

Quiz 8

Friday, April 21, 2017 8:44 AM

Using the generalized solution to find specific wavefunctions

The generalized LCAO energy eigenstates for an N -atom monatomic chain (assuming only one atomic orbital per atom, and periodic boundary conditions) are:

$$|k\rangle = \frac{1}{\sqrt{N}} \sum_{n=1}^N e^{ikna} |n\rangle$$

where $|n\rangle$ is the atomic orbital centered on the n^{th} nuclei.

For this quiz, assume $N=4$.

a) Write out the specific wavefn $|k=\frac{\pi}{2a}\rangle$ in terms of the basis states $|1\rangle, |2\rangle, |3\rangle$ and $|4\rangle$.

b) Write out the wavefunction $|k=\frac{\pi}{a}\rangle$ in terms of the basis states $|1\rangle, |2\rangle, |3\rangle$ and $|4\rangle$.