Lunds Universitet
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Spring 2016

Exercises to Quantum Mechanics FYSN17/FMFN01, Week 5

Homework to be handed in on February 23

Exercise 1: *Energy shifts of atoms in magnetic fields*

Aim: Understanding the Hamilton operator in a magnetic field

Let $\mathbf{B}$ be a constant magnetic field. Consider the Hamiltonian

$$\hat{H} = \frac{1}{2m}\left(\hat{\mathbf{p}} - q\mathbf{A}(\hat{\mathbf{r}})\right)^2 + q\phi(\hat{\mathbf{r}})\,.$$

It can be rewritten:

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta + q\phi(\hat{\mathbf{r}}) - \frac{q}{2m}B\hat{L}_z + \frac{q^2}{8m}B^2(\hat{x}^2 + \hat{y}^2)$$

where it is assumed that $\mathbf{B} = B\mathbf{e}_z$. Estimate the size of the last two terms for an electron in an atom if the field has the strength of 10 T.

Exercise 2 (Homework): *Electron in inversion layer with magnetic field*

Aim: Quantifying the energy splitting due to B; addressing a common task in solid state physics

In solid state physics one can establish two-dimensional systems at the interface of a semiconductor. Consider a single electron confined to such a layer, so that it can only move freely in x and y-direction. A magnetic field points in z-direction, perpendicular to the interface.

a) Construct the Hamiltonian for this particle.

b) Find the energy spectrum for a magnetic field of 5 T. Use the effective mass $m_{eff} = 0.067m_e$ which is appropriate for a conduction band electron in GaAs.

Exercise 3: *First-order correction of energy*

Aim: Learning how to apply the formalism of stationary perturbation theory

Consider a one-dimensional harmonic oscillator with frequency ω which is perturbed by $\hat{H}_p = \lambda e^{-\alpha\hat{x}^2}$. Calculate the first order correction to the ground state energy and to the energy of the first excited state.

Exercise 4: *Perturbation of two dimensional oscillator*

Aim: Getting familiar with degeneracies in perturbation theory

A two dimensional harmonic oscillator is perturbed by $\hat{H}_p = \lambda m\omega^2\hat{x}\hat{y}$.

a) Use first order perturbation theory to calculate the energy shift for the ground state and the first excited state.

b) Calculate the ground state energy to second order.

c) Solve the full problem exactly and compare the result with the approximation you obtained in a) and b).

See other side

Exercise 5 (Homework): *Molecule vibration*

Aim: Applying stationary perturbation theory; understanding basic features of molecular vibrations

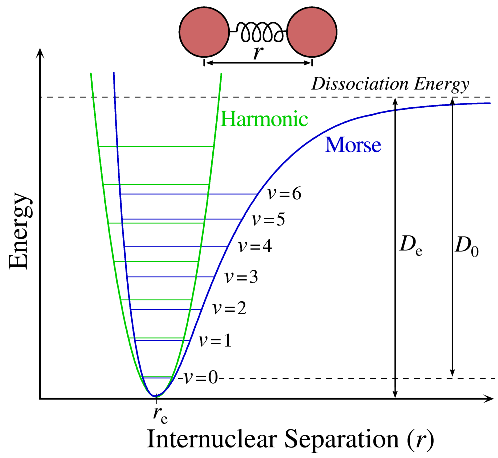
A diatomic molecule can rotate and vibrate. To describe vibrations one can use a potential as in the figure where r denotes the distance between the nuclei. As a first approximation we may consider this as a one-dimensional problem (in x direction) with the parabolic potential

$$V_0(x) = \frac{1}{2}m\omega^2 x^2 - D_e$$

where m is the reduced mass for the system of both atoms and x is the deviation from the equilibrium position r_e.

For higher excitation energies the potential deviates from the parabolic approximation and one can add a third order term:

$$\hat{H}_p = \alpha\hbar\omega\left(\frac{2m\omega}{\hbar}\right)^{\frac{3}{2}}\hat{x}^3.$$



Graphical depiction of the Morse potential with a harmonic potential for comparison, CC-BY-SA Mark Somoza (2006)

We shall in this exercise study the effect of $\hat{H}_p$ as a perturbation.

a) Express $\hat{H}_p$ in terms of a and $a^\dagger$ of the harmonic oscillator corresponding to $V_0(x)$.

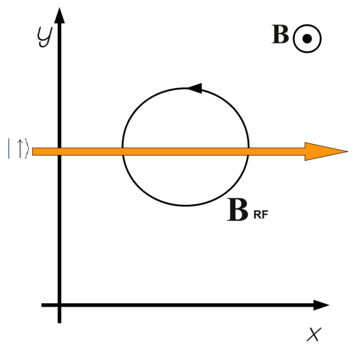
b) Determine all matrix elements $\langle m|\hat{H}_p|n\rangle$ between unperturbed harmonic oscillator states.

c) Consider the second excited state. Calculate the change in energy in second order perturbation theory and its state in the first order.

d) Calculate $\langle x\rangle$ with the new state and discuss its relation to thermal expansion of a crystal

Exercise 6: *Rabi's resonance experiment*

Aim: Getting familiar with an important feature of general two-level systems



We will in this example discuss Rabi's famous spin resonance experiment. The particles (say neutrons) enter the apparatus from the left with a selected spin. A magnet gives a homogeneous magnetic field in the $z-$direction, $\mathbf{B}_0 = B_0\mathbf{e}_z$. In the area where this magnetic field is, there is also a so called RF-loop which creates an oscillating field $\mathbf{B}_{RF} = B_1[\cos(\omega t)\mathbf{e}_x + \sin(\omega t)\mathbf{e}_y]$. When the particles enter the field $\mathbf{B} = \mathbf{B}_0 + \mathbf{B}_{RF}$ from the left side they are in the spin state $|\uparrow\rangle$. Only those particles that changed their spin directions (flips) will be detected on the right hand side by an appropriate detector.

a) The magnetic moment of the particles is given by $\hat{\mu} = \gamma\hat{\mathbf{S}}$. Write down the time-dependent Schrödinger equation valid in the magnetic field $\mathbf{B}$ in spinor representation, i.e. for the component $a(t)$, $b(t)$ of the time-dependent state $|\Psi\rangle(t) = a(t)|\uparrow\rangle + b(t)|\downarrow\rangle$.

b) With the initial condition $|\Psi\rangle(0) = |\uparrow\rangle$ one finds (after tedious but straightforward algebra – not required)

$$a(t) = \left[\cos(\Omega t) + \mathrm{i}\frac{\gamma B_0 + \omega}{2\Omega}\sin(\Omega t)\right]\mathrm{e}^{-\mathrm{i}\omega t/2} \quad \text{and} \quad b(t) = \mathrm{i}\frac{\gamma B_1}{2\Omega}\sin(\Omega t)\mathrm{e}^{\mathrm{i}\omega t/2}$$

with the Rabi frequency $\Omega = \sqrt{\gamma^2 B_1^2 + (\gamma B_0 + \omega)^2}/2$. For which field B_0 can the probability to observe a spin flip be equal to one? How does the probability evolve in time?

c) In an experiment with neutrons one observes the maximal signal at $B_0 = 0.54$T for a frequency of $\omega_{resonance} = 9.92 \times 10^7$ rad/s. Determine γ and deduce the Landé factor g_n of the neutron.