Quantum Mechanics: Set 1

1. Show that the matrix $U_{ni} \equiv \langle r_n|q_i\rangle$ is unitary, where $\{|r_n\rangle\}$ and $\{|q_i\rangle\}$ are the eigenkets of two different observables, R and Q.

2. Use operator methods to calculate the correctly normalized wavefunction $\langle x|2\rangle$ of the second excited state of harmonic oscillator of mass m and spring constant $k = \omega^2 m$.

3. Show that when the above oscillator is in a state of well defined energy, the expectation value of x, $\langle x\rangle$, vanishes. Show that when it's in a generic state (energy not well defined), $\langle x\rangle$ oscillates with period $2\pi/\omega$.

4. For the above oscillator we have

$$x = \sqrt{\frac{\hbar}{2m\omega}}(A + A^\dagger)$$

Use this result to write out the first 16 entries of the matrix x_{mn}. Similarly calculate part of the matrix p_{mn}

5. Show that for any two $N \times N$ matrices A, B, trace$[A, B] = 0$. Comment on this result in the light of the results of the last exercise and the canonical commutation relations.

6. Imagine a system with Hamiltonian H for which the set $\{|u\rangle, |d\rangle\}$ is a complete set of states. Let

$$\begin{array}{ll}\langle u|H|u\rangle = \mathcal{E}_0 & \langle u|H|d\rangle = -A \\ \langle d|H|u\rangle = -A & \langle d|H|d\rangle = \mathcal{E}_0\end{array}$$

Find the eigenvalues $\mathcal{E}_\pm$ and eigenvectors $|\pm\rangle$ of H in the $\{|u\rangle, |d\rangle\}$ basis. Show that $\mathcal{E}_\pm \to \mathcal{E}_0$ as $A \to 0$. At time $t = 0$ the system is known to be in the state $|\psi(0)\rangle = |u\rangle$. Solve the TDSE for the subsequent evolution of the system. Show that after a time $t = \frac{1}{2}\pi\hbar/A$ the system is in the state $|d\rangle$.

7. The classical picture of an ammonia molecule NH_3 consists of three H atoms at the vertices of a triangle and an N atom that lies some distance s away from the triangle either 'above' or 'below' it – see §4.5 of Townsend or §9-1 of Feynman vol III. Explain the relevance of the formalism explored in the last problem for NH_3. Given that $A > 0$, which state is the ground state? Give a physical explanation for this choice of ground state.

8. The N atom carries a slight -ve charge $-q$ with a corresponding +ve charge on the triangle. We switch on an electric field of strength E perpendicular to the plane of the triangle. How does this field modify the Hamiltonian in the $|u\rangle, |d\rangle$ basis? Find the eigenvalues $\mathcal{E}'_\pm$ of this new Hamiltonian as a function of $\delta \equiv qEs/A$ and plot them as functions of E.

Find as a function of δ the ground state in the $|u\rangle, |d\rangle$ basis. Plot as a function of E the molecule's electric dipole moment P. [The $|u\rangle$ and $|d\rangle$ states have a dipole moments of $\pm qs$, respectively.]

9. The electric field increases in strength in the direction of $\mathbf{E}$. (Describe an experimental setup that would generate such a field gradient.) Explain why the results you obtained in the last problem imply that molecules in one eigenstate of H experience a force in the direction of $\mathbf{E}$ while molecules in the other eigenstate feel a force in the opposite direction.

10. The Hamiltonian of a particle that moves in a magnetic field is

$$H = \frac{1}{2m}(\mathbf{p} - Q\mathbf{A})^2,$$

where $\mathbf{A}(\mathbf{x})$ is a vector potential for the field. Show that $\mathbf{A}$ and $\mathbf{A}' = \mathbf{A} + \nabla\Lambda$ generate identical magnetic fields, where $\Lambda(\mathbf{x})$ is any scalar function. Let $\psi(\mathbf{x})$ be an eigenfunction of H for the potential $\mathbf{A}$. Show that $\phi(\mathbf{x}) \equiv \psi(\mathbf{x})\mathrm{e}^{\mathrm{i}Q\Lambda/\hbar}$ is an eigenfunction for the same energy and the vector potential $\mathbf{A}'$.

11. Find the magnetic field that is generated by $\mathbf{A} = \frac{1}{2}\mathbf{B} \times \mathbf{r}$. Find the form of the vector potential $\mathbf{A}'$ defined above when $\Lambda = -\frac{1}{2}\mathbf{r}.(\mathbf{B} \times \mathbf{a})$, where $\mathbf{a}$ is a constant vector. Hence adapt the derivation of a wavefunction for the lowest Landau level that is given in the lectures to find the wavefunction for a particle that spirals around the line $(x = x_0, y = y_0)$ in the lowest Landau level of the magnetic field $\mathbf{B} = (0, 0, B)$.

12. Prove that if A and B are any two Hermitian operators, then AB is in general not Hermitian, but $(AB + BA)$ is. Hence show that

$$p_r \equiv -\mathrm{i}\left(\frac{\mathrm{d}}{\mathrm{d}r} + \frac{1}{r}\right)$$

is an Hermitian operator. [Hint: show that $p_r = \frac{1}{2\hbar}(\hat{\mathbf{r}} \cdot \mathbf{p} + \mathbf{p} \cdot \hat{\mathbf{r}})$, where $\hat{\mathbf{r}} = r^{-1}\mathbf{r}$.]

13. Let $\mathbf{r}$ be the vector from the proton to the electron in hydrogen and $\psi(\mathbf{r}) = R(r)Y_l^m(\theta, \phi)$ be an energy eigenfunction of hydrogen. Then to a good approximation and with $\alpha \equiv e^2/(4\pi\epsilon_0\hbar c)$ the fine-structure constant, R satisfies

$$\left[-\frac{a_0^2}{2r^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}}{\mathrm{d}r}\right) + l(l+1)\frac{a_0^2}{2r^2} - \frac{a_0}{r}\right]R = \epsilon R \quad \text{where} \quad \begin{cases} a_0 \equiv \dfrac{\hbar}{\alpha m_e c} \\ \epsilon \equiv \dfrac{E}{\alpha^2 m_e c^2}. \end{cases}$$

With p_r defined as in the last problem, show that this can be written

$$H_l R = \epsilon R \quad \text{where} \quad H_l \equiv \left[\frac{a_0^2}{2}\left(p_r^2 + \frac{l(l+1)}{r^2}\right) - \frac{a_0}{r}\right]R.$$

14. Show that

$$A_l^\dagger A_l = H_l + \frac{1}{2(l+1)^2},$$

where H_l is defined in the previous question and

$$A_l \equiv \frac{a_0}{\sqrt{2}}\left(\mathrm{i}p_r - \frac{l+1}{r} + \frac{1}{a_0(l+1)}\right).$$

Show also that

$$[A_l, A_l^\dagger] = H_{l+1} - H_l,$$
$$[H_l, A_l] = [A_l^\dagger, A_l]A_l,$$
$$[H_l, A_{l-1}^\dagger] = [A_{l-1}, A_{l-1}^\dagger]A_{l-1}^\dagger.$$

15. Let $|\epsilon, l\rangle$ be such that $H_l|\epsilon, l\rangle = \epsilon|\epsilon, l\rangle$. Show that

$$H_{l+1}A_l|\epsilon, l\rangle = \epsilon A_l|\epsilon, l\rangle.$$

What feature of the energy-level structure of the hydrogen atom follows from this relation? Show similarly that $H_{l-1}A_{l-1}^\dagger|\epsilon, l\rangle = \epsilon A_{l-1}^\dagger|\epsilon, l\rangle$.

16. Explain why for given value of ϵ there must be a value $l_{\rm m}$ of l such that $A_{l_{\rm m}}|\epsilon, l_{\rm m}\rangle = 0$. Hence show that $\epsilon = -1/\{2(l_{\rm m}+1)^2\}$ and thus deduce the energy eigenvalues of the hydrogen atom.

17. Write down a first-order differential equation satisfied by the radial part of the wavefunction that represents $|\epsilon, l_{\rm m}\rangle$. Solve this equation and explain how any radial eigenfunction of the hydrogen atom may be obtained by an extension of this procedure. Illustrate this procedure by obtaining the radial wavefunctions of the $n = 1$ and $n = 2$ levels.