

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

5.73 Quantum Mechanics I
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Problem Set #2

Reading: Merzbacher “Quantum Mechanics”, 3rd Edition: Chapter 7.

Problems:

1. $\psi_1(x) = \frac{a^2}{b^2(x-x_0)^2 + c^2}$ a, b, and c are real
 - A. Normalize $\psi_1(x)$ in the sense $\int_{-\infty}^{\infty} |\psi|^2 dx = 1$.
 - B. Compute values for $\langle x \rangle$, $\langle x^2 \rangle$, and Δx for $\psi_1(x)$.
 - C. (*optional*) Compute values for $\langle k \rangle$ and Δk for $\bar{\psi}_1(k)$, where $\bar{\psi}_1(k)$ is the Fourier transform of $\psi_1(x)$.
[If you choose not to do this problem, state what you expect for the form of $\Psi_1(k)$ and the magnitude of Δk .]

2. $\psi_2(x) = e^{-c^2(x-b)^2} e^{i\alpha(x)}$ where c , b , and $\alpha(x)$ are real. Use the stationary phase idea to design $\alpha(x)$ in the region of x near $x = b$ so that $\langle k \rangle = k_0 \neq 0$.

3. (*optional*) Consider a potential $V = 0$ for $x > a$, $V = -V_0$ for $a \geq x \geq 0$, and $V = +\infty$ for $x < 0$. Show that for $x > a$ the positive energy solutions of the Schrödinger equation have the form [taken from Merzbacher (3rd Ed.), page 111, problem 2]
$$e^{i(kx + 2\delta)} - e^{-ikx}$$
Calculate the scattering coefficient $|1 - e^{2i\delta}|^2$ and show that it exhibits maxima (resonances) at certain discrete energies if the potential is sufficiently deep and broad.

4. The following problem is one of my “patented” magical mystery tours. It is a very long problem which absolutely demands the use of a computer for parts F

and G. There are many separate computer programs that you will need to write for this problem. I urge you to divide the labor into smaller groups, each responsible for a different piece of programming. I believe that the insights you will obtain from working together on this problem will be more than worth the effort expended.

Consider the simplest possible symmetric double minimum potential:

$$\begin{aligned} V(x) &= a\delta(x) & a > 0 & & -L/2 < x < L/2 \\ V(x) &= \infty & & & |x| \geq L/2. \end{aligned}$$

- A. Solve for all of the eigenstates and eigen-energies for states that have odd reflection symmetry about $x = 0$. (This part of the problem is very easy.)
- B. Solve for the energy eigenstates and eigen-energies for the 5 lowest energy even-symmetry states. Choose $a = 400\hbar^2/Lm$. I suggest you use trial functions of form

$$\begin{aligned} \psi_n(x) &= N \sin[k_n(x + L/2)] & -L/2 \leq x < 0 \\ \psi_n(x) &= -N \sin[k_n(x - L/2)] & 0 < x \leq L/2 \end{aligned}$$

One way to find the eigen-energies is to plot the quantities $y = \tan(kL/2)$ and $y = -kL/400$ and to determine eigen-energies from the k -values at intersections. Each E_n (odd n , even symmetry) is located at an intersection. Note there will be exactly one value of E_n below the lowest odd-symmetry eigenstate (E_2) and one value of E_n between each consecutive pair of odd-symmetry eigenstates.

- C. For an ordinary infinite square well, the ratio of the spacing between the two lowest levels to that between the two lowest odd-symmetry levels, is

$$R_{21;42} \equiv \frac{E_2 - E_1}{E_4 - E_2} = \frac{4 - 1}{16 - 4} = \frac{3}{12} = 0.25.$$

For your double minimum potential, this level spacing ratio will decrease from 0.25 at $a = 0$ toward 0 as a increases. For the value of a that I suggested, this ratio should be about 0.003.

Repeat the calculation of $R_{21;42}$ using a -values a factor of 3 and 9 smaller than the one you decided on above.

Suggest a functional relationship between a and $R_{21;42}$.

D. The ratio

$$R_{43;42} = 7/3$$

is for an ordinary infinite square well. Is the E_4-E_3 spacing you obtained for $a = 400\hbar^2/Lm$ larger or smaller than E_2-E_1 ? Why?

E. For $a = 400\hbar^2/Lm$, plot

$$\Psi_+(x) \equiv 2^{-1/2}(\psi_1 + \psi_2)$$

and

$$\Psi_-(x) \equiv 2^{-1/2}(\psi_1 - \psi_2).$$

What does this suggest about the possibility of creating a state localized on the left or right side of the well?

F. Note that, to obtain a solution to the TDSE for a time-independent \mathbf{H} ,

$\Psi(x,t) = \sum_n a_n \psi_n e^{-iE_n t/\hbar}$. Construct $\Psi_+(x,t)$ and $\Psi_-(x,t)$ and compute the following three quantities (you should be able to get the answers for parts (ii) and (iii) from your answer to part (i)):

(i). Survival Probability of $\Psi_+(x,0)$

$$P_+(t) = \left| \int \Psi_+^*(x,t) \Psi_+(x,0) dx \right|^2$$

(ii). Survival Probability of $\Psi_-(x,0)$

$$P_-(t) = \left| \int \Psi_-^*(x,t) \Psi_-(x,0) dx \right|^2$$

(iii). $\Psi_+(x,t) \rightarrow \Psi_-(x,0)$ Transfer Probability

$$P_{+-}(t) = \left| \int \Psi_+^*(x,t) \Psi_-(x,0) dx \right|^2.$$

G. Now construct a more elaborate wavepacket from

$$\Psi_L(x,0) = 6^{-1/2} [\psi_1 - \psi_2 + \psi_3 - \psi_4 + \psi_5 - \psi_6]$$

There may be several critical times in the evolution of $\Psi_L(x,t)$. These will likely include:

- (i) t_g , the global recurrence time for the even-n levels of the infinite box without the δ -function barrier

$$t_g = \frac{2mL^2}{h};$$

- (ii) probably the longest critical time, t_t , the tunneling round trip time for the $\Psi_+(x)$ and $\Psi_-(x)$ states in part E,

$$t_t = \frac{h}{(E_2 - E_1)};$$

- (iii) probably the shortest critical time, t_s , the time corresponding to the largest energy difference in the superposition state

$$t_s = \frac{h}{(E_6 - E_1)}.$$

- (a) Plot $|\Psi_L(x,0)|^2$, $\left| \Psi_L\left(x, \frac{2mL^2}{h}\right) \right|^2$, and $\left| \Psi_L\left(x, \frac{h}{(E_2 - E_1)}\right) \right|^2$.

Comment on what you see in these 3 plots. There is a huge amount of information. “Assign” as many features or families of features as you can. You may need to make additional plots to verify your assignment hypotheses.

- (b) Calculate the following quantities and plot the following quantities twice, once over a short $0 \leq t \leq 2t_s$ and once over a long $0 \leq t \leq 2t_t$ time interval,

$$\langle x \rangle_t = \int \Psi_L^*(x,t)x\Psi_L(x,t)dx$$

$$\langle x^2 \rangle_t = \int \Psi_L^*(x,t)x^2\Psi_L(x,t)dx$$

$$\Delta x_t = \left[\langle x^2 \rangle_t - \langle x \rangle_t^2 \right]^{1/2}.$$

- (c) Compare $\langle x \rangle_t$ and Δx_t and propose a reason for why the position variance exhibits periodic crashes toward 0. What might account for such a focussing of the wavepacket?

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