

## 351-1 Problems

1. Newton's Laws Can be derived from Hamilton's equations.

- (a) Identify the Hamiltonian from conservation of energy using only momentum  $p$  (for Kinetic Energy) and position  $x$  (for potential Energy):

$$H = KE + PE$$

Use the Hamiltonian for a particle in a 1-D quadratic potential like a mass on a spring. What is  $KE, PE$ ?

- (b) Hamilton's equations are

$$\frac{dp}{dt} = -\frac{\partial H}{\partial x}$$

$$\frac{dx}{dt} = \frac{\partial H}{\partial p}$$

Show these give Newton's laws of motion for the mass on a spring.

- (c) Derive the 1-D differential equation of motion from Hamilton equation. For a particle of total energy  $E$  and spring constant  $k, x = 0$  at  $t = 0$ , what is the equation of motion  $x(t)$ . what is  $p(t)$ . show the region of Phase Space ( $p$  vs  $x$ ) that describes the particle throughout its motion.
- (d) Use the equipartition theorem (where  $\langle A \rangle$  is time average of  $A$ , and  $i$  is index for each spatial dimension):

$$\left\langle p_i \frac{\partial H}{\partial p_i} \right\rangle = \left\langle x_i \frac{\partial H}{\partial x_i} \right\rangle = k_B T$$

to derive the relationship between thermal velocity and temperature  $\frac{1}{2} m v_{th}^2 = \frac{3}{2} k_B T$

- (e) Derive the Dulong-Petit law for atoms in a 3-D potential from the equipartition theorem:

$$\langle E \rangle = 3k_B T$$

- (f) What is the heat capacity  $C = dE/dT$  in this case?

2. Problem 1.1 from Solymar and Walsh:

A 10 mm cube of germanium passes a current of 6.4 mA when 10 mV is applied between two of its parallel faces. Calculate the resistivity of the sample. Assuming that the charge carriers are electrons that have a mobility of  $0.39 \text{ m}^2 \text{ V}^{-1} \text{ s}^{-1}$ , calculate the density of carriers. What is their collision time if the electron's effective mass in germanium is  $0.12 m_e$  where  $m_e$  is the free electron mass?

3. Give a one line description of each of these experiments and their significance to modern physics: Photoelectric Effect, Compton Effect, Black Body Radiation, Rutherford Backscattering (Bohr model), Electron Diffraction, Atomic spectra.

Classical: <https://www.youtube.com/watch?v=yXsHf1XB7QM>

Bohr Atom: <https://www.youtube.com/watch?v=ydPzEZTd-98>

Wave Particle Duality - photoelectric effect: <https://www.youtube.com/watch?v=frNLTEm1glg>

Schrödinger waves: <https://www.youtube.com/watch?v=C8XGIYz1PCw>

Probability interpretation: <https://www.youtube.com/watch?v=p7xIKoBdViY>

Compton Effect: <https://www.youtube.com/watch?v=0Y648TNGAIo>

4. Problem 2.1 from Solymar and Walsh.

Find the de Broglie wavelength of the following particles, ignoring relativistic effects:

(i) an electron in a semiconductor having average thermal velocity at  $T = 300\text{K}$  and an effective mass of  $m_e^* = am_o$ ,

(ii) a helium atom having thermal energy at  $T = 300\text{K}$

(iii) an  $\alpha$  particle ( $He^4$  nucleus) of kinetic energy 10 MeV.

Hint: See question 1. For a gas of non-interacting particles,  $\frac{1}{2} m v_{th}^2 = \frac{3}{2} k_B T$ .

5. A particle of mass,  $m$ , is confined to a 1-D region  $0 \leq x \leq L$ . In class, we derived the following stationary state wavefunctions and energies for this 1-D infinite square well potential:

$$\psi_n(x) = A \sin\left(\frac{\pi n}{L}x\right)$$

- (a) Normalize the wave function to find the value of  $A$ .  
 (b) Find the Energy of these stationary states

Assuming that the initial normalized wavefunction of this particle at  $t = 0$  is:

$$\Psi(x, t = 0) = \sqrt{\frac{8}{5L}} \left[ 1 + \cos\left(\frac{\pi}{L}x\right) \right] \sin\left(\frac{\pi}{L}x\right)$$

- (a) Derive an expression for the wavefunction  $\Psi(x, T)$ , at all later times  $t > 0$ .  
 (b) Show that the probability of finding the particle in the left half of the box (i.e., in the region  $0 \leq x \leq L/2$ ) at time  $t > 0$  is:  $\frac{1}{2} + \frac{16}{15\pi} \cos\left(\frac{3\pi^2 \hbar t}{2mL^2}\right)$
6. Assuming that  $\Psi(x, t)$  is a solution of the 1-D Schrödinger Equation, the current density is defined as:

$$J(x) = -\frac{i\hbar e}{2m} \left[ \Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x} \right]$$

In this problem, consider the potential barrier of height ( $V$ ) and width ( $d$ ) that is depicted in Fig. 3.3 of Solymar and Walsh. Assume that the electron energy ( $E$ ) is less than  $V$ .

- (a) By applying suitable boundary conditions and your knowledge of quantum mechanics, develop a system of equations that could be solved to determine the transmitted current through the barrier ( $J_t$ ) in terms of the incident current on the barrier ( $J_i$ ).  
 (b) By solving your system of equations from part (a), show that:

$$\frac{J_t}{J_i} = \frac{1}{1 + \frac{V^2}{4(V-E)E} \sinh^2(\gamma d)}$$

where  $\gamma = \frac{\sqrt{2m(V-E)}}{\hbar}$  and  $\sinh(\gamma d) = \frac{1}{2}(e^{\gamma d} - e^{-\gamma d})$

- (c) In the limit where  $\gamma d \gg 1$ , show that:  $\frac{J_t}{J_i} = \frac{16(V-E)E}{V^2} e^{-2\gamma d}$   
 (d) The exponential dependence of the "tunneling" current on distance is utilized for atomic resolution imaging of conductive surfaces with the scanning tunneling microscope (STM). Conservatively assume that the STM can detect changes in the tunneling current of 1%. Under typical tunneling conditions (e.g.,  $V - E = 1\text{eV}$ ,  $d \sim 10 \text{ \AA}$ ), estimate the vertical spatial resolution of the STM. Hint: The answer can be expressed in picometers ( $10^{-12} \text{ m}$ )!
7. Derive the solution of the 2-D particle in a box (particle is constrained in both  $x$ , and  $y$  directions;  $V \rightarrow \infty$  at the boundaries).
- (a) Solve for the energies and wave functions of the ground and first excited states.  
 (b) What is the degeneracy of the first excited state?  
 (c) Plot the probability distributions  $2|\psi|^2$  of the first excited states as surface plots.  
 (d) Optional: plot probability distributions of the ground state, first excited states, and 2nd excited states, and comment on the evolution.

8. Consider the infinite spherical well:  $V(r) = 0$  if  $r \leq a$ ,  $V(r) = \infty$  if  $r > a$ .

- (a) For  $l = 0$ , determine the allowed energies ( $E_n$ ).
- (b) For  $l = 0$ , show that the corresponding wavefunctions are:

$$\Psi_n(r) = \frac{1}{\sqrt{2\pi a}} \frac{\sin(n\pi r/a)}{r}$$

In class, we worked through the Schrödinger equation in spherical coordinates for spherically symmetric potentials by breaking the solution into radial and angular functions. You should be able to solve the radial equation for the conditions given here.

9. Consider the infinite spherical well:  $V(r) = 0$  if  $r \leq a$ ,  $V(r) = V_0$  if  $r > a$ .
- (a) For  $l = 0$ , show that there is no bound state if:  $V_0 a^2 < \frac{\pi^2 \hbar^2}{8m}$ . This can be shown without resorting to numerical computation.
- (b) Given  $V_0 = \frac{2\hbar\pi^2}{ma^2}$ , find the energies of the two bound states by graphing in MATLAB or Excel. You can also use MATLAB to check your solution by solving the transcendental equation directly.

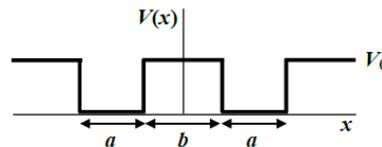
This problem is analogous to the finite square well problem solved in 3.8 of Solymar and Walsh, but in the spherical coordinate system. Through the appropriate application of boundary conditions, you should arrive at a transcendental equation whose argument can be analyzed to establish the condition for the existence of bound states.

10. Suppose that the nucleus of a hydrogen atom is located at a distance  $d$  from a two-dimensional infinite potential wall which, of course, tends to distort the hydrogen atom. As  $d$  approaches zero, determine the following items:
- (a) The ground state wavefunction.
- (b) The degeneracy of the first excited state (ignore degeneracy due to spin).
- (c) The wavelength of light that is emitted upon transition between the first excited state and the ground state (express your answer in nanometers).

With the exception of part (c), this problem does not involve mathematical calculation. The proper choice of coordinate system can make the relationship between these solutions and the usual hydrogen atom solutions clear. Bear in mind that the ground state refers to the lowest energy state that exists.

11. Consider a double finite potential well in one dimension. Suppose that the depth  $V_0$  and the width  $a$  are fixed such that the following equation is obeyed:

$$\beta^2 = \frac{V_0 m a^2}{2\hbar^2} = 4\pi^2$$



12. Qualitatively sketch the ground state wavefunction  $\psi_1$  and the first excited state wavefunction  $\psi_2$  for: (i)  $b = 0$ , (ii)  $b = a/2$ , and (iii)  $b \gg a$ .

- (a) For  $b = 0$ , show that the ground state energy ( $E_1$ ) is given by:  $E_1 = \frac{\hbar^2 x_1^2}{2ma^2}$ , where  $x_1$  is the solution of the following equation:  $\tan x_1 = \sqrt{\left(\frac{2\beta}{x_1}\right)^2 - 1}$ . Calculate  $E_1$  in units of  $\frac{\hbar^2}{ma^2}$ .

- (b) For  $b = 0$ , show that the first excited state energy ( $E_2$ ) is given by:  $E_2 = \frac{\hbar^2 x_2^2}{2ma^2}$  where  $x_2$  is the solution of the following equation:  $-\cot x_2 = \sqrt{\left(\frac{2\beta}{x_2}\right)^2 - 1}$ . Calculate  $E_2$  in units of  $\frac{\hbar^2}{ma^2}$ .
- (c) For  $b \gg a$ , estimate  $E_1$  and  $E_2$  in units of  $\frac{\hbar^2}{ma^2}$ .
- (d) Use the MATLAB code derived from Garcia, R., Zozulya, A. & Stickney, J. MATLAB codes for teaching quantum physics: Part 1. *arXiv physics.ed-ph*, (2007). <http://arxiv.org/pdf/0704.1622.pdf>

Consult the original publication for background on the code, which is reproduced below.

- What is the Heaviside function? How is it used in this code (for what purpose)?
  - Using the MATLAB code, generate the plots you sketched in part (a) (ground and first excited states for  $b=0$ ,  $b=a/2$ , and  $b \gg a$ ). You should have three graphs with two curves on each. Label the graphs and the wave functions.
  - Generate 2 more plots with intermediate barrier widths, and sketch the trends in  $E_1$  and  $E_2$  as a function of barrier width (you should have 5 different widths).
- Note: in the code, you can change the potential profile quite easily (e.g. the quadratic harmonic oscillator potential or single square well). Parameters can be varied to develop insight into how the wavefunctions vary with the potentials.*
- (e) Provide a physical explanation for the variation of  $E_1$  with  $b$  that you observed in part (e).
- (f) The double well is a primitive one dimensional model for the potential experienced by an electron in a diatomic molecule (the two wells represent the attractive force of the nuclei). If the nuclei are free to move, they will adopt the configuration of minimum energy. In view of your conclusions in (b), does the electron in the ground state ( $E_1$ ) tend to draw the nuclei together or push them apart? What about  $E_2$ ? Provide a physical reason for these behaviors, considering your answer to the previous question.

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1 % Program 4: Find several lowest eigenmodes V(x) and
2 % eigenenergies E of 1D Schrodinger equation
3 % -1/2*hbar^2/m(d2/dx2)V(x) + U(x)V(x) = EV(x)
4 % for arbitrary potentials U(x)
5 % Parameters for solving problem in the interval -L < x < L
6 % PARAMETERS:
7 L = 5; % Interval Length
8 N = 1000; % No of points
9 x = linspace(-L,L,N)'; % Coordinate vector
10 dx = x(2) - x(1); % Coordinate step
11
12 % POTENTIAL, choose one or make your own
13 U = 1/2*100*x.^2; % quadratic harmonic oscillator potential
14 %U = 1/2*x.^4; % quartic potential
15
16 % Finite square well of width 2w and depth given
17 %w = L/50;
18 %U = -500*(heaviside(x+w)-heaviside(x-w));
19
20 % Two finite square wells of width 2w and distance 2a apart
21 %w = L/50; a=3*w;
22 %U = -200*(heaviside(x+w-a) -heaviside(x-w-a) ...
23 % + heaviside(x+w+a) -heaviside(x-w+a));
24
25 % Three-point finite-difference representation of Laplacian
26 % using sparse matrices, where you save memory by only
27 % storing non-zero matrix elements
28 e = ones(N,1); Lap = spdiags([e -2*e e],[-1 0 1],N,N)/dx^2;
29
30 % Total Hamiltonian hbar = 1; m = 1;
31 % constants for Hamiltonian H = -1/2*(hbar^2/m)*Lap + spdiags(U,0,N,N);
32
33 % Find lowest nmodes eigenvectors and eigenvalues of sparse matrix

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34 nmodes = 3; options.disp = 0;
35 [V,E] = eigs(H,nmodes,'sa',options);% find eigs
36 [E,ind] = sort(diag(E));% convert E to vector and sort low to high
37 V = V(:,ind); % rearrange corresponding eigenvectors
38
39 % Generate plot of lowest energy eigenvectors V(x) and U(x)
40 Usc = U*max(abs(V(:)))/max(abs(U)); % rescale U for plotting
41 plot(x,V,x,Usc,'-k'); % plot V(x) and rescaled U(x)
42
43 % Add legend showing Energy of plotted V(x)
44 lgnd_str = [repmat('E = ',nmodes,1),num2str(E)];
45 legend(lgnd_str) % place legend string on plot

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13. Consider a cesium chloride crystal where the potential energy per formula unit is:

$$E(r) = \frac{A}{r^n} - \frac{Me^2}{4\pi\epsilon_0 r}$$

where  $A$  is a constant,  $n > 1$ ,  $r$  is interionic distance, and  $M$  is the Madelung constant.

- Express the binding energy ( $E_0$ ) in terms of  $M$ ,  $n$ ,  $r_0$ , and fundamental constants. *Hint: first express  $A$  in terms of these constants by considering the equilibrium condition.*
- The cesium chloride crystal structure consists of cations located on a simple cubic lattice (lattice constant =  $a$ ) with an anion located at the center of the cube. What is the volume per formula unit ( $v$ ) in terms of  $r$ ?
- From thermodynamics, the bulk modulus ( $B$ ) is known to be:  $B = v \frac{\partial}{\partial v} \left( \frac{\partial E}{\partial v} \right)$ . Show that  $B_0$  is of the form  $B_0 = \frac{C}{r_0} \frac{d^2 E}{dr^2} \Big|_{r=r_0}$ , and find  $C$ . *Hint: use your result from the previous problem to rewrite the derivatives in terms of  $r$ .*
- Using the result from part (c), express the equilibrium bulk modulus ( $B_0$ ) in terms of  $M$ ,  $n$ ,  $r_0$ , and fundamental constants.
- The experimentally determined values of  $B_0$  and  $r_0$  for CsCl are 19.8 GPa and 3.571 Å respectively. Calculate  $E_0$  for CsCl in eV. Note:  $M = 1.7627$  for CsCl.