Quantum Mechanics A
Solutions
Problem Set 4.

Problem 1

First, we will need the following general integration

$$I_{\alpha,\beta}(\vec{r}_a,\vec{r}_b) = \int d^3r_M \; e^{-\alpha(\vec{r}_a-\vec{r}_M)^2} \, e^{-\beta(\vec{r}_M-\vec{r}_b)^2} =$$

$$= e^{-(\alpha r_a^2+\beta r_b^2)} \int d^3r_M \; e^{-(\alpha+\beta)\left[r_M^2 - 2\frac{(\alpha\vec{r}_a+\beta\vec{r}_b)}{\alpha+\beta}\cdot\vec{r}_M\right]}$$

in order to do this, we need to complete the square as follows

$$I_{\alpha,\beta}(\vec{r}_a,\vec{r}_b) = e^{-(\alpha r_a^2+\beta r_b^2)} \, e^{(\alpha+\beta)\left[\frac{\alpha\vec{r}_a+\beta\vec{r}_b}{\alpha+\beta}\right]^2} \int d^3r_M \; e^{-(\alpha+\beta)\left[r_M - \frac{\alpha\vec{r}_a+\beta\vec{r}_b}{\alpha+\beta}\right]^2}$$

$$\boxed{I_{\alpha\beta}(\vec{r}_a,\vec{r}_b) = \left(\frac{\pi}{\alpha+\beta}\right)^{3/2} e^{-\frac{\alpha\beta}{\alpha+\beta}(\vec{r}_a-\vec{r}_b)^2}}$$

we are going to use -1- repeatedly:

1) Integration over $\vec{r}_1$

$$\int d^3r_1 \; e^{\frac{i}{2}\frac{m}{\hbar\Delta t}(\vec{r}_0-\vec{r}_1)^2} \; e^{\frac{i}{2}\frac{m}{\hbar\Delta t}(\vec{r}_1-\vec{r}_2)^2}$$

in this case $\alpha = \beta = -\frac{i\,m}{2\hbar\Delta t} = \zeta$

The result is

$$\left(\frac{\pi}{2\zeta}\right)^{3/2} \; e^{-\frac{\zeta}{2}(\vec{r}_0-\vec{r}_2)^2}$$

2) Integration over $\vec{r}_2$

$$\int d^3\vec{r}_2 \; e^{-\frac{\zeta}{2}(\vec{r}_0-\vec{r}_2)^2} \; e^{-\zeta(\vec{r}_2-\vec{r}_3)^2}$$

$$= \left(\frac{\pi}{\frac{\zeta}{2}+\zeta}\right)^{3/2} \; e^{-\frac{\zeta(\zeta/2)}{\zeta+\zeta/2}(\vec{r}_0-\vec{r}_3)^2}$$

$$= \left(\frac{2\pi}{3\zeta}\right)^{3/2} \; e^{-\frac{\zeta}{3}(\vec{r}_0-\vec{r}_3)^2}$$

3) Integration over $\vec{r}_3$ gives

$$\left(\frac{3\pi}{4J}\right)^{3/2} \quad e^{-\frac{J}{4}\left(\vec{r}_0-\vec{r}_4\right)^2}$$

⋮

N) Integration over $\vec{r}_N$ gives.

$$\left(\frac{N\pi}{(N+1)J}\right)^{3/2} \quad e^{-\frac{J}{N+1}\left(\vec{r}_0-\vec{r}_f\right)^2}$$

Including all prefacter we have

$$C\left(\frac{\pi}{\cancel{2}J}\;\frac{\cancel{2}\pi}{\cancel{3}J}\;\frac{\cancel{3}\pi}{\cancel{4}J}\;\cdots\;\frac{\cancel{N}\pi}{(N+1)J}\right)^{3/2} e^{\frac{im}{2\hbar\underbrace{\Delta t(N+1)}_{t_f-t_0}}\left(\vec{r}_0-\vec{r}_f\right)^2}$$

$$= C\left(\frac{\pi}{J}\right)^{3N/2}\left(\frac{1}{N+1}\right)^{3/2} e^{\frac{im}{2\hbar}\frac{\left(\vec{r}_0-\vec{r}_f\right)^2}{t_f-t_0}}$$

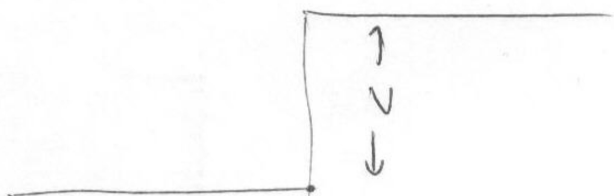
$$= C\left(\frac{\pi}{J}\right)^{\frac{3(N+1)}{2}}\left(\frac{J}{\pi(N+1)}\right)^{3/2} e^{\frac{im}{2\hbar}\frac{\left(\vec{r}_0-\vec{r}_f\right)^2}{t_f-t_0}} =$$

$$= \left(\frac{\cancel{m}}{2\pi \cancel{i}\cancel{\hbar\Delta t}}\;\frac{-\pi\, 2\cancel{\hbar\Delta t}}{i\cancel{m}}\right)^{\frac{3(N+1)}{2}}\left(-\frac{im}{2\hbar\,\Delta t\,\pi(N+1)}\right)^{3/2} e^{\frac{im}{2\hbar}\frac{\left(\vec{r}_0-\vec{r}_f\right)^2}{t_f-t_0}}$$

$$= \left(\frac{m}{2\hbar i \pi (t_f - t_0)} \right)^{3/2} e^{\frac{im}{2\hbar} \frac{(\vec{r}_0 - \vec{r}_f)^2}{t_f - t_0}}$$

and we have used the fact that $t_f - t_0 = (N+1)\Delta t$.

Problem 2



The incident wave packet @ $t=0$ has a wave function of the form

$$\psi_{inc}(x, t=0) = \int \frac{dp}{2\pi\hbar} f(p) \, e^{\frac{i}{\hbar}px} \, e^{-\frac{i}{\hbar}E_p t} \Big|_{t=0} \quad (2.1)$$

The reflected wave packet @ $t=0$ has a wave function of the following

$$\psi_{ref}(x, t=0) = \int \frac{dp}{2\pi\hbar} f(p) \left(\frac{p - \bar{p}}{p + \bar{p}} \right) e^{\frac{i}{\hbar}(-px - Et)} \Big|_{t=0}$$

however, as discuss in class

$$\frac{p-\bar{p}}{p+\bar{p}} = -e^{i2\delta} = e^{i[2\delta+\pi]}$$

where

$$\tan\delta = \frac{p}{\hbar K} = \sqrt{\frac{E}{V-E}}$$

Therefore

$$\psi_{refl}(x,t) = \int \frac{dp}{2\pi\hbar} f(p)\, e^{\frac{i}{\hbar}\left(-px+(2\delta+\pi)\hbar - E_p t\right)}$$

For a wave packet with $f(p)$ peaked around some $p=p_0$ or for a single well-defined momentum $p=p_0$ we can write this as

$$\psi_{refl}(x,t) = \int \frac{dp}{2\pi\hbar} f(p)\, e^{\frac{i}{\hbar}\left(-p(x-x_0) - E_p t\right)} \qquad (2.2)$$

where

$$x_0 = \frac{(2\delta+\pi)\hbar}{p_0}$$

by comparing (2.2) and (2.1) we find that

$$\psi_{reflected}(x,t) = \psi_{incident}(-x+x_0, t)$$

However, if the process of reflection, were instantaneous we would have had

$$\psi_{refl}(x,t) = \psi_{inc}(-x,t)$$

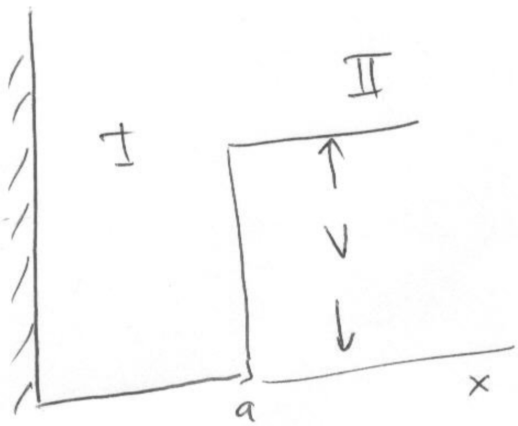
Thus there is a distance of travel within the step of size $x_0 = \frac{(2\delta+\pi)\hbar}{p}$

similarly we could write

$$\psi_{refl}(x,t) = \int \frac{dp}{2\pi\hbar} f(p)\, e^{\frac{i}{\hbar}\left(-px - E_p(t-t_0)\right)}$$

where $t_0 = \frac{(2\delta+\pi)\hbar}{E_p}$

Problem 3



a)

$$\psi(x) = \begin{cases} A \sin kx , & 0 < x < a , \quad k = \frac{\sqrt{2mE}}{\hbar} \\ B e^{-\bar{k} x} & x > a , \quad \bar{k} = \frac{\sqrt{2m(V-E)}}{\hbar} \end{cases}$$

Boundary Condition

$$\psi_I(a) = \psi_{II}(a) \Rightarrow A \sin ka = B e^{-\bar{k} a} \quad (3.1)$$

$$\psi'_I(a) = \psi'_{II}(a) \Rightarrow A k \cos ka = -\bar{k} B e^{-\bar{k} a} \quad (3.2)$$

dividing (3.2) by (3.1) we obtain

$$\bar{k} \tan ka = -k \quad (3.3)$$

(b) Eq. 3.2 can be written in terms of k as follows:

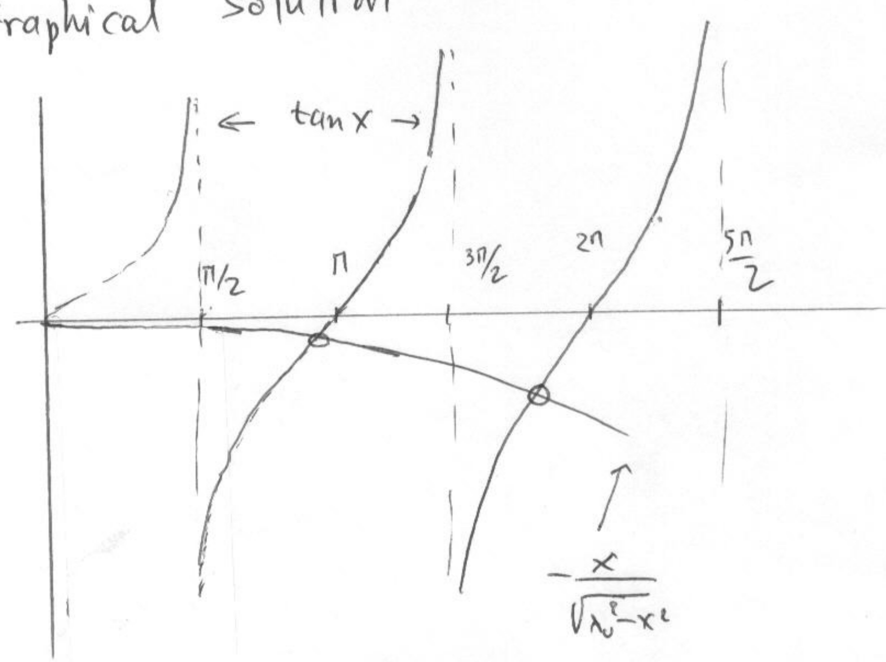
$$\tan ka = -\frac{ka}{\sqrt{\lambda_0^2 - (ka)^2}} \qquad (3.4)$$

where $\lambda_0^2 = \dfrac{2mVa^2}{\hbar^2}$

Let's call $x = ka$, then

$$\tan x = -\frac{x}{\sqrt{\lambda_0^2 - x^2}} \qquad (3.5)$$

Graphical solution



c) For large V λ_0 is large and

$$-\frac{x}{\sqrt{\lambda_0^2-x^2}} \approx -\frac{x}{\lambda_0} \quad \text{for } \frac{x}{\lambda_0} \text{ small}$$

In this case the intersection is just below π.

i.e

$$x \approx \pi - \varepsilon \qquad \varepsilon \to 0^+$$

and

$$\tan x = -\tan \varepsilon \approx -\varepsilon$$

and in order to determine ε we can use (3.5) as follows:

$$-\varepsilon = -\frac{\pi-\varepsilon}{\sqrt{\lambda_0^2-(\pi-\varepsilon)^2}}$$

we need to expand the rhs in power of ε and we find that

$$\text{rhs} = -\frac{\pi}{\sqrt{\lambda_0^2-\pi^2}} + \frac{\varepsilon}{\sqrt{\lambda_0^2-\pi^2}} + O(\varepsilon^2)$$

which implies that

$$\varepsilon \approx \frac{\pi}{1+\sqrt{\lambda_0^2-\pi^2}} \overset{\lim \lambda_0 >> 1}{\approx} \frac{\pi}{\lambda_0} = \frac{\pi \hbar}{\sqrt{2mV}\, a}$$

d) we need to normalize ψ as follows

$$\int_0^\infty |\psi(x)|^2 dx = 1 \Rightarrow \int_0^a |\psi(x)|^2 dx + \int_a^\infty |\psi(x)|^2 dx = 1$$

$$\Rightarrow |A|^2 \int_0^a \sin^2 kx\, dx + |B|^2 \int_a^\infty e^{-2\bar{k}x} dx = 1$$

$$|A|^2 \left[\frac{a}{2} - \frac{1}{4k}\sin 2ka\right] + |B|^2 \frac{e^{-2\bar{k}a}}{2\bar{k}} = 1$$

using eq. 3,1 we can write

$$|B|^2 \left[\frac{e^{-2\bar{k}a}}{2\bar{k}} + e^{-2\bar{k}a}\left(\frac{a}{2} - \frac{1}{4k}\sin 2ka\right)\right] = 1$$

The first term is small in the large V limit

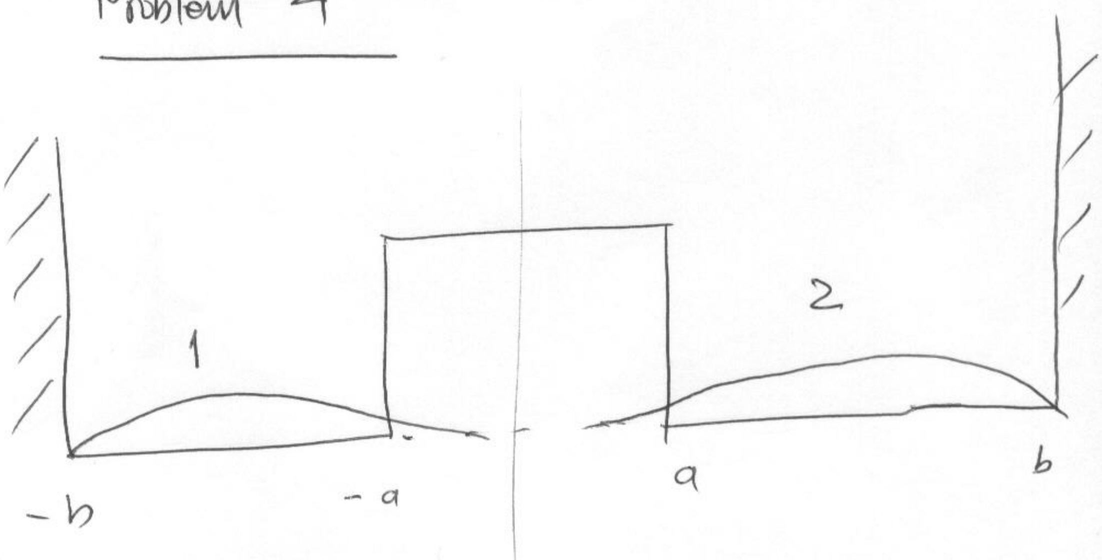
Therefore $|B|^2 \simeq e^{2\bar{k}a} \frac{2}{a} \frac{1}{1 - \frac{\sin 2ka}{2ka}}$

Thus

$$\psi(x>a) \cong \sqrt{\frac{2}{a}} \frac{1}{\sqrt{1-\frac{\sin 2ka}{2ka}}} e^{-\bar{k}(x-a)}$$

Problem 4

a)



$$\psi_1(x) = \begin{cases} A \sin k(x+b) & a<|x|<b \\ B\, e^{-\bar{k}(x+b)} & |x|<a \end{cases}$$

in addition A and B are related to those of the previous problem by replacing a with $|b-a|$.

$$\psi_2(x) = \begin{cases} A \quad \sin\left[k(-x+b)\right] & a<|x|<b \\ B \quad e^{-\bar{k}(-x+b)} & |x| \not> a \end{cases}$$

namely $\quad \psi_2(x) = \psi_1(-x)$ (it is the mirror image of 1).

b) $\quad h_{11} = \int dx \; \psi_1^*(x) \, H \, \psi_1(x) \approx E$

where E is the ground state of the left problem.

$$h_{22} = \int dx \; \psi_2^*(x) \, H \, \psi_2(x) \approx E$$

$$h_{12} = \int dx \; \psi_1^*(x) \, H \, \psi_2(x) = E \int dx \, \psi_1^*(x) \, \psi_2(x)$$

$$\simeq E \, |B|^2 \int_{-a}^{a} e^{-\bar{k}(x+b)} \; e^{-\bar{k}(-x+b)} \, dx =$$

$$= 2a \, E \, |B|^2 \, e^{-2\bar{k}b}$$

c) Therefore, the matrix is

$$\begin{pmatrix} E & 2aE|B|^2 e^{-2\bar{k}b} \\ 2aE|B|^2 e^{-2\bar{k}b} & E \end{pmatrix} =$$

$$E \begin{pmatrix} 1 & \alpha \\ \alpha & E \end{pmatrix} \qquad \text{where } \alpha = 2a|B|^2 e^{-2\bar{k}b}$$

The eigenvalues of this are

$E(1 \pm \alpha)$ and the corresponding eigenstates

$$\psi_{\pm}(x) = \frac{1}{\sqrt{2}}\left(\psi_1 \mp \psi_2\right) = \frac{1}{\sqrt{2}}\left(|1\rangle \mp |2\rangle\right)$$

d) The initial state can be expressed in terms of the two eigenstates as follows:

$$|1\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle + |-\rangle\right)$$

Therefore, the initial state can be written as follows

$$|\psi(t=0)\rangle = |1\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle + |-\rangle\right)$$

where $|+\rangle$ and $|-\rangle$ are the eigenstates of H. Thus, at time $t>0$

$$|\psi(t>0)\rangle = \frac{1}{\sqrt{2}}\left[e^{-\frac{i}{\hbar}E_+ t}|+\rangle + e^{-\frac{i}{\hbar}E_- t}|-\rangle\right]$$

$$= \frac{1}{\sqrt{2}}\, e^{-\frac{i}{\hbar}Et}\left(e^{-\frac{i}{\hbar}E\alpha t}|+\rangle + e^{\frac{i}{\hbar}E\alpha t}|-\rangle\right)$$

The amplitude to go to state $|2\rangle$ at time t is given by the inner product:

$$\langle 2|\psi(t>0)\rangle$$

and $|2\rangle = \frac{1}{\sqrt{2}}\left(|+\rangle - |-\rangle\right)$

Thus,

$$\langle 2|\psi(t)\rangle = \frac{1}{2}\left(e^{-\frac{i}{\hbar}E\alpha t} - e^{\frac{i}{\hbar}E\alpha t}\right) = -i\sin(E\alpha t)$$

The probability is

$$\left|\langle 2|\psi(t)\rangle\right|^2 = \sin^2(E\alpha t)$$

where

E, α have been defined earlier.