

§ 0.1 Infinite Linear Chain

The first idea of solid we can imagine is the direct generalization of cyclic molecules, obtained by increasing the number N of atoms.

We begin considering N atoms positioned on a regular polygon, we can approximate this system with a circle with circumference $2\pi R \simeq Na$ where a is the distance between two atoms. Taking a single atom of the chain as our coordinate origin we see easily that a finite rotation of $2\pi N^{-1}$, for $N \rightarrow \infty$ is almost indistinguishable from a discrete translation of a along a closed infinite chain.

From this symmetry we can immediately say, that if we define a translation operator \hat{T}_a that moves this chain, if we write the Hamiltonian of the system as $\hat{\mathcal{H}}$, we have that $[\hat{\mathcal{H}}, \hat{T}_a] = 0$, where the operator \hat{T}_a acts on eigenstates as follows

$$\hat{T}_a^m |\alpha\rangle = e^{\frac{2i\pi m}{N}} |\alpha\rangle \quad (1)$$

We can now define a new quantum number that depends from the interatomic distance a and the integer m , that we will call k_m , defined as follows

$$k_m = \begin{cases} \frac{2\pi m}{Na} = 0, \dots, \pm \left(\frac{N-1}{N} \right) \frac{\pi}{a} & N = 2k+1, \quad k \in \mathbb{N} \\ \frac{2\pi m}{Na} = 0, \dots, \pm \left(\frac{N-2}{N} \right) \frac{\pi}{a} + \frac{\pi}{a} & N = 2k \end{cases} \quad (2)$$

This quantum number has physical dimensions of an inverse length, and it's usually called the *wavenumber*. This wavenumber, with the previous definition, is contained in the closed set $[-\pi/a, \pi/a]$, called the *First Brillouin Zone*.

As a first approximation, for very large N , we can write this quantum number as a continuous variable k . The eigenstates of the Hamiltonian now depend explicitly on this quantum number k , and with a new notation we can write, analogously to the homonuclear trimer, the projection to the eigenstates $|n\rangle$ of our Hamiltonian

$$|k\rangle = \frac{1}{\sqrt{N}} \sum_{n=1}^N e^{ikna} |n\rangle \quad (3)$$

$$\hat{\mathcal{H}} |k\rangle = \epsilon_k |k\rangle = (\epsilon - 2\mathcal{H}_{ij} \cos(ka)) |k\rangle \quad i \neq j = 1, \dots, N$$

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