Quantum Fysica B

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5 opgaven (totaal van 90 punten).
Iedere uitwerking op een apart vel papier met naam en studie nummer.
Maak gebruik van de bijgevoegde formulelijst waar dat nodig lijkt.

Opgave 1 (20 pnts in total)

The electron in a hydrogen atom occupies the combined spin and position state

$$\Psi = R_{21}\left(\sqrt{2}Y_1^{-1}\chi_+ + \sqrt{3}Y_1^0\chi_-\right)/\sqrt{10} + R_{20}Y_0^0\chi_-/\sqrt{2}$$

5 pnts a. What values might you get and with what probabilty if the following quantities are measured:

(i) L^2.
(ii) S^2.
(iii) S_z.
(iv) J_z (where $\vec{J} = \vec{L} + \vec{S}$).

5 pnts b. Calculate the expectation value of:

(a) L_z.
(b) S_x.
(c) r.

3 pnts c. Calculate $\Phi = J_-\Psi$ where $J_- = L_- + S_-$.

3 pnts d. Calculate the expectation value of J^2.

4 pnts e. In a measurement r as well as m_s (the z-projection of the electron spin) are measured. Give the probability density for finding the electron with $m_s = +1/2$ at a distance r from the origine.

Opgave 2. (20 pnts in total)

2 pnts a. Give the time independent Schrödinger equations for the problem of an infinite square well in 2 dimensions,

$$V(x,y) = \begin{cases} 0 & \text{for } 0 < x < a \text{ and } 0 < y < a \\ \infty & \text{otherwise} \end{cases} .$$

Do not forget to specify also the boundary conditions.

6 pnts b. Solve for the energies and wave functions.

2 pnts c. Specify the degeneracy of the first and second excited states.

5 pnts d. We add now a perturbation H' to the Hamiltonian,

$$H' = \begin{cases} V_0, & \text{for } 0 < x < a/4 \text{ and } 0 < y < a/4 \\ 0, & \text{otherwise} \end{cases} .$$

Give the energy of the ground state in first order perturbation theory. (In case you could not solve part b, assume some reasonable sine or cosine functions for the ground state.)

5 pnts e. Same as the previous part, but now for the first excited state

Problem 3 (15 pnts in total)

A particle moves in a one-dimensional potential given by

$$V(x) = \begin{cases} V_o\left(\frac{1}{x^2} - \frac{2}{x}\right) & \text{for } x > 0 \\ \infty & \text{for } x < 0 \end{cases}$$

where $V_o > 0$. To find an approximation for the energy of the ground state we will use the following tryal function using a trial wave function of the form

$$\Psi(x) = \begin{cases} A\, x^2 e^{-bx} & \text{for } x > 0 \\ 0 & \text{for } x < 0 \end{cases} .$$

2 pnts a. Determine the normalization constant A.

5 pnts b. Calculate the expectation value of the kinetic energy $< T >$.

5 pnts c. Calculate the expectation value of the potential energy $< V >$.

3 pnts d. Use variational calculation to obtain the best approximation to the ground-state energy.

Opgave 4 (20 pnts in total)

The matrices representing S_x, S_y and S_z for a particle of spin 1 are:

$$S_x = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S_y = \frac{i\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S_z = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

5 pnts a. Calculate the commutator $[S_z, S_y]$ explicitly.

5 pnts b. In a measurement of S_y it is found to be $+\hbar$. What is the state vector immediately after the measurement?

c. Suppose that the particle is placed in a magnetic field of magnitude B_o which is parallel to the z-axis. The Hamiltonian in this case is given by $H = -\gamma \vec{B} \cdot \vec{S}$. At t=0 the the particle is the state $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$.

2 pnts (i) Express the Hamiltonian as a (3×3) matrix.

4 pnts (ii) Calculate the state of the system at a time $t > 0$.

4 pnts (iii) Calculate t-dependence of the expectation value of S_y.

Opgave 5 (15 pnts in total)

The rate for spontaneous emission of a photon with energy $\hbar\omega = E_a - E_b$ is given by

$$A_{a \to b} = \frac{4\omega^3 \alpha |\mathcal{P}|^2}{3c^2} \tag{1}$$

where $\mathcal{P} =< a|\vec{r}|b >$ and $\alpha = 1/137$ is the fine structure constant. Ignore spin for this problem. You may express all answers in terms of fundamental constants such as α, m_e, c.

2 pnts a. Show that the units in this equation work out correctly.

2 pnts b. To which level(s) can the 2s and the 2p levels in hydrogen decay?

3 pnts c. Specify the complete radial and angular dependence of the wave function for a 2s electron as well as for a 2p electron in hydrogen.

3 pnts d. Calculate the spontaneous-emission rate for the 2s level in hydrogen.

5 pnts e. Calculate the spontaneous-emission rate for one of the 2p levels in hydrogen.

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Bij de bovenstaande opgaven kunnen de volgende formules nuttig zijn.

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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 $\alpha = e^2/\hbar c = 1/137$.

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

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

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

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:

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

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

with $m = m_j - 1/2$.

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

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

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

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

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

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

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

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

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

$$\int_{0}^{\infty} x^{2n} e^{-ax^2} dx = \tfrac{1}{2}\frac{1\cdot 3\cdot 5\cdots(2n-1)}{(2a)^n}\sqrt{\pi/a} \text{ voor } \ n \geq 0\ , \tag{37}$$

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

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

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

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

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

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

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

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

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

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

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

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

$$\int_{-\infty}^{\infty} \frac{1}{(x^2+a^2)^n} dx = \frac{1\cdot 3\cdots(2n-3)}{2\cdot 4\cdots(2n-2)}\ \frac{\pi}{a^{2n-1}} \text{ voor } n \geq 2, \tag{50}$$

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

$$\Gamma(n+\tfrac{1}{2}) = 2^{-n}[1\cdot 3\cdot 5\cdots(2n-1)]\sqrt{\pi} \quad ; \quad \Gamma(\tfrac{1}{2}) = \sqrt{\pi} \quad ; \quad \Gamma(\tfrac{3}{2}) = \sqrt{\pi}/2\ , \tag{52}$$

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