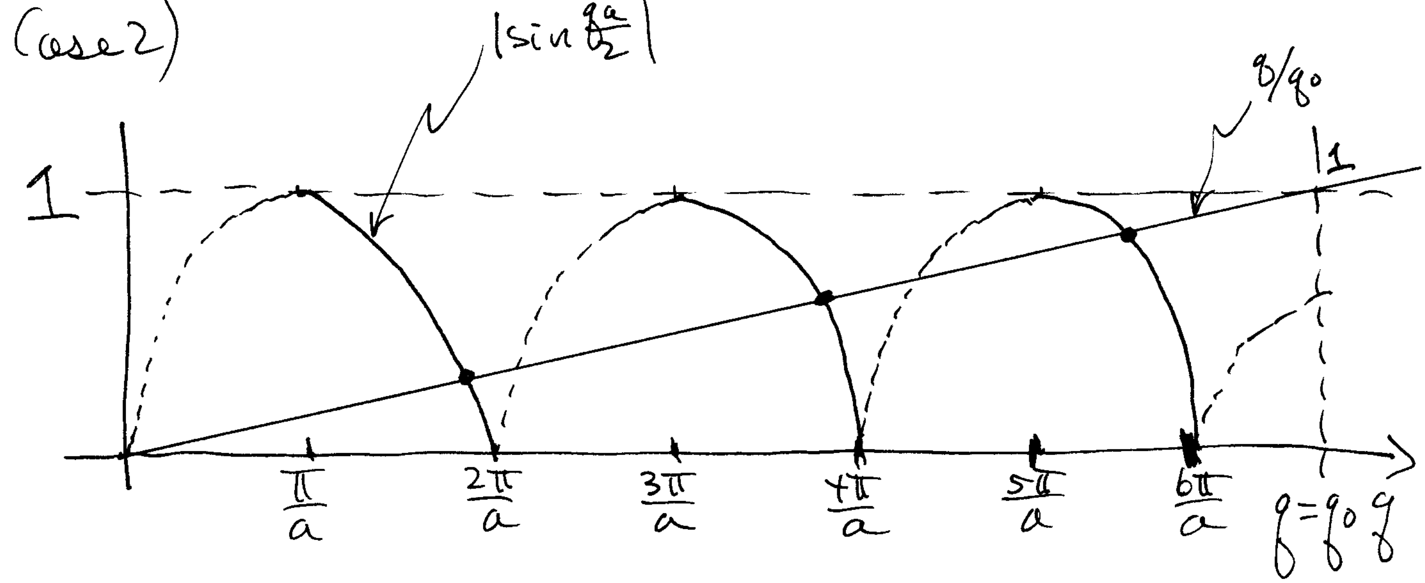
Since $q > 0$ this becomes

$$\boxed{\left|\sin\frac{qa}{2}\right| = \frac{q}{q_0}}$$

along with $\boxed{\tan\frac{qa}{2} < 0}$

Again we can solve this graphically

IV D) Case 2)



Again, the solid line $|\sin \frac{qa}{2}|$ curve is that part for which $\tan \frac{qa}{2} < 0$ also. The intersections of this curve with q/q_0 are the allowed values of q and hence E, the bound state energies. The solution to the bound state problem of our square well consists of both sets of these intersection points. Only discrete (quantized) values of the energy E lead to allowed solutions.

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

$$= \frac{\hbar^2}{2m}(q^2 - q_0^2).$$

ID) Suppose we consider the case where the well is infinitely deep $V_0 \to \infty$. As $V_0 \to \infty$ also $q_0 \equiv \sqrt{\frac{2mV_0}{\hbar^2}} \to \infty$. As $q_0 \to \infty$

we see that the solutions to our transcendental equation are those for which $q/q_0 \to 0$; that is

$$|\sin \tfrac{qa}{2}| = 0 = |\cos \tfrac{qa}{2}|$$

This is nothing but $\frac{qa}{2} = \frac{n\pi}{2}$, $n = 1, 2, 3, \ldots$.

The allowed values of q are

$$\boxed{q_n = \frac{n\pi}{a}, \; n = 1, 2, \ldots}$$

Hence the allowed values of the energy of the particle above the bottom of the potential V_0 are

$$\boxed{\begin{aligned} E_n = E + V_0 &= \frac{\hbar^2 q_n^2}{2m} \\ &= \frac{\hbar^2 \pi^2}{2ma^2} n^2, \quad n = 1, 2, \ldots \end{aligned}}$$

These are just the ~~allowed~~ allowed values we found explicitly in the infinite square well case.

II D) Suppose we next consider a very shallow well $q_0 \to 0$ so that there are less and less solutions to the transcendental equations — until finally $q_0 < \frac{\pi}{a}$ — only one solution persists: $\left|\cos\frac{qa}{2}\right| = q/q_0$; $\tan\frac{qa}{2} > 0$

and no matter how small $q_0 \to 0^+$, there is always this one solution — There is always a bound state.

The wavefunction is completely determined except for its normalization. Requiring $1 = \int_{-\infty}^{\infty} dx\, |\psi|^2$ will fix $B_<$ which was used to determine A, B and $A_>$.

Next consider the Scattering States $\boxed{E > 0}$

Now we define $E = \frac{\hbar^2 k^2}{2m}$, that is $k = \sqrt{\frac{2mE}{\hbar^2}} > 0$

and still $q \equiv \sqrt{\frac{2m(E+U_0)}{\hbar^2}} > 0$

The Schrödinger eq. becomes

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \text{for} \quad |x| > \frac{a}{2}$$

and

$$\frac{d^2\psi}{dx^2} + q^2\psi = 0 \quad \text{for} \quad |x| \le \frac{a}{2}$$

IID) So we have the solution

$$\psi(x) = N \begin{cases} e^{ikx} + r e^{-ikx} , & x < -\frac{a}{2} \\ A e^{iqx} + B e^{-iqx} , & -\frac{a}{2} \le x \le \frac{a}{2} \\ t e^{ikx} + C e^{-ikx} , & x > \frac{a}{2} \end{cases}$$

As usual in scattering problems, we must pick a direction for the incident beam of particles — take them coming in from the left - hence $\psi = \psi_{inc} + \psi_{scatt}$.

$$\psi_{incident} = N e^{ikx} \qquad (x < -\tfrac{a}{2})$$

These particles may be reflected off the potential well and this situation corresponds to the reflected wave in the region $(x < -\frac{a}{2})$

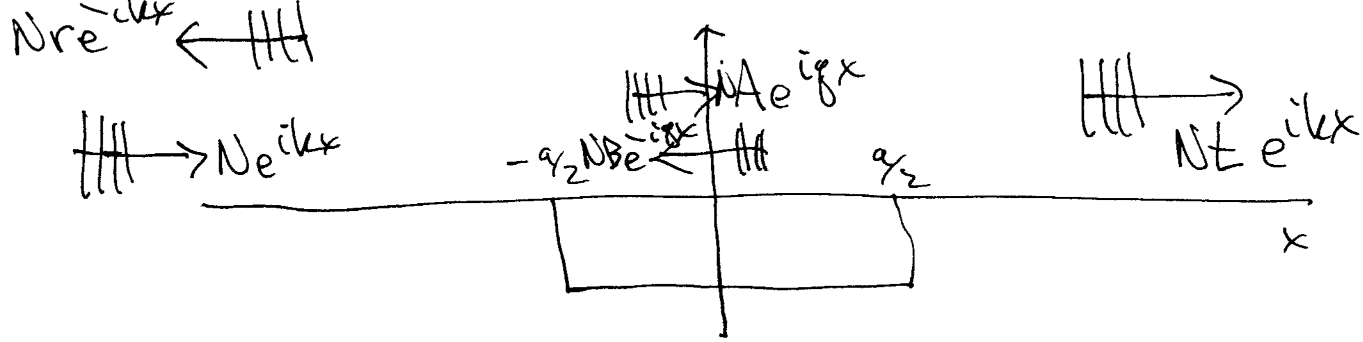
$$\psi_{reflect} = N r e^{-ikx} ,$$

After the well in the region $x > \frac{a}{2}$ we assume the particles are transmitted with corresponding wavefunction

$$\psi_{trans} = N t e^{ikx}$$

II D) and that there are no other particles incident from the right traveling towards the well. Thus we impose the

$$\boxed{C=0}$$ condition in order to describe this situation.



As before the BC will determine the relations between r, A, B, t and N.

BC: 1) $x=-a/2$

$$\psi\left(x=-\tfrac{a}{2}-\right)=\psi\left(x=-\tfrac{a}{2}+\right)$$

$$\Rightarrow \boxed{e^{-ik\frac{a}{2}}+re^{+ik\frac{a}{2}}=Ae^{-iq\frac{a}{2}}+Be^{+iq\frac{a}{2}}}$$

$$\psi'\left(x=-\tfrac{a}{2}-\right)=\psi'\left(x=-\tfrac{a}{2}+\right)$$

$$\Rightarrow \boxed{k\left[e^{-ik\frac{a}{2}}-re^{ik\frac{a}{2}}\right]=q\left[Ae^{-iq\frac{a}{2}}-Be^{+iq\frac{a}{2}}\right]}$$

III D) Thus

$$\boxed{\begin{aligned} A &= \tfrac{1}{2}\left[\left(1+\tfrac{k}{q}\right)e^{i(q-k)\frac{a}{2}} + \left(1-\tfrac{k}{q}\right) r e^{i(q+k)\frac{a}{2}}\right] \\ B &= \tfrac{1}{2}\left[\left(1-\tfrac{k}{q}\right)e^{-i(q+k)\frac{a}{2}} + \left(1+\tfrac{k}{q}\right) r e^{-i(q-k)\frac{a}{2}}\right] \end{aligned}}$$

2) $x = +\frac{a}{2}$

$$\psi(x = \tfrac{a}{2}^-) = \psi(x = \tfrac{a}{2}^+)$$

$$\Rightarrow \boxed{A e^{iq\frac{a}{2}} + B e^{-iq\frac{a}{2}} = t e^{ik\frac{a}{2}}}$$

$$\psi'(x = \tfrac{a}{2}^-) = \psi'(x = \tfrac{a}{2}^+)$$

$$\Rightarrow \boxed{q\left[A e^{iq\frac{a}{2}} - B e^{-iq\frac{a}{2}}\right] = k t e^{ik\frac{a}{2}}}$$

So analogously we find

$$\boxed{\begin{aligned} A &= \tfrac{1}{2}\left(1+\tfrac{k}{q}\right) t e^{-i(q-k)\frac{a}{2}} \\ B &= \tfrac{1}{2}\left(1-\tfrac{k}{q}\right) t e^{+i(q+k)\frac{a}{2}} \end{aligned}}$$

II. D) Now eliminating A & B from these two sets of equations yields the r & t coefficients

$$t = e^{i(q-k)a} + \frac{(q-k)}{(q+k)} r e^{iqa}$$

$$t = e^{-i(q+k)a} + \frac{(q+k)}{(q-k)} r e^{-iqa}$$

$$\Rightarrow \boxed{r = \frac{i(q^2-k^2)e^{-ika}\sin qa}{2qk\cos qa - i(q^2+k^2)\sin qa}}$$

And mutatis mutandis

$$r = \left(\frac{q+k}{q-k}\right)\left[e^{-iqa}t - e^{-ika}\right]$$

$$r = \left(\frac{q-k}{q+k}\right)\left[e^{+iqa}t - e^{-ika}\right]$$

$$\Rightarrow \boxed{t = \frac{2qk\, e^{-ika}}{2qk\cos qa - i(q^2+k^2)\sin qa}}$$

II D) Of course A&B are now known also.

The reflection and transmission coefficients may now be calculated.

$$R = \left| \frac{J_{ref.}}{J_{inc}} \right| = |r|^2$$

$$= \frac{(q^2-k^2)^2 \sin^2 qa}{4q^2k^2\cos^2 qa + (q^2+k^2)^2 \sin^2 qa}$$

$$\boxed{R = \frac{(q^2-k^2)^2 \sin^2 qa}{4q^2k^2 + (q^2-k^2)^2 \sin^2 qa}}$$

$$T = \left| \frac{J_{trans}}{J_{inc}} \right| = |t|^2$$

$$= \frac{4q^2k^2}{4q^2k^2\cos^2 qa + (q^2+k^2)^2 \sin^2 qa}$$

$$\boxed{T = \frac{4q^2k^2}{4q^2k^2 + (q^2-k^2)^2 \sin^2 qa}}$$

iii) So first note that

1) $R+T=1$, as required.

2) Recall $k^2 = \frac{2mE}{\hbar^2}$

$$q^2 = \frac{2m(E+V_0)}{\hbar^2}$$

Hence $(q^2-k^2) = \frac{2m}{\hbar^2} V_0$

$\Rightarrow$

$$\boxed{R = \frac{V_0^2 \sin^2\left(\sqrt{\frac{2m(E+V_0)}{\hbar^2}}\, a\right)}{4E(E+V_0) + V_0^2 \sin^2\left(\sqrt{\frac{2m(E+V_0)}{\hbar^2}}\, a\right)}}$$

$$\boxed{T = \frac{4E(E+V_0)}{4E(E+V_0) + V_0^2 \sin^2\left(\sqrt{\frac{2m(E+V_0)}{\hbar^2}}\, a\right)}}$$

Hence T can be plotted as a function of energy. The maximum T occurs at

$$\sqrt{\frac{2m(E+V_0)}{\hbar^2}}\, a = n\pi, \quad n=1,2,\ldots$$

-II δ) at which $T = 1$, and hence $R = 0$, the well is said to "become transparent". The minimum of T occurs at

$$\sqrt{\frac{2m(E+V_0)}{\hbar^2}}\, a = \left(n+\tfrac{1}{2}\right)\pi \,, \quad n = 0, 1, 2, \ldots$$

where

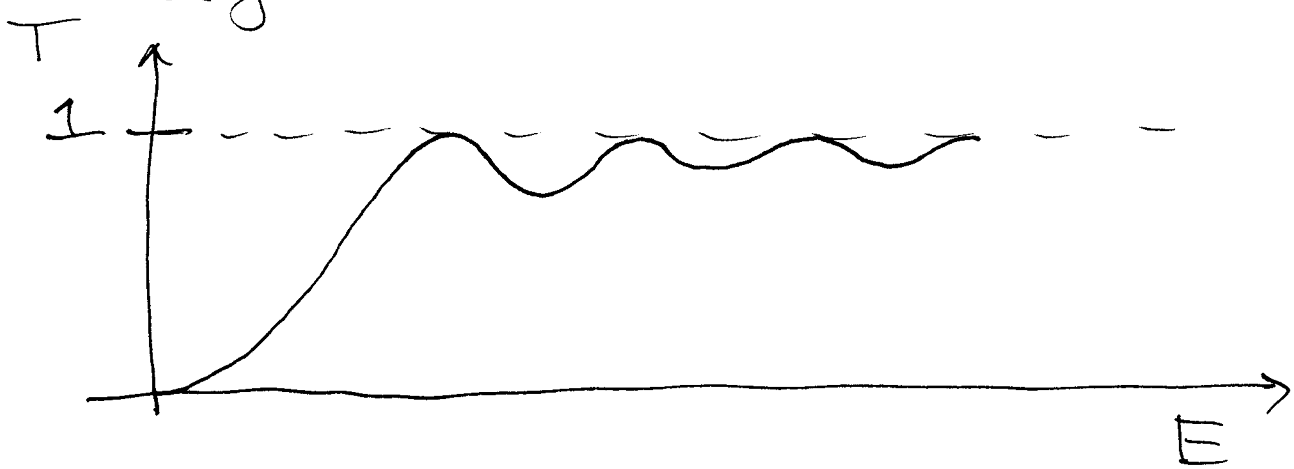
$$T = \frac{4E(E+V_0)}{4E(E+V_0)+V_0^2}$$

and hence

$$R = \frac{V_0^2}{4E(E+V_0)+V_0^2}$$

, its maxima.

In general



Note that $T = 1$ when

$$E_n - V_0 = \frac{\hbar^2 \pi^2}{2m\, a^2} n^2 \,, \quad n = 1, 2, \ldots ,$$

just the ∞ square well energies (resonance scattering)