Uitwerking Final Exam Kwantumfysica 1 27 April 2007

Problem 1

a) Time-independent Schrödinger equation for a one-dimensional particle, in x-representation:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\varphi(x) = E\,\varphi(x) \Rightarrow$$

$$\frac{\partial^2}{\partial x^2}\varphi(x) = -\frac{2m(E-V)}{\hbar^2}\varphi(x)$$

This differential equation has solutions of the form $\varphi(x) = e^{ikx}$ (plane waves with wave number k)

This is consistent with the schrodinger equation for

$$k = \frac{\sqrt{2m(E-V)}}{\hbar} \Rightarrow k_i = \frac{\sqrt{2m(E-V_i)}}{\hbar}$$

b) During the scatter event $\varphi(x)$ should have $\varphi(x)$ $\frac{\partial \varphi}{\partial x}$ continuous at $x=0$, where $\varphi(x)$ the wavefunction of the particle. Here $\varphi(x)$ is:

In region 1, $\varphi(x) = \varphi_1(x) = Ae^{ik_1x} + Be^{-ik_1x}$
(an incoming and reflected plane wave)

In region 2, $\varphi(x) = \varphi_2(x) = Ce^{ik_2x}$
(only a transmitted plane wave)

A description of those plane waves only is appropriate because the uncertainty in velocity is very small.

Working this out gives

$$\begin{cases}\varphi_1(0) = \varphi_2(0)\\ \frac{\partial\varphi_1(0)}{\partial x} = \frac{\partial\varphi_2(0)}{\partial x}\end{cases} \Rightarrow \begin{cases} A + B = C\\ k_1\cdot A - k_1\cdot B = k_2\cdot C\end{cases} \Rightarrow$$

Solve for B and C normalized to A

$$\begin{cases}\frac{B}{A} - \frac{C}{A} = -1\\ \frac{k_2}{k_1}\frac{C}{A} - \frac{B}{A} = -1\end{cases} \Rightarrow \begin{cases}\frac{B}{A} = \frac{1-k_2/k_1}{1+k_2/k_1}\\ \frac{C}{A} = \frac{2}{1+k_2/k_1}\end{cases}$$

The probability for the particle to be reflected is then $\left|\frac{B}{A}\right|^2$, which gives

$$R = \left|\frac{B}{A}\right|^2 = \left|\frac{1-k_2/k_1}{1+k_2/k_1}\right|^2 \Rightarrow$$

$$R = \left|\frac{1-\sqrt{\frac{E_0-V_2}{E_0-V_1}}}{1+\sqrt{\frac{E_0-V_2}{E_0-V_1}}}\right|^2$$

c) With $V_2 = V_1 - V_0$ follows from b)

$$R = \left|\frac{1-\sqrt{\frac{(E_0-V_1)+V_0}{(E_0-V_1)}}}{1+\sqrt{\frac{(E_0-V_1)+V_0}{(E_0-V_1)}}}\right|^2$$

Only differences in energy matter, absolute values of energy have little meaning.

d) Use c) and substitute

CASE	$(E_0 - V_1)$	V_0	R
$V_2 = 0.5\,V_1$	V_1	$0.5\,V_1$	0.01
$V_2 = 1\,V_1$	V_1	0	0
$V_2 = 1.5\,V_1$	V_1	$-0.5\,V_1$	0.029

$\boxed{V_2 = 0.5 V_1}$ $$R = \left|\frac{1-\sqrt{1.5}}{1+\sqrt{1.5}}\right|^2 \approx 0.01$$

$\boxed{V_2 = V_1}$ $$R = \left|\frac{1-\sqrt{1}}{1+\sqrt{1}}\right|^2 = 0$$

$\boxed{V_2 = 1.5 V_1}$ $$R = \left|\frac{1-\sqrt{0.5}}{1+\sqrt{0.5}}\right|^2 \approx 0.029$$

Problem 2

a) Normalized if $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 2A^2 \int_0^{\infty} e^{-2x/a} dx = -\frac{a}{2} 2A^2 \left[e^{-\frac{2x}{a}} \right]_0^{\infty}$$

$$= -a A^2 (0 - 1) = aA^2 = 1 \Rightarrow A = \sqrt{\frac{1}{a}}$$

b) Answer is $\psi(x)$ in k-representation $\Rightarrow$

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

$$= \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{0} e^{+x/a} e^{-ikx} dx + \frac{A}{\sqrt{2\pi}} \int_0^{\infty} e^{-x/a} e^{-ikx} dx$$

$$= \frac{A}{\sqrt{2\pi}} \int_{-\infty}^{0} e^{(\frac{1}{a} - ik)x} dx + \frac{A}{\sqrt{2\pi}} \int_0^{\infty} e^{-(\frac{1}{a} + ik)x} dx$$

$$= \frac{A}{\sqrt{2\pi}} \frac{1}{(\frac{1}{a} - ik)} \left[e^{(\frac{1}{a} - ik)x} \right]_{-\infty}^{0} + \frac{A}{\sqrt{2\pi}} \frac{-1}{(\frac{1}{a} + ik)} \left[e^{-(\frac{1}{a} + ik)x} \right]_0^{\infty}$$

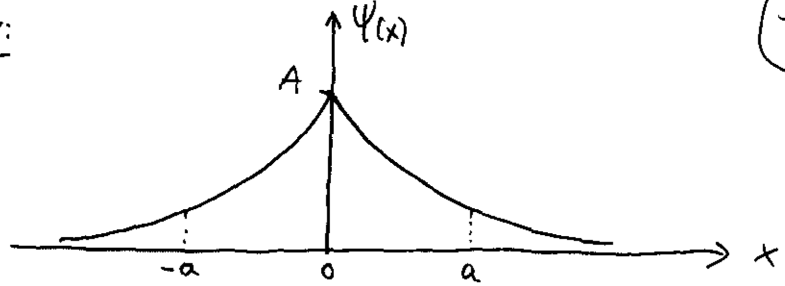
$$= \frac{A}{\sqrt{2\pi}} \frac{1}{\frac{1}{a} - ik} (1 - 0) + \frac{A}{\sqrt{2\pi}} \frac{-1}{(\frac{1}{a} + ik)} (0 - 1)$$

$$= \frac{A}{\sqrt{2\pi}} \left(\frac{1}{\frac{1}{a} - ik} + \frac{1}{\frac{1}{a} + ik} \right) = \frac{A}{\sqrt{2\pi}} \left(\frac{\frac{1}{a} + ik}{\frac{1}{a^2} + k^2} + \frac{\frac{1}{a} - ik}{\frac{1}{a^2} + k^2} \right)$$

$$= \frac{A}{\sqrt{2\pi}} \left(\frac{2\,\frac{1}{a}}{\frac{1}{a^2} + k^2} \right) = \frac{2aA}{\sqrt{2\pi}} \cdot \frac{1}{1 + a^2 k^2} \Rightarrow \text{with } A = \frac{1}{\sqrt{a}}$$

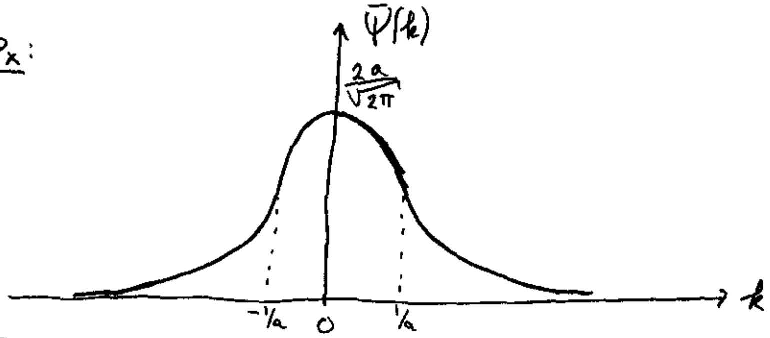
$$\bar{\psi}(k) = \frac{2\sqrt{a}}{\sqrt{2\pi}} \cdot \frac{1}{1 + a^2 k^2}$$

, **ΔX:**



$\psi(x)$ drops to $\frac{1}{e}\cdot A$ for $x = \pm a \Rightarrow$ Width of this state $\approx a \Rightarrow \Delta x \approx a$

ΔP_x:



$\bar{\psi}(k)$ drops to $\frac{1}{2}\cdot\frac{2a}{\sqrt{2\pi}}$ for $k = \pm\frac{1}{a} \Rightarrow$ Width of this state $\approx \frac{1}{a} \Rightarrow \Delta k \approx \frac{1}{a}$

$p_x = \hbar k \Rightarrow \Delta P_x \approx \frac{\hbar}{a}$

Heisenberg: $\Delta x \Delta P_x \geq \frac{\hbar}{2}$

Here we find $\Delta x \cdot \Delta P_x \approx a \cdot \frac{\hbar}{a} \approx \hbar \Rightarrow$ No violation

d) Velocity is proportional to k, $v = \frac{P_x}{m} = \frac{\hbar k}{m} \Rightarrow$

Use k-representation to evaluate this probability

$$P_{40\text{-}50} = \int_{k_{40}}^{k_{50}} |\bar{\psi}(k)|^2\, dk = \int_{k_{40}}^{k_{50}} \left(\frac{2\sqrt{a}}{\sqrt{2\pi}}\right)^2 \left(\frac{1}{1+a^2k^2}\right)^2 dk$$

$$= \frac{2a}{\pi}\int_{k_{40}}^{k_{50}} \left(\frac{1}{1+a^2k^2}\right) dk = \frac{2a}{\pi}\left[\frac{1}{2}\,\frac{k}{1+a^2k^2} + \frac{1}{2}\,\frac{\arctan(ak)}{a}\right]_{k_{40}}^{k_{50}}$$

$$= \frac{1}{\pi}\left[\frac{ak}{1+a^2k^2} + \arctan(ak)\right]_{k_{40}}^{k_{50}}$$, with

$$a k_{40} = \frac{a m v_{40}}{\hbar} = \frac{1\cdot 10^{-9}\cdot 9.1\cdot 10^{-31}\cdot 40\cdot 10^{3}\ \text{m kg m/s}}{1.055\cdot 10^{-34}\ \text{Js}} = 0.345$$

$$a k_{50} = \frac{a m v_{50}}{\hbar} = \frac{1\cdot 10^{-9}\cdot 9.1\cdot 10^{-31}\cdot 50\cdot 10^{3}\ \text{m kg m/s}}{1.055\cdot 10^{-34}\ \text{Js}} = 0.431$$

$$\Rightarrow P_{40\text{-}50} = \frac{1}{\pi}\left(\frac{0.431}{1+(0.431)^2} - \frac{0.345}{1+(0.345)^2} + \arctan(0.431) - \arctan(0.345)\right)$$

$$= 0.041 \Rightarrow \approx 4\%$$

Problem 3

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a) E_g and E_e should be consistent with $|\varphi_g\rangle$ and $|\varphi_e\rangle$ in the Schrödinger equation $\hat{H}|\varphi_i\rangle = E_i|\varphi_i\rangle$

For $\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$ this gives

$$\begin{pmatrix} E_0 & T \\ T & E_0 \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = E_+\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \Rightarrow E_+ = E_0 + T$$

For $\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix}$ this gives

$$\begin{pmatrix} E_0 & T \\ T & E_0 \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{-1}{\sqrt{2}} \end{pmatrix} = E_-\begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} \Rightarrow E_- = E_0 - T$$

Given that T real and $T<0$, it must be that

$$\begin{cases} E_g = E_+ = E_0 + T, & \text{for } |\varphi_g\rangle \\ E_e = E_- = E_0 - T, & \text{for } |\varphi_e\rangle \end{cases}$$

b) $\langle\varphi_g|\varphi_g\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{2} + \frac{1}{2} = 1 \Rightarrow$ Normalized

$\langle\varphi_e|\varphi_e\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{2} + \frac{1}{2} = 1 \Rightarrow$ Normalized

$\langle\varphi_e|\varphi_g\rangle = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{pmatrix}\begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{2} - \frac{1}{2} = 0 \Rightarrow$ Orthogonal

c) For $\hat{H}_0$:

0/.

$$[\hat{A}, \hat{H}_0] = \hat{A}\hat{H}_0 - \hat{H}_0\hat{A} = \begin{pmatrix} -a & 0 \\ 0 & a \end{pmatrix}\begin{pmatrix} E_0 & 0 \\ 0 & E_0 \end{pmatrix} - \begin{pmatrix} E_0 & 0 \\ 0 & E_0 \end{pmatrix}\begin{pmatrix} -a & 0 \\ 0 & a \end{pmatrix}$$

$$= \begin{pmatrix} -aE_0 & 0 \\ 0 & aE_0 \end{pmatrix} - \begin{pmatrix} -aE_0 & 0 \\ 0 & aE_0 \end{pmatrix} = 0 \Rightarrow \hat{A} \text{ and } \hat{H}_0 \text{ commute}$$

For $\hat{H}$:

$$[\hat{A}, \hat{H}] = \hat{A}\hat{H} - \hat{H}\hat{A} = \begin{pmatrix} -a & 0 \\ 0 & a \end{pmatrix}\begin{pmatrix} E_0 & T \\ T & E_0 \end{pmatrix} - \begin{pmatrix} E_0 & T \\ T & E_0 \end{pmatrix}\begin{pmatrix} -a & 0 \\ 0 & a \end{pmatrix}$$

$$= \begin{pmatrix} -aE_0 & -aT \\ aT & aE_0 \end{pmatrix} - \begin{pmatrix} -aE_0 & aT \\ -aT & aE_0 \end{pmatrix} = \begin{pmatrix} 0 & -2aT \\ -2aT & 0 \end{pmatrix} \neq 0$$

$\Rightarrow \hat{A}$ and $\hat{H}$ do not commute.

d) $\hat{A}$ is a diagonal matrix, so the eigenvalues are on the diagonal.
$\hat{H}_0$ and $\hat{A}$ commute (but $\hat{H}_0$ degenerate), so the eigenvectors of $\hat{A}$ are the same or a linear superposition of those of $\hat{H}_0$.

$\hat{A}|\varphi_i\rangle = \pm a|\varphi_i\rangle \Rightarrow$

$\begin{pmatrix} -a & 0 \\ 0 & a \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = +a\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ is consistent for $|\varphi_i\rangle \leftrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}$

$\Rightarrow$ eigenvalue $+a$ has eigenvector $|\varphi_R\rangle$

$\begin{pmatrix} -a & 0 \\ 0 & a \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = -a\begin{pmatrix} 1 \\ 0 \end{pmatrix}$ is consistent for $|\varphi_i\rangle \leftrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix}$

$\Rightarrow$ eigenvalue $-a$ has eigenvector $|\varphi_L\rangle$

e) Ground state of $\hat{H}$ is $|\varphi_g\rangle = \frac{1}{\sqrt{2}}(|\varphi_L\rangle + |\varphi_R\rangle)$ 9/11

So, a measurement of $\hat{A}$ can gives both $+a$ and $-a$ as answer

measurement outcome	Probability	state after measurement
$-a$	$\|\langle\varphi_L\|\varphi_g\rangle\|^2 = \frac{1}{2}$	$\|\varphi_L\rangle$
$+a$	$\|\langle\varphi_R\|\varphi_g\rangle\|^2 = \frac{1}{2}$	$\|\varphi_R\rangle$
	1 +	

f) $|\psi\rangle = \sqrt{\frac{1}{3}}|\varphi_g\rangle + \sqrt{\frac{2}{3}}|\varphi_e\rangle = \left(\sqrt{\frac{1}{6}}|\varphi_L\rangle + \sqrt{\frac{1}{6}}|\varphi_R\rangle\right) + \left(\sqrt{\frac{2}{6}}|\varphi_L\rangle - \sqrt{\frac{2}{6}}|\varphi_R\rangle\right)$

$= \frac{1+\sqrt{2}}{\sqrt{6}}|\varphi_L\rangle + \frac{1-\sqrt{2}}{\sqrt{6}}|\varphi_R\rangle \Rightarrow$ Both $|\varphi_L\rangle$ and $|\varphi_R\rangle$ have non-zero probability amplitude, so a measurement can give both $+a$ and $-a$ as answer.

Probability for $-a$ is $|\langle\varphi_L|\psi\rangle|^2$,
for $+a$ is $|\langle\varphi_R|\psi\rangle|^2$

measurement outcome	Probability	State after measurement
$-a$	$\left(\frac{1+\sqrt{2}}{\sqrt{6}}\right)^2$	$\|\varphi_L\rangle$
$+a$	$\left(\frac{1-\sqrt{2}}{\sqrt{6}}\right)^2$	$\|\varphi_R\rangle$
	1 +	

g) The state is $|\varphi_L\rangle = \frac{1}{\sqrt{2}}(|\varphi_g\rangle + |\varphi_e\rangle)$ 10/11

since $|\varphi_g\rangle = \frac{1}{\sqrt{2}}(|\varphi_L\rangle + |\varphi_R\rangle)$ and $|\varphi_e\rangle = \frac{1}{\sqrt{2}}(|\varphi_L\rangle - |\varphi_R\rangle)$

h) $\langle\varphi_g|\hat{A}|\varphi_g\rangle = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}-a & 0\\ 0 & a\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix} = 0$ $\Rightarrow$ expectation value for position is zero for system in state $|\varphi_g\rangle$

$\langle\varphi_e|\hat{A}|\varphi_e\rangle = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}-a & 0\\ 0 & a\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}}\\ -\frac{1}{\sqrt{2}}\end{pmatrix} = 0$ $\Rightarrow$ expectation value for position is zero for system in state $|\varphi_e\rangle$

$\langle\varphi_g|\hat{A}|\varphi_e\rangle = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}-a & 0\\ 0 & a\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}}\\ -\frac{1}{\sqrt{2}}\end{pmatrix} = -a$

$\langle\varphi_e|A|\varphi_g\rangle = \begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}-a & 0\\ 0 & a\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix} = -a$

When the system is in a superposition of $|\varphi_g\rangle$ and $|\varphi_e\rangle$ the expectation value for position can be different from zero.

i) State at $t=0$ denoted as $|\psi_0\rangle = |\varphi_L\rangle = \frac{1}{\sqrt{2}}(|\varphi_g\rangle + |\varphi_e\rangle)$

For investigating time evolution of $\hat{A}$, describe the state of the system as a superposition of energy eigen states.

$\langle\hat{A}(t)\rangle = \langle\psi(t)|\hat{A}|\psi(t)\rangle = \langle\psi_0|\hat{U}^+\hat{A}\hat{U}|\psi_0\rangle$

with $\hat{U} = e^{-\frac{i}{\hbar}\hat{H}t}$ $\Rightarrow$

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$$\langle \hat{A}(t) \rangle = \frac{1}{2}\left(\langle \varphi_g| + \langle \varphi_e|\right)\hat{U}^{+}\hat{A}\,\hat{U}\left(|\varphi_g\rangle + |\varphi_e\rangle\right)$$

$$= \frac{1}{2}\left(e^{+i\omega_g t}\langle \varphi_g| + e^{+i\omega_e t}\langle \varphi_e|\right)\hat{A}\left(e^{-i\omega_g t}|\varphi_g\rangle + e^{-i\omega_e t}|\varphi_e\rangle\right)$$

$$= \frac{1}{2}\left(\langle \varphi_g|\hat{A}|\varphi_g\rangle + \langle \varphi_e|\hat{A}|\varphi_e\rangle + e^{+i(\omega_g-\omega_e)t}\langle \varphi_g|\hat{A}|\varphi_e\rangle + e^{+i(\omega_e-\omega_g)t}\langle \varphi_e|\hat{A}|\varphi_g\rangle\right)$$

$$= \frac{1}{2}\left(0 + 0 + e^{-i(\omega_e-\omega_g)t}(-a) + e^{+i(\omega_e-\omega_g)t}(-a)\right)$$

$$= -\frac{1}{2}a \cdot 2\cos\left((\omega_e-\omega_g)\,t\right)$$

$$= -a\cos\left((\omega_e-\omega_g)\,t\right)$$

Where we used $\omega_e = \frac{E_e}{\hbar}$ and $\omega_g = \frac{E_g}{\hbar}$

$$E_e - E_g = \underbrace{-2T}_{>0} \Rightarrow$$

$$\langle \hat{A}(t) \rangle = -a\cos\left(\frac{|2T|}{\hbar}\cdot t\right)$$

The system oscillates between the two wells, from position $-a$ to $+a$ and back, and starts (as it should) indeed at $-a$ for $t=0$.

The angular frequency of the oscillations is $\frac{E_e - E_g}{\hbar} = \frac{|2T|}{\hbar}$