

6.728 Applied Quantum and Statistical Physics:

Department of Electrical Engineering and Computer Science  
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PROBLEM SET 3

Problem Set Out: 9/20/06

Problem Set Due: 9/27/06 at the beginning of class

PROBLEMS

**Problem 3.1** Spread of Gaussian Wave packet in time. This problem uses the `Matlab` scripts `ps3p1.m` and `cyclelines.m`. These are available on the course website in the `Assignments` section.

Read the `ps3p1.m` script carefully, and be sure that you understand it. You will be asked below to make some modifications of the scripts to solve new problems. (The `cyclelines.m` script is just for beautifying the graphs, and is not relevant to the “physics” of the problem.)

(a) Run script `ps3p1.m`. Explain the calculations being performed, and the resulting graphs. Also type the command `waterfall(psi_t_pdf')` to see another view of how the wave function changes in time. Also plot  $A(q)$  vs.  $q$ .

(b) Modify the script `ps3p1.m` to study the time evolution of a wavepacket which at  $t = 0$  has the form:

$$\Psi(x, 0) = \left( \frac{1}{\pi L^2} \right)^{1/4} e^{-x^2/2L^2} e^{i\pi x/(4L)}$$

with  $L = 1$  nm. Suppress the plotting of the “analytic solution”, which will otherwise clutter up your graphs (or, if you wish, modify the “analytic solution” so it matches the case you are working on). Also type the command `waterfall(psi_t_pdf')` to see another view of how the wave function changes in time. Also plot  $A(q)$  vs.  $q$ . Comment.

(c) Using the results from part (b), plot the expectation value of the displacement versus time (which, for a Gaussian, is the peak position) and determine the group velocity of the wave packet. Compare it to what you would predict analytically.

**Problem 3.2** Text Problem 6.2

The wave function should be corrected to read:

$$\psi(x, t) = Ae^{[k_0x - \omega(k_0)t]} + Be^{[-k_0x - \omega(-k_0)t]}$$

Also, read Problem 6.1.

**Problem 3.3** (This problem counts double.)

Consider a particle confined to a one dimensional box in the interval  $-L/2 \leq x \leq L/2$ . Assume that the particle is initially in the state

$$\Psi(x, 0) = \begin{cases} \sqrt{\frac{8}{L}} & \text{if } |x| \leq \frac{L}{16} \\ 0 & \text{otherwise} \end{cases}$$

This function can be written as a linear combination of basis (eigen) functions as

$$\Psi(x, t) = \sum_{\text{even}} a_n \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L} e^{-iE_n t/\hbar} + \sum_{\text{odd}} a_n \sqrt{\frac{2}{L}} \cos \frac{n\pi x}{L} e^{-iE_n t/\hbar}$$

where  $E = \frac{\hbar^2 \pi^2 n^2}{2mL^2}$ .

- (a) Find the coefficients  $\{a_n\}$  analytically.
- (b) Develop a `Matlab` script based on the results of the script in Problem 1 to compute  $\Psi(x, t)$  at later times using a finite number of basis functions. Be sure to write your script to include both the sine and cosine terms, even though for this part of the problem one set of terms is needed.  
Show the approximated wave function at time zero for 2, 10, 20 lowest energy basis functions at time zero and a few later times. Compare with the coefficients  $\{a_n\}$  analytically.
- (c) Plot the probability density for the wave function using your script in part (b) at a few later times. With 10 terms, find the time the wave function numerically “reconstructs” itself. Discuss why this “reconstruction” occurs.
- (d) Find (numerically) the average energy  $\langle E \rangle$  and width  $\Delta E = \sqrt{\langle E^2 \rangle - \langle E \rangle^2}$ .
- (e) Give the initial wave function a velocity and plot its probability distribution at later times.