Book of assignments for CHM421A (2022)

Quantum mechanics practice set

Mainak Sadhukhan

Dedicated to the memory of
those who were harmed in solving them : None

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Contents

Chapter 1

On the basics

1. I have kept a grain of sand in the otherwise empty(considering I have perished with the rest of the universe!) universe. This grain of sand is kept at rest with respect to a chosen frame of reference. After any given amount of time, the grain does not appear to start moving with respect to that frame of reference. Which property of the space, can you deduce from this observation?
   (a) Isotropicity of space
   (b) Homogeneity of space
   (c) None of the above
2. What name have we given for such a reference frame?
3. My friend Thomas argues that the time kept by his uncle at Greenwich should be considered as the definitive values of time and should be used to write the laws of mechanics. I am arguing the same for the time kept by my uncle in New Delhi. Which property of time dictates that both of us are wrong?
4. Expand the following functions of x in Taylor expansion with respect to a
   (a) e^{-x} and $a = 0$
   (b) e^{-x^2} and $a = 0$
   (c) e^{ikx} and $a = 0$ where $i = \sqrt{-1}$ and k is a constant real number.
   (d) $e^{-\alpha(x-a)^2}$ where α is a constant real number.
   (e) $\sin(x)$ and $a = 0$
   (f) $\cos(x)$ and $a = 0$
   (g) $\cos(x) + i\sin(x)$ and $a = 0$ where $i = \sqrt{-1}$
   (h) $\ln(x)$ and $a = 1$

(i) $\ln(1+x)$ and $a=0$
(j) $\ln(1-x)$ and $a=0$
(k) $\frac{1}{1-x}$ and $a=0$
(l) $\frac{1}{1+x}$ and $a=0$
(m) $(x+a)^2$ and $a=0$
(n) $(x+a)^4$ and $a=0$
(o) $\cos(x)e^{-x}$ and $a=0$
(p) $(1-e^{|(x-a)|})^2$.

5. Expand the following functions of x and y with respect to $x=0$ and $y=0$
   (a) $e^{x^2+y^2}$
   (b) $\sin(x)\cos(y)$
   (c) $\sin(x+y)$

6. Plot the following functions of x with respect to x. The domain of definition for all functions are $-5 \leq x \leq 5$. (A plot is not a plot unless labels are explicitly mentioned)
   (a) x
   (b) $\frac{1}{x}$
   (c) $\frac{1}{|x|}$
   (d) $\sin(x)$
   (e) $\sin(2x)$
   (f) $\cos(x)$
   (g) $\cos(2x)$
   (h) e^x
   (i) e^{-x}
   (j) e^{-x^2}
   (k) e^{x^2}
   (l) x
   (m) x^2
   (n) x^3
   (o) x^4
   (p) x^2-x^4
   (q) x^2+x^4
   (r) $-x^2+x^4$
   (s) $\frac{\sin(x)}{x}$
   (t) kx^2 where $k=1,2,3$. Plot all three functions (for three values of k) in a single plot and compare.
   (u) $(1-e^{|(x-a)|})^2$ where a is a real constant.

Chapter 2

On the classical mechanics

1. Two particles are moving in the x-direction. Their masses are m_1 and m_2. They are positioned at $x_1(t)$ and $x_2(t)$ at time t with respect to a given inertial reference frame. Correspondingly,their velocities are v_1 and v_2 which are constants. There is no interaction between them. See Fig.2.1 below.

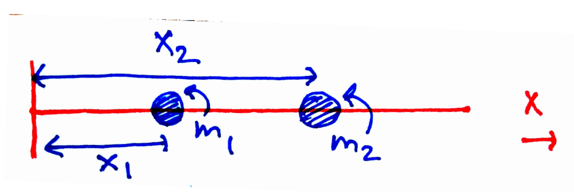

Figure 2.1: Two particles moving *freely* along x-direction.

   (a) Write down the Lagrangian for this system.

   (b) Using Lagrangian EOM, find out the relation between $v_1(t)$ and $v_2(t)$.

   (c) If you are sitting on m_1 (i.e. you have attached a reference frame on m_1) what will be the relative velocity of m_2 with respect to you? Write your answer using only v_1. (*Hint: Use the answer of the previous question*)

   (d) If $m_1 >> m_2$, and you are sitting on m_1 what will be the relative velocity of m_2 now? (*Hint: Take $m_2 \to \infty$ limit of the answer of the previous question.*)

   (e) Write the Hamiltonian function for this system (*Hint: Remember that the basic variables for Hamiltonian function are generalized positions and momenta, not velocities.*)

(f) Write the Hamiltonian EOMs for this system.

(g) What kind of curve are we describing by the Lagrangian vs. velocity space if the Hamiltonian and Lagrangian functions are same? (*Hint: Use the interpretation given in terms of the geometrical meaning of Legendre transformation*)

(h) Consider $v_1 = 0$ in your reference frame. Draw the phase space trajectory for the m_2 for a constant value of total energy.(*Remember: A phase space is defined by position and momentum, not velocity.*)

2. Consider the particles described above are moving in an arbitrary direction in 3-dimensional space.

(a) Compute the system's Lagrangian and Hamiltonian functions. (*Hint: These functions will be straightforward extensions for one-dimensional motion you already described above*)

(b) Find out the degrees of freedom for this system

3. Two particles are aligned along the x-direction. Their masses are m_1 and m_2. The particle with mass m_1 is positioned at the origin of a reference frame and at rest with respect to this reference frame. The other particle (with mass m_2) is initially at rest at a distance x_e. There is an interaction between these two masses such that if the position of m_2 is changed to a new position x, it experiences a **restoring force** which is proportional to the displacement $(x - x_e)$. See Fig.2.2 below.

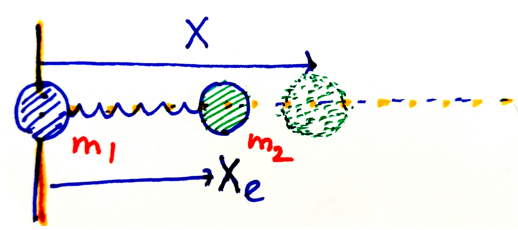

Figure 2.2: The particle with mass m_2 (green) moving *under the force law* given above, along x-direction. Mass m_1 is tethered to the origin of the reference frame (i.e. its position is $x = 0$ always). When at rest, the particle with mass m_2 is at x_e. When perturbed, this particle is at x.

(a) Write an expression for the restoring force experienced by the mass m_2 if the force per unit displacement is measured as k. (*Hint: Remember Hook's law?*)

(b) Find out the potential between these two particles.(*Hint:* $F(x) = -\frac{dV(x)}{dx}$ *and the force on* m_2 *at* x_e *is zero.*)

(c) What is the degrees of freedom for the system?

(d) Find out the Lagrangian function for the system.

(e) Write down the equation of motion for the system.

(f) Does m_1 appears in your EOM? What does that physically mean?

(g) Find out the Hamiltonian function for the system and write down the Hamiltonian equation of motion.

(h) If the system is **conservative**[1] then sketch the phase space trajectory for the system.

(i) If the total energy of the system is doubled to $2E$ redraw the phase space trajectory. Compare this shape with the shape obtained for total energy E.

(j) The shape is a well-known conic section. What is it called?

(k) Calculate the area J enclosed by the phase space trajectory for a given energy E in terms of k and m_2.

(l) If one considers only those phase space trajectories whose J are integer multiples of a constant number h, find out the difference between the two consecutive, allowed energy value in terms of k and m_2.

(m) What is the dimension of J?

‘ ‘ ‘

[1] It means that the total energy of the system E is constant for the system over time.

Chapter 3

On the classical mechanics and waves

1. If a classical mechanical property $A(q, p, t)$ is explicitly dependent on time t apart from generalized position q and generalized momentum p, write down its equation of motion (*Hint: There will be an extra term in the EOM derived in the class.*)

2. For any classical mechanical quantities $f(q, p), g(q, p), h(q, p)$ and real numbers a, b show that

   (a) $\{f, g\} = -\{g, f\}$

   (b) $\{af + bg, h\} = a\{f, h\} + b\{g, h\}$

   (c) $\{h, af + bg\} = a\{h, f\} + b\{h, g\}$

   (d) $\{fg, h\} = f\{g, h\} + g\{f, h\}$

   (e) $\{f, \{g, h\}\} + \{g, \{h, f\}\} + \{h, \{f, g\}\} = 0$

   (*Hint: Use the definition of Poisson bracket in terms of q and p*)

3. The Hamiltonian function of a system is given by

$$H(p, q) = \frac{p^2}{2m} + \frac{m\omega^2}{2} q^2$$

   Obtain the time-evolution equation (EOM) for the classical mechanical properties

   (a) $A = p$

   (b) $A = p^2$

   (c) $A = p^3$

   (d) $A = q$

   (e) $A = q^2$

(f) $A = q^3$

(g) $A = pq$

(h) $A = q^2 p$

(i) $A = p^2 q$

(*Hint: Use* $\frac{dA}{dt} = \{A, H\}$ *where* H *is the hamiltonian function*)

4. The Hamiltonian function of a system is given by

$$H(p, q) = \frac{p^2}{2m} + \frac{1}{q}$$

Obtain the time-evolution equation (EOM) for the classical mechanical properties

(a) $A = p$

(b) $A = p^2$

(c) $A = p^3$

(d) $A = q$

(e) $A = q^2$

(f) $A = q^3$

(g) $A = pq$

(h) $A = q^2 p$

(i) $A = p^2 q$

5. The Hamiltonian function of a system is given by

$$H(p, q) = \frac{p^2}{2m} + V(q)$$

Obtain the time-evolution equation (EOM) for the classical mechanical properties in terms of $V(q)$

(a) $A = p$

(b) $A = p^2$

(c) $A = p^3$

(d) $A = q$

(e) $A = q^2$

(f) $A = q^3$

(g) $A = pq$

(h) $A = q^2 p$

(i) $A = p^2 q$

6. Use the last question's Hamiltonian and equation of motion for $A(t) = q(t)p(t)$.

   (a) Show that
   $$\frac{dA(t)}{dt} = 2\frac{p^2}{2m} - q\frac{\partial V(q)}{\partial q}$$
   .

   (b) Show that for a periodic motion with time period T where $q(t) = q(t+T)$ and $p(t) = p(t+T)$
   $$2\frac{1}{T}\int_0^T \frac{p^2}{2m}dt = \frac{1}{T}\int_0^T q\frac{\partial V(q)}{\partial q}dt$$

   (c) Show that
   $$\frac{m}{2}\frac{d^2(q^2)}{dt^2} = 2\frac{p^2}{2m} - q\frac{\partial V(q)}{\partial q}$$

   (d) Consider $f(\lambda q) = \lambda^n f(q)$ where λ is a constant number and n is another number. Show that for such functions
   $$q\frac{\partial f(q)}{\partial q} = nf(q)$$

   [1]. *(Hint: Step 1: Take derivative of the $f(\lambda q) = \lambda^n f(q)$ with respect to λ. Step 2: Convert the LHS to $q'\frac{\partial f(q')}{\partial q'}$ where $q' = \lambda q$. Step 3: Write the whole equation in terms of q'.)*

7. Suppose a plane wave is moving through the string in x direction (see Fig.3.1).

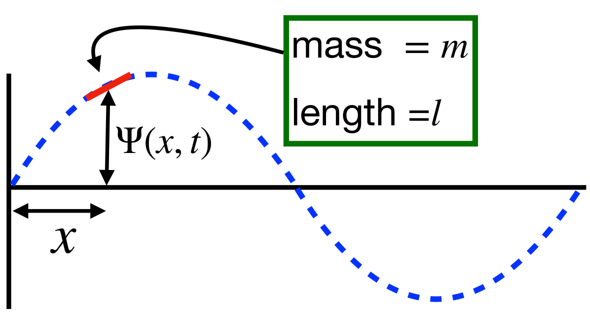

Figure 3.1: Wave is moving in the x direction.

The red patch of string has mass m and length l. The red patch is undergoing a simple harmonic motion in the perpendicular direction of wave

[1]Such functions are known as Euler homogeneous functions of degree n and $q\frac{\partial}{\partial q}$ is known as Euler operator.

propagation. The potential experienced by this patch is $= \frac{m\omega^2}{2}\psi^2(x,t)$ where x denotes the center position of the red patch. Note that $\psi(x,t)$ is the displacement from the equilibrium position of the string.

(a) Calculate the kinetic energy of the red patch in terms of $\psi(x,t)$.

(b) Calculate the total energy of the read patch in terms of $\psi(x,t)$.

(c) Considering

$$\psi(x,t) = A\sin(kx - \omega t)$$

calculate the total energy carried by of the red patch in terms of A, ω and m.

8. Can the function

$$\phi(x,t) = A\exp\big(-\alpha(x - vt)^2\big)$$

represent a travelling wave? Here A, v and α are positive real numbers.

9. A wave is moving at a velocity $v = 10$ m s^{-1}. Its wave length is $\lambda = 1$ cm.

(a) Compute the frequency ν in Hertz.

(b) Compute the wave number $\bar{\nu} = 1/\lambda$.

(c) Compute the angular wave number $k = 2\pi/\lambda$

(d) Compute its angular frequency $\omega = 2\pi\nu$.

10. A wave is moving at a velocity $c = 3 \times 10^8$ m s^{-1}. Its wave length is $\lambda = 400$ nm.

(a) Compute the frequency ν in Hertz.

(b) Compute the wave number $\bar{\nu} = 1/\lambda$.

(c) Compute the angular wave number $k = 2\pi/\lambda$

(d) Compute its angular frequency $\omega = 2\pi\nu$.

11. A wave is moving at a velocity $c = 3 \times 10^8$ m s^{-1}. Its wave length is $\lambda = 800$ nm.

(a) Compute the frequency ν in Hertz.

(b) Compute the wave number $\bar{\nu} = 1/\lambda$.

(c) Compute the angular wave number $k = 2\pi/\lambda$

(d) Compute its angular frequency $\omega = 2\pi\nu$.

Chapter 4

On the old quantum theory

1. Using the Planck's expression for spectral density

$$u(\nu) = \frac{8\pi h\nu^3}{c^3}\frac{1}{e^{\frac{h\nu}{K_B T}} - 1}$$

   (a) Derive the expression for frequency (ν_{max}) for which the $u(\nu)$ is maximum.
   *(**Hint:***
   Step 1: Obtain a transcendental equation involving ν_{max} and T.
   Step 2: Show the transcendental equation can be written in the form

$$xe^x = c$$

   where c is a constant
   Step 3: The solution for such equation ($x = W(c)$) is obtained by Lambert's W function such that

$$W(c) \approx c - c^2$$

   for $|c| << 1$
   Step 4: Using the previous step, show $\nu_{max} \propto T$ and compute the proportionality constant.)

   (b) Derive total energy emitted by the black body as a function of temparature.
   *(**Hint:***
   Step 1: Total energy per unit volume $E(T)$ emitted by the blackbody kept at temparature T is $= \int_0^\infty u(\nu)d\nu$
   Step 2: Convert one integral to a series (which one? - figure it out!) $\zeta(4) = \sum_{k=1}^{\infty} \frac{1}{k^4}$
   Step 3: Use $\zeta(4) = \frac{\pi^4}{90}$. See footnote [1]

[1] $\zeta(m)$ is Riemann Zeta function and can be computed from Fourier series expansion very easily.

Setp 4: Show $E(T) \propto T^4$
Step 5: Find out the proportionality constant.)

(c) A star is glowing yellow. Its peak intensity occurs at 550 nm. Calculate its surface temperature considering the star as a black body.

(d) Calculate the total energy radiated by the yellow star if its radius is 696000 km.

(e) A planet around the star has average surface temparature 14° C. Considering it as a blackbody, find out its peak emission frequency ν_{max}.[2]

2. Consider a H atom in its ground state. Using Bohr's model,

(a) Calculate the energy required to ionize it in (a) Joules, (2) atomic units, (3) Rhydberg, (4) wave number, (5) angular wave number, (6) frequency (7) wave length.[3]
*(**Hint:** If one provides exactly this energy, the electron will become a free particle and the final energy stored by the atom becomes zero.*

(b) Calculate radius of lowest two Bohr orbits in (1)pm, (2) Å, (3) m, (4) au

(c) Consider the electron is jumping from its lowest energy state to 3^{rd} and 5^{th} excited states. Compute the ratio of frequencies of absorbsion lines for these two transitions.
(***Remember:*** 1^{st} *excited state means quantum number* $n = 2$.)

(d) Calculate the velocity of the electron in the lowest energy orbit according to the Bohr's model.

(e) Calculate the ratio of this velocity and the velocity of light in vacuum.

(f) Show that the change of energy E_n with the small change of quantum number n is proportional to $r_n^{-3/2}$ for very large n where r_n is the radius of n^{th} orbit.

(g) Considering the relation between time period T related to the jump from state n to $n-1$ and transition energy $\Delta E_n = E_n - E_{n-1}$ find out the relation between T and r_n. ***Recognize this result?!***

(h) Compute the time-period of an electron moving in innermost Bohr orbit.

(i) Compute the de Broglie wave length of the electron in the innermost Bohr orbit.

(j) Compute the ratio of the circumference of the innermost Bohr orbit and the de Broglie wavelength computed above.

(k) Compute this ratio for n^{th} Bohr orbit. (Note: Both the circumference and de Broglie wavelength are determined by n. The second one is dependent on the velocity at that orbit.)

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[2] T in all equations are measured in Kelvin.
[3] Consider the proprtionality between the energy and frequency

3. A beam of electrons have been created in such a way that the avaerage spead of these electrons is 65% of the speed of light in vacuum.

   (a) Calculate the de Broglie wavelength for these electrons.

   (b) Does this wavelength depend on the temparature of the surrounding?

   (c) In double-slit experiment, the spacing between two consecutive fringes are given by $x = \frac{h\lambda}{d}$ where h, λ and d are distance between the slits and the detector screen, the wavelength of the wave and the distance between two slits, respectively. We heat a bunch of Buckminister fullerene molecules (C_{60}) to a temparature 1000 K. Assuming its thermal energy $\frac{3}{2}k_BT$ is converted to the kinetic energy of these molecules, calculate the fringe spacing created by the beams of C_{60} molecules if $h = 10$ m and $d = 5$ μm.

   (d) Usain Bolt weighs 94 Kg. Compute his de Broglie wavelength when he ran 100 m in 9.58 seconds.

4. The work function Φ of a few metals are given below.

Metal	W	Cu	Pd	Au	Ag
Φ/eV	4.35	4.75	5.40	5.25	4.50

   (a) Calculate maximum speed of ejected electrons if one shines these metals with a light with wavelength 600 nm.

   (b) Compute these electrons' de Broglie wavelengths for each cases.

5. Consider a neutral atom X with two electrons. Both of them are in the lowest Bohr orbit and they do not interact amongst each other (a hypothetical situation).

   (a) Calculate the radius of inner most orbit in (1) a.u. and (2) m

   (b) Calculate the largest frequency of the absorption lines in its absorption spectra.

   (c) We add one neutron in the nucleus of this atom. According to Bohr's model, compute the energy difference between the original atom and this isotope in their ground states.

   (d) Compute the energy required for the process $X \to X^+$ in eV, au and Joules.

   (e) Compute the energy required for the process $X^+ \to X^{2+}$ in eV, au and Joules.

   (f) The experimental ionization potentials for this atom are 24.6 eV and 54.4 e V respectively. Explain the discrepancies with your calculated values and the experiemntal values, if any.

Chapter 5

On the formalism and mathematical preliminaries

1. Show that for a self-adjoint operator[1] $\hat{\mathcal{A}}$
$$\langle\Psi|\chi\rangle = \langle\Phi|\alpha\rangle$$
where
$$|\chi\rangle = \hat{\mathcal{A}}\,|\alpha\rangle$$
$$|\Phi\rangle = \hat{\mathcal{A}}\,|\Psi\rangle$$

2. Show that the previous statement can be written as
$$\int_{-\infty}^{\infty}\left(\hat{\mathcal{A}}(x)\Psi(x)\right)^*\alpha(x)\mathrm{d}x = \int_{-\infty}^{\infty}\Psi^*(x)\left(\hat{\mathcal{A}}(x)\alpha(x)\right)\mathrm{d}x$$
in position representation.

3. Find out if the following operators are Hermitian for the functions $\{f(x)\}$ such that $f(x) \to 0; \frac{d^n f(x)}{dx^n} \to 0; n = 1, 2, \ldots$ for $|x| \to \infty$.
   - $\frac{d}{dx}$
   - $\frac{d^2}{dx^2}$
   - $x\frac{d}{dx}$
   - $e^{i\frac{d}{dx}}$
   - $e^{-\frac{d}{dx}}$
   - $e^{i\frac{d^2}{dx^2}}$
   - $\ln(\hat{x})$

[1]Notice, we are assuming here that the domain of definition of $\hat{\mathcal{A}}$ is same as that of $\hat{\mathcal{A}}^\dagger$

- $-i\frac{d}{dx}$

*(**Hint:** Use integration by parts)*

4. Find out if the following sets form vector spaces under the given binary operation. If yes, find the inverse and identity elements for them.

Set	Binary operation
$\mathbb{M} = \{\begin{pmatrix} a & b \\ c & d \end{pmatrix}; a, b, c, d \in \mathbb{C}\}$	Matrix addition
$\mathbb{M} = \{\begin{pmatrix} a & b \\ c & d \end{pmatrix}; a, b, c, d \in \mathbb{C}\}$	Matrix multiplication
$\mathbb{Q}$	Arithmetic addition
$\{f : \mathbb{R} \to \mathbb{R}; \lvert f(x)\rvert < \infty \forall x \in \mathbb{R}\}$	Function addition
$f(x) = Ae^{ikx} \lvert (A, k, x) \in \mathbb{R}$	Function multiplication

*(**Note:** Remember that some matrices are singular matrices)*

5. [2] For a set of all continuous functions $f : \mathbb{R} \to \mathbb{C}$ for which $|f(x)| < \infty$ and $\frac{d^n f(x)}{dx^n}$ exists for $n \in \mathbb{Z}^+$,
   (a) can $\mathcal{B} = \{e^{ikx} | k, x \in \mathbb{R}\}$ be considered a basis?
   (b) what should be the dimensionality of that space?
   (c) are the elements of $\mathcal{B}$ orthonormal?

   *(**Hint:** Think Fourier!)*

6. Show that
$$\langle \sigma_A^2 \rangle = \left\langle \hat{A}^2 \right\rangle - \left\langle \hat{A} \right\rangle^2$$
[3]

7. Consider,
$$\sigma_1 = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right), \sigma_2 = \left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right), \sigma_3 = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$$
.
   (a) Show that they are Hermitian
   (b) Show that they are unitary
   (c) Show that
$$[\sigma_k, \sigma_l] = 2i\epsilon_{klm}\sigma_m$$
   where Levi-Civita symbol is defined as[4]
$$\epsilon_{klm} = \begin{cases} 1 & \text{if } (k, l, m) \text{ is an even permutation} \\ -1 & \text{if } (k, l, m) \text{ is an odd permutation} \\ 0 & \text{if } k = l \text{ or } k = m \text{ or } l = m \end{cases}$$

[2] This question is only for students who are mathematically oriented. Rests can ignore it.
[3] Meaning of symbols as used in the class
[4] If you permute 1, 2, 3 **cyclically**. (1, 2, 3),(2, 3, 1), (3, 1, 2) are cyclic. If this order is broken, it is an odd permutation.

where $(k, l, m) \in (1, 2, 3)$

8. Show that the Heisenberg operator $\hat{A}_H(t)$ is related to Schrödinger operator $\hat{A}_s$ by
$$\hat{A}_H(t) = \hat{U}^\dagger(t, t_0)\hat{A}_S\hat{U}(t, t_0)$$

9. Using Ehrenfest theorem, show that for an one-dimensional potential $V(x)$,
$$\frac{d\langle\hat{p}\rangle}{dt} = -\left\langle\frac{dV(x)}{dx}\right\rangle$$

10. Using Ehrenfest theorem for potential $V(x) = x^2$, find out the expressions for
    (a) $\frac{d\langle\hat{p^2}\rangle}{dt}$
    (b) $\frac{d\langle\hat{x}\rangle}{dt}$

11. Starting from
$$i\hbar\frac{\partial\,|\psi(t)\rangle}{dt} = \hat{H}\,|\psi(t)\rangle = \varepsilon\,|\psi(t)\rangle$$
, show that the norm of wave function may not be conserved if $\hat{H}$ is not Hermitian.

Chapter 6

On the Toy model systems I

1. For a particle moving under a potential
$$V(x) = -\frac{\lambda(\lambda+1)}{2}\,\mathrm{sech}^2(x)$$
where $x \in (-\infty, \infty)$ and $\lambda \in \mathbb{N}$. For three bound eigenstates $|m\rangle, |l\rangle$ and $|n\rangle$, find out
$$\langle m|\,x\,|n\rangle\,\langle n|\,x\,|l\rangle\,\langle l|\,x\,|m\rangle$$
2. If the energy for the system is given by $E = -\frac{m^2}{2}$ where $m \in [1, \lambda]$, find out the energy eigenfunctions for the above potential.

   *(**Hint:** Substitute $\xi = \tanh(x)$)*
3. A particle is moving under potential
$$V(x) = V_0\Theta\left(\frac{a}{2} - |x|\right)$$
where $a > 0$ and Θ is Heaviside step function.
   (a) For $V_0 > 0$, plot $V(x)$ *vs* x.
   (b) For $V_0 < 0$, plot $V(x)$ *vs* x.
   (c) For both $V_0 > 0$ and $V_0 < 0$, find the eigenvalues and eigenfunctions in all regions for energy $E > 0$.
   (d) $V_0 < 0, E > 0$ in above problem defines a particle moving over a potential well. Define an effective mass $\tilde{m}$ for the motion above the potential well such that the wave function retains the same form as that for $x > a/2$.
   (e) For both $V_0 > 0$ and $V_0 < 0$, find the eigenvalues and eigenfunctions in all regions for energy $E < 0$.
   (f) Find the reflection and transmission *probabilities* at $x = \pm\frac{a}{2}$ for all possibilities considered above.

(g) Plot the wave functions as a function x in the region $x \in (-\infty, \infty)$ for all cases above.

4. A particle is trapped in a potential

$$V(x) = \begin{cases} 0 & \text{if } -\frac{a}{2} < x < \frac{a}{2} \\ \infty & \text{otherwise} \end{cases}$$

   (a) Find out the wave function and energy eigenvalues for the system. *(**Hint:** Set up the boundary conditions properly.)*

   (b) A coordinate transformation of $x = x' + \frac{a}{2}$ in the potential gives the potential function discussed in the class. Is it possible to do the same for wave functions?

   (c) Does the energy change?

   (d) Find out the total wave function $\Psi_n(x,t)$ for n^{th} energy state. *(**Hint:** $\Psi_n(x,t)$ is a stationary state.)*

   (e) Find out the number and positions of nodes in wavefunction for n^{th} energy state.

   (f) Find out the position-momentum uncertainty product for n^{th} energy state.

5. A polyacetylene ($[C_2H_2]_n$; $n > 1$) molecule has N π-electrons. Each energy states can be occupied by maximum two electrons. Consider C-C bond-length is d. Also, consider them non-interacting (!).

   (a) Modelling the π-system as independent particles in a box, find out the minimum amount of energy required to promote one electron to a higher excited state (promotion energy ΔE).

   (b) Find the total energy for this system. (You have to add *them*.)

   (c) Plot the total energy E with n keeping N fixed.

   (d) Plot the total energy E with N keeping n fixed.

   (e) Plot the ΔE versus n considering each addition of C atom brings in a new bond.

6. Compute the minimum wavelength of absorption of Pyridine molecule considering only π electrons and modelling it as a particle in a ring. The bond lengths are given in `https://cccbdb.nist.gov/exp2x.asp?casno=110861`

7. The actual spectrum of Pyridine is given in `https://webbook.nist.gov/cgi/cbook.cgi?ID=C110861&Mask=400`. To match the prediction with the actual result, calculate the "effective mass" of the electron under the same model. Is it larger or smaller than the mass of the electrons found in literature?

8. Compute the energy eigenvalues and eigenfunctions of a particle trapped in a 3-dimensional box defined by a potential which does not allow the particle to escape beyond its boundaries such that $x \in [0, a_x], y \in [0, a_y], z \in [0, a_z]$.
   (a) If $a_x \neq a_y \neq a_z$, calculate the degree of degeneracy in states with three lowest energies.
   (b) If $a_x = a_y \neq a_z$, calculate the degree of degeneracy in states with three lowest energies
   (c) If $a_x = a_y = a_z$, calculate the degree of degeneracy in states with three lowest energies.
9. Consider a quantum harmonic oscillator with mass m, angular frequency ω moving in x-direction. Starting from $a^\dagger |n\rangle = \sqrt{n+1}\,|n+1\rangle$,
   (a) find out the wavefunction in position representation for three lowest energy states.
   (b) If n^{th} energy eigenfunctions is
   $$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right) e^{\frac{m\omega x^2}{2\hbar}}$$
   where H_n is the Hermite polynomial, compute the form of $H_n(\xi)$ by comparing results from the previous question.
   (c) Find out the position-momentum uncertainty product for the n^{th} eigenstate.
   (d) Compute
   $$\langle n| x^4 |n\rangle$$
   where $|n\rangle$ is the n^{th} energy eigenstate of the quantum harmonic oscillators.
   (e) Compute the tunneling probability for $n = 2, 3$ states. Note that the CTP changes based on the n value.
10. A particle is moving under the potential
   $$V(x, y) = \frac{m\omega_x^2}{2}x^2 + \frac{m\omega_y^2}{2}y^2$$
   .
   (a) Find out the eigenfunctions and eigenvalues of the system.
   (b) Find out the degree of degeneracy for states with four lowest energies if $\omega = \omega_x = \omega_y$.
11. Consider a particle is moving freely on the surface of a sphere of radius r. We consider $\left[L^2, L_z\right] = 0$.

(a) Find out the uncertainty product for $\hat{\phi}$ and $\hat{L}_z$ at ground state.

(See (1)Uncertainty principle for angular position and angular momentum by Sonja Franke-Arnold *et al*, New Journal of Physics 6, 103 (2004) and (2) Quantum theory of rotation angles by Stephen M. Barnett and D. T. Pegg, Phys. Rev. A 41, 3427(1990) for very interesting outlooks.)

(b) Show

$$C_{\pm} = \sqrt{(j \mp m)(j \pm m + 1)}\hbar$$

. All symbols carry same meaning as used in class.

(c) What is the lowest energy allowed for this particle?

(d) A radiation of frequency ν shines on the particle and it is gets excited from $j = l$ to $j = l + 1$ state. Compute the relation between l and ν. Consider the mass of the particle is μ.

Chapter 7

On the Toy model systems II: Hydrogenic atom

If not mentioned otherwise, we are considering $Z = 1$.

1. Compute the radial probability distribution function for the following states.
    - $1s$ orbital
    - $2s$ orbital
    - $2p_x$ orbital
    - $2p_z$ orbital
    - $3d_z^2$ orbital
2. Compute the $\langle r \rangle$ and $\langle r^2 \rangle$ for
    (a) $1s$ orbital
    (b) $2s$ orbital
    (c) $2p_z$ orbital
3. Compute the most probable distance from a nucleus for an electron to hang around if it is in
    (a) $1s$ orbital
    (b) $2s$ orbital
    (c) $2p_z$ orbital
4. Compute the average potential energy and average kinetic energies of an electron in
    (a) $1s$ orbital

   (b) $2s$ orbital
   (c) $2p_z$ orbital

   Also find the ratios of these two quantities for each cases.

5. Find out the degree of degeneracy of the ground state of H atom. Consider all degrees of freedom.

6. Plot the electron density of a hydrogen atom as a function of Cartesian component z, keeping $x = 0$ ***and*** $y = 0$ for

   (a) $1s$ orbital
   (b) $3s$ orbital
   (c) $2p_z$ orbital

   Note: (a) Electron density $\rho_{nlm}(\mathbf{r}) = |\psi_{nlm}(\mathbf{r})|^2$ and (b) $z \in (-\infty, \infty)$

7. Compute the ratio of $\frac{\partial}{\partial r}\rho_{nlm}(r)|_{r=0}$ and $\rho_{nlm}(0)$ for a hydrogenic atom with nuclear charge Z in

   (a) $1s$ orbital
   (b) $3s$ orbital
   (c) $2p_z$ orbital

8. Compute and plot radial probability distribution function $g(r)$ for a hydrogen atom for

   (a) $1s$ orbital
   (b) $2s$ orbital
   (c) $2p_z$ orbital
   (d) $3d_z^2$ orbital

9. Find out the radius r_{max} of a sphere which is centred at nuclear site and contains $4/5$ fraction of total electron density.

10. Schematically sketch the polar plots for the angular part of

   (a) $2s$ orbital
   (b) $2p_x$ orbital
   (c) $3d_{z^2}$ orbital