PH 427, 2013

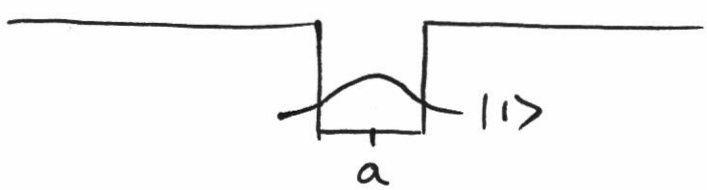
DAY 8

Quiz: Why do I prefer k (which is $\frac{2\pi}{\lambda}$) for describing 1d normal modes, rather than wavelength, λ?

Comment on HW #3: Penetration depth concept.
e⁻ hits barrier
light wave hits metal etc.

Last time... Following section 15.1 McIntyre

$V^{sq}(x-a)$



$V^{sq}(x-2a)$

The error from this approx is analyzed in §15.9

Use $|1\rangle$ and $|2\rangle$ as "nearly orthogonal" basis states to analyze the low-energy states of the double-~~po~~well potential.

$V^{sq}(x-a) + V^{sq}(x-2a)$

Write the Hamiltonian for the double-well potential in this simplified basis

$$H \doteq \begin{bmatrix} \langle 1|H|1\rangle & \langle 2|H|1\rangle \\ \langle 1|H|2\rangle & \langle 2|H|2\rangle \end{bmatrix} = \begin{bmatrix} \alpha & \beta \\ \beta & \alpha \end{bmatrix}$$

Eigenstates	$\frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\end{bmatrix} \doteq \frac{1}{\sqrt{2}}\left(\vert 1\rangle + \vert 2\rangle\right)$	$\frac{1}{\sqrt{2}}\begin{bmatrix}1\\-1\end{bmatrix} \doteq \frac{1}{\sqrt{2}}\left(\vert 1\rangle - \vert 2\rangle\right)$
Eigenvalues	$\alpha + \beta$	$\alpha - \beta$

These approximate eigenstates are called
"Linear combinations of atomic orbitals"
L C A O

Since $|1\rangle$ & $|2\rangle$ are orbitals of isolated "atoms"

To complete the LCAO analysis I need to calculate the two energies

$$\langle 1|H|1\rangle \quad \& \quad \langle 2|H|1\rangle$$

Proceedure: 1 Write $\hat{H}$ in differential operator form.

2 Write $\langle 1 | \hat{H} | 1 \rangle$ as an integral.

White board

Show me $\langle 1 | \hat{H} | 1 \rangle$ as an integral

$$\hat{H} = \frac{\hat{p}^2}{2m} + V^{sq}(x-a) + V^{sq}(x-2a)$$

$$\langle 1 | H | 1 \rangle = \langle 1 | \frac{\hat{p}^2}{2m} + V^{sq}(x-a) | 1 \rangle + \langle 1 | V^{sq}(x-2a) | 1 \rangle$$

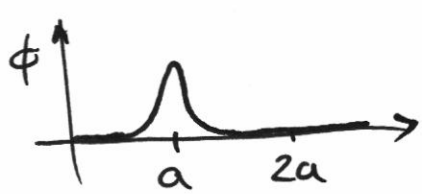
$$= E_g + \int_{-\infty}^{\infty} \phi^{g*}(x-a)\, V^{sq}(x-2a)\, \phi^{g}(x-a)\, dx$$

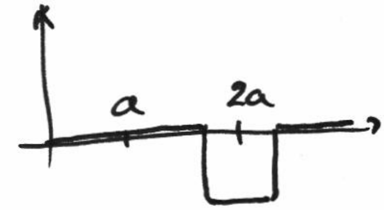
Gnd state energy of the "atomic orbital"

$$= E_g + \int_{-\infty}^{\infty} |\phi(x-a)|^2\, V^{sq}(x-2a)\, dx$$

Probability density

Potential energy





$$= E_g + \text{small correction}$$

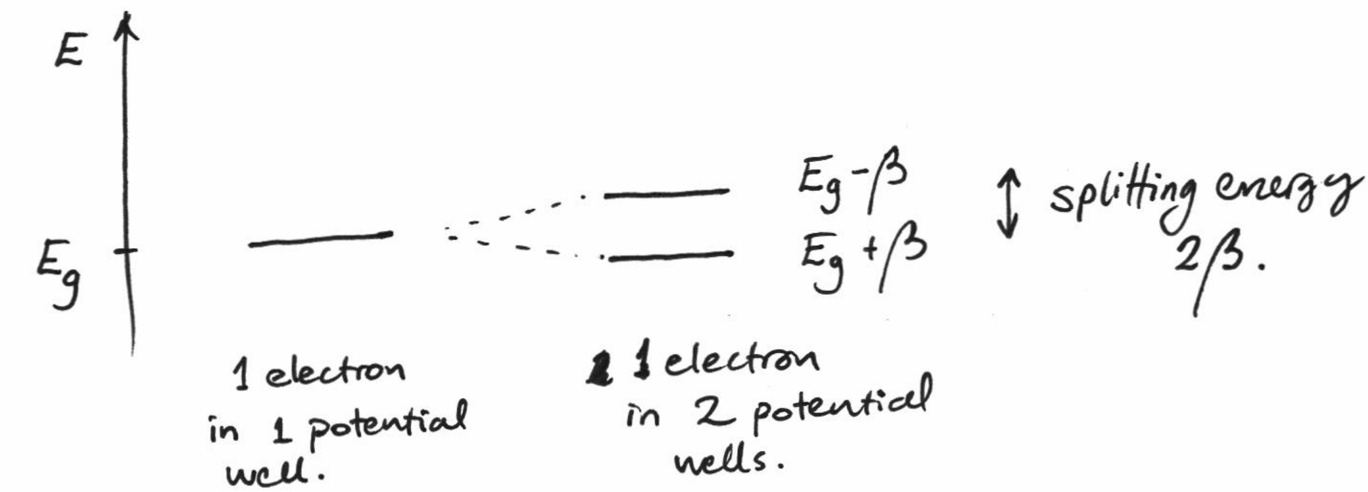
much smaller than β.

$\langle 2|H|1\rangle = \beta$ is called the overlap integral.

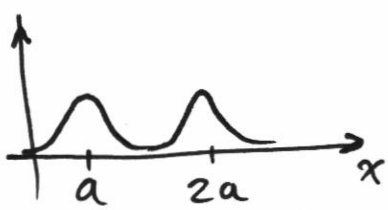
$\langle 2|H|1\rangle$ will be calculated in HW #5. See §15.8 for help.

$\langle 2|H|1\rangle < 0$ since $V^{sq}(x-2a)$ & $V^{sq}(x-a)$ are either zero or negative.

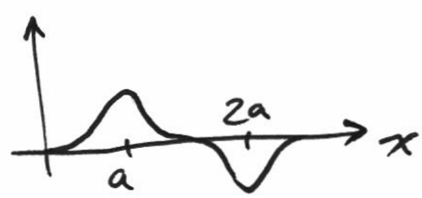
Sumarry



The two LCAO states made from $|1\rangle$ & $|2\rangle$ are



Eigenenergy $E_g + \beta$



Eigenenergy $E_g - \beta$