Body frame dipole moment NaK → 2.7 D (Z65 D)

electric field $\vec{E} \parallel \hat{z}$

What is lab-frame $|\vec{d}|$ for state $X^1\Sigma\ |N=0, J=0\rangle$?

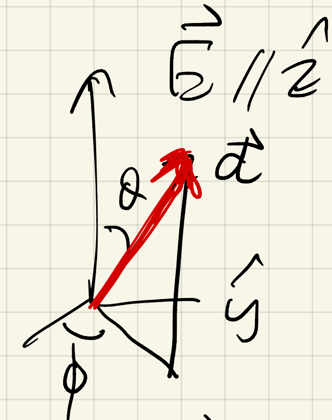
(neglect hf)

→ here $J = N$ = rotational quantum

basis $\{ \overset{J\ m_J}{|00\rangle}\ |1\,{-1}\rangle\ |10\rangle\ |11\rangle\ |2\,{-2}\rangle \ldots \}$

truncate @ $J=2$

$\vec{d} = e\vec{r}, \quad \hat{r} = \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix}$



$\vec{E}$ mixes basis states (strong field, m_J is only good q.n.)

$$H = \underbrace{H^{stark}}_{-\vec{d}\cdot\vec{E}} + \underbrace{H^{rotation}}_{\cancel{2}B_{rot}J(J+1)}$$

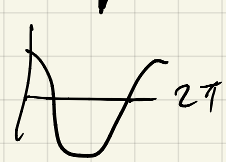
$$H^{rot} = B_{rot}\begin{pmatrix} 0 & & & & & & & & \\ & 2 & & & & & & & \\ & & 2 & & & & & & \\ & & & 2 & & & & & \\ & & & & 6 & & & & \\ & & & & & 6 & & & \\ & & & & & & 6 & & \\ & & & & & & & 6 & \\ & & & & & & & & 6 \end{pmatrix}$$

$H^{stark} = ?$ consider $\langle 00|\vec{d}|00\rangle \propto \langle 00| \begin{matrix}\hat{x}\\ \hat{y}\\ \hat{z}\end{matrix} |00\rangle$

$$\underbrace{\langle 00|\hat{x}|00\rangle}_{\text{even parity}} = \int d\Omega\, \underline{Y^{00}(\theta,\phi)}\, \hat{x}\, \underline{Y^{00}(\theta,\phi)}$$

$$= \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin\theta \frac{1}{4\pi} \sin\theta \cos\phi$$

$= 0$, so $\vec{d} = 0$



However

$\langle 00|\vec{d}|10\rangle = |d|\int d\Omega\, Y^{00} Y^{10} \begin{pmatrix}\hat{x}\\ \hat{y}\\ \hat{z}\end{pmatrix} \neq \vec{0}$

even, odd, odd → nonzero

MW

2652

J=1

σ^+, $\omega = 2B_{rot}$

J=0

$$H = H_{mol} + H_{MW} + H_{mol+light\ interaction}$$

$$H_{mol} \rightarrow \begin{bmatrix} 0 & & & \\ & 2B & & \\ & & 2B & \\ & & & 2B \end{bmatrix} \qquad H_{MW} \rightarrow \hbar\omega\left(\bar{N} + \tfrac{1}{2}\right) = \hbar\omega\left(a^\dagger a + \tfrac{1}{2}\right)$$

$H_{mol+light\ interaction} \rightarrow$ coupling $\Omega_r \hbar$

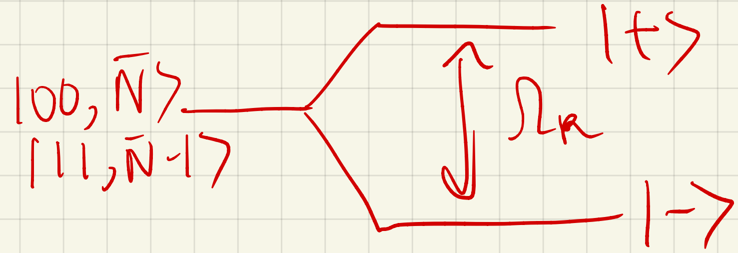
→ consider only $\bar{N}, \bar{N}-1$ manifold

2×2 hamiltonian in dressed frame

$$H = \begin{bmatrix} 2B & & & \\ & 2B & & \\ & & 2B & \Omega_r \\ & & \Omega_r & 2B \end{bmatrix}$$

→ eigenstates $|\pm\rangle = \frac{1}{\sqrt{2}}\left(|00\bar{N}\rangle \pm |11\bar{N}\rangle\right)$

Dressed picture



Go back to Lab frame

let's say we consider state

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|00\rangle - e^{-i\omega t}|11\rangle\right)$$

(non rotating frame)

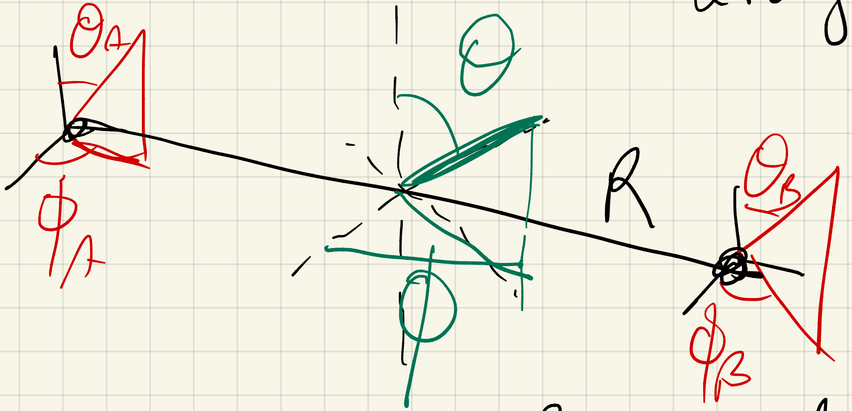
$$\langle\psi|\vec{d}|\psi\rangle = \frac{1}{2}\Big\{\cancel{\langle 00|\vec{d}|00\rangle}^{\,0} + \cancel{\langle 11|\vec{d}|11\rangle}^{\,0} - \langle 00|\vec{d}|11\rangle e^{-i\omega t} - \langle 11|\vec{d}|00\rangle e^{i\omega t}\Big\}$$

$$= \frac{d}{\sqrt{6}}\begin{pmatrix} (e^{i\omega t} + e^{-i\omega t})/2 \\ (ie^{-i\omega t} - ie^{i\omega t})/2 \\ 0 \end{pmatrix} = \frac{d}{\sqrt{6}}(\cos\omega t, \sin\omega t, 0)$$

Key point: can induce $\frac{d}{\sqrt{6}} \sim 1.1\,D$ rotating dipole!

2 body V_{dd}

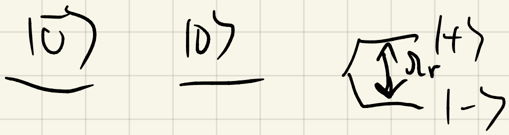
ZG53



$$\frac{\vec{d}_A \cdot \vec{d}_B - 3\,\vec{d}_A \cdot \hat{R}\,\vec{d}_B \cdot \hat{R}}{|R|^3}$$

basis states

A B internal	external (2 fermions)
$\lvert --\rangle$	$L = 1, 3, 5, \ldots$
$\lvert ++\rangle$	$\lvert 1\ -1\rangle$ (with m_L)
$\lvert -+\rangle + \lvert +-\rangle$	$\lvert 1\ 0\rangle$
~~$\lvert -+\rangle - \lvert +-\rangle$~~	$\lvert 1\ 1\rangle$



$$4 \times 3 = 12 \text{ states}$$

$$|\Psi\rangle = |\Psi\rangle^{internal}_{\hookrightarrow SYM}\ |\Psi\rangle^{ext}_{\hookrightarrow ASYM}$$

But wait, there's more!

"spectators" $|0\rangle \equiv |1\ 0\rangle$ ($|J\ m_J\rangle$)
$|\bar{0}\rangle \equiv |1\ -1\rangle$ } participate in 2nd order

so ... $4^2 \cdot 3 = 48$ basis states

Can ignore some stuff!

interchange Mol $A \leftrightarrow B$, V_{dd} unaffected

so internal part $|\Psi_A\ \Psi_B\rangle$ must be symmetric under exchange

$\rightarrow$ actually $10 \cdot 3 = 30$ basis states

Compute example

ZGS 3B

$$\langle -|_A \langle -|_B \langle L m_L | \; V_{dd} \; |+\rangle_A |+\rangle_B |L' m_L'\rangle$$

first do internal bit: $\langle --| \dfrac{\vec{d}_A \cdot \vec{d}_B - 3\vec{d}_A \cdot \vec{R}\, \vec{d}_B \cdot \vec{R}}{R^3} |++\rangle$

$$|\mp\rangle = \frac{1}{\sqrt{2}}\left(|\overset{J m_J}{00}\rangle \mp e^{-i\omega t} |\overset{J m_J}{11}\rangle\right)$$

$$\langle AB|V_{dd}|AB\rangle = \frac{1}{2}\frac{|d|^2}{R^3}\Big[\langle 00|\, \hat{r}_A \cdot \hat{r}_B - 3(\hat{r}_A\cdot\hat{r})(\hat{r}_B\cdot\hat{r})\,|00\rangle$$

$$+ \langle 11| \quad \text{''} \quad |11\rangle$$

$$\star_1 \quad - e^{-i\omega t}\langle 00| \quad \text{''} \quad |11\rangle$$

$$\star_2 \quad - e^{i\omega t}\langle 11| \quad \text{''} \quad |00\rangle\Big]$$

$\star_1 = \star_2$ under exchange

$\star_1 + \star_2 = -2\cos\omega t \; \langle 00| \text{''} |11\rangle$

time-averages to zero!

$$= \frac{|d|^2}{2R^3} \iiiint d\Omega_A d\Omega_B \, Y^{*}_{00}(\theta\phi_{A}) \left\{ \begin{pmatrix} \sin\theta_A\cos\phi_A \\ \sin\theta_A \sin\phi_A \\ \cos\theta_A \end{pmatrix} \cdot \begin{pmatrix} \hat{x}_B \\ \hat{y}_B \\ \hat{z}_B \end{pmatrix} \right.$$

$$\int_0^{2\pi}\int_0^{\pi}\int_0^{2\pi}\int_0^{\pi} d(\cos\theta_A)\, d\phi_A\, d(\cos\theta_B)\, d\phi_B \qquad - 3 \begin{pmatrix} \hat{x}_A \\ \hat{y}_A \\ \hat{z}_A \end{pmatrix} \cdot \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix} \times$$

$$\left. \begin{pmatrix} \hat{r}_B \end{pmatrix} \cdot \begin{pmatrix} \hat{r} \end{pmatrix} \right\}$$

$$\times \; Y^{11}(\theta_B \phi_B)$$

$$= \frac{|d|^2}{R^3}\left(\frac{-1}{6} + \frac{\sin^2\theta}{4}\right)$$

$$= \frac{-|d|^2}{R^3} C_{20}(\theta,\phi)$$

In fact, all nonzero $\langle AB|V_{dd}|A'B'\rangle$ have form $C_{2q}(\theta,\phi), q=-1,0,1$

What about external? $|L' m_L'\rangle$ "=" $Y^{L' m_L'}(\theta,\phi)$

$$\boxed{V_{dd}^{lab} = \frac{\langle d_1\rangle\langle d_2\rangle}{R^3}\langle L M_L| \underbrace{C_{2q}(\theta,\phi)}_{\text{Racah-normalized Sph harmonic}} |L' M_L'\rangle}$$

for $q=1$, eg, $\langle -\overset{AB}{-}| V_{dd} | \overset{AB}{(0\,-\!\!\!>\!+1\,-0>)}/2) \propto C_{2,1}$ 2654

then $\langle 1\, m_L | \ C_{2,1}(\theta,\phi) | 1\, m_L' \rangle$

$$= \begin{array}{c|c} & m_L' \quad -1 \quad 0 \quad 1 \\ \begin{array}{c} m_L \\ -1 \\ 0 \\ 1 \end{array} & \begin{bmatrix} & -\frac{\sqrt{3}}{5} & \\ \frac{\sqrt{3}}{5} & & \\ & & \end{bmatrix} \end{array}$$

need $m_L = m_L' - 1$

for $q=0$, eg $\langle --| V_{dd} | --\rangle$

then $\langle 1\, m_L | \ C_{20}(\theta,\phi) | 1\, m_L' \rangle$

$$= \begin{array}{c|c} & m_L' \rightarrow \\ m_L \downarrow & \begin{bmatrix} & & 1/5 \\ & 2/5 & \\ 1/5 & & \end{bmatrix} \end{array}$$

need $m_L = m_L'$

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fastest single-channel scattering?

from loss $\leftrightarrow$ scattering X-section

$\sigma = \lambda_{dB}^2$

$= \dfrac{h}{2\pi M K T}$, M = reduced mass 2 molecules

$\beta = \langle \sigma v \rangle$

$\langle v \rangle = \sqrt{\dfrac{8}{\pi}\dfrac{KT}{M}}$ (MB)

$\langle \sigma v \rangle = \dfrac{\hbar}{MKT}\sqrt{\dfrac{8}{\pi}}\sqrt{\dfrac{KT}{M}}$

$= \sqrt{\dfrac{8}{\pi}}\dfrac{\hbar}{M}\dfrac{1}{\sqrt{MKT}}\dfrac{\sqrt{2\pi\hbar^2}}{\sqrt{2\pi\hbar^2}}$

$= \sqrt{4}\,\dfrac{\hbar}{M}\lambda_{dB}$

$\langle \sigma v \rangle \overset{\text{unitarity}}{=} \dfrac{2\hbar\lambda_{dB}}{M}$ $\longrightarrow$ limit for u.c. bosons (s-wave $L=0$ scattering only)

for p-wave, 3 channels

$\Rightarrow$ each saturated $\Rightarrow \beta = \dfrac{6\hbar\lambda_{dB}}{M}$