Quantum Mechanics of Atoms and Molecules (PC 3602)
Exercise 1

1. (a) Verify in details that
$$[\hat{x},\ \hat{p}_x] = i\hbar\ .$$
(b) Determine the transposed operator of $\hat{p}_x$ and prove that $\hat{p}_x$ is a Hermitian operator.
(c) Exponential operator of $\hat{A}$ is defined as
$$e^{\hat{A}} = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \left(\hat{A}\right)^n\ .$$
Prove that if Φ is an eigenstate of $\hat{A}$ with eigenvalue α, Φ is also an eigenstate of $e^{\hat{A}}$. Determine the corresponding eigenvalue.

2. Use Schrödinger equation
$$i\hbar\frac{\partial}{\partial t}\Psi\left(\mathbf{r},t\right) = \left[-\frac{\hbar^2}{2m}\nabla^2 + V\left(\mathbf{r}\right)\right]\Psi\left(\mathbf{r},t\right)$$
to obtain the equivalent of classical continuity equation
$$\frac{\partial}{\partial t}\rho\left(\mathbf{r},t\right) + \nabla\cdot\mathbf{j}\left(\mathbf{r},t\right) = 0$$
with the density and current defined as
$$\rho\left(\mathbf{r},t\right) \equiv \left|\Psi\left(\mathbf{r},t\right)\right|^2, \quad \mathbf{j}\left(\mathbf{r},t\right) = \frac{i\hbar}{2m}\left(\Psi\nabla\Psi^* - \Psi^*\nabla\Psi\right)\ .$$
For hints, see Mandl's *QM*, Hint for Problem 1.6.

3. (a) Given the definition of creation and destruction operators as
$$\hat{a}^\dagger \equiv \sqrt{\frac{m\omega}{2\hbar}}\hat{x} - \frac{i\hat{p}}{\sqrt{2m\hbar\omega}}, \quad \hat{a} \equiv \sqrt{\frac{m\omega}{2\hbar}}\hat{x} + \frac{i\hat{p}}{\sqrt{2m\hbar\omega}}$$
Prove their commutation is
$$[\hat{a},\ \hat{a}^\dagger] = 1\ .$$
(b) If state $|n\rangle$ is an eigenstate state of operator $\hat{n} \equiv \hat{a}^\dagger\hat{a}$ with eigenvalue n,
$$\hat{n}\,|n\rangle = n\,|n\rangle$$

prove that the state

$$|n+1\rangle \equiv \frac{\hat{a}^\dagger}{\sqrt{n+1}}\,|n\rangle$$

is also an eigenstate of $\hat{n}$ with eigenvalue $(n+1)$.
(c) Prove that state $|n+1\rangle$ is normalized if $|n\rangle$ is normalized.

4. Three-dimensional (3D) harmonic oscillator has the following Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2 r^2 \; .$$

(a) Show that this Hamiltonian can be separated into three independent parts, each of which is a 1D harmonic oscillator.
(b) Determine its ground state and ground-state energy.
(c) Show that the next two energy levels are degenerate and determine the energies and their degeneracies.

5. (a) Consider a spin-1/2 system. Use eigenstates of S^z as basis, show spin raising and lowering operators S^+ and S^- can be written in matrices as

$$\hat{S}^+ = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \hat{S}^- = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$

Hint: You may use general angular momentum formula

$$\hat{L}^\pm|l,m\rangle = \hbar\sqrt{l(l+1)-m(m\pm 1)}\;|l,m\pm 1\rangle \; .$$

(b) Consider an electron in a magnetic field. Suppose the field makes an angle θ with the z axis and is given by $\mathbf{B} = (B\sin\theta, 0, B\cos\theta)$. The magnetic energy potential is, using magnetic moment $\mu_s = -e\hat{\mathbf{S}}/m$, $\hat{H}_m = -\mu_s\cdot\mathbf{B} = \frac{e}{m}\hat{\mathbf{S}}\cdot\mathbf{B} = \frac{eB}{m}(\sin\theta\hat{S}_x + \cos\theta\hat{S}_z)$. Find its eigenvalues and eigenstates.