Principles of Quantum Mechanics: Example Sheet 1

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1. Let $\mathbf{n}$ be a unit vector with polar coordinates (θ, ϕ) and let $\boldsymbol{\sigma}$ denote the Pauli matrices. Find the eigenvectors of $\mathbf{n} \cdot \boldsymbol{\sigma}$. Hence show that the state of a spin-$\frac{1}{2}$ particle for which a measurement of spin along $\mathbf{n}$ yields $\hbar/2$ with certainty is

$$|\mathbf{n}\rangle = \sin\left(\frac{\theta}{2}\right) e^{i\phi/2} |\downarrow\rangle + \cos\left(\frac{\theta}{2}\right) e^{-i\phi/2} |\uparrow\rangle.$$

where $|\uparrow\rangle$ and $|\downarrow\rangle$ are the usual eigenstates of $\hat{S}_z$. Obtain the corresponding expression for the eigenstate of $\mathbf{n} \cdot \boldsymbol{\sigma}$ with eigenvalue $-\hbar/2$. Explain why $\langle \uparrow | \mathbf{n} \rangle = 0$ at $\theta = \pi$, and why both coefficients have modulus $1/\sqrt{2}$ when $\theta = \pi/2$.

2. Write the 3×3 matrix for $\hat{S}_x$ in the basis where $\hat{S}_z = \mathrm{diag}(\hbar, 0, -\hbar)$. An unpolarised spin-1 beam passes through:

- a Stern–Gerlach filter passing only $\hat{S}_z = \hbar$,
- then a filter for $\hat{S}_x = \hbar$,
- then one for $\hat{S}_z = -\hbar$.

What fraction of the initial particles emerge?

3. Consider a 1D quantum harmonic oscillator with classical frequency ω. Define the coherent state $|\alpha\rangle$ by

$$|\alpha\rangle = e^{\alpha \hat{a}^\dagger - \bar{\alpha} \hat{a}} |0\rangle,$$

where $\hat{a}^\dagger$, $\hat{a}$ are the raising and lowering operators, $|0\rangle$ is the ground state, and $\alpha \in \mathbb{C}$.

i) Show that $|\alpha\rangle$ is an eigenstate of $\hat{a}$ and find its eigenvalue. Compute the inner product between two different coherent states $|\alpha\rangle$ and $|\beta\rangle$. [*Hint: You may find it helpful to use the results of question 2.*] Does the set of statesl $|\alpha\rangle$ for all $\alpha \in \mathbb{C}$ form a basis of the Hilbert space?

ii) A quantum oscillator is prepared in state $|\alpha\rangle$ at $t = 0$. Show that it evolves to become a new coherent state $e^{-i\omega t/2} |e^{-i\omega t} \alpha\rangle$.

iii) Suppose $\alpha \in \mathbb{R}$. By expressing $\hat{a}$ and $\hat{a}^\dagger$ in terms of $\hat{x}$ and $\hat{p}$, sketch the position space wavefunction of $|\alpha\rangle$.

iv) Let $\alpha \in \mathbb{C}$ and compute $\langle\alpha|\hat{p}|\alpha\rangle$. Give a physical interpretation of the coherent state for general complex α. Without further calculation, describe the shape and motion of both the position space and momentum space wavefunctions as time passes.

4. In units where $\hbar = 2m = 1$, the relative motion of atoms in a diatomic molecule is modelled by the Hamiltonian

$$\hat{H}_\nu = \hat{p}^2 + \left(\nu + \frac{1}{2} - e^{-\hat{x}}\right)^2 ,$$

where ν is a real parameter.

i) Sketch the potential. Explain why it models molecular vibrations better than a harmonic oscillator.

ii) Find a non-Hermitian operator $\hat{a}_\nu$ such that

$$\hat{H}_\nu = \hat{a}_\nu^\dagger \hat{a}_\nu + \nu + \frac{1}{4} .$$

What is the ground state energy? Find the position-space wavefunction of the ground state. For what range of ν is this state normalizable?

iii) Let $|0, \nu\rangle$ be the ground state for parameter ν. Show that

$$\hat{a}_\nu \hat{a}_\nu^\dagger = \hat{a}_{\nu-1}^\dagger \hat{a}_{\nu-1} + 2\nu - 1,$$

and hence that $\hat{a}_\nu^\dagger|0, \nu - 1\rangle$ is an (unnormalized) eigenstate of $\hat{H}_\nu$.

iv) Deduce an expression for the unnormalized n^{th} eigenstate using raising operators. Find the bound state spectrum of $\hat{H}_\nu$. Show that the number of bound states is $\lfloor \nu + 1 \rfloor$. Do these form a basis of the Hilbert space?