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Answers: ADVANCED QUANTUM PHYSICS 2014

(a) Classical limits when

$$E_0 = \frac{1}{2}\hbar\omega = \frac{1}{2}m\omega^2 x^2$$
$$x = \pm\sqrt{\frac{\hbar}{m\omega}}$$

Probability, P, that particle is outside the classical limits is

[1]

$$P = \frac{\int_{\sqrt{\frac{\hbar}{m\omega}}}^{\infty} \exp\{-\frac{m\omega}{\hbar}x^2\} dx}{\int_{0}^{\infty} \exp\{-\frac{m\omega}{\hbar}x^2\} dx}$$

Substitute
$$y = \sqrt{\frac{m\omega}{\hbar}}x$$
, $dy = \sqrt{\frac{m\omega}{\hbar}}dx$, and $(x = 0, y = 0)$, $(x = \infty, y = \infty)$ and $x = \sqrt{\frac{\hbar}{m\omega}}$, $y = 1$ to obtain

$$P = \frac{\int_{1}^{\infty} \exp\{-y^2\} dy}{\int_{0}^{\infty} \exp\{-y^2\} dy}$$
$$= 1 - 0.843$$
$$= 0.16$$

[2]

(b) From first-order perturbation theory

$$c_{i\to f} = -\frac{i}{\hbar} \int_0^t \langle \psi_1 | \widehat{H}(t') | \psi_2 \rangle \exp\{i \frac{(E_1 - E_2)}{\hbar} t'\} dt'$$

[1]

Represent 2 states by matrix $\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$.

Then

$$c_{i \to f} = -\frac{\iota}{\hbar} \int_0^t \left(\psi_1 \quad 0 \right) \left(\begin{matrix} 0 & U \\ U & 0 \end{matrix} \right) \delta(t') \left(\begin{matrix} 0 \\ \psi_2 \end{matrix} \right) \exp\{\iota \frac{(E_1 - E_2)}{\hbar} t'\} dt'$$

$$= -\frac{\iota}{\hbar} \int_0^t \left(\psi_1 \quad 0 \right) \left(\begin{matrix} U \psi_2 \delta(t') \\ 0 \end{matrix} \right) \exp\{\iota \frac{(E_1 - E_2)}{\hbar} t'\} dt'$$

$$= -\frac{\iota}{\hbar} U \psi_1^* \psi_2 \int_0^t \delta(t') \exp\{\iota \frac{(E_1 - E_2)}{\hbar} t'\} dt'$$

$$= -\frac{\iota}{\hbar} U \psi_1^* \psi_2 \exp\{\iota \frac{(E_1 - E_2)}{\hbar} t\}$$

Therefore, probability $P_{i \to f}$ is given by

$$P_{i \to f} = |c_{i \to f}|^{2}$$

$$= \left(-\frac{\iota}{\hbar}U\psi_{1}^{*}\psi_{2}\exp\left\{i\frac{(E_{1} - E_{2})}{\hbar}t\right\}\right)\left(\frac{\iota}{\hbar}U\psi_{1}\psi_{2}^{*}\exp\left\{-i\frac{(E_{1} - E_{2})}{\hbar}t\right\}\right)$$

$$= \left(\frac{U}{\hbar}\right)^{2}$$

[1]

[1]

[2]

[2]

(c) 2 electrons in p^2 configuration.

$$s_1 = \frac{1}{2}, s_2 = \frac{1}{2} \Rightarrow S = 0, 1$$

 $l_1 = 1, l_2 = 1 \Rightarrow L = 0, 1, 2$

Using notation ${}^{2S+1}L_J$, all possible states are 1S_0 , 1P_1 , 1D_2 , 3S_1 , ${}^3P_{0,1,2}$, ${}^3D_{1,2,3}$. However, 1P_1 , 3S_1 , ${}^3D_{1,2,3}$ are not allowed due to identicle particle symmetry.

Therefore allowed states are ${}^{1}S_{0}$, ${}^{1}D_{2}$, ${}^{3}P_{0,1,2}$.

Hund's rules states that the level with the highest S and then the lowest J, for a sub-shell less than half full, has the lowest energy. Therefore, the ground state is ${}^{3}P_{0}$.

2 (a) Bookwork: Postulates of Quantum Mechanics

- •The state of a QM system is specified by the wavefunction $\Psi(\mathbf{r},t)$. The wavefunction must be single-valued, continuous and finite.
- •The probability of finding a particle in the volume element $d^3 \mathbf{r}$ at time t is $|\Psi(\mathbf{r},t)|^2 d^3 \mathbf{r}$. For a single particle, the net probability of finding it at some point in space must be unity leading to the normalization condition $\int_{-\infty}^{+\infty} |\Psi(\mathbf{r},t)|^2 d^3 \mathbf{r} = 1.$
- •To every observable in classical mechanics there corresponds a linear, Hermitian operator in QM. If the system is in an eignstate of the linear, Hermitian operator \widehat{A} with eigenvalue a, then any measurement of the quantity A will yield a. [2]
- •If a system is in a state described by a normalised wavefunction Ψ , then the average value of the observable corresponding to the operator \widehat{A} is $\langle A \rangle = \int_{-\infty}^{+\infty} \Psi^* \widehat{A} \Psi d^3 \mathbf{r}$. A linear, Hermitian operator leads to real expectation values.
- •An arbitrary state, describing the same system, can be expanded in the complete set of eigenfunctions of the operator \widehat{A} ($\widehat{A}\Psi_i = a_i\Psi_i$) as $\chi = \sum_i^n c_i\Psi_i$, where n may go to infinity. In this case, the probability of obtaining the result a_i from the measurement of \widehat{A} is $P(a_i) = |\langle \Psi_i | \chi \rangle|^2 = |c_i|^2$ and the expectation value is $\langle A \rangle = \sum_i a_i |c_i|^2$. [2]

- •A measurement of the state χ , which leads to the eigenvalue a_i , causes the wavefunction to "collapse" into the corresponding eigenstate Ψ_i .
- [2]
- •The wavefunction or state function os a system evolves in time according to the time-dependent SE $i\hbar \frac{\partial \Psi}{\partial t} = \widehat{H}\Psi(\mathbf{r},t)$, where \widehat{H} is the Hamiltonian. If χ is an eigenstate of \widehat{H} , it follows that $\Psi(\mathbf{r},t) = \Psi(\mathbf{r},0) \exp{-iEt/\hbar}$. [2]
- (b) Bookwork: Central field approximation and the Hartree method
 - •Hamiltonian for a multi-electron atom can be written as

$$\widehat{H} = \sum_{i} \left[-\frac{\hbar^2}{2m} \nabla_i^2 - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r_i} \right] + \sum_{i < j} \frac{1}{4\pi\epsilon_0} \frac{e^2}{r_{ij}}$$

where the last term represents the Coulomb interaction between constituent electrons.

[2]

[1]

- •The central-field approximation is based upon the observation that the electron interaction term contains a large central (spherically symmetric) component arising from the "core electrons". A closed shell has an electron density distributions that is isotropic.
- •Develop a perturbative scheme using $\widehat{H} = \widehat{H}_0 + \widehat{H}_1$, where

$$\widehat{H}_0 = \sum_i \left[-\frac{\hbar^2}{2m} \nabla_i^2 - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r_i} + U_i(r_i) \right]$$

and

$$\widehat{H}_1 = \sum_{i < j} \frac{1}{4\pi\epsilon_0} \frac{e^2}{r_{ij}} - \sum_i U_i(r_i).$$

The one-electron potential $U_i(r_i)$, which is assumed central incorporates the "average" effect of the other electrons. \widehat{H}_0 is separable into a sum of terms for each electron, so that the overall wavefunction can be factorized into components for each electron.

Basic idea is to solve the SE for \widehat{H}_0 and then to treat \widehat{H}_1 as a perturbation. [2]

- •The potentials $U_i(r_i)$ can be estimated using the "self-consistent field method"; a variational approach due to Hartree.
- •If electrons are considered independent, the wavefunction can be factorized

$$\Psi(\{\boldsymbol{r}_i\}) = \Psi_{i1}(\boldsymbol{r}_1)\Psi_{i2}(\boldsymbol{r}_2)\cdots\Psi_{iN}(\boldsymbol{r}_N)$$

with $i_k \equiv (n\ell m_\ell m_s)_k$. [1]

•Using this wavefunction as a trial state, the variational energy is given by

$$E = \langle \Psi | \widehat{H} | \Psi \rangle = \sum_{i} \int d^3 r \psi_i^* \left(-\frac{\hbar^2}{2m} \nabla^2 - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r} \right) \psi_i + \frac{1}{4\pi\epsilon_0} \sum_{i < j} \int d^3 r \int d^3 r' \psi_i^*(\mathbf{r}) \psi_j^*(\mathbf{r}') \frac{1}{|\mathbf{r}|^2} \left(-\frac{\hbar^2}{2m} \nabla^2 - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r} \right) \psi_i + \frac{1}{4\pi\epsilon_0} \sum_{i < j} \int d^3 r' \psi_i^*(\mathbf{r}) \psi_j^*(\mathbf{r}') \frac{1}{|\mathbf{r}|^2} \left(-\frac{\hbar^2}{2m} \nabla^2 - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r} \right) \psi_i + \frac{1}{4\pi\epsilon_0} \sum_{i < j} \int d^3 r' \psi_i^*(\mathbf{r}) \psi_j^*(\mathbf{r}') \frac{1}{|\mathbf{r}|^2} \left(-\frac{\hbar^2}{2m} \nabla^2 - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r} \right) \psi_i + \frac{1}{4\pi\epsilon_0} \sum_{i < j} \int d^3 r' \psi_i^*(\mathbf{r}) \psi_j^*(\mathbf{r}') \frac{1}{|\mathbf{r}|^2} \left(-\frac{\hbar^2}{2m} \nabla^2 - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r} \right) \psi_i + \frac{1}{4\pi\epsilon_0} \sum_{i < j} \int d^3 r' \psi_i^*(\mathbf{r}) \psi_j^*(\mathbf{r}') \frac{1}{|\mathbf{r}|^2} \left(-\frac{\hbar^2}{2m} \nabla^2 - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r} \right) \psi_i + \frac{1}{4\pi\epsilon_0} \sum_{i < j} \int d^3 r' \psi_i^*(\mathbf{r}) \psi_j^*(\mathbf{r}') \frac{1}{|\mathbf{r}|^2} \left(-\frac{\hbar^2}{2m} \nabla^2 - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r} \right) \psi_i + \frac{1}{4\pi\epsilon_0} \sum_{i < j} \int d^3 r' \psi_i^*(\mathbf{r}) \psi_j^*(\mathbf{r}') \frac{1}{|\mathbf{r}|^2} \left(-\frac{\hbar^2}{2m} \nabla^2 - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r} \right) \psi_i + \frac{1}{4\pi\epsilon_0} \sum_{i < j < j} \int d^3 r' \psi_i^*(\mathbf{r}) \psi_j^*(\mathbf{r}') \frac{1}{|\mathbf{r}|^2} \left(-\frac{\hbar^2}{2m} \nabla^2 - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r} \right) \psi_i + \frac{1}{4\pi\epsilon_0} \sum_{i < j < j < j} \int d^3 r' \psi_i^*(\mathbf{r}) \psi_i^*(\mathbf{r}') \psi_i^*(\mathbf{r$$

[2]

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• Variational principle - vary $E[\psi_i]$ wrt complex wavefunction ψ_i (normalised). Normalization can be imposed using Lagrange multipliers. Following the variation, get the Hartree equations:

$$\left(-\frac{\hbar^2}{2m}\nabla^2 - \frac{1}{4\pi\epsilon_0}\frac{Ze^2}{r}\right)\psi_i + \frac{1}{4\pi\epsilon_0}\sum_{j\neq i}\int d^3r'|\psi_j(\boldsymbol{r}')|^2\frac{e^2}{|\boldsymbol{r}-\boldsymbol{r}'|}\psi_i(\boldsymbol{r}) = \epsilon_i\psi_i(\boldsymbol{r}).$$

The 3rd term represents the electrostatic potential experienced by the individual electrons.

[2]

•The set of possible trial functions that minimizes the energy are determined by the effective potential

$$U_i(\mathbf{r}) = \frac{1}{4\pi\epsilon_0} \sum_{j \neq i} \int d^3r' |\psi_j(\mathbf{r}')|^2 \frac{e^2}{|\mathbf{r} - \mathbf{r}'|}$$

[1]

•One electron energies are given by (multiply Hartree equations by $\psi_i^*(r)$ and integrate):

$$\epsilon_i = \int d^3r \psi_i^* \left(-\frac{\hbar^2}{2m} \nabla^2 - \frac{1}{4\pi\epsilon_0} \frac{Ze^2}{r} \right) \psi_i + \frac{1}{4\pi\epsilon_0} \sum_{i \neq i} \int d^3r' d^3r |\psi_j(\boldsymbol{r'})|^2 \frac{e^2}{|\boldsymbol{r} - \boldsymbol{r'}|} |\psi_i(\boldsymbol{r})|^2.$$

and the variational energy by

$$E = \sum_{i} \epsilon_{i} - \frac{1}{4\pi\epsilon_{0}} \sum_{i < j} \int d^{3}r' d^{3}r |\psi_{j}(\mathbf{r}')|^{2} \frac{e^{2}}{|\mathbf{r} - \mathbf{r}'|} |\psi_{i}(\mathbf{r})|^{2}.$$

[2]

(c) Bookwork: Properties and operation of lasers

Laser - light amplification by stimulated emission of radiation. Properties:

- •Monochromaticity (one atomic transition, spectral line width,Q of the cavity)
- •Coherence, including discussion of spatial (irregularities in optical phase) and temporal coherence (time duration over which beam is well-defined). Coherence length for various light sources.
- •Brightness (high power per unit area, energy in narrow spectrum of atomic transition, example)
- •Ultra-short pulse generation (time duration of pulses, mode-locking, examples)

[5]

Operating principles (diagram,pumping energy, positive optical feedback, resonant cavity, mirrors, losses: useful(output coupling) and useless(absorption, scattering, refelctivity))

[4]

Gain mechanism (population inversion, rate equations and laser threshold condition)

[4]

3 Bookwork:

The spin raising and lowering operators are $\hat{\sigma}_{\pm} = \hat{\sigma}_{x} \pm i \hat{\sigma}_{y}$. Therefore,

$$\widehat{\sigma}_{+} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \iota \begin{pmatrix} 0 & -\iota \\ \iota & 0 \end{pmatrix} = \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix}$$

$$\widehat{\sigma}_{-} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \iota \begin{pmatrix} 0 & -\iota \\ \iota & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix}$$

[4]

$$\widehat{\sigma}_x = \frac{1}{2} (\widehat{\sigma}_+ + \widehat{\sigma}_-)$$

$$\widehat{\sigma}_y = \frac{1}{2i} (\widehat{\sigma}_+ - \widehat{\sigma}_-)$$

and

$$\begin{split} \widehat{\sigma}_{1} \cdot \widehat{\sigma}_{2} &= \widehat{\sigma}_{1x} \widehat{\sigma}_{2x} + \widehat{\sigma}_{1y} \widehat{\sigma}_{2y} + \widehat{\sigma}_{1z} \widehat{\sigma}_{2z} \\ &= \frac{1}{4} \left(\widehat{\sigma}_{1+} + \widehat{\sigma}_{1-} \right) \left(\widehat{\sigma}_{2+} + \widehat{\sigma}_{2-} \right) - \frac{1}{4} \left(\widehat{\sigma}_{1+} - \widehat{\sigma}_{1-} \right) \left(\widehat{\sigma}_{2+} - \widehat{\sigma}_{2-} \right) + \widehat{\sigma}_{1z} \widehat{\sigma}_{2z} \\ &= \frac{1}{2} \left(\widehat{\sigma}_{1+} \widehat{\sigma}_{2-} + \widehat{\sigma}_{1-} \widehat{\sigma}_{2+} \right) + \widehat{\sigma}_{1z} \widehat{\sigma}_{2z} \end{split}$$

In matrix form

$$\widehat{\sigma}_{+} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \iota \begin{pmatrix} 0 & -\iota \\ \iota & 0 \end{pmatrix} = \begin{pmatrix} 0 & 2 \\ 0 & 0 \end{pmatrix}$$

$$\widehat{\sigma}_{-} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} - \iota \begin{pmatrix} 0 & -\iota \\ \iota & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 2 & 0 \end{pmatrix}$$

Hence,

$$\begin{aligned}
\widehat{\sigma}_{+} | \uparrow \rangle &= 0 = \widehat{\sigma}_{-} | \downarrow \rangle \\
\widehat{\sigma}_{-} | \uparrow \rangle &= 2 | \downarrow \rangle \\
\widehat{\sigma}_{+} | \downarrow \rangle &= 2 | \uparrow \rangle \\
\widehat{\sigma}_{z} | \uparrow \rangle &= | \uparrow \rangle \\
\widehat{\sigma}_{z} | \downarrow \rangle &= - | \downarrow \rangle
\end{aligned}$$

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and

$$\widehat{\sigma}_{1} \cdot \widehat{\sigma}_{2} | \uparrow_{1} \uparrow_{2} \rangle = | \uparrow_{1} \uparrow_{2} \rangle
\widehat{\sigma}_{1} \cdot \widehat{\sigma}_{2} | \downarrow_{1} \uparrow_{2} \rangle = 2 | \uparrow_{1} \downarrow_{2} \rangle - | \downarrow_{1} \uparrow_{2} \rangle
\widehat{\sigma}_{1} \cdot \widehat{\sigma}_{2} | \uparrow_{1} \downarrow_{2} \rangle = 2 | \downarrow_{1} \uparrow_{2} \rangle - | \uparrow_{1} \downarrow_{2} \rangle
\widehat{\sigma}_{1} \cdot \widehat{\sigma}_{2} | \downarrow_{1} \downarrow_{2} \rangle = | \downarrow_{1} \downarrow_{2} \rangle$$

Matrix elements of Hamiltonian are then given by

$$\begin{split} \widehat{H}|\uparrow_{1}\uparrow_{2}\rangle &= \frac{\Delta E}{4}|\uparrow_{1}\uparrow_{2}\rangle - \left(\frac{g_{1}\mu_{0}}{\hbar}\frac{\hbar}{2}|\uparrow_{1}\uparrow_{2}\rangle + \frac{g_{2}\mu_{0}}{\hbar}\frac{\hbar}{2}|\uparrow_{1}\uparrow_{2}\rangle\right)B\\ &= \left[\frac{\Delta E}{4} - (g_{1} + g_{2})\frac{\mu_{0}B}{2}\right]|\uparrow_{1}\uparrow_{2}\rangle\\ &= H_{11}|\uparrow_{1}\uparrow_{2}\rangle \end{split}$$

$$\begin{split} \widehat{H}|\downarrow_{1}\downarrow_{2}\rangle &= \frac{\varDelta E}{4}|\downarrow_{1}\downarrow_{2}\rangle + \left(\frac{g_{1}\mu_{0}}{\hbar}\frac{\hbar}{2}|\downarrow_{1}\downarrow_{2}\rangle + \frac{g_{2}\mu_{0}}{\hbar}\frac{\hbar}{2}|\downarrow_{1}\downarrow_{2}\rangle\right)B\\ &= \left[\frac{\varDelta E}{4} + (g_{1} + g_{2})\frac{\mu_{0}B}{2}\right]|\downarrow_{1}\downarrow_{2}\rangle\\ &= H_{44}|\downarrow_{1}\downarrow_{2}\rangle \end{split}$$

$$\widehat{H}|\downarrow_{1}\uparrow_{2}\rangle = \frac{\Delta E}{4} (2|\uparrow_{1}\downarrow_{2}\rangle - |\downarrow_{1}\uparrow_{2}\rangle) - \left(-\frac{g_{1}\mu_{0}}{\hbar}\frac{\hbar}{2}|\downarrow_{1}\uparrow_{2}\rangle + \frac{g_{2}\mu_{0}}{\hbar}\frac{\hbar}{2}|\downarrow_{1}\uparrow_{2}\rangle\right) B$$

$$= \frac{\Delta E}{2}|\uparrow_{1}\downarrow_{2}\rangle + \left[(g_{1} - g_{2})\frac{\mu_{0}B}{2} - \frac{\Delta E}{4}\right]|\downarrow_{1}\uparrow_{2}\rangle$$

$$= H_{23}|\uparrow_{1}\downarrow_{2}\rangle + H_{22}|\downarrow_{1}\uparrow_{2}\rangle$$

$$\begin{split} \widehat{H}|\uparrow_{1}\downarrow_{2}\rangle &= \frac{\varDelta E}{4} \left(2|\downarrow_{1}\uparrow_{2}\rangle - |\uparrow_{1}\downarrow_{2}\rangle\right) - \left(\frac{g_{1}\mu_{0}}{\hbar}\frac{\hbar}{2}|\uparrow_{1}\downarrow_{2}\rangle - \frac{g_{2}\mu_{0}}{\hbar}\frac{\hbar}{2}|\uparrow_{1}\downarrow_{2}\rangle\right) B \\ &= \frac{\varDelta E}{2}|\downarrow_{1}\uparrow_{2}\rangle + \left[-(g_{1}-g_{2})\frac{\mu_{0}B}{2} - \frac{\varDelta E}{4}\right]|\uparrow_{1}\downarrow_{2}\rangle \\ &= H_{32}|\downarrow_{1}\uparrow_{2}\rangle + H_{33}|\uparrow_{1}\downarrow_{2}\rangle \end{split}$$

Eigenvalues: we already have two diagonal elements, so that

$$E_{1} = \left[\frac{\Delta E}{4} - (g_{1} + g_{2})\frac{\mu_{0}B}{2}\right]$$

$$E_{2} = \left[\frac{\Delta E}{4} + (g_{1} + g_{2})\frac{\mu_{0}B}{2}\right]$$

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[9]

We obtain the characteristic equation for the other two eigenvalues from the 2×2 matrix. We have

$$\left[(g_1 - g_2) \frac{\mu_0 B}{2} - \frac{\Delta E}{4} - E \right] \left[-(g_1 - g_2) \frac{\mu_0 B}{2} - \frac{\Delta E}{4} - E \right] - \left[\frac{\Delta E}{2} \right]^2 = 0$$

$$E^2 + \frac{\Delta E}{2} E + \left[\frac{\Delta E}{4} \right]^2 - \frac{1}{4} \left[(g_1 - g_2) \mu_0 B \right]^2 = 0$$

$$E_{\pm} = -\frac{\Delta E}{4} \pm \frac{1}{2} \sqrt{\left(\frac{\Delta E}{2}\right)^2 + ((g_1 - g_2)\mu_o B)^2 + \frac{3}{4}(\Delta E)^2}$$
$$= -\frac{\Delta E}{4} \left(1 \mp 2\sqrt{1 + x^2}\right)$$

where

$$x = \frac{\mu_0 B (g_1 - g_2)}{\varDelta E}$$

[4]

Energy levels for a

•zero **B** field:

$$E_{1} = E_{4} = \frac{\Delta E}{4}$$

$$E_{+} = \frac{\Delta E}{4}$$

$$E_{-} = -\frac{3}{4}\Delta E$$

Degeneracy 2

•high **B** field:

$$E_{1} = -\frac{\mu_{0}B}{2}(g_{1} + g_{2})$$

$$E_{+} = \frac{\mu_{0}B}{2}(g_{1} - g_{2})$$

$$E_{-} = -\frac{\mu_{0}B}{2}(g_{1} - g_{2})$$

$$E_{4} = \frac{\mu_{0}B}{2}(g_{1} + g_{2})$$

Degeneracy 4

[4]

Sketch of energy levels. Use some convenient numbers $\Delta E = 1.0$, $g_1 = 2.0$, $g_2 = 1.0$ and $\mu_0 = 1.0$. [4]

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4 *TODO: Bookwork* [8] Molecule, state $|J,m\rangle$ with rotational energy BJ(J+1), dipole moment p in field E.

$$H_1 = -pE\cos\theta$$

 $\langle i|H_1|i\rangle = 0$ from parity, since H_1 odd and $|i\rangle$ has parity $(-1)^J$. [4] Second order corrections to state $|J,m\rangle$ come from

$$|\langle J, m | \cos \theta | J - 1, m |^2 = \left(\frac{J^2 - m^2}{4J^2 - 1} \right)$$

with

$$E_i - E_k = B[J(J+1) - (J-1)J] = 2BJ$$

and

$$|\langle J, m | \cos \theta | J + 1, m |^2 = \left(\frac{(J+1)^2 - m^2}{4(J+1)^2 - 1} \right)$$

with

$$E_i - E_k = B[J(J+1) - (J+1)(J+2)] = -2B(J+1)$$

Therefore,

$$\Delta E_i = \frac{(pE)^2}{2B} \left[\frac{J^2 - m^2}{(4J^2 - 1)J} - \frac{(J+1)^2 - m^2}{(4(J+1)^2 - 1)(J+1)} \right]$$

$$[...] = \frac{J^2 - m^2}{(4J^2 - 1)J} - \frac{(J+1)^2 - m^2}{(4(J+1)^2 - 1)(J+1)}$$

$$=$$

$$= \frac{J(J+1) - 3m^2}{J(2J-1)(J+1)(2J+3)}$$

Hence,

$$\Delta E_i = \frac{(pE)^2}{2B} \left[\frac{J(J+1) - 3m^2}{J(2J-1)(J+1)(2J+3)} \right]$$

When J = 0, only the $|\langle 0, 0| \cos \theta | 1, 0 \rangle|^2 = \frac{1-0}{4-1}$ term contributes. Therefore,

$$\Delta E_i(0 \to 0) = (pE)^2 \left[\frac{|\langle 0, 0 | \cos \theta | 1, 0 \rangle|^2}{0 - 2B} \right]$$
$$= -\frac{(pE)^2}{6B}$$
(1)

[8]

For the OCS molecule, the unperturbed transition $J=0 \rightarrow J=1$ occurs at 12.16 GHz.

$$\Delta E = 12.16 \text{ GHz} = B \times 1 \times 2 - B \times 0 \times 1 = 2B$$

In the static field of 10^5 Vm⁻¹, tranistion splits due to transitions from $|1,\pm 1\rangle \rightarrow |0,0\rangle$ or $|1,0\rangle \rightarrow |0,0\rangle$. The energy split is given by

$$\Delta E_{|1,\pm 1\rangle} - \Delta E_{|1,0\rangle} = \frac{3}{10} \frac{(pE)^2}{2B}$$

Hence, dipole moment

$$p = \frac{1}{E} \sqrt{\frac{10h^2}{3}} (12.16 \text{ GHz} \times 3.21 \text{ MHz})$$
$$= 2.39 \times 10^{-30} \text{ Cm}$$
$$= 14.95e \text{ pm}$$

[5]