

Exercise session 12 will be held on Wednesday 9th from 08:15 to 13:00.

Return your solutions to this exercise before Friday 11th 14:00.

763312A QUANTUM MECHANICS I Exercise 12 Autumn 2009

1. Derive the dipole selection rules $\Delta l = \pm 1$ and $\Delta m = \pm 1$ by calculating the matrix elements of the x - and y -components of the dipole operator $\mathbf{D} = e\mathbf{r}$. You may need the recurrence relation $(2\ell + 1)\sqrt{1 - t^2}P_\ell^{m-1}(t) = P_{\ell+1}^m(t) - P_{\ell-1}^m(t)$.
2. Consider a one-dimensional anharmonic oscillator. Let the perturbation be of the form $H_1 = \sigma\hbar\omega x^3$. Calculate the matrix elements

$$\langle \psi_{n+3} | x^3 | \psi_n \rangle = \sqrt{\frac{(n+3)(n+2)(n+1)}{8}},$$

$$\langle \psi_{n+1} | x^3 | \psi_n \rangle = 3 \left(\frac{n+1}{2} \right)^{\frac{3}{2}},$$

$$\langle \psi_{n-1} | x^3 | \psi_n \rangle = 3 \left(\frac{n}{2} \right)^{\frac{3}{2}},$$

$$\langle \psi_{n-3} | x^3 | \psi_n \rangle = \sqrt{\frac{n(n-1)(n-2)}{8}}.$$

3. Consider an anharmonic oscillator in which the perturbation is of the form $H_1 = \sigma\hbar\omega x^3$. First, show that the energy levels are (to the second order in σ)

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega - \sigma^2 \left[\frac{15}{4} \left(n + \frac{1}{2}\right)^2 + \frac{7}{16} \right] \hbar\omega.$$

Then, show that the energy difference

$$E_n - E_{n-1} = \left(1 - \frac{15}{2}\sigma^2 n\right) \hbar\omega.$$

Finally, determine the energy eigenfunctions to the first order in σ .

Hint: See the lecture notes section 17.2.3.

4. Calculate the van der Waals constant

$$\begin{aligned} C &= -\frac{e^4}{2E_{1s}} \langle 1s; 1s | (x_A x_B + y_A y_B - 2z_A z_B)^2 | 1s; 1s \rangle \\ &= -\frac{e^4}{2E_{1s}} 6 \left| \langle 1s | \frac{r_A^2}{3} | 1s \rangle \right|^2 \\ &= 12a_0^6 \times Ry. \end{aligned}$$

5. Consider a system composed of noninteracting spin- $\frac{1}{2}$ fermions in a three-dimensional harmonic oscillator potential. First, describe the shell structure of the system. Then, suppose that there are a total of 100 particles in the system and that all the energy states of the system are filled up to energy $E_F = 1$ Ry. Estimate the strength of the potential $V(r) = \frac{1}{2}m\omega^2r^2$ by calculating the value of $\hbar\omega$.

6. Consider a hydrogen, a helium and a lithium atom and assume that there is no Coulomb interaction between the electrons. Calculate the binding energies of the outmost electrons. Does this model give the correct shell structure for these atoms, or for heavier atoms?
Hint: Since we assume that there is no Coulomb interaction between the electrons, the shell structures of all the three atoms can be solved in a similar manner.