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Quantum Mechanics I 7th Nov. '03.

2nd Midterm Exam Solutions T. Hübsch

DISCLAIMER: This solution set presents more detail than was required of the Student, and is meant as an additional resource for learning. Please *do* study not just the solutions as presented, but try also to understand the rationale behind the approach. Although none of the questions pertained to the linear harmonic oscillator and the $\hat{a}, \hat{a}^\dagger$ operator formalism *per se*, much of the calculations in this test are related to it. This also means that you will probably have a good opportunity to show off your $\hat{a}, \hat{a}^\dagger$-mastery on the Final, where it will count twice as much.

1. For a particle of mass M moves freely within a box (as in HW#4.2) of size L:

a. calculate $\triangle_P = \sqrt{\langle n|(\vec{P} - \langle n|\hat{P}|n\rangle)^2|n\rangle}$, the indeterminacy of observing $\hat{P}$.

Solution

For the particle in a box (using the results of HW#4.2),

$$\langle n'|\hat{\mathcal{O}}|n\rangle = \int \mathrm{d}x\, \psi^*_{n'}(x)\hat{\mathcal{O}}\psi_n(x) = \frac{2}{\pi}\int_0^L \mathrm{d}x\, \sin\left(n'\pi\tfrac{x}{L}\right)\hat{\mathcal{O}}\sin\left(n\pi\tfrac{x}{L}\right)\ .$$

Therefore (using $\phi = \frac{\pi}{L}x$),

$$\begin{aligned}\langle n|\hat{P}|n\rangle &= \frac{2\hbar}{iL}\int_0^L \mathrm{d}x\, \sin(n\pi\tfrac{x}{L})\frac{\mathrm{d}}{\mathrm{d}x}\sin(n\pi\tfrac{x}{L}) = -\frac{2n\hbar}{iL}\int_0^\pi \mathrm{d}\phi\, \sin(n\phi)\cos(n\phi)\ ,\\ &= -\frac{n\hbar}{iL}\int_0^\pi \mathrm{d}\phi\, \sin(2n\phi)\ =\ 0\ .\end{aligned}$$

Then: [=10pt]

$$\begin{aligned}\triangle_P &= \langle n|(\hat{P} - \langle n|\hat{P}|n\rangle)^2|n\rangle = \langle n|\hat{P}^2|n\rangle = -\frac{2\hbar^2}{L}\int_0^L \mathrm{d}x\, \sin(n\pi\tfrac{x}{L})\frac{\mathrm{d}^2}{\mathrm{d}x^2}\sin(n\pi\tfrac{x}{L})\ ,\\ &= \frac{n^2\pi^2\hbar^2}{L^2}\frac{2}{\pi}\int_0^\pi \mathrm{d}\phi\, \sin^2(n\phi) = \frac{n^2\pi^2\hbar^2}{L^2}\ .\end{aligned}$$

In fact, quite a bit more can be calculated using the integrals given in the test:

$$\begin{aligned}\langle n'|\hat{P}|n\rangle &= \frac{2\hbar}{iL}\int_0^L \mathrm{d}x\, \sin(n'\pi\tfrac{x}{L})\frac{\mathrm{d}}{\mathrm{d}x}\sin(n\pi\tfrac{x}{L}) = \frac{2\hbar}{iL}\int_0^L \mathrm{d}x\, \sin(n'\pi\tfrac{x}{L})\big[(-\tfrac{n\pi}{L})\cos(n\pi\tfrac{x}{L})\big]\ ,\\ &= -\frac{2n\hbar}{iL}\int_0^\pi \mathrm{d}\phi\, \sin(n'\phi)\cos(n\phi) = -\frac{2n^2\hbar}{iL}\begin{cases}\frac{1-(-1)^{n+m}}{(n-m)(n+m)}\ , & \text{if } n'{\neq}n,\\ 0\ , & \text{if } n'{=}n;\end{cases}\\ &= -\frac{4n^2\hbar}{iL}\begin{cases}\frac{1}{n^2-m^2}\ , & \text{if } n'{\pm}n \text{ is odd},\\ 0\ , & \text{if } n'{\pm}n \text{ is even}.\end{cases}\end{aligned}$$

Also:

$$\langle n'|\hat{P}^2|n\rangle = -\frac{2\hbar^2}{\pi}\int_0^L \mathrm{d}x\ \sin(n'\pi\tfrac{x}{L})\frac{\mathrm{d}^2}{\mathrm{d}x^2}\sin(n\pi\tfrac{x}{L}) = -\frac{2\hbar^2}{\pi}\int_0^L \mathrm{d}x\ \sin(n'\pi\tfrac{x}{L})\Big[(-\tfrac{n^2\pi^2}{L^2})\sin(n\pi\tfrac{x}{L})\Big]\ ,$$
$$= \frac{n^2\pi^2\hbar^2}{L^2}\frac{2}{\pi}\int_0^\pi \mathrm{d}\phi\ \sin(n'\phi)\sin(n\phi) = \frac{n^2\pi^2\hbar^2}{L^2}\delta_{n',n}\ ,$$

b. Calculate $\triangle_E$, the indeterminacy of observing $\hat{H}$. Compare with $\triangle_P$ and explain.

Solution____________________________________.

Since $\hat{H} = \frac{1}{2M}\hat{P}^2$, $\triangle_H = \frac{1}{2M}\triangle_P = \frac{n^2\hbar^2\pi^2}{2ML^2}$. Note that this indeterminacy in fact equals the value of the n^{th} energy level: $E_n = \frac{n^2\hbar^2\pi^2}{2ML^2}$, so that, for a particle in a box, the energy of the n^{th} state is predicted to be $E_n \pm E_n = E_n(1\pm 1)$! [=5pt]

c. Calculate the expectation value $\langle n|\frac{1}{2}(\hat{Q}\hat{P}+\hat{P}\hat{Q})|n\rangle$ for all n.

Solution____________________________________.

First, use $[\hat{Q},\hat{P}] = i\hbar$ to simplify:

$$\langle n'|\tfrac{1}{2}(\hat{Q}\hat{P}+\hat{P}\hat{Q})|n\rangle = \langle n'|\tfrac{1}{2}(\hat{Q}\hat{P}-i\hbar)|n\rangle = \tfrac{1}{2}\langle n'|\hat{Q}\hat{P}|n\rangle - \tfrac{i}{2}\hbar\delta_{n',n}\ .$$

So, now:

$$\langle n'|\hat{Q}\hat{P}|n\rangle = \frac{2\hbar}{iL}\int_0^L \mathrm{d}x\ \sin(n'\pi\tfrac{x}{L})\,x\,\frac{\mathrm{d}}{\mathrm{d}x}\sin\big(n\pi\tfrac{x}{L}\big) = \frac{2\hbar}{iL}\int_0^L \mathrm{d}x\ \sin\big(n'\pi\tfrac{x}{L}\big)\,x\,\big[(-\tfrac{n\pi}{L})\cos(n\pi\tfrac{x}{L})\big]\ ,$$
$$= -\frac{n\hbar}{i}\frac{2}{\pi}\int_0^\pi \mathrm{d}\phi\ \sin\big(n'\phi\big)\,\phi\,\cos(n\phi) = \frac{n\hbar}{i}\begin{cases}\frac{2n(-1)^{n+m}}{(n-m)(n+m)})\ , & \text{if } n'{\neq}n,\\ \frac{1}{2n}\ , & \text{if } n'{=}n.\end{cases}$$

Therefore, $\langle n|\frac{1}{2}(\hat{Q}\hat{P}+\hat{P}\hat{Q})|n\rangle = \frac{\hbar}{2i}+\frac{\hbar}{2i} = -i\hbar$. [=15pt]

2. Consider a particle of mass M, moving freely within a 2-dimensional box, specified by the potential $W(x,y) = 0$ if $|x|,|y|{<}L$ but $W(x,y) = \infty$ otherwise.

a. Specify the boundary conditions on the wave-function (if any) and state the nature (discrete/continuous) of the energy spectrum.

Solution____________________________________.

The boundary conditions on $\psi(x,y)$ are as follows:

$$\psi(x,y) = 0\ ,\quad \text{if } |x{-}\tfrac{L}{2}| \geq \tfrac{L}{2} \text{ or } |y{-}\tfrac{L}{2}| \geq \tfrac{L}{2}\ ,$$

that is, $\psi(x,y) = 0$ when (x,y) are outside the square $x,y \in (0,L)$. [=10pt]

b. Using separation of Cartesian coordinates, determine the energy levels in terms of the excitation numbers of the x- and y-directional motion, n_x and n_y.

Solution____________________________________.

Since $\hat{H} = \frac{1}{2M}(\hat{p}_x^2+\hat{p}_y^2) = \hat{H}_x+\hat{H}_y$, where $\hat{H}_x = \frac{1}{2M}\hat{p}_x^2$ and $\hat{H}_y = \frac{1}{2M}\hat{p}_y^2$, we have that $E_{n_x,n_y} = E_{n_x}+E_{n_y}$, where the two summands are just the energies from HW#4.2. Thus:[=10pt]

$$E_{n_x,n_y} = \frac{n_x^2\pi^2\hbar^2}{2ML^2}+\frac{n_y^2\pi^2\hbar^2}{2ML^2} = \frac{\pi^2\hbar^2}{2ML^2}(n_x^2+n_y^2)\ .$$

c. Using separation of Cartesian coordinates, determine the Hilbert space of this 2-dimensional system, *i.e.*, list all the eigenstates of $\hat{H}$, and state the orthonormality and the completeness conditions.

Solution

As standard in the separation of variables procedure, we have that $\psi_{n_x,n_y}(x,y) = \psi_{n_x}(x)\psi_{n_y}(y) = \langle x|n_x\rangle\langle y|n_y\rangle$, and so also $|n_x,n_y\rangle = |n_x\rangle \otimes |n_y\rangle$. Using the solutions from HW#4.2 again, the eigenstates of $\hat{H}$ are:

$$\psi_{n_x,n_y}(x,y) = \langle x,y|n_x,n_y\rangle = \frac{2}{L}\sin(n_x\pi\frac{x}{L})\sin(n_y\pi\frac{y}{L}) \ .$$

The orthogonality relation is

$$\langle n'_x,n'_y|n_x,n_y\rangle = \frac{4}{L^2}\int_0^L \mathrm{d}x \int_0^L \mathrm{d}y \ \psi^*_{n'_x,n'_y}(x,y)\psi_{n_x,n_y}(x,y) = \delta_{n'_x,n_x}\delta_{n'_y,n_y} \ , \qquad (o)$$

and the completeness relation is

$$\sum_{n_x,n_y} |n_x,n_y\rangle\langle n_x,n_y| = \frac{4}{L^2}\sum_{n_x,n_y} \psi_{n_x,n_y}(x,y)\int_0^L \mathrm{d}x \int_0^L \mathrm{d}y \ \psi^*_{n_x,n_y}(x,y)\big(\cdots\big) = \mathbb{1} \ , \quad (c)$$

where the ellipses in the parentheses indicate that the integral is to be appllied as an integral transform on a function of x, y. Thus, the Hilbert space is: [=20pt]

$$\mathcal{H} = \big\{ \ |n_x,n_y\rangle \ : \ n_x,n_y = 1,2,3,\ldots, \ \text{Eq. } (o), \ \text{Eq. } (c) \ \big\} \ .$$

d. Tabulate (in 2D) the energies of states with $1 \le n_x, n_y \le 10$, in units of $\frac{\hbar^2\pi^2}{2ML^2}$ and determine their degeneracy (the number of states with that energy).

Solution

Let's begin with the table, as instructed:

$n_y \backslash n_x$:	1	2	3	4	5	6	7	8	9	10
1	2	5	10	17	26	37	50	65	82	101
2	5	8	13	20	29	40	53	68	85	104
3	10	13	18	25	34	45	58	73	90	109
4	17	20	25	32	41	52	65	80	97	116
5	26	29	34	41	50	61	74	89	106	125
6	37	40	45	52	61	72	85	100	117	136
7	50	53	58	65	74	85	98	113	130	149
8	65	68	73	80	89	100	113	128	145	164
9	82	85	90	97	106	117	130	145	162	181
10	101	104	109	116	125	136	149	164	181	200

Table 1: The table of energy values, in units of $\frac{\pi^2\hbar^2}{2ML^2}$.

From the table it is clear that for every $n' \neq n$, the states $|n', n\rangle$ and $|n, n'\rangle$ have the same energy, $\frac{\pi^2\hbar^2}{2ML^2}(n'^2+n^2)$. However, notice that there are additionally degenerate states, which do not follow this pattern. For example, *three* different states, $|1,7\rangle$, $|7,1\rangle$ and $|5,5\rangle$, have the energy $\frac{\pi^2\hbar^2}{2ML^2}\cdot 50$, owing to the arithmetic accident $5^2+5^2=1^2+7^2$. States on the diagonal of the above table, $|n,n\rangle$, are non-degenerate unless they are, owing to an arithmetic accident such as $5^2+5^2=1^2+7^2$. Oh, by the way, if you got about half of the entries above the diagonal (reflected below), you'd get full credit for this part. [=25pt]

e. Identify all the states that are degenerate owing to the $x \leftrightarrow y$ symmetry.

Solution.

These are indeed the $|n',n\rangle$–$|n,n'\rangle$ pairs. This follows from observing that [=10pt]

$$\hat{\mathcal{P}}_{x\leftrightarrow y}\,\psi_{n_x,n_y}(x,y) = \hat{\mathcal{P}}_{x\leftrightarrow y}\,\frac{2}{L}\sin(n_x\pi\frac{x}{L})\sin(n_y\pi\frac{y}{L}) = \frac{2}{L}\sin(n_x\pi\frac{y}{L})\sin(n_y\pi\frac{x}{L})\ ,$$
$$= \psi_{n_y,n_x}(x,y) = \hat{\mathcal{P}}_{n_x\leftrightarrow n_y}\,\psi_{n_x,n_y}(x,y)\ .$$

f. Does the $x \leftrightarrow y$ symmetry cause all the degeneracy in this system or not? Justify your answer, and give at least one example if your answer is "not."

Solution.

As stated above, the $x \leftrightarrow y$ symmetry does not account for all of the degeneracy. The remaining degenerate states are degenerate owing to arithmetic accidents, such as $5^2+5^2=1^2+7^2$, or $6^2+7^2=2^2+9^2$, *etc.* [=10pt]

3. A Helium atom has its two electrons in a $j_1=\frac{3}{2}$ and a $j_2=\frac{1}{2}$ state, respectively.

a. Calculate all the possible values of the (composite) total angular momentum of the 2-electron system, j, its projection, m, and the degeneracy (multiplicity) of each.

Solution.

This pretty much follows the procedure done in class, so we list only the end result, in the familiar tabular form:

$j_1=\frac{3}{2}$	$j_2=\frac{1}{2}$	$j=2$	$j=1$
m_1	m_2	m	m
$+\frac{3}{2}$	$+\frac{1}{2}$	$+2$	
$+\frac{1}{2}$	$-\frac{1}{2}$	$+1$	$+1$
$-\frac{1}{2}$		0	0
$-\frac{3}{2}$		-1	-1
		-2	

Table 2: The addition of angular momenta table: the data in the top-left quadrant were given; those in the bottom-left quadrant are the possible projections of the angular momenta in the column heading; those in the bottom-right quadrant are all the possible sums of projections, one from each of the columns in the bottm-left quadrant; those in the top-right quadrant are deduced to be the "magnitudes" of the angular momenta the projections of which appear in the columns of the bottom-right quadrant.

So, the possible values of angular momenta are $(j = 2, 1)$. Their projections (m) and degeneracies (d) are: $(m, d) = (\pm 2, 1), (\pm 1, 2), (0, 2)$. [=15pt]

b. Calculate the possible eigenvalues of the operator $\hat{\mathbf{J}}_1\cdot\hat{\mathbf{J}}_2$. (A formula similar to (7.105) may be derived and should simplify the task.)

Solution____.

As directed:

$$\langle\hat{\mathbf{J}}_1\cdot\hat{\mathbf{J}}_2\rangle = \tfrac{1}{2}\big[\langle\hat{\mathbf{J}}^2\rangle - \langle\hat{\mathbf{J}}_1^2\rangle - \langle\hat{\mathbf{J}}_2^2\rangle\big]\ ,$$

$$= \begin{cases} \tfrac{1}{2}\big[2(2{+}1) - \tfrac{3}{2}(\tfrac{3}{2}{+}1) - \tfrac{1}{2}(\tfrac{1}{2}{+}1)\big] = \tfrac{3}{4}\ , & \text{if } j=2; \\ \tfrac{1}{2}\big[1(1{+}1) - \tfrac{3}{2}(\tfrac{3}{2}{+}1) - \tfrac{1}{2}(\tfrac{1}{2}{+}1)\big] = -\tfrac{5}{4}\ , & \text{if } j=1. \end{cases}$$

[=10pt]

c. Is the complete total angular momentum of the Helium atom (including the nucleus) integral of half-integral? Explain and justify.

Solution____.

The atom of the standard isotope of Helium, ${}^2_4$He, has two electrons, two protons and two neutrons. All of these have spin $\frac{1}{2}\hbar$, and since there is an even number of them, their composite spin must be integral. Orbital angular momenta are always integral, so the total, composite, complete angular momentum of ${}^2_4$He-atom is integral. However, its adjacent isotopes, ${}^2_3$He and ${}^2_5$He both have half-integral total angular momentum, on account of the odd number (1 and 3, respectively) of spin-$\frac{1}{2}$ neutrons. Finally, once ionized Helium atoms have a single electron, so that the total angular momentum of ${}^2_4\mathrm{He}^+$, ${}^2_3\mathrm{He}^+$ and ${}^2_5\mathrm{He}^+$ is half-integral, integral and integral, respectively. [=10pt]