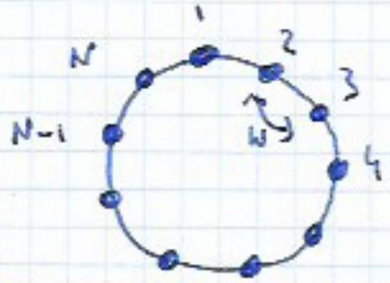
CHAIN OF ATOMS

P.B.C. $|N+1\rangle = |1\rangle$



$$\boxed{\hat{H} = \sum_{n=1}^{N} E_0 |n\rangle\langle n| + \sum_{n=1}^{N} w \left[|n\rangle\langle n+1| + |n+1\rangle\langle n| \right]}$$

let

$$\boxed{\hat{A} \equiv \sum_{n=1}^{N} |n\rangle\langle n+1| \quad , \quad \hat{A}^{+} \equiv \sum_{n=1}^{N} |n+1\rangle\langle n|}$$

$$\boxed{\hat{H} = E_0 \hat{\mathbb{1}} + w \hat{A} + w \hat{A}^{+}}$$

properties of $\hat{A}$ and $\hat{A}^+$

$$\hat{A}|n\rangle = \sum_{m=1}^{N} |m\rangle \underbrace{\langle m+1|n\rangle}_{\delta_{m,n-1}} = |n-1\rangle$$

$$\hat{A}^{+}|n\rangle = \sum_{m=1}^{N} |m+1\rangle \underbrace{\langle m|n\rangle}_{\delta_{mn}} = |n+1\rangle$$

$$A_{mn} = \langle m|\hat{A}|n\rangle = \langle m|n-1\rangle = \delta_{m,n-1}$$

$$A^{+}_{mn} = \langle m|\hat{A}^{+}|n\rangle = \langle m|n+1\rangle = \delta_{m,n+1}$$

$$\hat{A} = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & & & & & \\ 0 & 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & 0 & \cdots & 0 \end{pmatrix}$$

$$\hat{A}^{+} = \begin{pmatrix} 0 & 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 1 & 0 & \cdots & 0 \\ \vdots & & & & & \\ 0 & 0 & 0 & 0 & \cdots 1 & 0 \end{pmatrix}$$

$$\hat{A}^{+}\hat{A} = \sum_{m,m'=1}^{N} |m+1\rangle \underbrace{\langle m|m'\rangle}_{\delta_{mm'}} \langle m'+1| = \sum_{n=1}^{N} |n\rangle\langle n| = \hat{\mathbb{1}}$$

If $\hat{A}|v\rangle = a|v\rangle$ eigensystem then

$$\hat{A}^{+}|v\rangle = \frac{1}{a}|v\rangle \qquad a \in \mathbb{C} \qquad \hat{A} \neq \hat{A}^{+}$$

proof

$$|v\rangle = \underbrace{\hat{A}^{+}\hat{A}}_{\hat{\mathbb{1}}}|v\rangle = a\hat{A}^{+}|v\rangle \to \hat{A}^{+}|v\rangle = \frac{1}{a}|v\rangle \quad \square$$

$$\boxed{\text{conclusion, if } |v\rangle \text{ - eigenvector of } \hat{A} \text{ with eigenvalue } a \text{ then } |v\rangle \text{ is an eigenvector of } \hat{H} \text{ with eigenvalue } E_0 + w(a + a^{-1}).}$$

proof

$$\hat{H}|v\rangle = (E_0\hat{\mathbb{1}} + w\hat{A} + w\hat{A}^{+})|v\rangle = E_0|v\rangle + wa|v\rangle + \frac{w}{a}|v\rangle =$$

$$= (E_0 + wa + w/a)|v\rangle$$

$\square$

<u>We need to find eigenvalues of $\hat{A}$:</u>

$$\det(\hat{A} - \lambda\hat{\mathbb{1}}) = \det\begin{pmatrix} -\lambda & 1 & 0 & 0 \dots 0 \\ 0 & -\lambda & 1 & 0 \dots 0 \\ \vdots & & & \\ 1 & 0 & 0 & 0 \dots -\lambda \end{pmatrix} = \begin{pmatrix} \text{Laplace} \\ \text{expansion} \\ \text{in 1st column} \end{pmatrix}$$

$$= (-1)^{N+1} \underbrace{\det\begin{pmatrix} 1 & 0 & & \\ -\lambda & 1 & & 0 \\ 0 & -\lambda & \ddots & \\ \vdots & & \ddots & \\ 0 & \dots & -\lambda & 1 \end{pmatrix}}_{1} + (-\lambda)\underbrace{\det\begin{pmatrix} -\lambda & 1 & 0 & 0 \dots & 0 \\ 0 & -\lambda & 1 & 0 \dots & 0 \\ 0 & 0 & -\lambda & 1 & 0 \dots 0 \\ \vdots & & & \ddots & 1 \\ 0 & \dots & & & -\lambda \end{pmatrix}}_{(-\lambda)^{N-1}} =$$

$$= (-1)^{N+1} + (-\lambda)^{N} = (-1)^{N}(\lambda^{N} - 1) = 0$$

$$\Rightarrow |\lambda|e^{Ni\varphi} = \lambda^{N} = 1 = e^{2\pi n i} \qquad n \in \mathbb{Z}$$

N - different eigenvalues

$$\boxed{\lambda = e^{\frac{2\pi n}{N}i} \qquad n = 0, 1, \dots, N-1}$$

Hence, eigenvalues of $\hat{H}$

$$E_n = E_0 + W\left(e^{2\pi \frac{n}{N} i} + e^{-2\pi \frac{n}{N} i}\right) =$$

$$\boxed{E_n = E_0 + 2W \cos\left(2\pi \frac{n}{N}\right)}$$

Remark

The same result can be obtained via discrete Fourier transform

$$|n\rangle = \frac{1}{\sqrt{N}} \sum_k e^{ikn} |k\rangle$$

PBC $\quad |N+1\rangle = |1\rangle \Leftrightarrow \frac{1}{\sqrt{N}} \sum_k e^{ikN} e^{ik} |k\rangle = \frac{1}{\sqrt{N}} \sum_k e^{ik} |k\rangle$

$$\rightarrow e^{ikN} = 1 = e^{2\pi n i} \Rightarrow \boxed{k = \frac{2\pi n}{N}}$$

$$\hat{H} = \sum_{kk'} \frac{1}{N} \sum_n E_0 e^{i(k-k')n} |k\rangle\langle k'| +$$

$$+ W \sum_{kk'} \frac{1}{N} \sum_n \left(e^{ikn - ik'(n+1)} + e^{ik(n+1) - ik'n}\right) |k\rangle\langle k'|$$

Lattice sum $\quad \frac{1}{N} \sum_n e^{i(k-k')n} = \delta_{kk'}$

$$\hat{H} = E_0 \sum_k |k\rangle\langle k| + W \sum_k \left(e^{-ik} + e^{ik}\right) |k\rangle\langle k| =$$

$$= \sum_k \left(E_0 + 2W \cos k\right) |k\rangle\langle k| =$$

$$= \sum_{\tilde{n}} \left(E_0 + 2W \cos\left(\frac{2\pi \tilde{n}}{N}\right)\right) |\tilde{n}\rangle\langle \tilde{n}|$$

$\square$