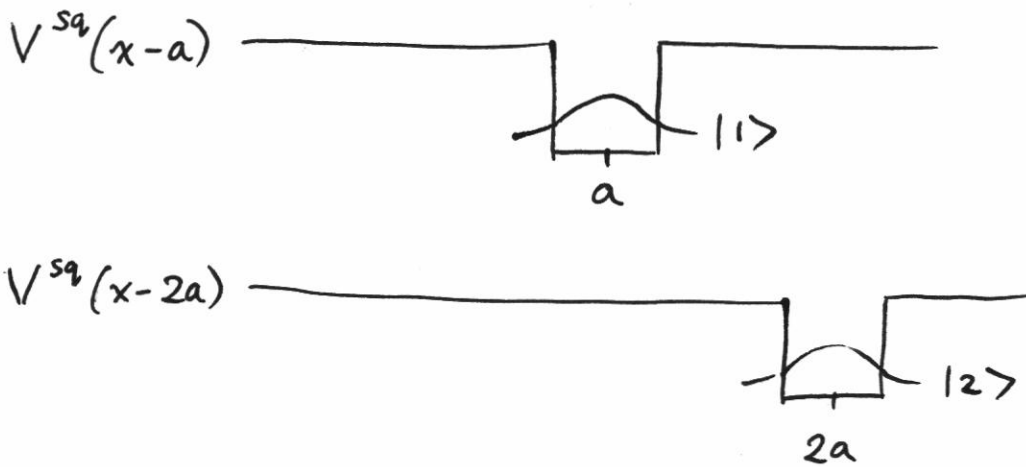


Quiz: why do I prefer k (which is $\frac{2\pi}{\lambda}$)
for describing 1d normal modes, rather than
wavelength, λ ?

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

Last time... Following section 15.1 McIntyre



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-well potential.



(2)

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	$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix} \doteq \frac{1}{\sqrt{2}} (1\rangle + 2\rangle)$	$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \doteq \frac{1}{\sqrt{2}} (1\rangle - 2\rangle)$
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 ~~finish~~ complete the LCAO analysis I need to calculate the two energies

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

③

Procedure: 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

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

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

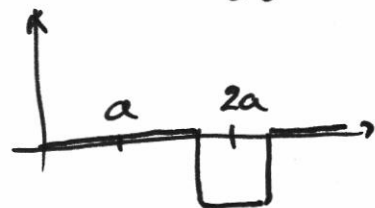
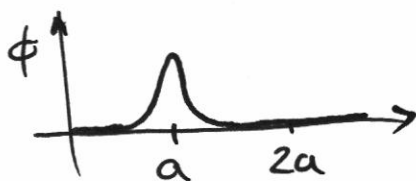
$$= E_g + \int_{-\infty}^{\infty} \phi^g(x-a) V^{sq}(x-2a) \phi^g(x-a) dx$$

↑
 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 .

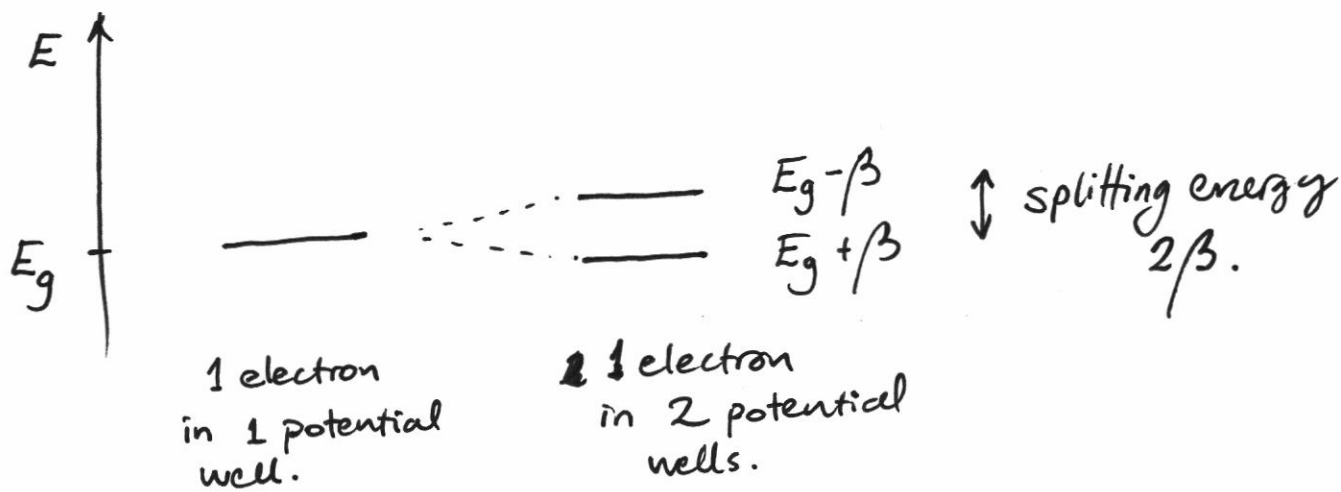
(4)

$\langle 2|H|1 \rangle = \beta$ 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.

Summary



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

