PC3130 W10L2 AY24

Thursday, 24 October 2024 11:53 am

$n=2$ (continue example from W10L1)

Find the 1st order corrections to the eigenvalues for $n=2$.

Degeneracy ⇒ Find the submatrix for V in the degenerate subspace.

Please state your basis.

Let
$$|1\rangle = |2\,0\,0\rangle \quad (n\ \ell\ m)$$
$$|2\rangle = |2\,1\,0\rangle$$
$$|3\rangle = |2\,1\,{-1}\rangle$$
$$|4\rangle = |2\,1\,1\rangle$$

$V_{13}=0$, $V_{14}=0$

In the basis $\{|1\rangle, |2\rangle, |3\rangle, |4\rangle\}$, V is given by:?

$$V = \begin{array}{c} \\ \langle 1| \\ \langle 2| \\ \langle 3| \\ \langle 4| \end{array} \begin{array}{c} \begin{array}{cccc} |1\rangle & |2\rangle & |3\rangle & |4\rangle \end{array} \\ \begin{pmatrix} 0 & V_{12} & 0 & 0 \\ V_{21} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{array}$$

need to diagonalize

still diagonal

$V_{11}=0$ because $|1\rangle$ has definite parity & V is odd.

Similarly, $V_{22}=V_{33}=V_{44}=0$

For off-diagonals, we use $[V, L_z]=0$

Since $[V, L_z]=0$, $L_z|n\ell m\rangle = m\hbar|n\ell m\rangle$,

we know that

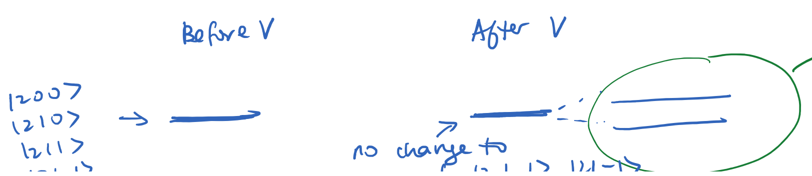
$$\langle n_1 \ell_1 m_1 | V | n_2 \ell_2 m_2\rangle = 0 \quad \text{when } m_1 \neq m_2 \quad ☆$$

Therefore, $V_{ij}=0$ for all $i\neq j$,
except for V_{12} & V_{21}
because $m=0$ for both $|1\rangle$ & $|2\rangle$

V is diagonal in the subspace spanned by $\{|3\rangle, |4\rangle\}$.
Therefore 1st order corrections are V_{33}, V_{44} which are both zero.
subspace spanned by the

For the $m=0$ states $\{|1\rangle, |2\rangle\}$
the 1st order corrections are the eigenvalues of
$$\tilde{V} = \begin{pmatrix} 0 & V_{12} \\ V_{21} & 0 \end{pmatrix}.$$

$$\det(\tilde{V} - \lambda I) = 0$$
$$\lambda^2 - V_{12}.V_{21} = 0$$
$$\lambda = \pm\sqrt{|V_{12}|^2} \qquad (V_{21} = V_{12}^*)$$
$$= \pm |V_{12}|$$



Note that $|200\rangle$ and $|210\rangle$ are not the states that give these corrections.
To know the states, ... eigenstates of $\tilde{V}$.

$|200\rangle$
$|210\rangle$
$|211\rangle$
$|21{-1}\rangle$ $\rightarrow$

no change to energy of $|211\rangle, |21{-1}\rangle$

give these corr…
To know fine states,
find the eigenstates of $\tilde{V}$.

$$\tilde{V} = \begin{pmatrix} 0 & \alpha \\ \alpha^* & 0 \end{pmatrix} \qquad \alpha = V_{12}.$$

suppose $\alpha > 0$, real.

Eigenvalues $\lambda = \pm\alpha$

$$(\tilde{V} - \lambda \mathbb{1})\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$\lambda = \alpha$:

$$\begin{pmatrix} -\alpha & \alpha \\ \alpha & -\alpha \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$\left.\begin{array}{l} -\alpha x + \alpha y = 0 \\ \alpha x - \alpha y = 0 \end{array}\right\} \quad x = y$$

Eigenstate : $|\psi_\alpha\rangle = \frac{1}{\sqrt{2}}\left(|200\rangle + |210\rangle\right)$

$$|\psi_{-\alpha}\rangle = \frac{1}{\sqrt{2}}\left(|200\rangle - |210\rangle\right)$$

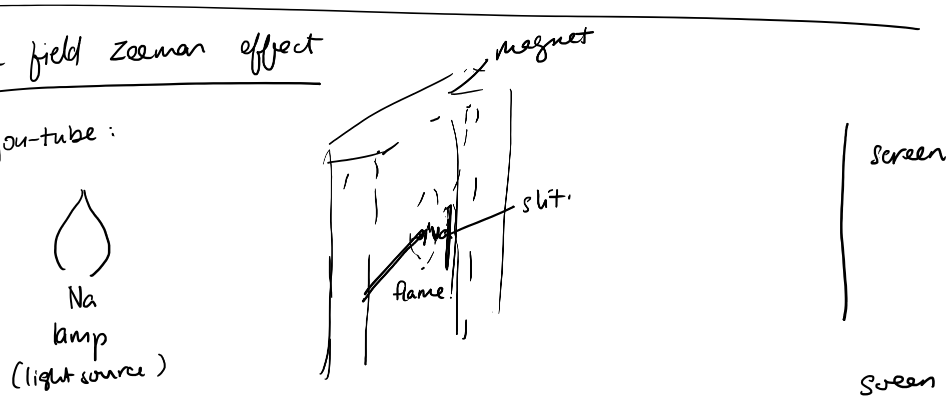
More examples

- Fine structure for hydrogen atom (see tutorial)
- Weak field Zeeman effect.

Zeeman Effect - Control light with magnetic fields

Weak field Zeeman effect

you-tube :



screen

Case : magnet off

ΔE_{Na} $\rightarrow h\nu$

Na lamp.

$h\nu$ ΔE_{Na}

Na in flame absorbs photon from Na lamp — resonance condition.

Na flame blocks some of the light from the Na lamp.

Case : magnet on.

→ Energy levels for Na in the flame shift (or split?)

– no longer exactly in resonance.

absorb less light from the Na lamp.

Screen

less blockage of light from the Na lamp.

Now we work it out

Interaction with an electromagnetic field.

Classical: $$H = \frac{p^2}{2m} + V(r)$$

Add an EM field:

$$H = \frac{1}{2m}(\vec{p} - q\vec{A})^2 + q\phi + V(r),$$ q is the charge. (eg. $q = -e$, $e>0$ for electrons)

$$\vec{B} = \vec{\nabla} \times \vec{A}$$
$$\vec{E} = -\vec{\nabla}\phi - \frac{\partial \vec{A}}{\partial t} \quad \text{(SI units)}$$

QM: $$\hat{H} = \frac{1}{2m}(\hat{p} - q\vec{A})^2 + q\phi + \hat{V}(r)$$

Weak field Zeeman effect

uniform constant external magnetic field.

Coulomb gauge $\phi = 0$, $\nabla \cdot \vec{A} = 0$, $\vec{A} = \frac{1}{2}(\vec{B} \times \vec{r})$

$$\hat{H} = \frac{1}{2m}(\hat{p} - q\vec{A})^2 + \underbrace{\cancel{q\phi}}_{0} + \hat{V}(r)$$

$$= \frac{\hat{p}^2}{2m} - \frac{q}{2m}(\hat{p}\cdot\vec{A} + \vec{A}\cdot\hat{p}) + \hat{V}(r) + \underbrace{\frac{q^2}{2m}\vec{A}\cdot\vec{A}}_{\simeq 0 \text{ for weak fields (for 1st order effect)}}$$

$$= H_0 + V'$$

$$V' = \frac{e}{2m}(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}) \quad \text{, taking } q = -e \text{ now.}$$

$$\vec{p} = -i\hbar\vec{\nabla}$$

Apply $(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p})$ to an arbitrary $\psi(\vec{r})$.

$$(\vec{p}\cdot\vec{A} + \vec{A}\cdot\vec{p}) = -i\hbar(\vec{\nabla}\cdot(\vec{A}\psi) + \vec{A}\cdot\vec{\nabla}\psi)$$
$$= -i\hbar\left((\underbrace{\vec{\nabla}\cdot\vec{A}}_{=0 \text{ from choice of gauge. (Coulomb gauge)}})\psi + \vec{A}\cdot\vec{\nabla}\psi + \vec{A}\cdot\vec{\nabla}\psi\right)$$
$$= -i\hbar\, 2\vec{A}\cdot\vec{\nabla}\psi$$
$$= 2(\vec{A}\cdot\vec{p})\psi.$$

$$\boxed{H = H_0 + \underbrace{\frac{e}{m}(\vec{A}\cdot\vec{p})}}$$

- Perturbation for an external magnetic field.
- We can also rewrite this using $\vec{A} = \frac{1}{2}(\vec{B} \times \vec{r})$

$$\frac{e}{m}(\vec{A}\cdot\vec{p}) = \frac{e}{2m}((\vec{B}\times\vec{r})\cdot\vec{p})$$

$$= \frac{e}{2m} \left(\vec{B} \cdot (\vec{r} \times \vec{p}) \right)$$

$$= -\vec{B} \cdot \vec{\mu}_L \,, \quad \vec{\mu}_L = -\frac{e}{2m} \vec{L} \quad \text{in SI units.}$$

$$\vec{\mu}_L = -\frac{e}{2m} \vec{L} = -\mu_B \frac{\vec{L}}{\hbar} \,, \quad \mu_B = \frac{e\hbar}{2m}$$

Bohr magneton $\sim 10^{-5}$ eV/T.

So $$\boxed{H = H_0 + \frac{e}{m} \vec{A} \cdot \vec{p} = H_0 - \vec{\mu}_L \cdot \vec{B}}$$

Normal Zeeman effect $-\vec{\mu}_L \cdot \vec{B}$.

Historically, scientists sometimes observed a Zeeman effect that was different from what was expected from $-\vec{\mu}_L \cdot \vec{B}$.

– Called the anomalous Zeeman effect.

Now we know there is a term $-\vec{\mu}_s \cdot \vec{B}$ in general (from Dirac's equation & Pauli's equation)

Let's add it in.

$$\boxed{H = H_0 + \frac{e}{2m} \vec{B} \cdot (\vec{L} + g_e \vec{S}) \,,}$$

$$-\vec{\mu}_s \cdot \vec{B} = \frac{e}{2m} g_e \vec{S} \cdot \vec{B} \,, \quad g_e \simeq 2.$$

Landé g-factor for an electron.

Perturbation $$V' = \frac{e}{2m} \vec{B} \cdot (\vec{L} + g_e \vec{S})$$

Now let's be specific. –

Consider the hydrogen atom, and $\vec{B} = B\hat{z}$, $\hat{z} = \frac{\vec{z}}{|\vec{z}|}$

$$V' = \frac{e}{2m} B\hat{z} \cdot (\vec{L} + g_e \vec{S})$$

$$= \frac{e}{2m} B (L_z + g_e S_z)$$

Weak field Zeeman effect, $B_{ext} \ll B_{soc}$ spin-orbit coupling.

~ 10T.

$$H_0 = \frac{p^2}{2m} - \frac{e^2}{r} + U_{soc} \quad —(1)$$

(incl. relativistic terms)

From tutorial 3,

$\{ H_0 \text{ in } (1), \; J^2, \; J_z, \; L^2, \; S^2 \}$ form a complete set of commuting observables

$\uparrow j \quad \uparrow m_j \quad \uparrow l \quad \uparrow s$

$\vec{J} = \vec{L} + \vec{S}$.

So the eigenstates of (1) can be written as $|n, j, m_j, l, s\rangle$

From slides on the fine structure of the hydrogen atom,

we know that the states $|n, j, m_j, l, s\rangle$ with different j have different energies.

we know that the states $|n, j, m_j, l, s\rangle$

with different j have different energies,

but degeneracies occur for different m_j and l (s = $\frac{1}{2}$ always)

$m_j \uparrow J_z$, $l \uparrow L^2$

We need degenerate perturbation theory.

We can try to use this :

$\hat{p}$ Hermitian, $[\hat{p}, V] = 0$. $\hat{p}|\psi_a\rangle = p_a|\psi_a\rangle$, $\hat{p}|\psi_b\rangle = p_b|\psi_b\rangle$

$\langle\psi_a|V|\psi_b\rangle = 0$ whenever $p_a \neq p_b$.

$$V' = \frac{e}{2m} B\,(L_z + g_e S_z)$$

(degeneracies for m_j)

$[J_z, V] = ?$ (is it zero?)

$[J_z, L_z] = [L_z + S_z, L_z] = 0$

similarly, $[J_z, S_z] = 0$

$\Big\}$ so $[J_z, V] = 0$

$$\Rightarrow \langle n\, j\, m_j\, l\, s\,|V'|\,n'\, j'\, m_j'\, l'\, s'\rangle = 0 \quad \text{when } m_j \neq m_j'$$

Note we are only interested in $n = n'$, $j = j'$, and $s = \frac{1}{2}$ always.

(degeneracies for l)

$[L^2, V] = ?$ (is it zero?)

$[L^2, L_z] = 0$ (by definition)

$[L^2, S_z] = 0$ (operate in different spaces)

$\Big\}$ So $[L^2, V] = 0$.

$$\Rightarrow \langle n\, j\, m_j\, l\, s\,|V'|\,n\, j\, m_j'\, l'\, s\rangle = 0 \quad \text{when } m_j \neq m_j' \text{ or } l \neq l'.$$

So $$\boxed{E^{(1)}_{njm_jls} = \frac{e}{2m} B \langle n\, j\, m_j\, l\, s\,|L_z + g_e S_z|\,n\, j\, m_j\, l\, s\rangle}$$