Homework 3 - Quantum Mechanics I

NAME: ____ **SCORE:** _____________

Deadline: Friday 21 November 2025 by 21:00
Credits: 20 points **Number of problems:** 5 **Type of evaluation:** Formative Evaluation

This assignment is individual and consists of 5 problems related to units 2 and 3 of quantum mechanics. Please justify all calculations and highlight the answers.

1. **(4 points) Finite square well potential**

   In class we studied the finite square well potential and found that this potential admits both scattering states (when $E > 0$) and bound states (when $E < 0$). For the latter, we derived the even solutions and numerically solved a transcendental equation for the allowed energies.

   (a) Following the same approach we followed in class, find the odd bound state wave functions, $\psi(x)$, for the finite square well.

   (b) Derive the transcendental equation for the allowed energies of these odd bound states.

   (c) Solve it graphically and numerically (using your favourite programming tool). Study and discuss the two limiting cases and how the energy levels compare to those found for the even bound state wave functions studied in class.

   (d) Is there always an odd bound state? Normalise the odd bound state wave functions.

2. **(4 points) Mathematical formalism of quantum mechanics**

   (a) Consider the orthonormal states: $|1\rangle$, $|2\rangle$, $|3\rangle$, $|4\rangle$. For which value(s) of the phase θ are the following states, $|\Psi_1\rangle = 4\,|1\rangle - 3\,|2\rangle + 7\,|3\rangle + |4\rangle$ and $|\Psi_2\rangle = 2\,|1\rangle + 5\,|2\rangle - |x|e^{i\theta}\,|3\rangle - 2\,|4\rangle$, orthogonal? For $\theta = 0$, find the value of $|x|$ that ensures orthogonality.

   (b) Let $|n\rangle$ be the normalised n-th energy eigenstate of the 1D harmonic oscillator. We know that $\hat{H}\,|n\rangle = \hbar\omega(n + \frac{1}{2})\,|n\rangle$. If $|\psi\rangle$ is a normalised ensemble state that can be expressed as a linear combination of the eigenstates as follows: $|\psi\rangle = \frac{1}{\sqrt{14}}\,|1\rangle - \frac{2}{\sqrt{14}}\,|2\rangle + \frac{3}{\sqrt{14}}\,|3\rangle$, what is the expectation value of the energy operator in this ensemble state?

   (c) Consider the state $\Psi = \frac{1}{\sqrt{5}}\Psi_{-1} + \frac{1}{\sqrt{4}}\Psi_{+1} + \frac{1}{\sqrt{20}}\Psi_{+2} + \frac{1}{\sqrt{2}}\Psi_{+3}$, which is a linear combination of four orthonormal eigenstates of the operator $\hat{Q}$ corresponding to eigenvalues -1, $+1$, $+2$, and $+3$. Calculate the expectation value of the operator $\hat{Q}$ for this state.

   (d) Assuming that $\gamma \in \mathbb{R}$, for what range of γ is the function $f(x) = x^{\gamma-1}\ln(x)$ in Hilbert space on the interval $(0, 1)$? What about $x\,f(x)$ and $\frac{d}{dx}f(x)$?

3. **(4 points) Vectors and operators in QM formalism**

(a) Compute the momentum-space wave function, $\Phi(p,t)$, of a quantum particle in the ground state of the harmonic oscillator.

(b) For the same particle considered in (a), calculate the probability that a measurement of momentum, p, returns a value outside the classical range for the same energy, E.

(c) Find the normalised eigenvectors and the corresponding eigenvalues of a quantum mechanical observable described by the matrix below:

$$\hat{Q} = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

(d) For the same observable considered in (c), is there any degeneracy? Could you provide a physical example where these results would be relevant?

4. **(4 points) Dirac notation: brakets and dual basis**

Consider that $|e_1\rangle$, $|e_2\rangle$, $|e_3\rangle$ is an orthonormal basis. In this basis, let the $|\Psi_\alpha\rangle$ and $|\Psi_\beta\rangle$ kets be:

$$|\Psi_\alpha\rangle = i\,|e_1\rangle - 4\,|e_2\rangle + 2\,i\,|e_3\rangle$$

$$|\Psi_\beta\rangle = 2\,|e_1\rangle - 3\,|e_2\rangle + 5\,|e_3\rangle$$

(a) Are these kets normalised? If not, normalise them.

(b) Write $\langle\Psi_\alpha|$ and $\langle\Psi_\beta|$ in terms of the dual basis $\langle e_1|$, $\langle e_2|$, $\langle e_3|$.

(c) Compute the inner products $\langle\Psi_\alpha|\Psi_\beta\rangle$ and $\langle\Psi_\beta|\Psi_\alpha\rangle$, and confirm that $\langle\Psi_\beta|\Psi_\alpha\rangle = \langle\Psi_\alpha|\Psi_\beta\rangle^*$.

(d) Find all the matrix elements of the operators $\hat{M}_{\alpha\beta} = |\Psi_\alpha\rangle\langle\Psi_\beta|$, $\hat{M}_{\alpha\alpha} = |\Psi_\alpha\rangle\langle\Psi_\alpha|$, and $\hat{M}_{\beta\beta} = |\Psi_\beta\rangle\langle\Psi_\beta|$ in this basis, and construct their respective matrices. Are they Hermitian?

5. **(4 points) Hamiltonian, eigenvalues and eigenvectors**

Consider a two-state quantum mechanical system in the basis:

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

whose Hamiltonian is represented by the matrix shown below (in the $\{|0\rangle, |1\rangle\}$ basis):

$$\hat{H} = \begin{bmatrix} 1 & 0.5 \\ 0.5 & 1 \end{bmatrix}$$

(a) Find the eigenvalues of $\hat{H}$. What do the eigenvalues represent?

(b) Find the eigenvectors of $\hat{H}$, and express them in terms of $|0\rangle$ and $|1\rangle$.

(c) Find $\langle H \rangle$, $\langle H^2 \rangle$, and σ_H for $|\Psi(t=0)\rangle = |1\rangle$.

(d) If $|\Psi(t=0)\rangle = |1\rangle$, find the state of the system at any time t, $|\Psi(t)\rangle$, described by the Schrödinger equation: $i\hbar \dfrac{\partial |\Psi\rangle}{\partial t} = \hat{H}\, |\Psi\rangle$. What physical role does each matrix element in $\hat{H}$ play in the system and why?