

Quiz: Three potential wells



Atomic orbitals  $|1\rangle$ ,  $|2\rangle$  &  $|3\rangle$

$$\hat{H} \equiv \begin{bmatrix} \langle 1|H|1\rangle & \langle 1|H|2\rangle & \langle 1|H|3\rangle \\ \langle 2|H|1\rangle & \langle 2|H|2\rangle & \langle 2|H|3\rangle \\ \langle 3|H|1\rangle & \langle 3|H|2\rangle & \langle 3|H|3\rangle \end{bmatrix}$$

Which matrix elements can you approximate as zero?

Note: HW#4, Q1 complete this problem.

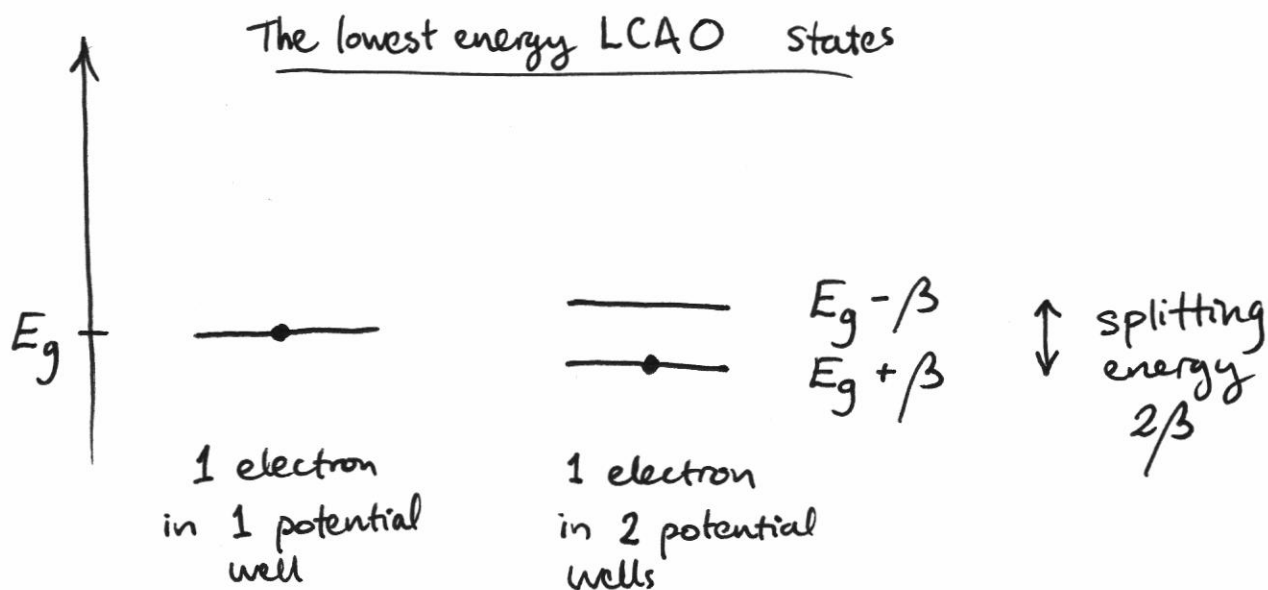
Discussion of journal club assignment.

- Hand out the grading rubric.
- you grade my talk.

Start the worksheet. Note that the band structure simulator is calculating exact ~~the~~ eigenenergies of the ~~potenti~~ periodic potentials. No LCAO approximation.

(2)

Last time



Start the worksheet

Note that the band structure simulator is calculating exact eigenstates/eigenenergies. Not ~~the~~ using the LCAO approx that we employ to simplify the math.