§ 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 $N \to \infty$ 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 $\left[\hat{\mathcal{H}}, \hat{T}_a\right] = 0$, where the operator $\hat{T}_a$ acts on eigenstates as follows

$$\hat{T}_a^m \left|\alpha\right\rangle = e^{\frac{2i\pi m}{N}} \left|\alpha\right\rangle \tag{1}$$

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

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

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, analoguously to the homonuclear trimer, the projection to the eigenstates $\left|n\right\rangle$ of our Hamiltonian

$$\begin{aligned} \left|k\right\rangle &= \frac{1}{\sqrt{N}} \sum_{n=1}^{N} e^{ikna} \left|n\right\rangle \\ \hat{\mathcal{H}} \left|k\right\rangle &= \epsilon_k \left|k\right\rangle = (\epsilon - 2\mathcal{H}_{ij} \cos(ka)) \left|k\right\rangle \qquad i \neq j = 1, \cdots, N \end{aligned} \tag{3}$$

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