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Quantum Physics B

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Exam, Friday 24 October, 2003
4 problems (total of 50 points) + one bonus problem for additional points.
The solution of every problem on a separate piece of paper with name and study number.
Use the attached formula list where necessary.

Problem 1 (20 pnts in total)
The electron in a hydrogen atom occupies the combined spin and position state

$$\Psi = R_{32}\left(\sqrt{3}Y_2^{-1}\chi_+ + \sqrt{2}Y_2^0\chi_-\right)/\sqrt{5} \quad (1)$$

1 pnts — a. If you measured the orbital angular momentum squared (L^2), what values might you get, and what is the probability of each?

1 pnts — b. Same for the z-component of orbital angular momentum (L_z).

1 pnts — c. Same for the z-component of spin angular momentum (S_z).

2 pnts — d. Same for the z-component of total angular momentum, $J_z = L_z + S_z$.

3 pnts — e. Calculate for this wave function the expectation value $<\vec{S}\cdot\vec{n}>$ where $\vec{n} = \hat{x}\cos\alpha + \hat{z}\sin\alpha$.

4 pnts — f. If you measured J^2, what values might you get and what is the probability of each? (you may use the table of Clebsch-Gordan coefficients).

4 pnts — g. Calculate $\Phi = J_-\Psi$ where $J_- = L_- + S_-$.

4 pnts — h. In an experiment one measures r, the distance to the origin, as well as m_s, the z-projection of the electron spin. Give the probability density to find the electron with $m_s = -1/2$ at a distance r.

Problem 2 (15 pnts in total)
The two outermost electrons in the neutral Ti (Z=22, 2 electrons in the 3d shell) atom are in the $(3d)^2\ {}^{2s+1}L_J$ configuration.

5 pnts — a. Show that the coupled wave function in coordinate space is symmetric for L=4 (G) and anti-symmetric for L=3 (F). (Hint: use the lowering operator for total angular momentum).

2 pnts — b. Which configurations are allowed for the two electron $(3d)^2$ configuration in the notation ${}^{2s+1}L_J$ for L=4 and L=3 and why?

4 pnts — c. Show which of the configurations, ${}^3F_4$ or ${}^3F_2$, is lower in energy due to the spin-orbit force, $H' = \frac{\alpha}{2m^2}\frac{1}{r^3}L\cdot S$.

4 pnts — d. What is the ground state configuration for the V (Z=23, 3 electrons in the 3d shell) atom and give arguments.

Problem 3 (10 pnts in total) An electron is at rest in an oscillating magnetic field

$$\vec{B} = B_0 \cos(\omega t)\hat{y} \ . \qquad (2)$$

The hamiltonian for the particle is now given by $H = g\vec{B}\cdot\vec{S}$, where $\vec{S}$ are the spin matrices.

3 pnts a. Write the (time-dependent) Hamiltonian for this system explicitly as a 2×2 matrix.

3 pnts b. Write the time-dependent Schrödinger equation for each of the two components of the spinor-wavefunction for this problem. (Hint: there are 2 solutions, one with time dependence $e^{+\frac{gB_0}{\hbar\omega}\sin\omega t}$, the other with $e^{-\frac{gB_0}{\hbar\omega}\sin\omega t}$.

4 pnts c. The electron starts out (at t=0) in the spin-up state with respect to the x-axis ($\chi(0) = \chi_+^{(x)}$). Determine $\chi(t)$ at any subsequent time.

Problem 4 (15 pnts in total)
To the Hamiltonian of a one-dimensional harmonic-oscillator,

$$H_0(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 \ ,$$

a perturbation is added.

$$H'(x) = -\lambda x^3 \ .$$

3 pnts a. Calculate the first order correction to the energies of the lowest 2 states.

6 pnts b. Calculate the second-order correction to the energy of the ground state.

6 pnts c. Calculate $< x >$ for the ground state using first order perturbation theory for the wave function.

Problem 5 (10 pnts in total) N.B. This exercise is for Bonus points
The Hamiltonian for a certain problem is given by

$$H(x) = H_0(x) + H'(x) = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 - \lambda x^3 \ ,$$

the same as in the previous problem. Use

$$\psi(x;b) = A\,\pi)^{-1/4}(1 + 2b\sqrt{\alpha}x)e^{-\alpha x^2} = A\,(<x|0> + b<x|1>) \qquad (3)$$

as a variational wave function with $\alpha = \frac{m\omega}{2\hbar}$. The states $|0>$ and $|1>$ denote the ground, respectively the first exited state of H_0.

2 pnts a. Show that the trial wave function is properly normalized for $A = \sqrt{\frac{1}{1+b^2}}$.

4 pnts b. Calculate the expectation value of H for the state $\psi(x;b)$. (Hint: use that $\psi(x;b)$ is a superposition of eigenstates of H_0)

4 pnts c. Use the variational principle to calculate the best approximation to the ground state energy.

$$\int_{-a}^{a} e^{i\alpha x}\,dx = \frac{2}{\alpha}\sin(\alpha a)\ , \tag{28}$$

$$\int_{-a}^{a} \cos\alpha x\; e^{ikx}\,dx = \left[\frac{\sin(\alpha+k)a}{\alpha+k} + \frac{\sin(\alpha-k)a}{\alpha-k}\right]\ , \tag{29}$$

$$\int_{-a}^{a} \sin\alpha x\; e^{ikx}\,dx = i\left[\frac{\sin(\alpha+k)a}{\alpha+k} - \frac{\sin(\alpha-k)a}{\alpha-k}\right]\ , \tag{30}$$

$$\int_{-\infty}^{\infty} e^{i(k-k')x}\,dx = 2\pi\,\delta(k-k')\ , \tag{31}$$

$$\int_{-\infty}^{\infty} f(p')\,\delta(p-p')\,dp' = f(p) \quad \text{(mits } f(p) \text{ differentieerbaar in } p\text{)}\ , \tag{32}$$

$$\int_{-\infty}^{\infty} e^{-a(x+b+ic)^2}dx = \sqrt{\pi/a}\ , \tag{33}$$

$$\int_{-\infty}^{\infty} x^2 e^{-a(x+b)^2}dx = (b^2+1/2a)\sqrt{\pi/a}\ , \tag{34}$$

$$\int_{-\infty}^{\infty} e^{-a(x+b)^2} e^{ikx}dx = \sqrt{\pi/a}\,e^{-ikb-k^2/4a}\ , \tag{35}$$

$$\int_{-\infty}^{\infty} e^{-ax^2}\cos(bx)\,dx = \sqrt{\pi/a}\;e^{-b^2/4a}\ , \tag{36}$$

$$\int_{0}^{\infty} x^{2n}e^{-ax^2}dx = \tfrac{1}{2}\frac{1\cdot3\cdot5\cdots(2n-1)}{(2a)^n}\sqrt{\pi/a} \text{ voor } \ n\geq 0\ , \tag{37}$$

$$= \tfrac{1}{2}\sqrt{\frac{\pi}{a}} \quad \text{voor} \quad n=0\ , \tag{38}$$

$$\int_{0}^{\infty} x^{2n+1}e^{-ax^2}dx = \frac{n!}{2\,a^{n+1}} \quad \text{met} \quad a>0\ , \tag{39}$$

$$\int_{0}^{\infty} x^{n}e^{-ax}dx = \frac{n!}{a^{n+1}} \quad \text{met} \quad a>0\ , \tag{40}$$

$$\int_{0}^{\infty} xe^{-ax}\sin(bx)\,dx = \frac{2ab}{(a^2+b^2)^2} \quad \text{met} \quad a>0\ , \tag{41}$$

$$\int_{0}^{\infty} xe^{-ax}\cos(bx)\,dx = \frac{a^2-b^2}{(a^2+b^2)^2} \quad \text{met} \quad a>0\ , \tag{42}$$

$$\int_{0}^{\infty} \frac{\sin^2(px)}{x^2}dx = \tfrac{1}{2}\pi p\ , \tag{43}$$

$$\int_{-\infty}^{\infty} \frac{1}{x^2+a^2}\,e^{ikx}dx = \frac{\pi}{a}e^{-a|k|}\ , \text{ ook geldig voor k=0 }\ , \tag{44}$$

$$\int_{0}^{a} x^2\,\sin^2 n\pi x/a\,dx = \frac{a^3}{4}\left[\frac{2}{3} - \frac{1}{(n\pi)^2}\right]\ , \tag{45}$$

$$\int_{0}^{a} x^2\,\cos^2(n-\frac{1}{2})\pi x/a\,dx = \frac{a^3}{4}\left[\frac{2}{3} - \frac{1}{((n-\frac{1}{2})\pi)^2}\right]\ , \tag{46}$$

$$\int_{0}^{\pi} \sin^m\theta\,d\theta = \sqrt{\pi}\Gamma(\frac{m+1}{2})/\Gamma(\frac{m+2}{2})\ , \tag{47}$$

$$\int_{0}^{\infty} \frac{x^a}{(x^b+q^b)^c}dx = \frac{q^{a+1-bc}}{b}\frac{\Gamma(\frac{a+1}{b})\Gamma(c-\frac{a+1}{b})}{\Gamma(c)}\ , \tag{48}$$

$$\int_{-\infty}^{\infty} \frac{1}{(x^2+a^2)^2}dx = \frac{\pi}{2\,a^3}\ , \tag{49}$$

$$\int_{-\infty}^{\infty} \frac{1}{(x^2+a^2)^n}dx = \frac{1\cdot3\cdots(2n-3)}{2\cdot4\cdots(2n-2)}\,\frac{\pi}{a^{2n-1}} \text{ voor } n\geq 2, \tag{50}$$

$$\Gamma(n) = (n-1)\Gamma(n-1) = (n-1)! \quad ; \quad \Gamma(1) = 0! = 1\ , \tag{51}$$

$$\Gamma(n+\tfrac{1}{2}) = 2^{-n}[1\cdot3\cdot5\cdots(2n-1)]\sqrt{\pi} \quad ; \quad \Gamma(\tfrac{1}{2}) = \sqrt{\pi} \quad ; \quad \Gamma(\tfrac{3}{2}) = \sqrt{\pi}/2\ , \tag{52}$$

$$\cos^2 x = \tfrac{1}{2}(1+\cos 2x)\ . \tag{53}$$

Spherical harmonics Y_l^m.

$$Y_0^0 = \frac{1}{\sqrt{4\pi}} \; ; Y_1^1 = -\sqrt{\frac{3}{8\pi}}\, e^{i\phi} \sin\theta \; ; Y_1^0 = \sqrt{\frac{3}{4\pi}} \cos\theta \; , \tag{21}$$

$$Y_2^2 = \sqrt{\frac{15}{32\pi}}\, e^{2i\phi} \sin^2\theta \; ; Y_2^1 = -\sqrt{\frac{15}{8\pi}}\, e^{i\phi} \sin\theta \cos\theta \; ; Y_2^0 = \sqrt{\frac{5}{16\pi}}\, (3\cos^2\theta - 1) \; , \tag{22}$$

with $Y_l^{-m} = (-1)^m [Y_l^m]^*$, and the normalization condition:

$$\int d\Omega\, [Y_l^m(\Omega)] * Y_{l'}^{m'}(\Omega) = \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\, [Y_l^m(\Omega)]^* Y_{l'}^{m'}(\Omega) = \delta_{l,l'}\, \delta_{m,m'} \; . \tag{23}$$

$$L_+ = L_x + iL_y \quad \text{and} \quad L_+\, Y_l^m = \hbar\sqrt{l(l+1) - m(m+1)}\; Y_l^{m+1} \; , \tag{24}$$

$$L_- = L_x - iL_y \quad \text{and} \quad L_-\, Y_l^m = \hbar\sqrt{l(l+1) - m(m-1)}\; Y_l^{m-1} \; . \tag{25}$$

$$L^2 = L_x^2 + L_y^2 + L_z^2 = L_+L_- + L_z^2 - \hbar L_z = L_-L_+ + L_z^2 + \hbar L_z$$

In addition:

$$|l, j, m_j> \;=\; \sqrt{\frac{l-m}{2l+1}} |Y_l^{m+1}\chi_- > + \sqrt{\frac{l+m+1}{2l+1}} |Y_l^m \chi_+ > \quad \text{for } j = l + 1/2 \tag{26}$$

$$|l, j, m_j> \;=\; \sqrt{\frac{l+m+1}{2l+1}} |Y_l^{m+1}\chi_- > - \sqrt{\frac{l-m}{2l+1}} |Y_l^m \chi_+ > \quad \text{for } j = l - 1/2 \tag{27}$$

with $m = m_j - 1/2$.

Table 4.7: Clebsch-Gordan coefficients. (A square root sign is understood for every entry; the minus sign, if present, goes *outside* the radical.)

1/2 × 1/2

m_1 m_2	1 +1
+1/2 +1/2	1

m_1 m_2	1 0	0 0
+1/2 −1/2	1/2	1/2
−1/2 +1/2	1/2	−1/2

m_1 m_2	1 −1
−1/2 −1/2	1

1 × 1/2

m_1 m_2	3/2 +3/2
+1 +1/2	1

m_1 m_2	3/2 +1/2	1/2 +1/2
+1 −1/2	1/3	2/3
0 +1/2	2/3	−1/3

m_1 m_2	3/2 −1/2	1/2 −1/2
0 −1/2	2/3	1/3
−1 +1/2	1/3	−2/3

m_1 m_2	3/2 −3/2
−1 −1/2	1

2 × 1

m_1 m_2	3 +3
+2 +1	1

m_1 m_2	3 +2	2 +2
+2 0	1/3	2/3
+1 +1	2/3	−1/3

m_1 m_2	3 +1	2 +1	1 +1
+2 −1	1/15	1/3	3/5
+1 0	8/15	1/6	−3/10
0 +1	6/15	−1/2	1/10

m_1 m_2	3 0	2 0	1 0
+1 −1	1/5	1/2	3/10
0 0	3/5	0	−2/5
−1 +1	1/5	−1/2	3/10

m_1 m_2	3 −1	2 −1	1 −1
0 −1	6/15	1/2	1/10
−1 0	8/15	−1/6	−3/10
−2 +1	1/15	−1/3	3/5

m_1 m_2	3 −2	2 −2
−1 −1	2/3	1/3
2 0	1/3	−2/3

m_1 m_2	3 −3
−2 −1	1

1 × 1

m_1 m_2	2 +2
+1 +1	1

m_1 m_2	2 +1	1 +1
+1 0	1/2	1/2
0 +1	1/2	−1/2

m_1 m_2	2 0	1 0	0 0
+1 −1	1/6	1/2	1/3
0 0	2/3	0	−1/3
−1 +1	1/6	−1/2	1/3

m_1 m_2	2 −1	1 −1
0 −1	1/2	1/2
−1 0	1/2	−1/2

m_1 m_2	2 −2
−1 −1	1

2 × 1/2

m_1 m_2	5/2 +5/2
+2 1/2	1

m_1 m_2	5/2 3/2	3/2 +3/2
+2 −1/2	1/5	4/5
+1 +1/2	4/5	−1/5

m_1 m_2	5/2 +1/2	3/2 +1/2
+1 −1/2	2/5	3/5
0 +1/2	3/5	−2/5

m_1 m_2	5/2 −1/2	3/2 −1/2
0 −1/2	3/5	2/5
−1 +1/2	2/5	−3/5

m_1 m_2	5/2 −3/2	3/2 −3/2
−1 −1/2	4/5	1/5
−2 +1/2	1/5	−4/5

m_1 m_2	5/2 −5/2
−2 −1/2	1

3/2 × 1/2

m_1 m_2	2 +2
+3/2 +1/2	1

m_1 m_2	2 +1	1 +1
+3/2 −1/2	1/4	3/4
+1/2 +1/2	3/4	−1/4

m_1 m_2	2 0	1 0
+1/2 −1/2	1/2	1/2
−1/2 +1/2	1/2	−1/2

m_1 m_2	2 −1	1 −1
−1/2 −1/2	3/4	1/4
−3/2 +1/2	1/4	−3/4

m_1 m_2	2 −2
−3/2 −1/2	1

3/2 × 1

m_1 m_2	5/2 +5/2
+3/2 +1	1

m_1 m_2	5/2 +3/2	3/2 +3/2
+3/2 0	2/5	3/5
+1/2 +1	3/5	−2/5

m_1 m_2	5/2 +1/2	3/2 +1/2	1/2 +1/2
+3/2 −1	1/10	2/5	1/2
+1/2 0	3/5	1/15	−1/3
−1/2 +1	3/10	−8/15	1/6

m_1 m_2	5/2 −1/2	3/2 −1/2	1/2 −1/2
+1/2 −1	3/10	8/15	1/6
−1/2 0	3/5	−1/15	−1/3
−3/2 +1	1/10	−2/5	1/2

m_1 m_2	5/2 −3/2	3/2 −3/2
−1/2 −1	3/5	2/5
−3/2 0	2/5	−3/5

m_1 m_2	5/2 −5/2
−3/2 −1	1

= =

The following formula's may be helpful in solving the problems.

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Sigma (spin) matrices.

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{1}$$

$$\sigma_{x,y,z} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{2}$$

$$(\vec{\sigma} \cdot \vec{A})(\vec{\sigma} \cdot \vec{B}) = \vec{A} \cdot \vec{B} + i\vec{\sigma} \cdot (\vec{A} \times \vec{B}) \tag{3}$$

Harmonic oscillator wave functions.

Solutions for a harmonic oscillator potential $V(x) = \frac{\omega^2 m}{2} x^2$

$$u_n = (2^n n! \sqrt{\pi})^{-1/2} H_n(y) e^{-y^2/2} \tag{4}$$

with $y = \sqrt{m\omega/\hbar}\, x$, where the Hermiet polynomials for $n \leq 4$ are given as

$$H_0(y) = 1 \tag{5}$$

$$H_1(y) = 2y \tag{6}$$

$$H_2(y) = 4y^2 - 2 \tag{7}$$

$$H_3(y) = 8y^2 - 12y \tag{8}$$

$$H_4(y) = 16y^4 - 48y^2 + 12 \tag{9}$$

Matrix elements:

$$< n|x^2|n > = < n|p^2|n > /(m\omega)^2 = (2n+1)\, \frac{\hbar}{2m\omega} \tag{10}$$

$$< n|x^2|n-2 > = - < n|p^2|n-2 > /(m\omega)^2 = \sqrt{n(n-1)}\, \frac{\hbar}{2m\omega} \tag{11}$$

$$< n|x^3|n-1 > = 3\, n^{3/2} \left(\frac{\hbar}{2m\omega}\right)^{3/2} \tag{12}$$

$$< n|x^3|n-3 > = \sqrt{n(n-1)(n-2)} \left(\frac{\hbar}{2m\omega}\right)^{3/2} \tag{13}$$

$$< n|x^4|n > = [2(n+1)(n+2) + (2n-1)(2n+1)] \left(\frac{\hbar}{2m\omega}\right)^2 \tag{14}$$

$$< n|x^4|n-2 > = 2(2n-1)\sqrt{n(n-1)} \left(\frac{\hbar}{2m\omega}\right)^2 \tag{15}$$

$$< n|x^4|n-4 > = \sqrt{n(n-1)(n-2)(n-3)} \left(\frac{\hbar}{2m\omega}\right)^2 \tag{16}$$

Hydrogen wave functions.

$R_{nl}(r)$ are hydrogen-like wave functions with $E_n = -\alpha^2 m_e c^2/2n^2 = -13.6\ eV/n^2$, $a_0 = \hbar/m_e c\alpha$ and $\alpha = e^2/\hbar c = 1/137$.

$$R_{10}(r) = 2 \left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}, \tag{17}$$

$$R_{20}(r) = 2 \left(\frac{Z}{2a_0}\right)^{3/2} \left(1 - \frac{Zr}{2a_0}\right) e^{-Zr/2a_0}, \tag{18}$$

$$R_{21}(r) = \frac{1}{\sqrt{3}} \left(\frac{Z}{2a_0}\right)^{3/2} \frac{Zr}{a_0} e^{-Zr/2a_0}, \tag{19}$$

$$R_{32}(r) = \frac{8}{81\sqrt{15}} \left(\frac{Z}{2a_0}\right)^{3/2} \left(\frac{Zr}{a_0}\right)^2 e^{-Zr/3a_0}. \tag{20}$$