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Quantum Mechanics I 2nd Dec. '02.
1st 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.

1. For a simple linear harmonic oscillator:

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

Sol'n: As shown in class, the fastest way to calculate this is using the creation-annihilation operator representation, with

$$\hat{P} = i\sqrt{\frac{M\omega\hbar}{2}}(\hat{a}^\dagger - \hat{a}) \ ,$$

so it easily follows that

$$\langle n|\hat{P}|n\rangle = i\sqrt{\frac{M\omega\hbar}{2}}\big(\langle n|\hat{a}^\dagger|n\rangle - \langle n|\hat{a}|n\rangle\big) = i\sqrt{\frac{M\omega\hbar}{2}}\big(\sqrt{n+1}\langle n|n+1\rangle - \sqrt{n}\langle n|n-1\rangle\big) \equiv 0 \ .$$

Then (this is a *simple linear* harmonic oscillator, so $\vec{P}$ was na obvious typo):

$$\triangle_P = \sqrt{\langle n|\hat{P}^2|n\rangle} = \sqrt{-\frac{M\omega\hbar}{2}\langle n|\big(\hat{a}^{\dagger 2} - \hat{a}^\dagger\hat{a} - \hat{a}\hat{a}^\dagger + \hat{a}^2\big)|n\rangle} \ .$$

Just as in the previous calculation, $\langle n|\hat{a}^{\dagger 2}|n\rangle = 0 = \langle n|\hat{a}^2|n\rangle$, and we use $\big[\hat{a}, \hat{a}^\dagger\big] = 1$ so $\hat{a}\hat{a}^\dagger = \hat{a}^\dagger\hat{a} + 1$ and [=10pt]

$$\triangle_P = \sqrt{\frac{M\omega\hbar}{2}\langle n|\big(2\hat{a}^\dagger\hat{a} + 1\big)|n\rangle} = \sqrt{ME_n} \ , \quad \text{where} \quad E_n = \hbar\omega(n+\tfrac{1}{2}) \ .$$

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

Sol'n: Using the general definition and that $\hat{H}\,|n\rangle = E_n\,|n\rangle$, we have that

$$\triangle_E = \sqrt{\langle n|(\hat{H} - \langle n|\hat{H}|n\rangle)^2|n\rangle} = \sqrt{\langle n|(\hat{H} - E_n)^2|n\rangle} = \sqrt{\langle n|(\hat{H}^2 - 2E_n\hat{H} + E_n^2)|n\rangle}$$
$$= \sqrt{\langle n|(E_n^2 - 2E_n\,E_n + E_n^2)|n\rangle} \equiv 0 \ .$$

The indeterminacy being zero implies that E_n, the eigenvalue of $\hat{H}$, may be measured with infinite precision — which had to be true, since the $|n\rangle$ are the eigenstates of $\hat{H}$; they however are not eigenstates of $\hat{P}$, whence $\triangle_P \neq 0$. [=10pt]

c. Calculate the matrix element $\langle n'|\frac{1}{2}(\hat{Q}\hat{P} + \hat{P}\hat{Q})|n\rangle$ for all n', n.

Sol'n: First, translate this operator into the $(\hat{a}, \hat{a}^\dagger)$ representation:

$$\tfrac{1}{2}(\hat{Q}\hat{P} + \hat{P}\hat{Q}) = \tfrac{1}{2}\sqrt{\frac{2\hbar}{M\omega}}\,i\sqrt{\frac{M\omega\hbar}{2}}\big[(\hat{a}^\dagger{+}\hat{a})(\hat{a}^\dagger{-}\hat{a}) + (\hat{a}^\dagger{-}\hat{a})(\hat{a}^\dagger{+}\hat{a})\big] \ ,$$
$$= \tfrac{\hbar}{2}\big[(\hat{a}^\dagger{+}\hat{a})(\hat{a}^\dagger{-}\hat{a}) + (\hat{a}^\dagger{-}\hat{a})(\hat{a}^\dagger{+}\hat{a})\big] = \hbar\big(\hat{a}^{\dagger 2} - \hat{a}^2\big) \ .$$

Now,

$$\tfrac{1}{2}\langle n'|(\hat{Q}\hat{P}+\hat{P}\hat{Q})|n\rangle = \hbar\big(\langle n'|\hat{\mathrm{a}}^{\dagger 2}|n\rangle - \langle n'|\hat{\mathrm{a}}^{2}|n\rangle\big)\ ,$$

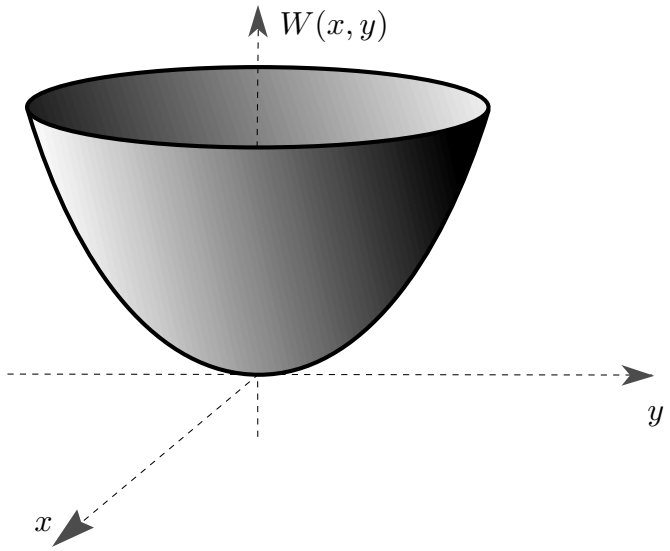
$$= \hbar\big(\sqrt{(n+1)(n+2)}\delta_{n',n+2} - \sqrt{n(n-1)}\delta_{n',n-2}\big)\ .$$

As usual: fill in the missing steps, please. [=15pt]

2. Consider a particle of mass M, moving in the potential $W(x,y) = \frac{1}{2}M\omega^2(x^2+y^2)$.

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

Sol'n:



The boundary conditions stem from the fact that, for large enough values of x, y, $V(x,y) > E$ for any (constant) value of E. Thus, the wave-function (*i.e.*, the probability density for finding the particle) must vanish as $r \stackrel{\text{def}}{=} \sqrt{x^2+y^2} \to \infty$. Therefore: $\lim_{r\to\infty}\psi(x,y) = 0$ is the required boundary condition. The wave-functions are thus localized, and the corresponding states will have discrete energy levels for all $E \geq 0$. $E < 0$ is not permitted, as $E < \min\big(W(x,y)\big)$ yields unnormalizably divergent wave-functions. [=5pt]

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

Sol'n: Writing

$$\hat{H} = \hat{H}_x + \hat{H}_y\ , \quad \text{where}$$

$$\hat{H}_x = \frac{1}{2M}\hat{P}_x^2 + \tfrac{1}{2}M\omega^2 x^2 \quad \text{and} \quad \hat{H}_y = \frac{1}{2M}\hat{P}_y^2 + \tfrac{1}{2}M\omega^2 y^2\ ,$$

we have that

$$E_{n_x,n_y} = E_{n_x} + E_{n_y} = \hbar\omega(n_x+\tfrac{1}{2}) + \hbar\omega(n_y+\tfrac{1}{2}) = \hbar\omega(n_x+n_y+1)\ .$$

[=5pt]

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

Sol'n: Writing

$$|n_x,n_y\rangle = |n_x\rangle_x\,|n_y\rangle_y\ , \qquad \text{where}$$

$$|n_x\rangle_x = \frac{\left(\hat{\mathrm{a}}^\dagger{}_x\right)^{n_x}}{n_x!}\,|0\rangle_x \quad \text{and} \quad |n_y\rangle_y = \frac{\left(\hat{\mathrm{a}}^\dagger{}_y\right)^{n_y}}{n_y!}\,|0\rangle_y \ ,$$

we have that

$$|n_x, n_y\rangle = \frac{\left(\hat{\mathrm{a}}^\dagger{}_x\right)^{n_x}\left(\hat{\mathrm{a}}^\dagger{}_y\right)^{n_y}}{n_x!\,n_y!}\,|0,0\rangle \ .$$

[=15pt]

d. Determine the degeneracy of *every* energy level (# of states with that energy).

Sol'n: Since $E_{n_x,n_y} = \hbar\omega(n_x{+}n_y{+}1)$, the value of the energy depends only on $N \stackrel{\text{def}}{=} (n_x{+}n_y)$, and not on $\nu \stackrel{\text{def}}{=} (n_x{-}n_y)$. Now, from the first definition, we have that $n_y = N{-}n_x$, so $\nu = 2n_x{-}N$, and it should be obvious that $\nu \in [-N, N]$: $\nu = N$ corresponds to $(n_x, n_y) = (N, 0)$ and $\nu = -N$ to $(n_x, n_y) = (0, N)$.

What is less obvious, is that (for a fixed N) ν can change only in increments of 2: to increase ν, we must increase n_x; but then, to keep N fixed, we must also decrease n_y by the same amount, so (for a fixed N) $\triangle\nu = 2\triangle n_x = -2\triangle n_y$.

Therefore, the number of values ν can take for a fixed value of N (and each defines a degenerate wave-function) is $N{+}1$. That is, the energy level $\hbar\omega(N{+}1)$ is $N{+}1$-fold degenerate: $|N, 0\rangle$, $|N{-}1, 1\rangle$, $\cdots$ $|0, N\rangle$ all have the that same energy. [=5pt]

e. Writing $\psi(r,\phi) = e^{-\frac{M\omega}{2\hbar}r^2} f(r)\, e^{im\phi}$, determine the boundary conditions on $f(r)$ and $e^{im\phi}$, and so the type of values m can have. (The sign in the exponent was an obvious typo; however, graded on consistency and correctness of their work.)

Sol'n: There are no real boundary conditions to be imposed on $e^{im\phi}$, since ϕ varies in a circle, without a boundary. However, we do have to require $\psi(r,\phi)$ to be periodic, *i.e.*, that $\psi(r, \phi{+}2\pi) \equiv \psi(r,\phi)$. Thus $e^{im(\phi+2\pi)} = e^{im\phi}$ implies that $e^{i2m\pi} = 1$, whence $m \in \mathbb{Z}$, *i.e.*, m must be an integer.

Since $W(r) > E$ when $r \to \infty$ for any E, we know that all states are localized, $\psi(r,\phi) \to 0$ as $r \to \infty$, and the boundary condition for $f(r)$ is that it may diverge, but not too badly so that $e^{-\frac{\alpha}{2}r^2} f(r) \to 0$ still holds. [=5pt]

f. Substituting this wave-function into the Schrödinger equation, determine and solve the differential equation for $f(r)$, subject to the boundary conditions. Show that this solution precisely corresponds to the Cartesian one.

Sol'n: In polar coordinates, the Schrödinger equation for our problem is

$$\Big[\frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial\phi^2} + k^2 - \alpha^2 r^2\Big]\psi(r,\phi) = 0 \ ,$$

where $k^2 = \frac{2ME}{\hbar^2}$ and $\alpha = \frac{M\omega}{\hbar}$. Since

$$\frac{\partial^2}{\partial\phi^2}\psi(r,\phi) = -m^2\psi(r,\phi) = -m^2 e^{\frac{\alpha}{2}r^2} f(r)\, e^{im\phi} \ ,$$

upon substituting $\psi(r,\phi) = e^{-\frac{M\omega}{2\hbar}r^2} f(r)\, e^{im\phi}$, the Schrödinger equation becomes

$$\Big[f'' + \big(\frac{1}{r} - 2\alpha r\big) f' + \big(k^2 - 2\alpha - \frac{m^2}{r^2}\big) f\Big] e^{-\frac{\alpha}{2}r^2} = 0 \ .$$

We seek solutions in the form $f(r) = \sum_{\ell=0}^{\infty} c_\ell r^{\ell+s}$, and obtain:

$$\sum_{\ell=0}^{\infty} c_\ell \big[(\ell{+}s)(\ell{+}s{-}1) + (\ell{+}s) - m^2\big] r^{\ell+s-2} - \sum_{\ell=0}^{\infty} c_\ell \big[2\alpha(\ell{+}s) + 2\alpha - k^2\big] r^{\ell+s} \;=\; 0 \;,$$

i.e.,

$$\sum_{\ell=0}^{\infty} c_\ell \big[(\ell{+}s)^2 - m^2\big] r^{\ell+s-2} - \sum_{\ell=0}^{\infty} c_\ell \big[2\alpha(\ell{+}s{+}1) - k^2\big] r^{\ell+s} \;=\; 0 \;.$$

To add up the two sums, we shift the summation index in the first sum, $\ell \to \ell{+}2$, and write the initial two terms separately:

$$c_0[s^2{-}m^2]r^{s-2} + c_1[(s{+}1)^2{-}m^2]r^{s-1} + \sum_{\ell=0}^{\infty} \Big\{ c_{\ell+2}\big[(\ell{+}s)^2{-}m^2\big] - c_\ell\big[2\alpha(\ell{+}s{+}1){-}k^2\big] \Big\} r^{\ell+s} \;=\; 0 \;.$$

Since different powers of any variable are linearly independent, the coefficient of each power of r must vanish separately. Starting with the coefficient of r^{s-2}, we conclude that $s = \pm m$ since $c_0 \neq 0$ (the series must have an initial term). Then, the vanishing of the coefficient of r^{s-1}, $c_1[(s{+}1)^2{-}m^2] = c_1(1 \pm 2m)$, implies that $c_1 = 0$ as $(1 \pm 2m) \neq 0$ for integer m. The vanishing of the remaining coefficients, enclosed in the curly braces, then implies that:

$$c_{\ell+2} = c_\ell \frac{2\alpha(\ell{+}s{+}1) - k^2}{(\ell{+}s)^2 - m^2} = c_\ell \frac{2\alpha(\ell{\pm}m{+}1) - k^2}{\ell(\ell{\pm}2m)} \;. \qquad (*)$$

Note: $c_1 = 0$ then implies that $c_\ell = 0$ for all odd ℓ; *i.e.*, we must restrict to even ℓ!

This defines $f(r) = \sum_{\ell=0}^{\infty} c_\ell r^{\ell+s}$, with the coefficients defined in Eq. $(*)$. We must ensure, however, that this solution does not destroy the expected behavior, $e^{-\frac{\alpha}{2}r^2} f(r) \to 0$. To this end, we need to determine how fast does this series diverge for $r \to \infty$. Since for large r, larger powers of it have larger values, we consider

$$c_{\ell+2} = c_\ell \frac{2\alpha(\ell{\pm}m{+}1) - k^2}{\ell(\ell{\pm}2m)} \xrightarrow{\ell\to\infty} \frac{2\alpha}{\ell}\, c_\ell \;,$$

which is the recursion relation for the function $F(r) = e^{+2\alpha r^2}$. That is,

$$\sum_{\ell=0}^{\infty} c_\ell r^{\ell+s} \sim e^{+2\alpha r^2} \;, \quad \text{for} \quad r \to \infty \;,$$

and this *does not* obey the stated boundary condition. The only solution is to choose $k^2 = 2ME/\hbar^2$ so that the recursion relation $(*)$ begins to produce zeroes after some ℓ. To that end, choose $k^2 = 2\alpha(N{+}1)$, and find that $c_{N\mp m}$ is the last non-zero coefficient. Then, the solution becomes a polynomial of $(\ell_{\max}{\pm}m){=}N$th order, and the boundary condition is obeyed. The relation $k^2 = 2\alpha(N{+}1)$ then implies that

$$\frac{2ME_N}{\hbar^2} = 2\frac{M\omega}{\hbar}(N{+}1) \;, \quad \Rightarrow \quad E_N = \hbar\omega(N+1) \;. \qquad (\diamond)$$

Since E_N does not depend on m, the values of m (for a fixed N) count the degeneracy of the energy level E_N. Recalling that $\ell_{\max} = N \mp m \geq 0$, it follows that $m \in [-N, +N]$, just like ν in the Cartesian solution above. Furthermore, remembering that $c_1 = 0$ and the recursion relation $(*)$ jointly imply that $c_\ell = 0$ for all odd ℓ, we require that $\ell_{\max} = N \mp m$ is even, whereupon m can only change in even units—just like ν in the Cartesian solution.

This almost proves the equivalence of the two solutions; what remains is to show that the actual wave-functions agree: $\psi_{N,m}(r,\phi) = \psi_{n_x,n_y}(x,y)$, with $N = n_x{+}n_y$ and $m = n_x{-}n_y$. We leave that to the diligent Student. [=20pt]

3. A Hydrogen atom has its electron in an "L orbital," *i.e.*, with $\ell = 1$. The spin of the electron is $\frac{1}{2}$, as is that of the proton (about which the electron orbits).

a. Calculate the possible values of the total angular momentum of the orbiting electron, $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}_e$.

Sol'n: Consider doing this first by using the triangle inequality:

$$\tfrac{1}{2} = |\ell{-}s_e| \le j \le \ell{+}s_e = \tfrac{3}{2} \ , \quad \text{so} \quad j = \tfrac{1}{2}, \tfrac{3}{2} \ .$$

[=10pt]

b. Calculate the possible values of the total angular momentum of the Hydrogen atom, $\hat{\mathbf{J}}_H = \hat{\mathbf{L}} + \hat{\mathbf{S}}_e + \hat{\mathbf{S}}_p$.

Sol'n: Consider doing this also first by using the triangle inequality:

$$0 = |\ell{-}s_e{-}s_p| \le j_H \le \ell{+}s_e{+}s_p = 2 \ , \quad \text{so} \quad j_H = 0, 1, 2 \ .$$

Now, the Student might complain: "Hold on, the *four* vector operators, $\hat{\mathbf{J}}_H, \hat{\mathbf{L}}, \hat{\mathbf{S}}_e, \hat{\mathbf{S}}_p$ don't form a triangle!" Indeed; they form a quadrangle. So the "triangle" rule needs to be iterated. Since $\hat{\mathbf{J}}_H = \hat{\mathbf{J}} + \hat{\mathbf{S}}_p$, we can write

$$\min\big(|j{-}s_p|\big) \le j_H \le \max\big(j{+}s_p\big) \ ,$$

so as to obtain the correct [=10pt]

$$0 = \min\big(|\tfrac{1}{2}{-}\tfrac{1}{2}|, |\tfrac{3}{2}{-}\tfrac{1}{2}|\big) \le j_H \le \max\big((\tfrac{1}{2}{+}\tfrac{1}{2}), (\tfrac{3}{2}{+}\tfrac{1}{2})\big) = 2 \ .$$

As far as obtaining the correct range, these relations suffice. However, they do not specify the number of times a particular value can be obtained. To this end, we do have to use the "table method" used in class; this is left for the diligent Student.

c. Calculate the possible eigenvalues of the operator $\hat{\mathbf{L}}{\cdot}\hat{\mathbf{S}}_e$.

Sol'n: As done in class, we square $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}_e$ to obtain

$$\hat{\mathbf{J}}^2 = \hat{\mathbf{L}}^2 + \hat{\mathbf{S}}_e^2 + 2\hat{\mathbf{L}}{\cdot}\hat{\mathbf{S}}_e \ ,$$

i.e.,

$$\hat{\mathbf{L}}{\cdot}\hat{\mathbf{S}}_e = \tfrac{1}{2}\big[\hat{\mathbf{L}}^2 + \hat{\mathbf{S}}_e^2 - \hat{\mathbf{J}}^2\big] \ ,$$

so that

$$\langle \hat{\mathbf{L}}{\cdot}\hat{\mathbf{S}}_e \rangle = \tfrac{1}{2}\big[\ell(\ell{+}1) + s_e(s_e{+}1) - j(j{+}1)\big] = \tfrac{1}{2}\Big[2 + \tfrac{3}{4} - \begin{cases} {}^3\!/_4 \\ {}^{15}\!/_4 \end{cases}\Big] = \begin{cases} 1 \\ -{}^1\!/_2 \end{cases} \ ,$$

for the two possible values, $j = \frac{1}{2}, \frac{3}{2}$. [=10pt]

d. Calculate the possible eigenvalues of the operator $\hat{\mathbf{L}}{\cdot}\hat{\mathbf{S}}_p$.

Sol'n: By the same token, we square $\hat{\mathbf{K}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}_p$ to obtain

$$\hat{\mathbf{L}}{\cdot}\hat{\mathbf{S}}_p = \tfrac{1}{2}\big[\hat{\mathbf{L}}^2 + \hat{\mathbf{S}}_p^2 - \hat{\mathbf{K}}^2\big] \ ,$$

so that

$$\langle \hat{\mathbf{L}}\cdot\hat{\mathbf{S}}_p\rangle = \left\{ \begin{array}{c} 1 \\ -1/2 \end{array} \right. ,$$

for the two possible values, $\langle \hat{\mathbf{K}}^2\rangle = \frac{3}{4}, \frac{15}{4}$, since all the numerics are the same as in the previous problem. [=10pt]

e. Calculate the possible eigenvalues of the operator $\hat{\mathbf{S}}_p\cdot\hat{\mathbf{S}}_e$.

Sol'n: By the same token, we square $\hat{\mathbf{S}} = \hat{\mathbf{S}}_p + \hat{\mathbf{S}}_e$ to obtain

$$\hat{\mathbf{S}}_p\cdot\hat{\mathbf{S}}_e = \tfrac{1}{2}\big[\hat{\mathbf{S}}_p^2 + \hat{\mathbf{S}}_e^2 - \hat{\mathbf{S}}^2\big] ,$$

and note that $\langle \hat{\mathbf{S}}^2\rangle = 0, 2$, *i.e.*, $s = 0, 1$ for this sum. Thus,

$$\langle \hat{\mathbf{L}}\cdot\hat{\mathbf{S}}_e\rangle = \tfrac{1}{2}\big[s_p(s_p{+}1) + s_e(s_e{+}1) - s(s{+}1)\big] = \left\{ \begin{array}{c} 3/4 \\ -1/4 \end{array} \right. ,$$

for the two possible values, $s = 0, 1$. [=10pt]

f. Is the total angular momentum of the Hydrogen atom half-integral? Explain.

Sol'n: First of all, (half-)integrality of an angular momentum (-like) operator $\hat{\mathbf{J}}$ refers to the (half-)integrality of the quantity j specifying the eigenvalues of $\hat{\cdot}^2$ as $j(j{+}1)$.

So, no, the total angular momentum of a Hydrogen atom is not half-integral; it's integral. The reason is that the Hydrogen atom system includes both one electron and one proton, and the total angular momentum of the whole Hydrogen atom system is then $\hat{\mathbf{J}}_H$, as defined above to include the (half-integral) spins of each of the proton and the electron, and the (integral) orbital angular momentum of the electron-proton system. For this j_H we have found integer eigenvalues, $j_H = 0, 1, 2$.

In general, a composite system consisting of an *even* number of separate subsystems (fermions) with half-integral spins and any number of separate subsystems (bosons) with integral spins will have an integral total angular momentum. Conversely, a composite system consisting of an *odd* number of separate subsystems (fermions) with half-integral spins and any number of separate subsystems (bosons) with integral spins will have a half-integral total angular momentum. Thus, the Hydrogen atom is bosonic, but the Deuterium atom is fermionic (it has an extra neutron, with spin $\frac{1}{2}$, in the nucleus), while the Tritium atom is again bosonic (it has two extra neutrons in the nucleus), *etc.* [=5pt]