Hamiltonian for n-particle have a form of nxn matrix with $\frac{n(n-1)}{2}$ distinct matrix elements. Depending on the problem at hand each element can take a number of possibilities:

• • • • •
• • • • • [45 unique elements] $_{10\times10}$

Traveling Salesman problem

$A \to B \to C \to \cdots \to A$

5. $\cdot^1$
6. $\cdot^2$ $\cdot^3$
7. $\cdot^8$ $\cdot^4$
9. $\frac{(n-1)!}{2}$

$10^3 \times 10^3$ matrices

But now consider a $\frac{1}{2}$ Spin System or a qubit:

• • • • •
• • • • •

10 qubit $\longrightarrow$ $2^{10} \cong 10^3$

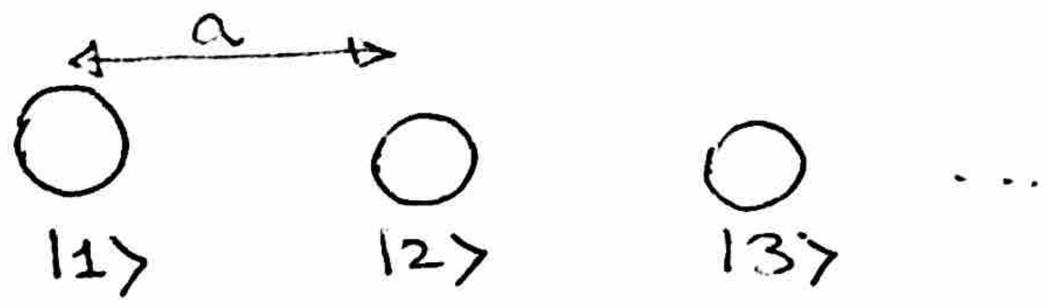
Quantum Size	Classical memory site	Simulate dynamics
50 Qubit	$2^{50} \equiv 10^{15}$	$10^{15} \times 10^{15}$
100	$2^{100} \equiv 10^{30}$	$10^{30} \times 10^{30}$

Dynamics: $\frac{1}{dt}\frac{d}{|\psi\rangle} = H|\psi\rangle$

H time-independent:

$|\psi(t)\rangle = e^{-iHt}|\psi_0\rangle$

LCAO: linear combination of atomic orbitals



In this picture there is a single orbital on atom n which we call $|n\rangle$.

and periodic boundary condition (site N is the same as site 0). Also we assume that all of the orbitals are orthogonal to each other: $\langle n|m\rangle = \delta_{n,m}$

General trial wavefunction: $|\psi\rangle = \sum_n \phi_n |n\rangle$

Similar to earlier this can be written as: $\sum_m H_{nm}\phi_m = E\phi_n$ } this equation is a variational approximation meaning that

where $H_{nm} = \langle n|H|m\rangle$

instead of finding the exact ground state, it finds the best possible ground state

made up of the orbitals that we have put in the model. instead of having only one orbital $|n\rangle$ at a given site, one could consider many $|n,\alpha\rangle$ where α runs from 1 to some number $\Rightarrow$ increasingly better approximate the exact Schroedinger equation $\Rightarrow$ one complication, typically have to give up our nice orthogonality assumption.

$H = K + \sum_j V_j$ where $K = P^2/2m$ & V_j is coulomb interaction of the electron with the nucleus at site j. $V_j = V(r - r_j)$ where r_j is the position of the j^{th} nucleus.

$H|m\rangle = (K + V_m)|m\rangle + \sum_{j\neq m} V_j|m\rangle$ as before $K+V_m$ is the Hamiltonian for a single nucleus (m^{th}) and no other nuclei in the system so $(K+V_m)|m\rangle = \varepsilon_{atomic}|m\rangle$

[energy of an $\bar{e}$ on nucleus m ← orbital
in absence of any other nuclei

$H_{n,m} = \langle n|H|m\rangle = \varepsilon_{atom}\delta_{n,m} + \underbrace{\sum_{j\neq m}\langle n|V_j|m\rangle}$

Similar to hopping term so $\sum_{j\neq m}\langle n|V_j|m\rangle = \begin{cases} V_0 & n=m \\ -t & n=m\pm1 \\ 0 & \text{o w} \end{cases}$

V_0 term does not hop an electron from one site to another (shifts energy)

$\Rightarrow H_{n,m} = \varepsilon_0\,\delta_{n,m} - t(\delta_{n+1,m} + \delta_{n-1,m})$ where $\varepsilon_0 = \varepsilon_{atomic} + V_0$

tight binding chain

t is the hopping term to move the $\bar{e}$ from one site to another $\Rightarrow$ large when orbitals are close together and decaying exponentially when they are far apart.

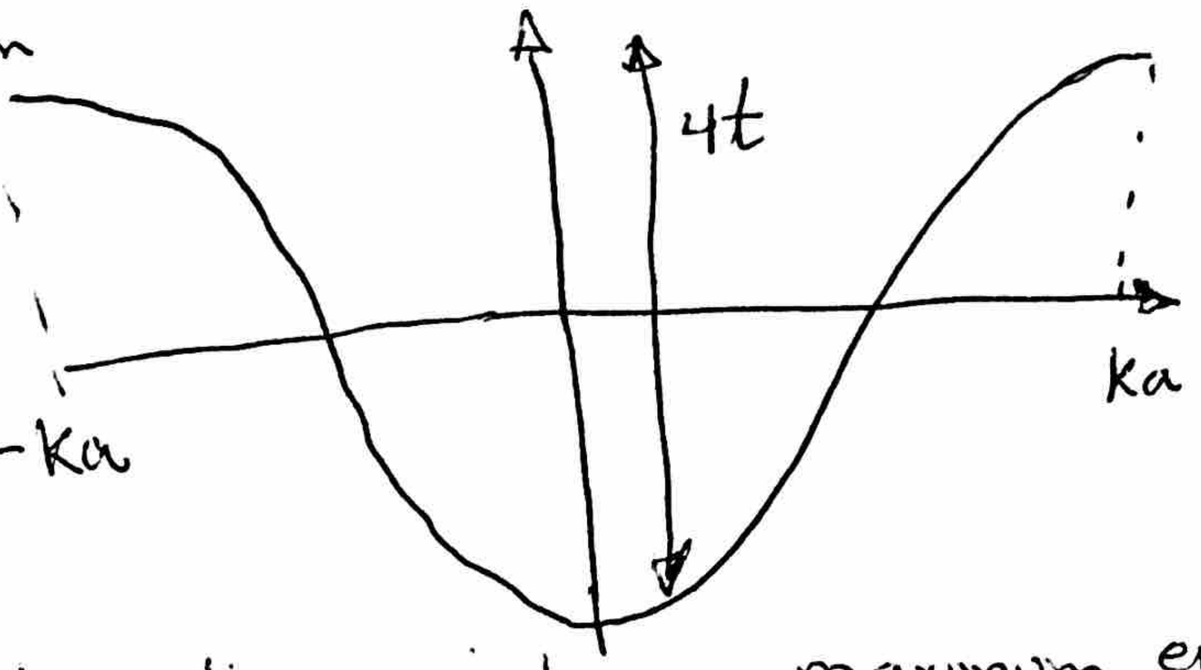
we propose a solution: $\phi_n = \frac{e^{-ikna}}{\sqrt{N}}$ $\Rightarrow$ $k \to k + \frac{2\pi}{a}$ we get the same solution

periodic bounding $\Leftrightarrow$ system has a length $L = Na$ $\Rightarrow$ allowed values of k are quantized in units of $\frac{2\pi}{L}$.

$$\sum_m H_{n,m}\phi_m = \varepsilon_0\frac{e^{-ikna}}{\sqrt{N}} - t\left(\frac{e^{-ik(n+1)a}}{\sqrt{N}} + \frac{e^{-ik(n-1)a}}{\sqrt{N}}\right) = E\phi_n = E\frac{e^{-ikna}}{\sqrt{N}}$$

$\Rightarrow E = \varepsilon_0 - 2t\cos(ka)$

Lets plot the dispersion



- dispersion always has zero group velocity for $k = \frac{n\pi}{a}$ for any n

- unlike free $\bar{e}$, electron dispersion has a maximum energy as well as a minimum energy. or electrons only have eigenstates within a certain energy bands.

- The energy difference from the bottom of the band to the top is known as the bandwidth. For energies outside of the bandwidth there are no k-states with that energy.

- The bandwidth (in this model 4t) is determined by the magnitude of the hopping which depends on the distance between nuclei.

- Near the bottom of the band, the dispersion is parabolic: $E(k) = const + ta^2k^2$ similar to free electron:

$E_{free}(k) = \frac{\hbar^2k^2}{2m}$ ← $\bar{e}$ momentum ⟹ except prefactor or a new effective mass (crystal momentum)

$\frac{\hbar^2k^2}{2m} = ta^2k^2$ which gives us $m^* = \frac{\hbar^2}{2ta^2}$

Filling Bands

Our model is made up of atoms and each atom "donates" one $\bar{e}$ into the band. Since there are N possible k-states in the band and $\bar{e}$ are fermions and have spin so bands are only half filled.