# MAT 265: PROBLEM SET 4

DUE TO FRIDAY NOV 13 AT 9:00PM

Abstract. This is the fourth problem set for the graduate course Mathematical Quantum Mechanics in the Fall Quarter 2020. It was posted online on Sunday Nov 1 and is due Friday Nov 13 at 9:00pm via online submission.

**Purpose**: The goal of this assignment is to review and practice the Schrödinger formulation of Quantum Mechanics, canonical quantization and the Heisenberg group, as learnt in Mathematical Quantum Mechanics (MAT265). In particular, we would like to become familiar with many examples of basic quantum mechanical systems, including the free particle, a harmonic oscillator and the hydrogen atom, and finding stationary states, expected values and standard deviations.

**Task and Grade**: Solve two of the six problems below. Each Problem is worth 50 points.The maximum possible grade is 100 points. Despite the task being two problems, I strongly encourage you to work on all the problems.

**Instructions**: It is perfectly good to consult with other students and collaborate when working on the problems. However, you should write the solutions on your own, using your own words and thought process. List any collaborators in the upper-left corner of the first page.

**Textbook**: We use "A Brief Introduction to Physics for Mathematicians" by I. Dolgachev, which is freely available in the course website.

**Problem 1**. (Standard Deviation as Uncertainty) Consider a state $\mu = P_\psi$, $\psi \in L^2(\mathbb{R}, \mathbb{C})$ for a quantum particle in a line and $A \in \mathcal{L}^{\in}(\mathbb{R}, \mathbb{C})$ an observable. By definition, its standard deviation is

$$\sigma_\mu(A) := \sqrt{E_\mu(A^2) - E_\mu(A)^2}.$$

(a) Show that $\sigma_\mu(A)^2 = E_\mu(A - E_\mu(A))^2$.

(b) Deduce from Part (a) that $\sigma_\mu(A) = \|(A - E_\mu(A))\psi\|_{L^2}$. Prove that the standard deviation vanishes $\sigma_\mu(A) = 0$ iff $\psi$ is an eigenstate of the observable $A$.

The basic lesson from Parts (a) and (b) is that the *standard deviation* is the mathematical quantity that models the physical idea of *uncertainty*. This is in line with Heisenberg's inequality, as described in class. We now continue with a simple example: an electron in the hydrogen atom in the simplest possible state.

(c) Let $a_0$ be the Bohr radius, which is about about half an $\mathring{A}$ngstrom[1]. An electron moves in $\mathbb{R}^3_{(x,y,z)}$ around a hydrogen nucleus, located at the origin. One of its ground states[2] $\mu$ is given by

$$\psi(x, y, z) = \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0}, \quad r \in \mathbb{R}^+,$$

where $r = \sqrt{x^2 + y^2 + z^2}$ is the distance from the electron to the nucleus.

Show that the expectations $E_\mu(\hat{x})$, $E_\mu(\hat{y})$ and $E_\mu(\hat{z})$ vanish, and thus the electron is expected to be at the origin $(x, y, z) = (0, 0, 0)$.[3]

(d) Show that Part (c) is not a problem. Namely, show that the uncertainty of finding the electron at the nucleus is strictly positive, i.e. $\sigma_\mu(\hat{x}) > 0$.

(e) Even better, show that the uncertainty of the position operator $\hat{x}$ is exactly the Bohr radius. (This is why this radius is important.)

(f) (Optional) Show that the same applies to the momentum operators, $\hat{p}_x$, $\hat{p}_y$ and $\hat{p}_z$, i.e. their expectation value at the ground state $\psi$ is zero, but again with positive uncertainty.

Physically, the lesson from Parts (c) through (f) is that in the simplest possible state $\psi$ for the electron, the expectation is to find the electron at origin and at rest. Nevertheless, since the standard deviation of the positions is Bohr radius $a_0$, the electron is actually somewhere at distance $a_0$ from the origin. (If you like the hydrogen atom, you are welcome to continue with Problem 7.)

**Problem 2**. (Free Particle in $\mathbb{S}^1_R$) Let $m, R \in \mathbb{R}^+$ and consider a free quantum particle of mass $m$ moving on an $R$-radius circle $\mathbb{S}^1_R := \{z \in \mathbb{C} : |z| = R)\} = \mathbb{R}_q/(2\pi R\mathbb{Z})$. Since the classical Hamiltonian is $H(q, p) = p^2/2m$, $(q, p) \in T^*\mathbb{S}^1_R$, the canonically quantized Hamiltonian is

$$\hat{H} : L^2(\mathbb{S}^1, \mathbb{C}) \longrightarrow L^2(\mathbb{S}^1_R, \mathbb{C}), \quad \hat{H}(f) := -\frac{\hbar}{2mR^2}\partial_q^2(f).$$

(a) Show that the possible energies of the system in a stationary state are

$$E_n = \frac{\hbar^2 n^2}{2mR^2}, \quad n \in \mathbb{N} \cup \{0\}.$$

(b) Prove that the corresponding stationary states can be written in the form

$$\psi_n(q, t) = C \cdot e^{in\theta} e^{-iE_n t/\hbar}, \quad n \in \mathbb{Z}, t \in \mathbb{R}^+,$$

and find the normalizing constant $C \in \mathbb{R}^+$.

(c) Consider the pure state $\mu_n = P_{\psi_n(q,t)}$. Compute the expected energies $E_{\mu_n}(\hat{H})$, expected momenta $E_{\mu_n}(\hat{p})$ and their standard deviations.

[1]Approximately $0.529177 \cdot 10^{-10} m$.
[2]The energy at this ground state is $E_1 \simeq -13.6057 eV$, the lowest possible energy.
[3]This would be a problem, as the nucleus is fixed to be there.

(d) What is the expected value when observing the position operators

$$\hat{q}_1\phi = (\cos\theta)\cdot\phi, \quad \hat{q}_2\phi = (\sin\theta)\cdot\phi$$

if the system is at the pure state $\mu_n$ ? What about the standard deviations $\sigma_{\mu_n}(\hat{q}_1)$ and $\sigma_{\mu_n}(\hat{q}_2)$ for these two observables ?

(e) Give an example of an eigenstate for the energy operator $\hat{H}$ which is *not* an eigenstate for the momentum operator $\hat{p}$.

(f) At $t = 0$, a quantum particle in a circle $\mathbb{S}^1_R$, $R = 1$, is at the state $P_\varphi$ where

$$\varphi(\theta,0) = \sqrt{2}\cdot\left(\frac{1}{\sqrt{3}}\cdot\sin\theta + \sqrt{\frac{2}{3}}\cdot\cos(3\theta)\right).$$

Show that $\varphi$ is a superposition of energy eigenstates $\psi_n(\theta,0)$. Compute the possible values of its momentum $\hat{p}$ and each of the probabilities for these values of being observed.

(g) Let the state in Part (f) evolve for one second, until $t = 1$. Compute the possible values of its momentum $\hat{p}$ and each of the probabilities for these values of being observed.

**Problem 3**. (The Heisenberg Group) Consider a quantum particle moving in a line $\mathbb{R}_q$, subject to a potential, the Hilbert space being $V = L^2(\mathbb{R},\mathbb{C})$. In this problem we study the algebraic framework behind the *canonical quantization* $\hat{q}$ and $\hat{p}$ of the position observable $q$, and the momentum observable $p$, both classical observables $q, p \in C^\infty(T^*\mathbb{R})$.

Consider the Heisenberg group

$$G := \{A \in GL_3(\mathbb{R}) : A = M_{\alpha\beta\gamma}, \alpha,\beta,\gamma \in \mathbb{R}\}, \quad \text{where } M_{\alpha\beta\gamma} = \begin{pmatrix} 1 & \alpha & \gamma \\ 0 & 1 & \beta \\ 0 & 0 & 1 \end{pmatrix}.$$

(a) Show that $G$ is a Lie group and its center is

$$Z(G) = \{A \in G : A = M_{00\gamma}, \gamma \in \mathbb{R}\}.$$

(b) Prove that the matrices

$$\mathfrak{q} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathfrak{p} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathfrak{z} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

generate the Lie algebra $\mathfrak{g} = T_eG$ of the Heisenberg group $G$, known as the Heisenberg Lie algebra. Show also that they satisfy the so-called *Heisenberg relations*:

$$[\mathfrak{q},\mathfrak{p}] = \mathfrak{z}, \quad [\mathfrak{z},\mathfrak{q}] = 0, \quad [\mathfrak{z},\mathfrak{p}] = 0.$$

This is the Lie algebra way of talking about the fact that in quantum mechanics we want $\{\hat{q},\hat{p}\}_\hbar = 1$ where $\mathfrak{z}$ plays the role of a constant (the *identity* operator), and it corresponds to the center $Z(G)$.

(c) Consider the vector space space $L^2(\mathbb{R}, \mathbb{C})$ and the map

$$\rho_\hbar : G \longrightarrow Aut(L^2(\mathbb{R}, \mathbb{C})), \quad \rho_\hbar(M_{\alpha\beta\gamma})\psi(q) := e^{i\hbar\gamma} e^{i\beta q}\psi(q + \hbar\alpha).$$

Show that $\rho_\hbar$ is a representation, i.e. a group morphism.
(*Optional*: Show that $\rho_\hbar$ is irreducible.)

(d) Compare the representation $\rho_\hbar$ with the *canonical quantization*:

$$\hat{q}\psi = q\psi, \quad \hat{p}\psi = -i\hbar\partial_q\psi, \quad \psi \in L^2(\mathbb{R}, \mathbb{C}).$$

Namely, compare the operators $\rho_\hbar(M_{1,0,0})$ and $\rho_\hbar(M_{0,1,0})$ with the unitary one-parametric groups associated to the Hermitian operators $\hat{q}, \hat{p} \in \mathcal{O}(L^2(\mathbb{R}, \mathbb{C}))$.[4]

(e) Consider the map $\mathfrak{A} : G \longrightarrow G$ given by $\mathfrak{A}(M_{\alpha,\beta,\gamma}) = M_{-\beta\hbar^{-1},\alpha\hbar,\gamma-\alpha\beta}$. Show that this is a Lie group automorphism, and it is the identity in the center $Z(G)$.

(f) By Part (d), the two representations $\rho_\hbar$ and $\mathfrak{A}^*(\rho_\hbar)$ coincide in the center, and thus by the Stone-Von Neumann Theorem, they must be equivalent. That is, there exists[5] a unitary operator $\mathfrak{F}$ acting on $L^2(\mathbb{R})$ such that

$$\mathfrak{F}\rho_\hbar(g)\mathfrak{F} = \mathfrak{A}^*(\rho_\hbar)(g), \quad \forall g \in G.$$

Show that $\mathfrak{F}$ is the classical Fourier transform.[6]

**Problem 4**. (Weyl's Canonical Quantization) Let us consider a classical system with a particle in $\mathbb{R}_q$, so that phase space is $T^*\mathbb{R} \cong \mathbb{R}^2_{q,p}$ and the algebra of observables is given by $\mathcal{O}(T^*\mathbb{R}^2) = C^\infty(T^*\mathbb{R}^2)$. As discussed in lecture, the canonical quantization of an observable $f \in \mathcal{O}(T^*\mathbb{R}^2)$ is given by the operator

$$A_f\psi(q) = \frac{1}{2\pi}\int_{\mathbb{R}}\int_{\mathbb{R}} \mathfrak{F}(f)(u,w)e^{iuq}e^{iw\partial_q}(e^{-i\hbar uw/2}\psi(q))dudw, \quad \psi = \psi(q) \in L^2(\mathbb{R}, \mathbb{C}),$$

where $\mathfrak{F}(f)$ denotes the Fourier transform of $f$. In the following Parts, $A_f$ is understood as an integral operator acting on distributions, and note that $\mathfrak{F}(f)$ typically will be a distribution.

(a) Compare the integral opeartors $A_q$ and $A_p$ with the canonical quantization $\hat{q}\psi(q) = q\psi(q)$ and $\hat{p}\psi(q) = -i\hbar\psi(q)$.

(b) Express the operators $A_{pq}$ and $A_{qp}$ in terms of a polynomial $G(q, -i\hbar\partial_q)$ on the formal variables $q, -i\hbar\partial_q$.

(c) Describe the quantization of the observable $f(q,p) = q^2p^2$.

(d) Let $c_1, c_2 \in \mathbb{C}$ be two constants and consider the polynomial

$$g(q,p) = (c_1q + c_2p)^n$$

[4]Recall Stone's Theorem, establishing a correpsondence between Hermitian operators $H$ and unitary 1-parametric subgroups $e^{iHt}$.

[5]In fact, since $\rho_\hbar$ is irreducible, Schur's lemma imples that the intertwiner must be unique.

[6]Note that Stone-Von Neumann also proves that the Fourier transform $\mathfrak{F}$ is unitary, which is Parseval's Theorem.

in the $q, p$ variables. Compare the quantization $A_{g(q,p)}$ of the polynomial $g$ with the (non-commutative) polynomial $G(q, \partial_q) = (c_1 q - i\hbar c_2 \partial_q)^n$.

(e) Let us consider a constant observable $f \in \mathcal{O}(T^*\mathbb{R})$, for instance $f(q,p) \equiv 1$. What is its quantization $A_1$ ?[7]

**Problem 5**. (The Harmonic Oscillator Revisited) The one-dimensional quantum harmonic oscillator consists of a particle of mass $m$ vibrating near the origin at frequence $\omega$ in a line $\mathbb{R}_q$, where $q$ denotes the distance to the origin. The Hilbert space if $V = L^2(\mathbb{R}, \mathbb{C})$ and the energy operator $\hat{H} \in \mathcal{O}(V)$ reads

$$\hat{H}\psi(q,t) = -\frac{\hbar}{2m}\partial_q^2\psi(q,t) + \frac{m\omega^2}{2}q^2 \cdot \psi(q,t).$$

In lecture, we solve this problem using *ladder operators*, which essentially brings algebraic methods from representation theory of Lie algebras to find all necessary quantities, including the stationary states $\psi_n(q,t)$. Instead, in this problem, we will find $\psi_n(q,t)$ directly via differential equations.

(a) The stationary states $\psi_{stat}(q,t)$ are solutions of the eigenvalue problem

$$-\frac{\hbar}{2m}\partial_q^2\psi_{stat}(q,t) + \frac{m\omega^2}{2}q^2 \cdot \psi_{stat}(q,t) = \Lambda \cdot \psi_{stat}(q,t), \quad \Lambda \in \mathbb{R}^+.$$

Show that the equation above rescales to

$$-\partial_x^2\psi_{stat}(x,t) + x^2\psi_{stat}(x,t) = \lambda \cdot \psi_{stat}(q,t),$$

if we perform the change of coordinates $x = q\sqrt{\frac{m\omega}{\hbar}}$ and re-write $\lambda := \frac{2\Lambda}{\hbar\omega}$.

(b) For $|x| \gg 1$, this equation tends to $-\partial_x^2\psi_{stat}(x,t) + x^2\psi_{stat}(x,t) \simeq 0$, and thus it makes sense to take the ansatz

$$\psi_{stat}(x,t) = e^{x^2/2}h(x), \quad h \in C^\infty(\mathbb{R}).$$

Show that, under the ansatz above, $h = h(x)$ must satisfy

$$-\partial_x^2 h + 2x\partial_x h + h = \lambda \cdot h.$$

(c) Find the possible (admissible) solutions for $h$ in Part (b). Here is a suggestion: expand $h(x)$ in a power series in $x$, conclude it must be a polynomial and find the possible coefficients.

(d) Conclude that, in fact, the stationary states are indexed by a natural number $n \in \mathbb{N} \cup \{0\}$, and are of the form

$$\psi_n(q,t) = e^{x^2/2} \cdot \left(\frac{1}{\sqrt{2^n n!}}\sqrt[4]{\frac{m\omega}{\pi\hbar}}\right) \cdot H_n(x),$$

where $H_n(x)$ is the $n$th Hermite polynomial.

[7]Note that the Fourier transform of 1 is a distribution, so it is crucial to understand $A_f$ as an integral operator for distributions.

(e) Plot the functions $\psi_n(x,0)$ and their probability distributions $\|\psi_n(x,0)\|^2$, as functions of $\mathbb{R}_x$, for the first few values $n = 0,1,2,3,4,5,6$. Describe the general pattern of $\|\psi_n(x,0)\|^2$.[8]

Deduce that a quantum particle with energy $\hbar\omega/2$ might be found in positions $x \in \mathbb{R}$ that a classical particle in that energy level would never be in.

(f) What is the expected value of the energy in the pure state $\mu_n = P_{\psi_n(x,t)}$ ?

(g) Classically, the lowest possible energy of a (classical) harmonic oscillator is $E = 0$, with the particle at the origin and at rest. Is this the case for the *quantum* harmonic oscillator ? Apart from a mathematical argument, give also a possible physics intuition based on the Heisenberg uncertainty principle.

Similarly, the possible energies for the classical harmonic oscillator form a continuum $E \in \mathbb{R}_{\geq 0}$, is this the case for the *quantum* harmonic oscillator ?

(h) (Optional) Find the expected position $E_{\mu_n}(\hat{x})$ and expected momenta $E_{\mu_n}(\hat{p}_x)$ in the two stationary states $\psi_0(x,t)$ and $\psi_1(x,t)$. (Or if you have a physical guess, go with it !)

**Problem 6**. (Free Particle in $\mathbb{S}^2$) Let us consider a quantum free particle of mass $m$ moving in the 2-sphere

$$\mathbb{S}^2 = \{(x,y,z) \in \mathbb{R}^3 : x^2 + y^2 + z^2 = 1\}.$$

Consider spherical coordinates $(r,\theta,\phi) \in \mathbb{R}^3$, given by

$$x = r\sin\theta\cos\phi, \quad y = r\sin\theta\cos\phi, \quad r\cos\theta,$$

where $r^2 = x^2 + y^2 + z^2$ is the distance to the origin.

(a) Show that the Laplacian operator $\Delta^2 = \partial_x^2 + \partial_y^2 + \partial_z^2$, which quantizes the kinetic energy (up to a constant), reads

$$\Delta^2\psi = \frac{1}{\sin^2\theta}\partial_\theta^2\psi + \frac{1}{\sin\theta}\partial_\theta(\sin\theta \cdot \partial_\theta\psi), \quad \psi = \psi(\theta,\phi) \in L^2(\mathbb{S}^2,\mathbb{C}).$$

when restricted to the sphere $\mathbb{S}^2$.

(b) Show that the equation for the stationary states $Y(\theta,\phi)$ is separable, and thus we can write

$$Y(\theta,\phi) = \Theta(\theta)\Phi(\phi),$$

for some solutions of the stationary eigenvalue problem.

(c) In the separation of Part (b), prove that the admissible solutions for $\Phi(\phi)$ are

$$\Phi_n(\phi) = \frac{1}{\sqrt{2\pi}}e^{in\phi}, \quad n \in \mathbb{Z}.$$

[8] Then go to our course website, and you will finally understand the picture !

(d) Show that $\Theta(\theta)$ satisfies

$$-\frac{n^2}{\sin^2\theta}\Theta(\theta)+\frac{2mE}{\hbar^2}\Theta(\theta)+\frac{1}{\sin\theta}\partial_\theta(\sin\theta\cdot\partial_\theta\Theta(\theta)),\quad n\in\mathbb{Z},$$

if $Y(\theta,\phi)$ is a stationary state with expected energy $E$. (The solutions to this classical ODE are Legendrian polynomials in $\cos\theta$.)

(e) Conclude that

$$\frac{2mE}{\hbar^2}=l(l+1),\quad l\in\mathbb{N}\cup\{0\},\quad n\in\mathbb{Z}\cap[-l,l],$$

and thus the possible energies are indexed as

$$E_l=\frac{\hbar^2}{2m}l(l+1),\quad l\in\mathbb{N}\cup\{0\}.$$

(f) (Optional) The stationary states $Y(\theta,\phi)_l^n\in L^2(\mathbb{S}^2,\mathbb{C})$ are called spherical harmonics. They are *not* harmonic functions, try to discover why they are called *harmonics*.

**Problem 7**. (The Hydrogen Atom)[9] In this problem we study an electron moving around a hydrogen nucleus. The former has mass $\mathfrak{m}\simeq 9.1\cdot 10^{-31}kg$ and is allowed to move in $\mathbb{R}^3$, whereas the latter lies at rest and is located at the origin $(0,0,0)\in\mathbb{R}^3$.[10] Let us consider spherical coordinates $(r,\theta,\phi)\in\mathbb{R}^3$ as in Problem 4, the potential energy for the electron (due to Coulomb's law) is given by

$$V(r,\theta,\phi)=\left(\frac{e^2}{4\pi\varepsilon_0}\right)\cdot\frac{-1}{r},$$

where $e\simeq 1.6\cdot 10^{-19}C$ is the magnitude of the electron's electric charge, and $\varepsilon_0\simeq 8.854\cdot 10^{-12}C^2/(Jm)$ is the vacuum permittivity[11].

(a) Show that the canonical quantization of the classical Hamiltonian is

$$\hat{H}\psi(r,\theta,\phi)=-\frac{\hbar}{2\mathfrak{m}r^2}\left(\partial_r(r^2\partial_r\psi)+\frac{1}{\sin^2\theta}\partial_\theta^2\psi+\frac{1}{\sin\theta}\partial_\theta(\sin\theta\cdot\partial_\theta\psi)\right)-\left(\frac{e^2}{4\pi\varepsilon_0}\right)\cdot\frac{1}{r},$$

where $\psi=\psi(r,\theta,\phi)\in L^2(\mathbb{R}^3,\mathbb{C})$.

(b) Let us find the stationary states using separation of variables, i.e. $\psi(r,\theta,\phi)=R(r)\Theta(\theta)\Phi(\phi)$. First, show that the quantity

$$E_{\theta,\phi}:=\frac{-\hbar^2}{\Theta(\theta)\Phi(\phi)}\cdot\left(\frac{1}{\sin^2\theta}\partial_\theta^2(\Theta(\theta)\Phi(\phi))+\frac{1}{\sin\theta}\partial_\theta(\sin\theta\cdot\partial_\theta(\Theta(\theta)\Phi(\phi)))\right)$$

[9] This is a heavily computational problem, only try if you have done Problem 4 and really like solving ODEs. The first four Parts (a)-(d) are reasonable, for Part (e) you should have also tried Problem 3.

[10] The understanding of the possible energy levels of this electron tells us the photons that a hydrogen atom may absorb or emit, which is crucial for many quantum experiments involving hydrogen atoms.

[11] That is, the capability of an electric field to permeate a vacuum.

is a constant. Similarly, show that

$$E_\phi := \frac{-\hbar^2}{\Phi}\partial_\phi(\Phi(\phi)),$$

is a constant.

(c) Use Part (b) to conclude that $\Phi(\phi) = e^{in\phi}$, $n \in \mathbb{Z}$, and thus $E_\phi = (n\hbar)^2$.

(d) Using Parts (b) and (c) deduce that

$$\Theta(\theta)\Phi(\phi) = Y_l^n(\theta, \phi),$$

are the spherical harmonics from Problem 4, and thus $E_{\theta\phi} = l(l+1)\hbar^2$. Note that in this case we also have the inequality $l \geq |n|$.

(e) Complete the study of the stationary states by finding $R(r)$, which will be indexed by two numbers $k, l \in \mathbb{Z}$ with $k > l$ and $l$ as above. These are often written as $R_{kl}$, so that the stationary states end up being written as

$$\psi_{k,l,n}(r, \theta, \phi) = R_{kl}(r)Y_l^n(\theta, \phi).$$

The main lesson here is that they are indexed by three numbers $k, l, n \in \mathbb{Z}$ such that $|n| < l < k$, and that the motion essentially breaks into the spherical harmonics (which govern the motion of a free particle in $\mathbb{S}^2$) and a radial component.

(f) Show that the possible energies of the stationary states are

$$E_k = \frac{E}{k^2}, k \in \mathbb{N},$$

where $E = -\hbar^2 \cdot (2\mathfrak{m}a_0^2)^{-1} \simeq -13.605eV$ is the lowest energy. Note that these only depend on $k$, and are much simpler than $\psi_{k,l,n}$. This is what you should remember the most from the hydrogen atom.