

Quantum Mechanics I
2nd Midterm Exam

26th Nov. '97.
Solutions (T. Hübsch)

1. Before we continue, note that the “Cartesian” wave-functions $|m, n\rangle = C_{m,n} e^{-\frac{1}{2}\beta^2(x^2+y^2)} H_m(\beta x) H_n(\beta y)$ are the stationary wave-functions, *i.e.*, the eigenfunctions of the Hamiltonian, and with eigenvalues $E_{m,n} = \hbar\omega(m+n+1)$. We will need those that have $E = 4\hbar\omega$, whence $m+n = 3$, which are:

$$|3, 0\rangle, \quad |2, 1\rangle, \quad |1, 2\rangle, \quad |0, 3\rangle.$$

a. It is easy to see that $\hat{Z}_2^2 = \mathbf{1}$, all of the eigenvalues of which are ± 1 . Obviously, it is easiest to calculate \hat{Z}_2^2 in a basis where \hat{Z}_2 itself is diagonal—in an eigenbasis. But then, \hat{Z}_2 is a diagonal matrix, with eigenvalues on the diagonal; for \hat{Z}_2^2 , these eigenvalues become squared, and we know must be equal to ± 1 . Hence, all eigenvalues of \hat{Z}_2 square to ± 1 , and so can only be ± 1 . This is clearly true for *any* operator which squares to $\mathbf{1}$: its eigenvalues *must be* ± 1 .

b. Since \hat{Z}_2 simply swaps $x \leftrightarrow y$, its action on the “Cartesian” wave-functions is $\hat{Z}_2 |m, n\rangle = |n, m\rangle$. Among the wave-functions of our interest, we have

$$\hat{Z}_2 |3, 0\rangle = |0, 3\rangle, \quad \hat{Z}_2 |0, 3\rangle = |3, 0\rangle; \tag{1a}$$

$$\hat{Z}_2 |1, 2\rangle = |2, 1\rangle, \quad \hat{Z}_2 |2, 1\rangle = |1, 2\rangle. \tag{1b}$$

Clearly then, the eigenvectors and eigenvalues of \hat{Z}_2 are

$$|3, 0; \pm\rangle \stackrel{\text{def}}{=} \frac{1}{\sqrt{2}} [|3, 0\rangle \pm |0, 3\rangle], \quad z_{3,0}^\pm = \pm 1; \tag{2a}$$

$$|1, 2; \pm\rangle \stackrel{\text{def}}{=} \frac{1}{\sqrt{2}} [|1, 2\rangle \pm |2, 1\rangle], \quad z_{1,2}^\pm = \pm 1. \tag{2b}$$

(Acting on any of these kets, \hat{Z}_2 produces the indicated eigenvalue.)

c. As a 90° -rotation in the x - y -plane, \hat{R}_4 acts as $\hat{R}_4: (x, y) \mapsto (y, -x)$. It is easy to see that $\hat{R}_4^2 = -\mathbf{1}$. Arguing as in part a., the eigenvalues of \hat{R}_4 thus must square to -1 . Thus, the eigenvalues of \hat{R}_4 *must be* $\pm i$.

d. Since the Hermite polynomials obey $H_n(-\beta x) = (-1)^n H_n(\beta x)$, the action on the “Cartesian” wave-functions is $\hat{R}_4 |m, n\rangle = (-1)^m |n, m\rangle$. Among the wave-functions of our interest, we have

$$\hat{R}_4 |3, 0\rangle = -|0, 3\rangle, \quad \hat{R}_4 |0, 3\rangle = +|3, 0\rangle; \tag{3a}$$

$$\hat{R}_4 |1, 2\rangle = -|2, 1\rangle, \quad \hat{R}_4 |2, 1\rangle = +|1, 2\rangle. \tag{3b}$$

The eigenvectors and corresponding eigenvalues of \hat{R}_4 are then

$$|0, 3; \pm\rangle \stackrel{\text{def}}{=} \frac{1}{\sqrt{2}} [|0, 3\rangle \pm i |3, 0\rangle], \quad r_{0,3}^\pm = \mp i; \tag{4a}$$

$$|2, 1; \pm\rangle \stackrel{\text{def}}{=} \frac{1}{\sqrt{2}} [|2, 1\rangle \pm i |1, 2\rangle], \quad r_{2,1}^\pm = \mp i; \tag{4b}$$

2. For this Hydrogen-like system, the Hamiltonian will be $\frac{1}{2m}\hat{p}^2 - \frac{e'^2}{r} [1 + e^{-3r/a_0}]$.

a. Writing $-\frac{e'^2}{r} [1 + e^{-3r/a_0}] = -\frac{e'^2}{r} + \hat{H}^{(1)}$, it follows that $\hat{H}^{(1)} = -e'^2 \left(\frac{e^{-3r/a_0}}{r}\right)$. We note that the screening function e^{-3r/a_0} rapidly vanishes: already at $r = a_0/2$ (half the Bohr radius), the screening function is just a bit over 22%; at $r = a_0$ (the Bohr radius), its less than 5%; at $r = 1.5375a_0$, it's less than 1%.

b. This perturbation will mix different states—those with same angular dependence (since $\hat{H}^{(1)}$ is independent of angles). That is to say, the correction to a given (unperturbed) wave-function will be a linear combination of *all* (unperturbed) wave-functions with same angular dependence. Since the wave-functions represent states, this is what is meant by saying that the perturbation mixes states. Indeed, already the first correction to the wave-function

$$|n, \ell, m\rangle^{(1)} = \sum_{n' \neq n} \left[\frac{\langle n', \ell, m | \hat{H}^{(1)} | n, \ell, m \rangle^{(0)}}{E_{n'}^{(0)} - E_n^{(0)}} \right] |n', \ell, m\rangle^{(0)} \quad (5)$$

is non-zero in general, since the matrix elements will be non-zero for some $n' \neq n$. The corrected wave-functions will then be mixtures of unperturbed wave-functions of *different energies* but same angular dependence (same ℓ, m).

c. Yes, one can use the ‘non-degenerate perturbation theory’, although the system is degenerate. This is because the sum in (5) extends only over states of the same angular dependence but different principal quantum number. For each principal quantum number (and so each energy level) there is only one state with any one fixed angular dependence (ℓ, m). Thus, no two states occurring in the sum (5) have the same energy, and no denominator vanishes.

d. The first order correction to energy equals $\langle n, \ell, m | \hat{H}^{(1)} | n, \ell, m \rangle^{(0)}$, which yields, for the ground state:

$$\begin{aligned} \langle 1, 0, 0 | \hat{H}^{(1)} | 1, 0, 0 \rangle^{(0)} &= -\frac{e'^2}{\pi a_0^3} \int_0^\infty r^2 dr \int_0^\pi \sin \theta d\theta \int_0^{2\pi} e^{-r/a_0} \frac{e^{-3r/a_0}}{r} e^{-r/a_0} \\ &= -\frac{4\pi e'^2}{\pi a_0^3} \int_0^\infty dr r e^{-5r/a_0} = -\frac{4e'^2}{a_0^3} \left(\frac{a_0}{5}\right)^2 1! = -4 \frac{e'^2}{25a_0} \end{aligned} \quad (6)$$

after changing variables, $t = \frac{2}{a_0}r$ in the first, and $t = (\frac{2}{a_0} + \xi)r$ in the second integral, and then using the Γ -function integral on p.558. Finally, in the last row, the fraction has been expanded in small ξ , keeping only the lowest order term.

e. The first order correction to the energy $E_{2,0,0}$ equals

$$\begin{aligned} \langle 2, 0, 0 | \hat{H}^{(1)} | 2, 0, 0 \rangle^{(0)} &= -\frac{e'^2}{2a_0^3} \int_0^\infty dr r e^{-2r/a_0} \left(1 - \frac{r}{2a_0}\right)^2 (e^{-3r/a_0}) \ , \\ &= -\frac{e'^2}{2a_0^3} \int_0^\infty dr r e^{-5r/a_0} \left[1 - \frac{r}{a_0} + \frac{r^2}{4a_0^2}\right] \ , \\ &= -\frac{e'^2}{2a_0^3} \left[\left(\frac{a_0}{5}\right)^2 1! - \frac{1}{a_0} \left(\frac{a_0}{5}\right)^3 2! + \frac{1}{4a_0^2} \left(\frac{a_0}{5}\right)^4 3! \right] = -\frac{1}{4} \frac{e'^2}{25a_0} \ . \end{aligned} \quad (7)$$

f. Note that $|E_{2,0,0}^{(1)}| = \frac{1}{16}|E_{1,0,0}^{(1)}|$ —to first order, the first excited level is shifted only $\frac{1}{16}$ of the shift to the ground state. This happens for a good reason: the perturbation $\hat{H}^{(1)}$ is exponentially decaying with growing distance from the origin and clearly affects more those states which are better localized around the origin. A quick glance at Fig. 6.8 will verify that this is indeed the case with lower states. Thus, the perturbation shifts lower states more than higher ones. Therefore, we expect $E_{171,0,0}$ to be shifted much, much less than $E_{1,0,0}$ and $E_{2,0,0}$.

3. Notice that the perturbation $\hat{H}^{(1)} = -e\mathcal{E}_0 \sin(\pi x/L)$ is antisymmetric with respect to the reflection $\hat{R}: x \mapsto -x$. That implies that the diagonal matrix elements W_{++} and W_{--} vanish for each k separately. However, the off-diagonal matrix elements ($n = 1, 2, \dots$)

$$W_{+-} \stackrel{\text{def}}{=} -e\mathcal{E}_0 \frac{2}{L} \int_{-L/2}^{+L/2} dx \cos(kx) \sin(\pi x/L) \sin(kx), \quad k = \frac{2n\pi}{L}, \quad (8)$$

are nonzero; manifestly, $W_{+-} = W_{-+}$.

a. It should then be clear from Eq. (7.12b) that the degeneracy *will* be lifted, as the discriminant under square-root is nonzero. Also, more generally, note that $\hat{R}|k, \pm\rangle = \pm|k, \pm\rangle$, but the perturbation $\hat{H}^{(0)}$ and so the perturbed (total) Hamiltonian $\hat{H} = \hat{H}^{(0)} + \hat{H}^{(1)}$ does not commute with the reflection operator \hat{R} : $\hat{H}^{(1)}\hat{R} = -\hat{R}\hat{H}^{(1)}$. This implies that the new eigenfunctions will no longer be degenerate.

b. Changing variables to $\varphi = 2\pi x/L$ and using the trigonometric addition formulae:

$$\begin{aligned} W_{+-} &\stackrel{\text{def}}{=} -\frac{e\mathcal{E}_0}{4\pi} \int_{-\pi}^{+\pi} d\varphi \left[\cos\left(\frac{4n-1}{2}\varphi\right) - \cos\left(\frac{4n+1}{2}\varphi\right) \right], \\ &= -\frac{e\mathcal{E}_0}{4\pi} \left[\frac{4}{4n-1} + \frac{4}{4n+1} \right] = -\frac{e\mathcal{E}_0}{4\pi} \frac{8n}{16n^2-1}. \end{aligned} \quad (9)$$

and $W_{+-} = W_{-+}$, whereupon Eq. (7.19b) produces

$$E_n^\pm = E_n^{(0)} \pm \sqrt{|W_{+-}|^2} = \frac{2\hbar^2 n^2 \pi^2}{mL^2} \pm \frac{e\mathcal{E}_0 L}{\pi} \frac{8n}{16n^2-1}. \quad (10)$$

Notice that while the energy without the perturbation is proportional to the square of the wave-vector (and so also of the mode number n), the first order correction is inversely proportional to the wave-vector (mode number): $E^{(1)} \sim \frac{1}{n}$. Thus, the energy of the lowest-lying states are corrected more than the energies of the higher, excited states.