

# Makroskopische Quantenzustände und kalte Gase

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Problem Set No 2

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## Problem 2.1 – Avoided Crossings (5 points)

The Frenkel two-state model provides a simple example where one can study the ‘cross-over’ from a linear to a quadratic Stark effect (or 1st to 2nd order perturbation theory). It is given by the Hamiltonian matrix

$$H = \begin{pmatrix} \varepsilon_1 & V \\ V^* & \varepsilon_2 \end{pmatrix} \quad (2.1)$$

The eigenvalues are given by

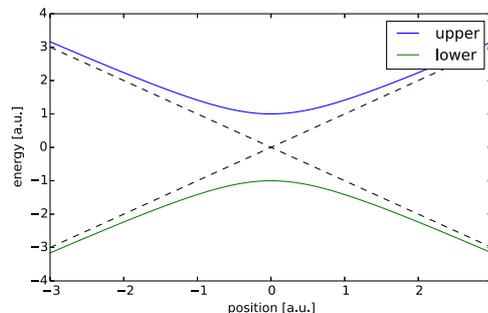
$$E_{1,2} = \frac{\varepsilon_1 + \varepsilon_2}{2} \pm \sqrt{\frac{\delta_{12}^2}{4} + |V|^2}, \quad \delta_{12} = \varepsilon_1 - \varepsilon_2 \quad (2.2)$$

(1) Make a plot of the eigenvalues and identify the regimes where the energy shifts  $E_a - \varepsilon_a$  ( $a = 1, 2$ ) are linear and quadratic in the perturbation  $V$ .

(2) In some cases, the coupling matrix elements  $V$  are complex. Make the following parametrisation of the eigenstate with energy  $E_1$

$$|\Psi_1\rangle = \cos(\theta/2)|1\rangle + e^{i\phi} \sin(\theta/2)|2\rangle \quad (2.3)$$

and find formulas that give  $\theta$  and  $\phi$ . ( $|1\rangle$  and  $|2\rangle$  are the basis states in which the matrix (2.2) is represented.) The angles  $\theta$  and  $\phi$  can be interpreted as spherical coordinates for a point on a sphere (‘Bloch vector’). Discuss how this point is moving as  $V$  changes in magnitude and phase.



(3) In the avoided crossing shown in the figure, the non-perturbed energies (dashed) vary linearly as a function of some control parameter. This can be the position  $z$  of

a particle (e.g., the inter-nuclear distance), and in that case  $\delta_{12} = -zF$  ( $F > 0$ ). At  $z = 0$ , the states  $|1\rangle$  and  $|2\rangle$  are degenerate: ‘the levels cross’. Due to the coupling  $V$ , the ‘degeneracy is lifted’. Landau and Zener have solved the time-dependent quantum dynamics when the particle is moving through the crossing with a fixed velocity  $v$ . They found that the following formula

$$p = \exp\left(-\frac{\pi |V|^2}{2 \hbar v F}\right) \quad (2.4)$$

describes a characteristic narrative: if the particle starts in the basis state  $|1\rangle$  (for  $z \rightarrow -\infty$ ), it ends on the other side in the same state  $|1\rangle$  with probability  $p$ . Or was it the other way round: if the particle starts in the upper eigenstate  $|\Psi_1\rangle$ , it ends on the other side in the upper eigenstate with probability  $p$ ? Discuss the limiting cases  $V \rightarrow 0$  and  $v \rightarrow 0$  to find out which case is the correct one.

Clarence Zener, ‘Non-adiabatic crossing of energy levels’, *Proc. R. Soc. London A* **137** (1932) 696 and L. D. Landau, *Phys. Z. USSR* (1932). See also Curt Wittig, ‘The Landau–Zener Formula’, *J. Phys. Chem. B* **109** (2005) 8428.

### Problem 2.2 – Rydberg state lifetimes (6 points)

With the Python script on the Moodle, you are invited to answer the following question: what is the lifetime of a Rydberg level like  $np$  with  $n \geq 10$ ? Into what states can this level decay? Which are the dominant ‘decay channels’?

(1) Make a sketch of the energy level  $np$  (choose hydrogen or some alkali atom) and connect it with lines to the ‘allowed’ lower states (recall the selection rules).

(2) The decay rate from  $np \rightarrow n'\ell'$  is proportional to

$$\gamma(np \rightarrow n'\ell') \sim |\langle n\text{p} || \hat{r} || n'\ell' \rangle|^2 (\varepsilon_{n\text{p}} - \varepsilon_{n'\ell'})^3 \quad (2.5)$$

where  $\langle n\text{p} || \hat{r} || n'\ell' \rangle$  is the matrix element of the radial distance operator (it depends *only* on the radial wave functions). Look up the energies of the lower states (you need quantum defects for the alkalis) and compute the matrix elements with the Python script. Plot your results as a function of  $n'$ .

### Problem 2.3 – Fluorescent or Förster resonant energy transfer (FRET) (4 points)

Consider a pair of atoms, one in the excited state ( $A^*$ ), another one in the ground state ( $B$ ). FRET is the process where atom  $A^*$  transfers its energy to atom  $B$  without emitting a photon. As a ‘chemical reaction’:



With the following model, you can compute the reaction rate.

(1) The transition  $A^* \rightarrow A$  is accompanied by an oscillating dipole moment  $\mathbf{d}_A e^{-i\omega_A t}$ . Compute the corresponding electric field  $\mathbf{E}(\mathbf{r}, t)$ , assuming that the distance between  $\mathbf{r}$  and atom  $A^*$  is much shorter than the wavelength. Find an expression for the ‘intensity’  $|\mathbf{E}(\mathbf{r}_B, t)|^2 \sim 1/R^6$  where  $R = |\mathbf{r}_B - \mathbf{r}_A|$ .

(2) Atom  $B$  absorbs this light field (and gets excited) with a rate given by the following expression

$$\gamma(A^* \rightarrow B) = \frac{\text{Im } \alpha_B(\omega_A)}{\hbar} |\mathbf{E}(\mathbf{r}_B, t)|^2 \quad (2.7)$$

Use the near-resonant approximation (1.5) for the polarisability in Problem 1.3 to find an estimate for  $\gamma(A^* \rightarrow B)$ . This process is used in chemistry and biology as a ‘ruler’ to determine the distance between two ‘chromophores’: measure the characteristic time  $1/\gamma(A^* \rightarrow B)$  for excitation transfer and infer the distance  $R$ .

**Problem 2.4** – Find a Förster resonance (5 points)

A Förster resonance appears when the sum of the energies of two Rydberg levels,  $E_n + E_{n'}$  is equal to twice the energy  $2E_{n^*}$  of another Rydberg level, provided the dipole selection rule allows for the transitions  $n \leftrightarrow n^*$  and  $n' \leftrightarrow n^*$ . (Here,  $n$  collects all relevant quantum numbers.) Then the states involved in the ‘chemical reaction’

$$n^* + n^* \leftrightarrow n + n' \quad (2.8)$$

have the same energy, and the dipole-dipole interaction gives a very strong energy shift.

(1) Check from the selection rules that the levels  $17s + 18d$  and  $17p$  may form a Förster resonance, while  $23f + 16d$  and  $21p$  may not.

(2) Find a Förster resonance by using the quantum defects in the Rb-85 atom. They can be parametrised by the following formula that goes back to Rydberg and Ritz

$$\delta_{ln,j} = a_0 + \frac{a_2}{(n - a_0)^2} + \frac{a_4}{(n - a_0)^4} + \dots \quad (2.9)$$

where the numbers  $a_0, a_2, \dots$  depend on the quantum numbers  $n, l, j$  (this is not shown for simplicity). They provide the energy dependence of the quantum defect, with the lowest approximation given by  $a_0$ . (This is *not* the Bohr radius in this problem!) The numbers are listed in the following table for the Rb-85 atom (taken from the document ‘Rydberg atoms in ten pages’ on the Moodle).

level	$a_0$	$a_2$	$a_4$	$a_6$	$a_8$
$(n \geq 14) s_{1/2}$	3.131 180 4(10)	0.1784(6)	-1.8		
$(n \geq 14) p_{1/2}$	2.654 884 9(10)	0.2900(6)	-7.9040	116.4373	-405.907
$(n \geq 14) p_{3/2}$	2.641 673 7(10)	0.2950(7)	-0.974 95	14.6001	-44.7265
$(n \geq 4) d_{3/2}$	1.348 091 71(40)	-0.602 86(26)	-1.505 17	-2.4206	19.736
$(n \geq 4) d_{5/2}$	1.346 465 72(30)	-0.596 00(18)	-1.505 17	-2.4206	19.736
$(n \geq 4) f$	0.016 312	-0.064 007	-0.360 05	3.2390	

Quantum defects for  $^{85}\text{Rb}$ , with expansion parameters in the Rydberg-Ritz formula (2.9). The data have been compiled by C.-J. Lorenzen and K. Niemax, ‘Quantum defects of the  $n^2P_{1/2,3/2}$  levels in  $^{39}\text{K I}$  and  $^{85}\text{Rb I}$ ’, Phys. Scr. 27 (1983) 300 and W. Li, I. Mourachko, M. Noel, and T. Gallagher, ‘Millimeter-wave spectroscopy of cold Rb Rydberg atoms in a magneto-optical trap: Quantum defects of the  $ns$ ,  $np$ , and  $nd$  series’ Phys. Rev. A 67 (2003) 052502. One may neglect the fine structure splitting of the  $f$  levels at this precision.

A possible solution with an energy difference  $\approx 7 \text{ MHz} \approx 2.3 \times 10^{-4} \text{ cm}^{-1}$  occurs for  $n = 56f_{5/2}$ ,  $n' = 60p_{1/2}$ , and  $n^* = 58d_{3/2}$ .