Problem Set #4: Due: Friday, February 16, 11:59pm

You are welcome to use Mathematica or similar tools in doing these problems

1. *Hermite polynomials:* We found by solving the HO Schrödinger equation directly that the solutions were

$$\phi_n(\xi) = \left(\frac{1}{\pi b^2}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} e^{-\xi^2/2} H_n(\xi)$$

And in our ladder operator work, we found that, for a raising operator normalized as below,

$$\phi_n(\xi) = \frac{1}{\sqrt{n}} \frac{1}{\sqrt{2}} \left[-\frac{d}{d\xi} + \xi \right] \phi_{n-1}(\xi)$$

Derive an expression for $H_n(\xi)$ in term of $H_{n-1}(\xi)$ and $H'_{n-1}(\xi)$. Starting with H_0, use this expression to generate H_1 through H_6.

2. *Visualizing Fourier transforms:* I have heard that some electrical engineers who probe chips with regular structures using light of different frequencies learn to "see" in Fourier transform space. We probably can't achieve that level of enlightenment, but let's try to gain a bit of insight into the momentum- or Fourier-world. To work this problem you will need a graphing routine, and it is also fine to ask MatLab or Mathematica to do the integral you need, which has an analytic form.

a) Consider the wave packet

$$f(x) = \cos\left(\frac{n\pi x}{2}\right) \left(\frac{1}{b^2 \pi}\right)^{1/4} e^{-\frac{x^2}{2b^2}}$$

which you will recognize as a normalized Gaussian whose width in x-space is governed by b, onto which is imposed periodic oscillations whose wave numbers are governed by n. Using a grid with fixed dimensions for all four cases – a good choice for the x-axis is the interval from $x = -6$ to $x = 6$ – plot the four wave packets defined by $(n, b) = \{(1, 1), (10, 1), (1, 1/2), (10, 1/2)\}$. It would be great to arrange your four graphs in a 2-by-2 pattern, grouping panels with the same b on the same row, and with the same n in the same column, to bring out what changes when you dial b or dial n. (But you need not do this, if difficult for you.)

b) Evaluate the Fourier transform - the coefficients of the expansion of $f(x)$ in terms of plane waves of definite momentum k - using

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$$

Be sure to use the fact that $f(x)$ is even under reflection to simplify this integral. Make another panel of graphs, just like above, but for $F(k)$. Use fixed axes, so visual comparisons are easy. A good choice for the range of ks displayed is -20 to 20.

c) What happens when n is fixed, but b is halved? What happens when b is fixed, but n is increased? What would you think the graphs would look like if n were kept fixed, but b were made very very large?

3. *Bound states - infinite and finite wells:* The energy levels of an infinite square well of width a are given by (as we derived)

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2}, \quad n = 1, 2, 3, ...$$

Thus the first level appears at an energy $E_1 = \frac{\hbar^2\pi^2}{2ma^2}$ above the bottom of the well. But we noted in class that a finite well of any small depth supports a bound state. Here we show that this is an aspect of a more general pattern.

a) Consider a finite potential well of depth $V_0 = 0.01E_1$. Determine the bound-state eigenvalue in units of V_0. (Helpful hint: remember that the parameters z and z_0 appearing in the eigenvalue equation are related by $z = z_0 \left[1 - \frac{|E|}{V_0}\right]^{1/2}$.)

b) Consider a finite potential well of depth $V_0 = 1.01E_1$. How many bounds states are there? Determine the bound-state eigenvalues in units of V_0.

c) Consider a finite potential well of depth $V_0 = 1.01E_2 = 4.04E_1$. How many bound states are there? Determine the bound-state eigenvalues in units of V_0.

d) On Figure 1, graph the states you have found for the appropriate wells, measuring energies in unit of E_1. (Be careful: you have calculated binding energies above, which are measured relative to the top of the well.) Connect the ground states of the four systems, and where they exist, the first excited states. What trends do you see, and how do you account for

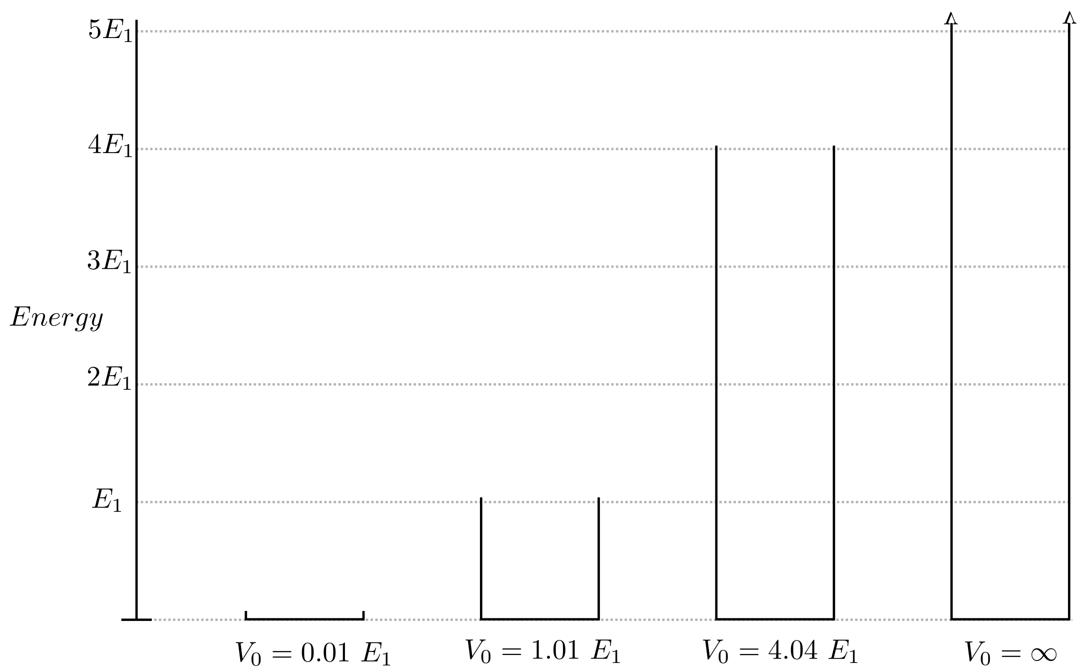


Figure 1: Finite and infinite wells..

them? If you have a well of depth $V_0 = n^2 E_1 + \epsilon,\ n = 0, 1, 2, ...,$, where ϵ is a small positive number, how many bound states are there?

4. *Solutions of the half-finite, half-infinite square well:* Consider the potential illustrated below.

   1. Consider bound solutions, for which $E < 0$. Write down appropriate solutions for the interior (in the well) and exterior regions.

   2. By matching the interior and exterior wave functions and their derivatives at the boundary, determine the wave function up to an overall normalization and the eigenvalue condition.

   3. If you are told that no bound state exists, what can you say about V_0 and a?

   4. Consider continuum solutions, for which $E > 0$. Write down the appropriate solutions for the interior and exterior regions.

5. By matching the interior and exterior solutions and their derivatives, determine the wave function. Show that the exterior wave function can be written in the form of $\sin(kr + \delta)$.

6. Find the conditions on $V_0 a^2$ such that, as the continuum energy $E \to 0$, $\delta = \pi$.

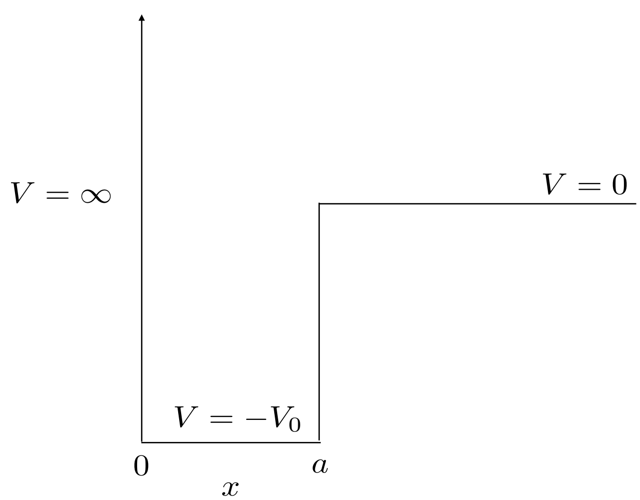


Figure 2: Half finite, half infinite square well.

Problem Set #4

Physics 137A

7. Hermite Polynomials

Solutions for harmonic oscillator

$$\phi_n(\xi) = \left(\frac{1}{\pi b^2}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} e^{-\xi^2/2} H_n(\xi)$$

$$= \frac{1}{\sqrt{n}} \frac{1}{\sqrt{2}} \left[-\frac{d}{d\xi} + \xi \right] \phi_{n-1}(\xi)$$

Therefore,

$$\cancel{\frac{1}{(\pi b^2)^{1/4}}} \frac{1}{\sqrt{2^n n!}} \cancel{e^{-\xi^2/2}} H_n(\xi) = \frac{1}{\sqrt{n}} \frac{1}{\sqrt{2}} \left[-\frac{d}{d\xi} + \xi \right]$$

$$\cancel{\frac{1}{(\pi b^2)^{1/4}}} \frac{1}{\sqrt{2^{n-1}(n-1)!}} \cancel{e^{-\xi^2/2}} H_{n-1}(\xi)$$

$$\frac{1}{\sqrt{2^n n(n-1)!}} H_n(\xi) = \frac{1}{\sqrt{2}\sqrt{n}} \frac{1}{\sqrt{2^{n-1}(n-1)!}} \left[-\frac{d}{d\xi} + \xi \right] H_{n-1}(\xi)$$

$$H_n(\xi) = \left(-\frac{dH_{n-1}(\xi)}{d\xi} + \xi H_{n-1}(\xi) \right)$$

$$= \left(-H'_{n-1}(\xi) + \xi H_{n-1}(\xi) \right)$$

Hermite Polynomial

Recursion Relation.

$$H_n(\xi) = -H_{n-1}'(\xi) + \xi H_{n-1}(\xi)$$

$$H_0(\xi) = 1 \quad (0)$$

$$H_1(\xi) = \xi \quad (1)$$

$$H_2(\xi) = -1 + \xi^2 \quad (2)$$

$$H_3(\xi) = -2\xi + \xi(-1 + \xi^2) = -3\xi + \xi^3 \quad (3)$$

$$H_4(\xi) = -(-3 + 3\xi^2) + \xi(-3\xi + \xi^3)$$

$$= 3 - 3\xi^2 - 3\xi^2 + \xi^4 = 3 - 6\xi^2 + \xi^4 \quad (4)$$

$$H_5(\xi) = -(4\xi^3 - 12\xi) + 3\xi - 6\xi^3 + \xi^5$$

$$= 15\xi - 10\xi^3 + \xi^5 \quad (5)$$

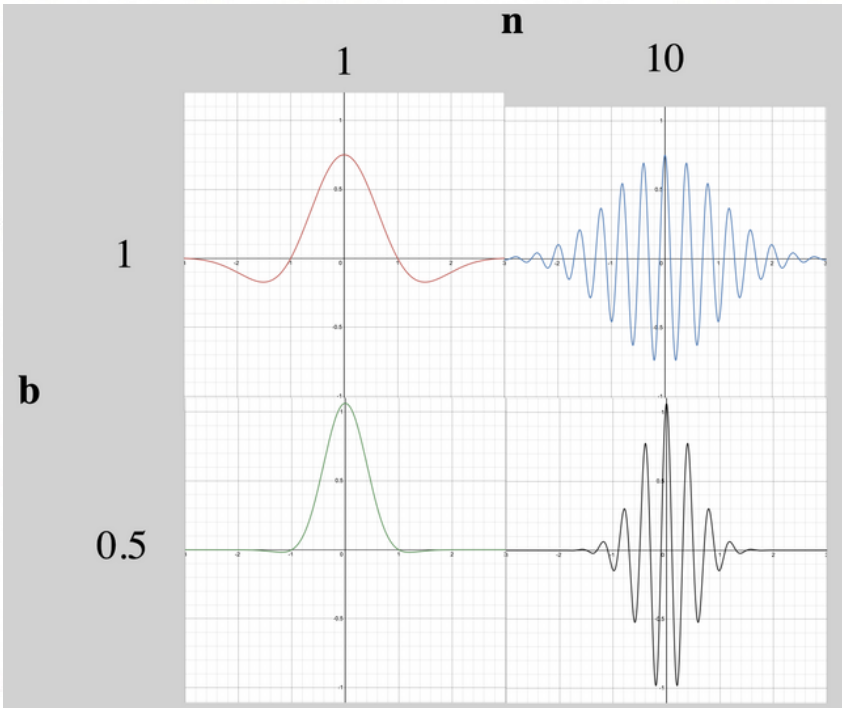
$$H_6(\xi) = -(15 - 30\xi^2 + 5\xi^4) + \xi^6 - 10\xi^4 + 15\xi^2$$

$$= -15 + 45\xi^2 - 15\xi^4 + \xi^6 \quad (6)$$

2. Numerical fourier transforms

a)

$$f(x) = \cos\left(\frac{n\pi x}{2}\right)\left(\frac{1}{b^2\pi}\right)^{1/4} e^{-x^2/2b^2}$$



b)

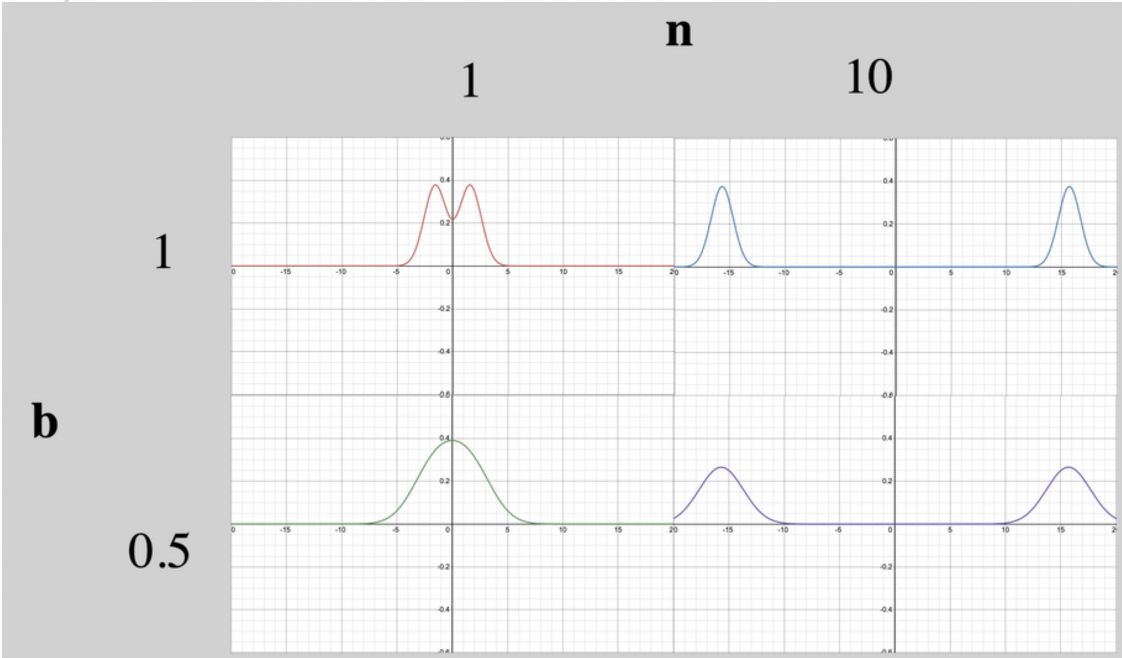
$$F(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)\, e^{-ikx}\, dx$$

$$= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \cos\left(\frac{n\pi x}{2}\right)\left(\frac{1}{b^2\pi}\right)^{1/4} e^{-x^2/2b^2} e^{-ikx}\, dx$$

$$= \frac{1}{\sqrt{2\pi}}\left(\frac{1}{b^2\pi}\right)^{1/4}\int_{-\infty}^{\infty} \cos\left(\frac{n\pi x}{2}\right) e^{-ikx - x^2/2b^2}\, dx$$

$$= \frac{\sqrt{b}}{2\pi^{1/4}}\left(e^{\pi b^2 k n} + 1\right) e^{\left[-\frac{\pi^2 b^2 n^2}{8} - \frac{\pi b^2 k n}{2} - \frac{b^2 k^2}{2}\right]}$$

plotting the fourier transforms



c)

for $f(x)$ when n is kept constant but b is $\frac{1}{2}$'d the graph "narrows" becomes pushed inward. The y axis bound remains constant. The x axis point gets squished.

for $F(x)$ if n is kept constant but b is $\frac{1}{2}$'d, the jumps in the curve do the opposite — get wider, but the location & altitude of the peaks remains constant.

3. Bound States

a) $V_0 = 0.01 E_1$

$$z_0 = \frac{a}{\hbar}\sqrt{\frac{mV_0}{2}} = \frac{a}{\hbar}\sqrt{\frac{m}{2}\left(0.01\frac{\hbar^2\pi^2}{2ma^2}\right)}$$

$$= \frac{a}{\hbar}\sqrt{0.01\frac{\hbar^2\pi^2}{4a^2}}$$

$$z_0 = \frac{\pi}{4}\sqrt{0.01}$$

Then,

$$z = \frac{\pi}{4}\sqrt{0.01}\left(1 - \frac{|E|}{V_0}\right)^{1/2}$$

$$\tan(z) = \sqrt{\frac{z_0^2}{z^2} - 1} \Longrightarrow z = 0.0783$$

Therefore,

$$0.0783 = \frac{\pi}{4}\sqrt{0.01}\left(1 - \frac{|E|}{V_0}\right)^{1/2}$$

$$\left[\left(\frac{0.0783(4)}{\pi\sqrt{0.01}}\right)^2 - 1\right]V_0 = |E| \Longrightarrow |E| = \underline{\underline{0.0061 V_0}}$$ — very near top

c) $V_0 = 4.04 E_1 \Longrightarrow z_0 = \frac{\pi}{4}\sqrt{4.04} \Longrightarrow$ 1 even ? 1 odd $\underline{\underline{2 \text{ sol's}}}$

Even solution : $z = 0.936 \Longrightarrow |E| = 0.6484\, V_0$ } 56% well below

Odd solution : $z = 1.5786 \Longrightarrow |E| = (3.89\times 10^{-5})\, V_0$ } basically free

b) is on next page

a)

~~for $V_0 = 9.0\,E_1$, $|E| = 0.00006\,E_1$~~

~~for $V_0 = 4.04\,E_1$, $|E| = 2.62\,E_1$~~

~~$|E| = 0.000157\,E_1$~~

b) $V_0 = 1.01 E_1 \Longrightarrow z_0 = \frac{\pi}{4}\sqrt{1.01}$

$z = 0.635$

Therefore,

$\underline{\underline{|E| = 0.3527\, V_0}}$ 65% well below

d) In terms of E_1,

$V_0 = 0.01 E_1$: $|E| = 6 \cdot 10^{-3}\, E_1$

$V_0 = 1.01 E_1$: $|E| = 0.0035\, E_1$

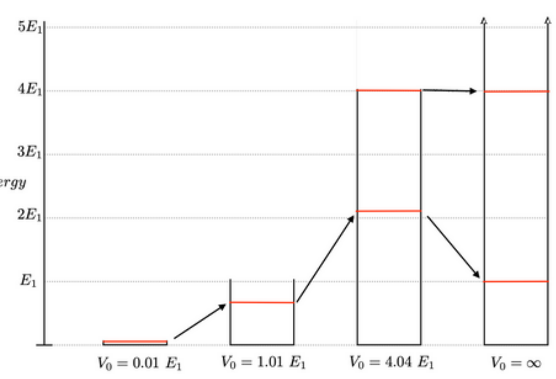
$V_0 = 4.04 E_1$: $|E| = 2.62 E_1$

$= 1.57 \cdot 10^{-4}\, E_1$

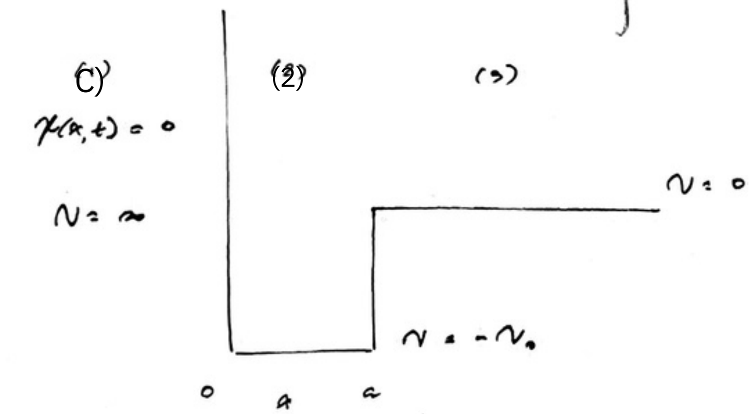
As $V_0 \uparrow$, the energy of the ground state increases except at $V_0 = \infty$ which I don't understand

for $V_0 \to \infty$ $z = z_0$

Infinite square well



4. Solutions of half-finite, half-infinite square well.



1)

for region (2),

$$\phi_2(x) = A\cos(kx) + B\sin(kx), \quad k = \sqrt{\frac{2m(V_0 - |E|)}{\hbar}} \qquad 0 < x < a$$

for region (3)

$$\phi_3(x) = Ce^{-\kappa x} \qquad x > a$$

for region (1)

$$\phi_1(x) = 0 \qquad x < 0$$

2) Matching $\phi_2(x)$ w/ $\phi_1(x)$,

$$\phi_2(0) = \phi_1(0) = 0$$

$$\phi_2(x) = B\sin(kx).$$

Matching $\phi_2(x)$ w/ $\phi_3(x)$

$$B\sin(ka) = Ce^{-\kappa a}$$
$$kB\cos(ka) = -\kappa Ce^{-\kappa a}$$

$k\cancel{B}\cos = -\kappa\cancel{B}\sin$

$k = -\kappa\tan(ka)$

$$\boxed{\begin{aligned} C &= B\sin(ka)e^{\kappa a} \\ k &= -\kappa\tan(ka) \end{aligned}}$$

Thus, the wave function,

$$\phi(x) = \begin{cases} 0 & x < 0 \\ B\sin(kx) & 0 < x < a \\ B\sin(ka)\, e^{\kappa a} e^{-\kappa x} & x > a \end{cases}$$

with the eigenvalue condition

$$k = -\kappa \tan(ka) \qquad B \text{ is normalization factor } \int_0^a \sin^2(kx)\, dx = 1/B^2$$

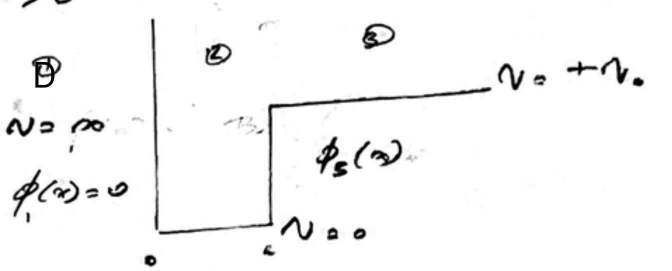
3) for no bound states to exist, $\kappa x = 0$, $\kappa a = 0$

$$\kappa = \sqrt{\frac{2m(V_0 - |E|)}{\hbar}}\, x = 0 \implies V_0 = |E| \text{ or } x = 0$$

$$\kappa a = 0 \implies V_0 = |E|,\ a = 0$$

Either V_0 equals the eigenvalue(s) or the well has no depth

4) $E > 0$



for $0 < x < a$

$$-\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2}\phi(x) = E\phi(x) \implies \phi_2(x) = A\sin(kx) + B\cos(kx) \qquad k = \sqrt{\frac{2m|E|}{\hbar}}$$

for $x > a$, $\phi_3(x) = Ce^{\kappa x} + De^{-\kappa x} \qquad \kappa = \sqrt{\frac{2m(V_0 - |E|)}{\hbar}}$

4) Continued.

$\phi_1(x) = 0$

$\phi_2(x) = A\sin(kx) + B\cos(kx)$, $k = \sqrt{\frac{2m|E|}{\hbar}}$

$\phi_3(x) = Ce^{Kx} + De^{-Kx}$, $K = \sqrt{\frac{2m(V_0 - |E|)}{\hbar}}$

$\phi_1(0) = \phi_2(0) \Longrightarrow \phi_2(x) = A\sin(kx)$

$\phi_3(\infty) \longrightarrow \phi_3(x) = De^{-Kx}$

$\phi_2(a) = \phi_3(a) \longrightarrow A\sin(ka) = De^{-Ka}$

$\phi_2'(a) = \phi_3'(a) \longrightarrow kA\cos(ka) = -KDe^{-Ka}$

$k\cancel{A}\cos(ka) = -K\cancel{A}\sin(ka)$

$k = -K\tan(ka)$

$D = A\sin(ka)e^{Ka}$

$k = -K\tan(ka)$

5)

Therefore

$$\phi(x) = \begin{cases} 0 & x < 0 \\ A\sin(kx) & 0 < x < a \\ A\sin(ka)e^{Ka}e^{-Kx} & x > a \end{cases}$$

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

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

$E > 0$

$\phi_3(x) = A\sin(ka)e^{K(a-x)}$

for spherical potential well. ???

22

6. a^2V_0 $E \to 0$, $\delta = \pi$ $\alpha \to 0$

$V_\delta = -\alpha V_0 \pi$ aV_0 constant, $\Longrightarrow$ $a^2V_0 = \pi^2a^2\alpha > 0$