Quantum Mechanics H.T. 2001

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Problem Set No. 7

Except for question 5, the questions in this set are on topics that are not included in the Part A quantum mechanics syllabus. For instance, it says "Knowledge of the properties of ladder operators will not be assumed" [those are the $\hat{L}_+$ and $\hat{L}_-$ operators of Q 2], and also "Knowledge of matrix representations will not be assumed" [that's what questions 1, 3, 4 and 6 are about]. Nevertheless.....similar questions have in fact been asked in Part A (sometimes as exercises on the matrix part of the maths syllabus); question 1 is good preparation for perturbation theory; and anyway it's nice to have some idea of the alternative ("matrix") formulation of q.m. which was discovered by Heisenberg, amazingly, before Schrödinger's wave mechanics.

Quantum mechanics as a matrix eigenvalue/eigenvector problem.

1. A certain quantum system can exist in just two states. The Hamiltonian for the system (which is in one dimension for simplicity) has the form $\hat{H} = \hat{H}_0 + V$, where we shall assume that we know the normalised eigenfunctions $\phi_1(x)$ and $\phi_2(x)$, and the corresponding eigenvalues E_1 and E_2, of the Hermitian operator $\hat{H}_0$: $\hat{H}_0\phi_1(x) = E_1\phi_1(x), \hat{H}_0\phi_2 = E_2\phi_2(x)$. We want to find the eigenvalues E and the eigenfunctions $\phi(x)$ of $\hat{H}$, as defined by $\hat{H}\phi(x) = E\phi(x)$.

   (i) Since the functions ϕ_1 and ϕ_2 form a complete set for this two-state problem, the solution $\phi(x)$ can be represented as a linear combination of them: $\phi(x) = a\phi_1(x) + b\phi_2(x)$. *If we can find* a *and* b *we will know* $\phi(x)$!

   So we have $\hat{H}(a\phi_1(x) + b\phi_2(x)) = E(a\phi_1(x) + b\phi_2(x))$. Show that this equation can be written as $(E_1 + V)a\phi_1(x) + (E_2 + V)b\phi_2(x) = Ea\phi_1(x) + Eb\phi_2(x)$. Now multiply this equation by $\phi_1^*(x)$ and integrate over all space to obtain the equation

   $$(E_1 + \epsilon)a + \epsilon\, b = Ea \tag{1}$$

   where you are given that $\int \phi_1^*(x)V(x)\phi_1(x)dx = \int \phi_1^*(x)V(x)\phi_2(x)dx = \epsilon$. Similarly, show that

   $$\epsilon a + (E_2 + \epsilon)b = Eb \tag{2}$$

   given that $\int \phi_2^*(x)V(x)\phi_2(x)dx = \int \phi_2^*(x)V(x)\phi_1(x)dx = \epsilon$.

(ii) Show that (1) and (2) are equivalent to

$$\boldsymbol{H}\boldsymbol{u} = E\boldsymbol{u}$$

where

$$\boldsymbol{H} = \begin{pmatrix} E_1 + \epsilon & \epsilon \\ \epsilon & E_2 + \epsilon \end{pmatrix}$$

and

$$\boldsymbol{u} = \begin{pmatrix} a \\ b \end{pmatrix}.$$

Verify that the elements of the matrix $\boldsymbol{H}$ are indeed the matrix elements $\langle i \mid \hat{H} \mid j \rangle \equiv \int \phi_i^*(x)\hat{H}\phi_j(x)dx$ for $i, j = 1, 2$.

(iii) Explain why the eigenvalues E are given by the roots of the equation $\det(\boldsymbol{H} - E\boldsymbol{I}) = 0$ where $\boldsymbol{I}$ is the unit 2×2 matrix. For the particular case $E_1 = -1$ and $E_2 = 1$ (in suitable units), show that the eigenvalues are $E_\pm = \epsilon \pm (1 + \epsilon^2)^{1/2}$, and find the ratios $(a/b)_+$ and $(a/b)_-$ for each of these two energy eigenvalues. Hence find the two energy eigenfunctions in terms of the "basis functions" $\phi_1(x)$ and $\phi_2(x)$.

So now you know the eigenvalues and the eigenfunctions without solving a differential equation! All you needed was the expression for $\hat{H}$ and the functions $\phi_1(x)$ and $\phi_2(x)$ plus (presumably) a machine for evaluating the matrix element integrals. Think about how this can be generalised to n - state systems.

Matrix representation of ang. mom. operators, column vector representation of states

2. The operator $\hat{L}_+$ is defined by $\hat{L}_+ = \hat{L}_x + i\hat{L}_y$ and the operator $\hat{L}_-$ by $\hat{L}_- = \hat{L}_x - i\hat{L}_y$. Show that
(a) $[\hat{L}_z, \hat{L}_+] = \hbar\hat{L}_+$
(b) $[\hat{L}_z, \hat{L}_-] = -\hbar\hat{L}_-$
(c) $[\hat{\mathbf{L}}^2, \hat{L}_+] = [\hat{\mathbf{L}}^2, \hat{L}_-] = 0$.

Suppose $\psi_{\ell m}$ is an eigenfunction of $\hat{\mathbf{L}}^2$ and $\hat{L}_z$ with eigenvalues $\ell(\ell+1)\hbar^2$ and $m\hbar$ respectively. Show that $\hat{L}_+\psi_{\ell m}$ and $\hat{L}_-\psi_{\ell m}$ are eigenfunctions of $\hat{\mathbf{L}}^2$ with eigenvalue $\ell(\ell+1)\hbar^2$ (use (c)).

By considering equation (a) applied to $\psi_{\ell m}$, show that $\hat{L}_+ \psi_{\ell m}$ is an eigenfunction of $\hat{L}_z$ with eigenvalue $(m+1)\hbar$, and by considering (b) show that $\hat{L}_-\psi_{\ell m}$ is an eigenfunction of $\hat{L}_z$ with eigenvalue $(m-1)\hbar$.

3. For states with $\ell = 1$, the three spherical harmonics $Y_{11}(\theta, \phi)$, $Y_{10}(\theta, \phi)$ and $Y_{1-1}(\theta, \phi)$ are a complete set of eigenfunctions. In this "three-dimensional space", the angular momentum operators $\hat{L}_x$, $\hat{L}_y$ and $\hat{L}_z$ are defined by the set of all their matrix

elements between different Y's (nine elements in all). For each of $\hat{L}_x, \hat{L}_y, \hat{L}_z$ these 9 matrix elements form the elements of a matrix, which represents the operator in this "space". Calculate the matrices representing $\hat{L}_x$, $\hat{L}_y$ and $\hat{L}_z$ in the $\ell = 1$ space as follows:-

Let $\hat{L}_+ = \hat{L}_x + i\hat{L}_y$. In spherical polars, this is given by (see McMurry p82 for example)

$$\hat{L}_+ = \hbar e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right).$$

Define $Y_{11} = -\sqrt{\frac{3}{8\pi}}e^{i\phi}\sin\theta, Y_{10} = \sqrt{\frac{3}{4\pi}}\cos\theta, Y_{1-1} = \sqrt{\frac{3}{8\pi}}e^{-i\phi}\sin\theta.$

Verify that

$$\hat{L}_+ Y_{1-1} = \sqrt{2}\hbar Y_{10}, \hat{L}_+ Y_{10} = \sqrt{2}\hbar Y_{11}, \hat{L}_+ Y_{11} = 0.$$

Multiply the first of these equations by Y_{11}^* and integrate over the solid angle $d\Omega = \sin\theta d\theta d\phi$ appropriate to 3-D spherical polars, and use the known orthogonality properties of the $Y_{\ell m}$, to show that

$$\langle 11 \mid \hat{L}_+ \mid 1-1\rangle \equiv \int\int Y_{11}^* L_+ Y_{1-1} d\Omega = 0.$$

Similarly, show that

$$\begin{aligned} \langle 10 \mid \hat{L}_+ \mid 1-1\rangle &= \sqrt{2}\hbar \\ \langle 1-1 \mid \hat{L}_+ \mid 1-1\rangle &= 0. \end{aligned}$$

Continue to show that the matrix representing $\hat{L}_+$ in this "$l = 1$ space" is

$$L_+^{(1)} \equiv \left(\begin{array}{ccc} \langle 11 \mid \hat{L}_+ \mid 11\rangle & \langle 11 \mid \hat{L}_+ \mid 10\rangle & \langle 11 \mid \hat{L}_+ \mid 1-1\rangle \\ \langle 10 \mid \hat{L}_+ \mid 11\rangle & \langle 10 \mid \hat{L}_+ \mid 10\rangle & \langle 10 \mid \hat{L}_+ \mid 1-1\rangle \\ \langle 1-1 \mid \hat{L}_+ \mid 11\rangle & \langle 1-1 \mid \hat{L}_+ \mid 10\rangle & \langle 1-1 \mid \hat{L}_+ \mid 1-1\rangle \end{array}\right) = \left(\begin{array}{ccc} 0 & \sqrt{2}\hbar & 0 \\ 0 & 0 & \sqrt{2}\hbar \\ 0 & 0 & 0 \end{array}\right).$$

$\hat{L}_-$ is given $\hat{L}_- = \hat{L}_x - i\hat{L}_y = (\hat{L}_x + i\hat{L}_y)^\dagger$ using $\hat{L}_x^\dagger = \hat{L}_x, \hat{L}_y^\dagger = \hat{L}_y$. So (this is the point of the definition of "Hermitian" for the differential operators!) we can write down the matrix for $\hat{L}_-$ straightaway:

$$L_-^{(1)} = \left(\begin{array}{ccc} 0 & 0 & 0 \\ \sqrt{2}\hbar & 0 & 0 \\ 0 & \sqrt{2}\hbar & 0 \end{array}\right), \text{ just the matrix dagger of } L_+^{(1)}.$$

So the matrix for $\hat{L}_x$ is

$$L_x^{(1)} = \frac{1}{2}(L_+^{(1)} + L_-^{(1)}) = \frac{1}{\sqrt{2}}\hbar\left(\begin{array}{ccc} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{array}\right)$$

and the matrix for $\hat{L}_y$ is

$$L_y^{(1)} = \frac{1}{2i}(L_+^{(1)} - L_-^{(1)}) = \frac{1}{\sqrt{2}}\hbar \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}.$$

(note that they are Hermitian matrices).

Finally, show that

$$L_z^{(1)} = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

in the same notation, and check that

$$[L_x^{(1)}, L_y^{(1)}] = i\hbar L_z^{(1)}.$$

What is the significance of this commutation relation? Evaluate $L_x^{(1)^2} + L_y^{(1)^2} + L_z^{(1)^2}$; what is the significance of the result?

Show that the column vectors

$$u_1^{(1)} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, u_0^{(1)} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, u_{-1}^{(1)} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

satisfy $L_z^{(1)} u_1^{(1)} = \hbar u_1^{(1)}, L_z^{(1)} u_0^{(1)} = 0, L_z^{(1)} u_{-1}^{(1)} = -\hbar u_{-1}^{(1)}$, so that they represent the states of definite $\hat{L}_z$ (eigenstates of $\hat{L}_z$) in this $\ell = 1$ space (the superscripts "(1)" indicate $\ell = 1$).

4. A particle with $\ell = 1$ is in the state represented by the column vector $u = \begin{pmatrix} a \\ b \\ c \end{pmatrix}$ where a, b, c are complex numbers. Show that the average value of L_z in this state is $\hbar(\mid a \mid^2 - \mid c \mid^2)$, assuming u is normalised such that $\mid a \mid^2 + \mid b \mid^2 + \mid c \mid^2 = 1$. What is the probability of obtaining the result $L_z = 0$ if L_z is measured?

Spin-$\frac{1}{2}$

5. In the Stern-Gerlach experiment, silver atoms with a kinetic energy of about 3×10^{-20}J each travelled a distance of 0.03 m through a non-uniform magnetic field of gradient $2.3 \times 10^3 \mathrm{Tm}^{-1}$. Calculate the separation of the two beams at a distance of 0.25 m downstream from the magnet (each atom behaves as if its magnetic moment, along any direction, takes only the two values $\pm\mu_B$ where μ_B is the Bohr magneton, with value $9.3 \times 10^{-24}\mathrm{JT}^{-1}$).

6. Find the eigenvalues, and corresponding normalised eigenvectors, of the three matrices
$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$
Verify that $S_x^2 + S_y^2 + S_z^2 = \frac{3}{4}\hbar^2 I$ where $I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and that $[S_x, S_y] = i\hbar S_z$.

[The matrices therefore have all the properties required to represent an angular momentum-like degree of freedom, of magnitude $j = \frac{1}{2}\hbar$].