Physics 137A

Spring 2014
University of California at Berkeley

Midterm 1

February 24, 2014, 7-9pm
1 LeConte Hall
120minutes ⋄ 50points

Problem 1 ⋄ Average Momentum *8points*

A particle's coordinate space wavefunction $\psi(x)$ is real and square integrable. Prove that the particle's average momentum is zero. Would the particle's average momentum be zero if $i\psi(x)$ were real?

Problem 2 ⋄ Properties of a Wavefunction *22points*

A particle of mass m moving under the influence of a one-dimensional potential $V(x)$ has the wavefunction:

$$\psi(x) = Nxe^{-\alpha x^2}.$$

⋄ A ⋄ Normalize $\psi(x)$. That is, find the value of N.
⋄ B ⋄ What is $\langle x \rangle$? What is $\langle p \rangle$?
⋄ C ⋄ What is $\langle x^2 \rangle$? What is $\langle p^2 \rangle$?
⋄ D ⋄ Does the uncertainty principle hold?
⋄ E ⋄ Suppose that you find out that $V(x) = 0$. What is $\langle H \rangle$? Is $\psi(x)$ an energy eigenstate?
⋄ F ⋄ Suppose instead that you only know that $V(0) = 0$ and you also do know that $\psi(x)$ is an energy eigenstate. Find the potential $V(x)$ and the energy eigenvalue E?
⋄ G ⋄ Explain why $\psi(x)$ is or is not the ground state wavefunction. That is, why E is or is not the lowest possible energy eigenvalue.

Problem 3 ⋄ Conserved Probability Current *10points*

Suppose $\psi(x,t)$ obeys the one-dimensional Schrödinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi(x,t).$$

⋄ A ⋄ Derive the conservation law for probability:

$$\frac{\partial\rho}{\partial t} + \frac{\partial j}{\partial x} = 0$$

where $\rho(x,t) = \psi^*\psi$ is the probability density and the probability current is given by:

$$j(x,t) = \frac{\hbar}{2im}\left(\psi^*\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^*}{\partial x}\right).$$

⋄ B ⋄ Explain why this equation is the conservation law for probability.
⋄ C ⋄ What is the current associated with a wavefunction $\psi(x)$ which is real? What is the current associated with a wavefunction such that $i\psi(x)$ is real?

Problem 4 ⋄ Qualitative Double Well (Griffiths Problem 2.47) *10points*

Note: No calculations are allowed in this problem. Sketches and descriptions only! If you are concerned that a qualitative feature which you intend to be visible in your sketch might not be clear, you can include a few descriptive sentences.

Consider the double square well potential as in Figure 1, where the depth V_0 and the width a are fixed, and large enough so several bound states occur while the separation b can vary.

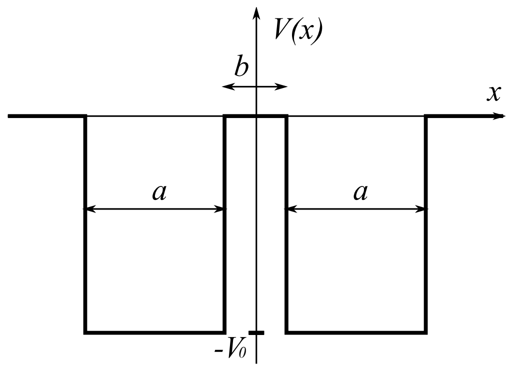


Figure 1: Double square well potential.

◇ A ◇ Sketch the ground state wavefunction ψ_1 and the first excited state ψ_2, (i) for case $b = 0$, (ii) for case $b \approx a$, and (iii) $b \gg a$.

◇ B ◇ Qualitatively, how do corresponding energies, E_1 and E_2, vary, as b goes from zero to infinity? Sketch $E_1(b)$ and $E_2(b)$ on the same graph.

◇ C ◇ The double well is a very primitive one-dimensional model for the potential experienced by an electron in an diatomic molecule where the two wells represent the attractive force of the two nuclei. If the nuclei are free to move, they will adopt the configuration of minimum energy. In view of your conclusions above, does the electron draw the nuclei together or push them apart?

Of course, there is also the internuclear repulsion to consider but that's a separate problem.

Mathematical Formulas

Trigonometry:

$$\sin(a \pm b) = \sin a \cos b \pm \cos a \sin b$$
$$\cos(a \pm b) = \cos a \cos b \mp \sin a \sin b$$

Law of cosines:

$$c^2 = a^2 + b^2 - 2ab\cos\theta$$

Integrals:

$$\int x \sin(ax)\; dx = \frac{1}{a^2}\sin(ax) - \frac{x}{a}\cos(ax)$$
$$\int x \cos(ax)\; dx = \frac{1}{a^2}\cos(ax) + \frac{x}{a}\sin(ax)$$

Exponential integrals:

$$\int_0^\infty x^n e^{-x/a}\; dx = n!\; a^{n+1}$$

Gaussian integrals:

$$\int_0^\infty x^{2n} e^{-x^2/a^2}\; dx = \sqrt{\pi}\;\frac{(2n)!}{n!}\;\left(\frac{a}{2}\right)^{2n+1}$$
$$\int_0^\infty x^{2n+1} e^{-x^2/a^2}\; dx = \frac{n!}{2}\; a^{2n+2}$$

Integration by parts:

$$\int_a^b f\frac{dg}{dx}\; dx = -\int_a^b \frac{df}{dx} g\; dx + fg\Big|_a^b$$

1.

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^* \frac{\hbar}{i} \frac{\partial}{\partial x} \psi \, dx \qquad \psi^* = \psi$$

0 for ψ to be integrable

$$= \int_{-\infty}^{\infty} \psi \frac{\hbar}{i} \frac{\partial}{\partial x} \psi \, dx = \frac{\hbar}{i} \cancel{\psi^2} \Big|_{-\infty}^{\infty} - \int \frac{\partial}{\partial x} \psi \frac{\hbar}{i} \psi \, dx = -\langle p \rangle$$

$$\langle p \rangle = -\langle p \rangle \Rightarrow \langle p \rangle = 0.$$

Since $i\psi \in \mathbb{R}$, $\psi_{(x)} = i f(x)$ where $f(x)$ is real.

Then $\psi^* = -i f(x) = -\psi$

$$\langle p \rangle = \int_{-\infty}^{\infty} \psi^* \frac{\hbar}{i} \frac{\partial}{\partial x} \psi \, dx \qquad \psi^* = -\psi$$

$$= -\int_{-\infty}^{\infty} \psi \frac{\hbar}{i} \frac{\partial}{\partial x} \psi \, dx$$

0 for ψ to be integrable

Technique 1: (by parts)

$$= -\frac{\hbar}{i} \cancel{\psi^2} \Big|_{-\infty}^{\infty} + \int \frac{\partial}{\partial x} \psi \frac{\hbar}{i} \psi \, dx$$

$$= \int \frac{\partial}{\partial x} \psi \frac{\hbar}{i} (-\psi^*) \, dx = -\langle p \rangle$$

Similarly, Yes. $\langle p \rangle = 0$

Technique 2: (total derivatives)

$$= -\int_{-\infty}^{\infty} \psi \frac{\hbar}{i} \frac{\partial}{\partial x} \psi \, dx = -\frac{\hbar}{i} \int_{-\infty}^{\infty} \psi \frac{\partial}{\partial x} \psi \, dx = -\frac{\hbar}{2i} \int_{-\infty}^{\infty} \frac{d}{dx} \psi^2 \, dx$$

$$= -\frac{\hbar}{2i} \psi^2 \Big|_{-\infty}^{\infty} = 0$$

2.

A) $$1 = \int_{-\infty}^{\infty} |\psi_{(x)}|^2 dx = N^2 \int_{-\infty}^{\infty} x^2 e^{-2\alpha x^2} dx$$

Using formula provided, $a = \frac{1}{\sqrt{2\alpha}}$, $n=1$

$$= 2N^2 \sqrt{\pi}\, \frac{2!}{1!} \cdot \frac{(2\alpha)^{-3/2}}{8} = N^2 \sqrt{\pi}\, \frac{(2\alpha)^{-3/2}}{2} \qquad N = \frac{\sqrt{2}}{\pi^{1/4}} (2\alpha)^{3/4} = \left(\frac{32\alpha^3}{\pi}\right)^{1/4}$$

↑ $-\infty$ to ∞ instead of 0 to ∞

B) $$\langle x \rangle = N^2 \int_{-\infty}^{\infty} \underbrace{x^3}_{\text{odd}} \cdot \underbrace{e^{-2\alpha x^2}}_{\text{even}} dx = 0 \quad ☑$$

$\langle p \rangle = 0$ as proven in Prob 1 above. ☑

C) $$\langle x^2 \rangle = N^2 \int_{-\infty}^{\infty} x^4 e^{-2\alpha x^2} dx$$

Using formula provided, $a = \frac{1}{\sqrt{2\alpha}}$, $n = 2$

$$= 2N^2 \sqrt{\pi}\, \frac{4!}{2!} \left(\frac{1}{2\sqrt{2\alpha}}\right)^5 = \left(\frac{32\alpha^3}{\cancel{\pi}}\right)^{1/2} \cancel{\sqrt{\pi}} \cdot \cancel{24}^{\,3} \cdot \frac{1}{\cancel{32}_{\,4} \cdot (2\alpha)^{5/2}} = \frac{3}{4} \cdot \frac{1}{\alpha} \quad ☑$$

$$\langle p^2 \rangle = N^2 \int_{-\infty}^{\infty} x e^{-\alpha x^2} \left(-\hbar^2 \frac{\partial^2}{\partial x^2}\right)\left(x e^{-\alpha x^2}\right) dx \qquad \hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}$$

$$= -\hbar^2 N^2 \int_{-\infty}^{\infty} x e^{-\alpha x^2} \left[2 e^{-\alpha x^2} \alpha x (2\alpha x^2 - 3)\right] dx$$

$$= -2\hbar^2 \alpha \underbrace{N^2 \int_{-\infty}^{\infty} (2\alpha x^4 - 3x^2)\, e^{-2\alpha x^2} dx}$$

$\to 1$ renormalization condition

$\to \langle x^4 \rangle$

$$= -2\hbar^2 \alpha \left(2\alpha \langle x^2 \rangle - 3\right) = -2\hbar^2 \alpha \left(\frac{3}{2} - 3\right) = 3\hbar^2 \alpha \quad ☑$$

D) $$\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{\frac{3}{4} \frac{1}{\alpha}} \qquad \sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \sqrt{3\hbar^2 \alpha}$$

$$\sigma_x \sigma_p = \frac{3}{2}\hbar > \frac{1}{2}\hbar$$

Yes. The uncertainty principle holds.

E) $V_{(x)} = 0 \quad \hat{H} = \frac{\hat{P}^2}{2m} \quad \langle H \rangle = \frac{\langle P^2 \rangle}{2m} = \frac{3\hbar^2\alpha}{2m}$

No, not an eigenstate because

$$\hat{H}\psi = \frac{\hat{P}^2}{2m}\psi = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\right)\left(Nx\,e^{-\alpha x^2}\right) = -\frac{\hbar^2}{2m}N2e^{-\alpha x^2}\alpha x(2\alpha x^2-3) \not\propto \psi$$

F) $\hat{H} = \frac{\hat{P}^2}{2m} + V_{(x)} \qquad \hat{H}\psi = E\psi$

$$\hat{H}\psi = -\frac{\hbar^2 N}{2m}2e^{-\alpha x^2}\alpha x(2\alpha x^2-3) + V_{(x)}Nxe^{-\alpha x^2} = E\left(Nxe^{-\alpha x^2}\right)$$

$$-\frac{\hbar^2 \cancel{N}}{\cancel{2}m}\cancel{2}\cancel{e^{-\alpha x^2}}\alpha \cancel{x}(2\alpha x^2-3) + V_{(x)}\cancel{N}\cancel{x}\cancel{e^{-\alpha x^2}} = E\left(\cancel{N}\cancel{x}\cancel{e^{-\alpha x^2}}\right)$$

$$-\frac{\hbar^2}{m}\alpha(2\alpha x^2-3) + V_{(x)} = E$$

indep. of x, so should be L.H.S.

$$\Rightarrow V_{(x)} = \frac{2\hbar^2}{m}\alpha^2x^2 + \cancel{C}^{\,0}$$ since $V_{(0)}=0$

$$\Rightarrow E = \frac{3\hbar^2\alpha}{m}$$

G) $\psi \propto x e^{-\alpha x^2}$

odd even → odd

Ground state wavefunctions should be even function but our ψ is odd. ψ is <u>not</u> a ground state.

Problem 3

A. $\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial t}(\psi^* \psi) = \frac{\partial \psi^*}{\partial t}\psi + \psi^* \frac{\partial \psi}{\partial t}$ substitute from Schrodinger's Eqn

$$\begin{cases} \frac{\partial \psi}{\partial t} = \frac{-\hbar}{2im}\frac{\partial^2 \psi}{\partial x^2} - \frac{iV}{\hbar}\psi \\ \frac{\partial \psi^*}{\partial t} = \frac{\hbar}{2im}\frac{\partial^2 \psi^*}{\partial x^2} + \frac{iV}{\hbar}\psi^* \end{cases}$$

$$= \frac{\hbar}{2im}\frac{\partial^2 \psi^*}{\partial x^2}\psi + \frac{iV}{\hbar}\psi^*\psi + \frac{-\hbar}{2im}\psi^*\frac{\partial^2 \psi}{\partial x^2} - \frac{iV}{\hbar}\psi^*\psi$$

$$= \frac{\hbar}{2im}\left(\frac{\partial^2 \psi^*}{\partial x^2}\psi - \psi^*\frac{\partial^2 \psi}{\partial x^2}\right)$$

$$\frac{\partial j}{\partial x} = \frac{\partial}{\partial x}\left(\frac{\hbar}{2im}\left(\psi^*\frac{\partial \psi}{\partial x} - \psi\frac{\partial \psi^*}{\partial x}\right)\right) = \frac{\hbar}{2im}\left(\frac{\partial \psi^*}{\partial x}\frac{\partial \psi}{\partial x} + \psi^*\frac{\partial^2 \psi}{\partial x^2} - \frac{\partial \psi}{\partial x}\frac{\partial \psi^*}{\partial x} - \psi\frac{\partial^2 \psi^*}{\partial x^2}\right)$$

$$= \frac{-\hbar}{2im}\left(\frac{\partial^2 \psi^*}{\partial x^2}\psi - \psi^*\frac{\partial^2 \psi}{\partial x^2}\right)$$

Hence $\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0$

B. Integrate over an interval: (a, b)

$$\int_a^b \frac{\partial \rho}{\partial t}dx = -\int_a^b \frac{\partial j}{\partial x}dx$$

$$\frac{d}{dt}\int_a^b \rho\, dx = +j(a) - j(b)$$

$\int_a^b \rho\, dx$ is

LHS: the probability that the particle will be found in (a, b)

RHS: The net flux of probability

The equation states that the probability change over an interval is equal to the net flux.

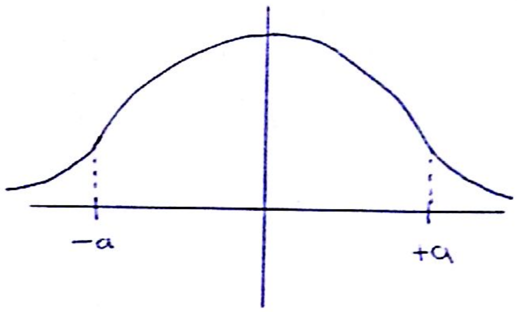
C. If $\psi(x)$ is real, then $\psi = \psi^*$, then $j = \frac{\hbar}{2im}\left(\psi\frac{\partial \psi}{\partial x} - \psi\frac{\partial \psi}{\partial x}\right) = 0$

If $\psi(x)$ is purely imaginary, then we can write $\psi = if$ for a real fcn f.

$$j = \frac{\hbar}{2im}\left(-if\, i\frac{df}{dx} - if(-i)\frac{df}{dx}\right) = 0$$

PROBLEM 4

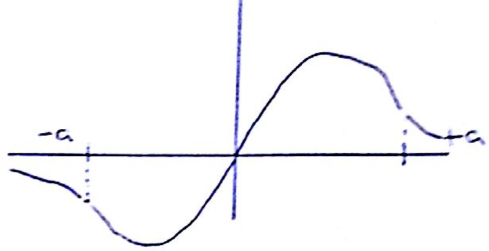
A. (i) $b=0$



Ground state

$[-a,a]$: cosine

outside $[-a,a]$: exponential decay



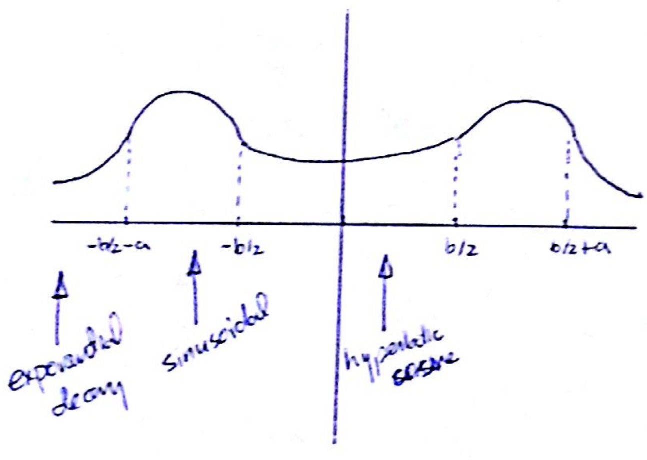
1st Excited State

$[-a,a]$: sine

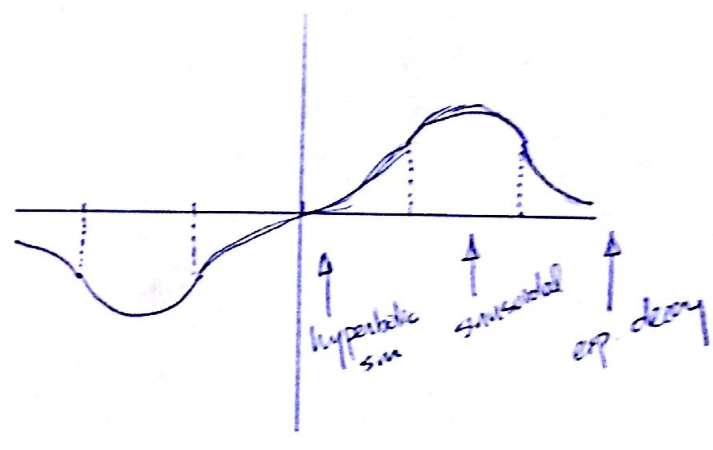
outside: exp. decay

(ii) $b \approx a$

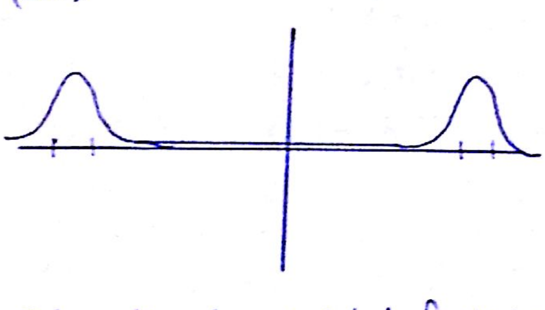
Ground State

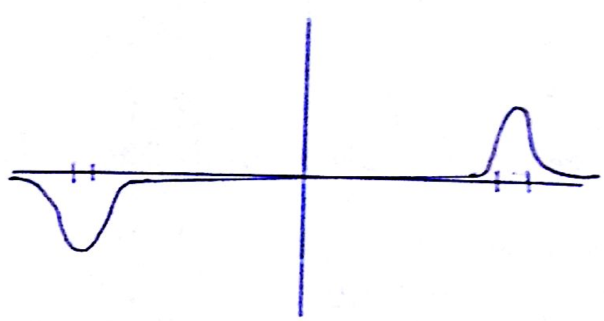


1st Excited State



(iii)

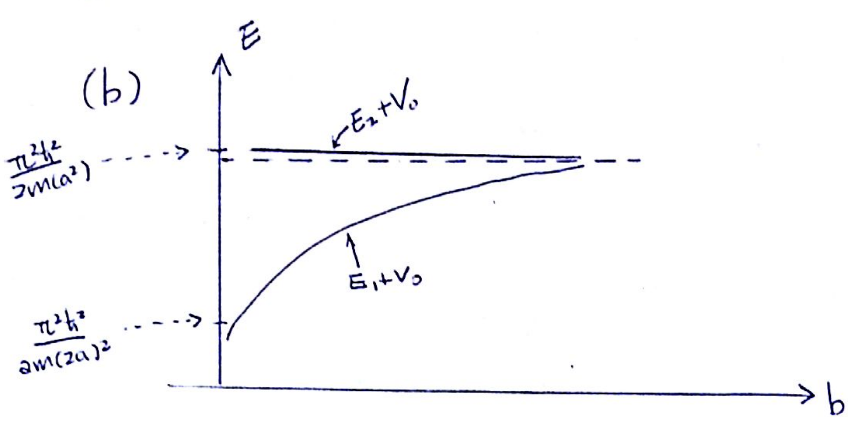




Behaves like two isolated finite square well.

Ground state of symmetric potential is even. 1st excited state is odd with one node.
(with 0 node)

(b)



For $b=0$, it is finite square well : $E_1+V_0 \approx \frac{\pi^2\hbar^2}{2m(2a)^2}$ $\left(\text{from } E_n+V_0 \approx \frac{n^2\pi^2\hbar^2}{2m(2a)^2}\right)$

$$E_2+V_0 \approx \frac{\pi^2\hbar^2}{2m(2a)^2}$$

For $b \gg a$, the wave function is an even or an odd linear combinations of the ground state wavefunction of the finite square well. Thus, $E_1+V_0 \approx \frac{\pi^2\hbar^2}{2ma^2}$ will satisfy $\frac{d^2\psi}{dx^2} = \frac{-2m}{\hbar^2}(V_0+E)\psi$ in both regions for both states.

(C) For the ground state, the energy is lowest for $b \to 0$, therefore e- draws the two nuclei together.