

Final Exam

The Cornell Code of Academic Integrity is in effect for this take-home exam as it is for all other components of this course. In addition, you are required to limit yourself to the following materials when completing the exam:

- documents on the course web site (homework assignments and solutions, notes)
- your own class notes and homework solutions
- a calculator

A computer may only be used to access the course web site. Other uses of a computer, as in evaluating mathematical expressions with Mathematica, is not permitted.

The exam has three problems of equal value. It is important to show your work. Any additional paper used for your calculations should be attached to your exam.

You are not required, or even encouraged, to complete the exam in one sitting. Your completed exam is due in the Physics office by 4 pm Thursday, December 6. To help us in returning the graded exams, please indicate your graduate department or undergraduate status.

Good Luck!

1. This problem examines the states of electrons bound to a **spherical droplet** of liquid helium (near the limit of zero temperature). The spherical shape of the droplet comes about from surface tension forces. In the limit of very large droplet radius R — the “flat-earth” approximation — the electron bound states are essentially the same as the bound states for the flat helium surface considered in homework assignment 5.

(a) By considering **length scales**, write down a criterion for the validity of the flat-earth approximation involving only the droplet radius R , the Bohr radius a_B , and the dimensionless parameter $\lambda \approx 0.0069$ that appears in the image charge potential: $V(z) = -\lambda e^2/z$ (z is distance above helium surface).

For the rest of this problem assume the flat-earth approximation is good.

(b) The electron bound states are rather fragile. In fact, the droplet is unable to bind two electrons unless its size exceeds a certain radius R_2 . Derive a **rough estimate** of R_2 and express your answer in terms of a_B and λ .

(c) Returning to the single bound electron, compare the energy scales of radial and angular excitations. For the radial scale use the definition $\Delta E_{\text{rad}} = E_{n=1} - E_{n=0}$, where n refers to the number of nodes in the radial wavefunction; for the angular scale use $\Delta E_{\text{ang}} = E_{l=1} - E_{l=0}$, where l is the standard total angular momentum quantum number.

You should find $\Delta E_{\text{rad}} \gg \Delta E_{\text{ang}}$. **For the rest of this problem you should assume that all electrons are in the $n = 0$ state and that only angular excitations are relevant.**

(d) Argue why the wavefunction for two electrons bound to the droplet will always be highly correlated — that is, the independent electron approximation that works for atoms never applies. **No detailed calculation please!**

You're probably thinking that you might get by on this problem without doing any real calculation! Sorry: here is where the fun begins. The **one-electron** droplet first becomes interesting when it is in an excited angular momentum state. As you saw in homework assignment 6 — which featured an inside-out version of this problem — the spherical shape can become unstable by the **Jahn-Teller mechanism**.

The quantum fairy has kindly provided you with the Hamiltonian $H = H_0 + H_{\text{int}}$ for analyzing this effect:

$$H_0 = \frac{1}{2mR^2}L^2 \qquad H_{\text{int}} = -2\lambda^3 \left(\frac{e^2}{a_B} \right) \frac{\delta R(\theta, \phi)}{a_B}.$$

Here L^2 is the standard total angular momentum operator and $\delta R(\theta, \phi)$ is the droplet surface perturbation.

(e) Calculate the energy shifts of the three $l = 1$ states for the (volume preserving) quadrupolar deformation $\delta R = \epsilon P_2(\cos \theta)$ to lowest order in ϵ and decide if the energy degeneracy is resolved for a prolate ($\epsilon > 0$) or oblate ($\epsilon < 0$) deformation.

2. This problem concerns a proposal for aligning macromolecules, where the torque has a quantum mechanical origin. The molecule is modeled as a charge-neutral rigid body which, through the magic of bio-engineering (or nature), has one quasi-free electron that can tunnel between two distant chemical sites on the molecule.

It is convenient to describe rotations of the molecule with the origin chosen to be the midpoint of the line that connects the two chemical sites. You should therefore consider an electron that tunnels between positions $\pm\mathbf{R}$, where \mathbf{R} is a fixed length vector that rotates with the molecule. If we now apply a (uniform) DC electric field \mathcal{E} to the molecule, the Hamiltonian for the electron two-level system is

$$H = \begin{pmatrix} E_1 + e\mathcal{E} \cdot \mathbf{R} & -t \\ -t & E_2 - e\mathcal{E} \cdot \mathbf{R} \end{pmatrix} .$$

Here $t > 0$ is the tunneling energy and E_1, E_2 are the electron energies at the two sites (for $\mathcal{E} = 0$). Since the chemistry at the two sites is in general different, $E_1 > E_2$.

In answering the questions below, please use the frequency equivalents of the various energies:

$$\omega_t = t/\hbar \quad \omega_{12} = (E_1 - E_2)/\hbar \quad \omega_{\mathcal{E}} = e|\mathcal{E}||\mathbf{R}|/\hbar .$$

The orientation of the molecule shows up as the angle θ between the fixed electric field \mathcal{E} and the variable vector \mathbf{R} .

(a) Find the energies of this two-level system and sketch them as a function of θ for $0 \leq \theta \leq \pi$. Your sketch should be for the case of **very weak tunneling** (small ω_t) and sufficiently strong field: $2\omega_{\mathcal{E}} > \omega_{12}$.

For small angular velocities of the molecule — in the adiabatic limit — the upper and lower energy curves you found in (a) define two potential energy functions, $V_+(\theta)$ and $V_-(\theta)$.

(b) **Describe in words** the physics that applies at the stable equilibrium point, $\theta = 0$, of the lower potential, $V_-(\theta)$. The stiffness is defined by the curvature of the potential: $\kappa_- = V_-''(0)$. **Also**, find the limit of κ_- for weak tunneling.

(c) When repeating the analysis in (b) for the upper potential $V_+(\theta)$, there is the interesting difference that the location of the stable equilibrium point can be varied by changing the strength of the electric field! To avoid mathematical complications, perform the analysis for the special case $E_1 = E_2$ (where the stable θ is easy to locate). **Compare the two stiffnesses, κ_+ and κ_- , in the limit of weak tunneling.**

It should seem from your analysis so far that a tunable, very stiff angular trapping is achieved simply by exciting the electron to the upper energy level. But as you know, the “no free lunch” theorem applies even to quantum lunches. In this case it is the adiabatic principle that must pay the bill.

(d) Reconsider your analysis in (c), also for the special case $E_1 = E_2$, but with the molecule rotating with uniform angular velocity $\Omega = \dot{\theta}$ through the stable equilibrium point. Interpret this scenario as an instance of the Landau-Zener problem and extract the corresponding LZ parameters α and β (express them in terms of the frequencies defined for this problem). Finally, write down a criterion involving frequencies that must hold for the trapping potential $V_+(\theta)$ to actually function as a trap. What goes wrong when the criterion fails?

3. A student in the McEuen lab has produced a beam of singly-charged carbon nanotubes of very uniform length L . These are semiconducting tubes, so that the electronic dynamics are confined to the single extra electron. Since the tube's length is much greater than its diameter, an excellent model of this electron's dynamics is that of a particle confined to a one dimensional box¹ of length L . The only thing we cannot know without further analysis (solid state physics) is the effective mass of the electron; in this problem you should use the standard free-space mass.

The student is considering an experiment where the nanotubes' electrons are excited to the first (particle-in-a-box) state above the ground state and the radiative decay rate is measured. She has approached you because she knows Physics 572 has taught you how to calculate such things.

(a) As a preliminary step, write down a condition on the tube length for the dipole approximation to be valid. Your condition should be expressed in terms of a_B , L , and α (fine structure constant). Verify that the dipole approximation is sound.

¹The infinite potential at the ends of the "box" is just a statement of the fact that the electron energy would become very large were it to wander beyond the ends of the tube.

(b) Calculate the radiative decay rate Γ summed over all final photon states (polarization and momentum) using the Golden Rule, the mode expansion of the radiation operator,

$$\mathbf{A} = \sqrt{\frac{2\pi\hbar c^2}{\omega_k V}} \boldsymbol{\epsilon} \left(e^{i\mathbf{k}\cdot\mathbf{r}} \mathbf{a} + e^{-i\mathbf{k}\cdot\mathbf{r}} \mathbf{a}^\dagger \right) ,$$

and the interaction (for single-photon processes),

$$H_{\text{int}} = \frac{e}{mc} \mathbf{A} \cdot \mathbf{p} .$$

Express your answer in terms of a_B , L , α and the frequency of the transition, ω .