III The quantum many-body problem

The central problem we want to solve is the Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle$$

with: (i) $|\psi\rangle \in \mathcal{H}$ the Hilbert space of the system

(ii) $\hat{H} : \mathcal{H} \to \mathcal{H}$ the Hamilton operator of the system

When & why do we need numerics?

Solvable problems are those for which we can determine the eigenstates / eigenvalues in a closed analytical form.

Examples:

- H-atom with one electron
- Potential well (box potential, δ-potential
- (An-) Harmonic oscillator

Note: These are all single-particle / non-interacting problems.

Be more precise:

Assume for some problem describing a degree of freedom "α", the eigenvalue-problem

$$\hat{H}_\alpha |\psi_{n_\alpha}\rangle = E_{n_\alpha} |\psi_{n_\alpha}\rangle$$

can be solved ($n_\alpha \in \mathbb{N}$ label the eigenstates/values)

Let $\mathcal{H}_\alpha$ be the corresponding Hilbert space, then the many-body Hilbert space for N degrees of freedoms labeled by α is defined by

$$\mathcal{H}^N = \mathcal{H}_{\alpha=1} \otimes \mathcal{H}_{\alpha=2} \otimes \cdots \otimes \mathcal{H}_{\alpha=N}.$$

Let us consider the total Hamiltonian

$$\hat{H}^{(1)} = \sum_{\alpha=1}^{N} \hat{H}_\alpha^{(1)}$$

Since $[\hat{H}^{(1)}_\alpha, \hat{H}^{(1)}_\beta] = 0$, the eigenstates of the many-body problem are

$$|\psi(n_1 \dots n_N)\rangle = |\psi_{n_1}\rangle \otimes |\psi_{n_2}\rangle \otimes \dots \otimes |\psi_{n_N}\rangle$$

with eigenvalues:

$$\hat{H}^{(1)}|\psi(n_1 \dots n_N)\rangle = \left(\sum_{\alpha=1}^{N} E_{n_\alpha}\right)|\psi(n_1 \dots n_N)\rangle$$

Now let us introduce an operator coupling two degrees of freedom:

$$\hat{V} : \mathcal{H}^N \to \mathcal{H}^N$$

& expand it in the $|\psi(n_1 \dots n_N)\rangle$:

$$\hat{V} = \sum_{n_1 \dots n_N} \sum_{n_1' \dots n_N'} \langle n_1 \dots n_N | \hat{V} | n_1' \dots n_N' \rangle \, |n_1 \dots n_N\rangle\langle n_1' \dots n_N'|$$

Now since $\hat{V}$ should only couple 2 degrees of freedom we must have:

$$\langle n_1 \dots n_N | \hat{V} | n_1' \dots n_N' \rangle = V_{n_\alpha n_\beta, n_\alpha' n_\beta'} \prod_{\gamma \neq \alpha,\beta} \delta_{n_\gamma, n_\gamma'}$$

for all pairs $\alpha \neq \beta \in \{1, \dots, N\}$.

Defining $(n_1 \dots n_N) \equiv \underline{n}_N$ & $\sum_{\alpha=1}^{N} E_{n_\alpha} \equiv E(\underline{n})$ we now ask, if the system with coupling described by:

$$\hat{H} = \hat{H}^{(1)} + \hat{V}$$ can be solved.

Therefore, calculate $[\hat{H}^{(1)}, \hat{V}]$ in basis of known eigenstates $|\psi(\underline{n})\rangle$:

$$[\hat{H}^{(1)}, \hat{V}] = \sum_{\{\underline{n}\}} \sum_{\{\underline{n}'\}} \sum_{\{\underline{n}''\}} \langle \underline{n} | \hat{H}^{(1)} | \underline{n}' \rangle \langle \underline{n}' | \hat{V} | \underline{n}'' \rangle \, |\underline{n}\rangle\langle \underline{n}''|$$

$$- \langle \underline{n} | \hat{V} | \underline{n}' \rangle \langle \underline{n}' | \hat{H}^{(1)} | \underline{n}'' \rangle \, |\underline{n}\rangle\langle \underline{n}''|$$

we have:

$$\langle \underline{n} | \hat{H}^{(1)} | \underline{n}' \rangle = \delta_{\underline{n}, \underline{n}'} \, E(\underline{n})$$

& thus (relabeling indices):

$$[\hat{H}^{(1)}, \hat{V}] = \sum_{\underline{n}} \sum_{\underline{n}'} \Big(E(\underline{n}) \langle \underline{n} | \hat{V} | \underline{n}' \rangle - E(\underline{n}') \langle \underline{n} | \hat{V} | \underline{n}' \rangle \Big) \, |\underline{n}\rangle\langle \underline{n}'|$$

$$= \sum_{\alpha \neq \beta} \Big\{ \sum_{n_\alpha n_\beta} \sum_{n'_\alpha n'_\beta} \left(E_{n_\alpha} + E_{n_\beta} - E_{n'_\alpha} - E_{n'_\beta} \right) V_{n_\alpha n_\beta, n'_\alpha n'_\beta} \, |n_\alpha n_\beta\rangle\langle n'_\alpha n'_\beta| \Big\}$$

$$\prod_{\gamma \neq \alpha, \beta} |n_\gamma\rangle\langle n_\gamma|$$

Thus, if $\hat{V}$ is diagonal in the $|\psi_{n_\alpha}\rangle$, i.e.

$$V_{n_\alpha n_\beta, n'_\alpha n'_\beta} = \delta_{n_\alpha n'_\alpha} \delta_{n_\beta n'_\beta} V_{n_\alpha n_\beta} ,$$

then $\hat{H}$ is also diagonalized by $|\psi(\underline{n})\rangle$.

Consequence:

Interacting many-particle problems in general can not be solved :(

Good news: Numerics helps!

III.1 Second quantization

We need a convenient way to describe many-body systems, i.e., compact representations of $\hat{H}^{(1)}$ & $\hat{V}$, especially not in real space!

Idea: Use eigenfunctions of solvable single-particle problems $|\psi_{n_\alpha}\rangle$

as basis!

We introduce occupation number representation. Consider single particle problem first. We have eigenstates $|\psi_{k_\alpha}\rangle$ labeled by k_α. The occupation number n_{k_α} characterizes, how often that state is occupied.

Bosonic system: $n_{k_\alpha} \in \mathbb{N}_0$

Fermionic system: $n_{k_\alpha} \in \{0, 1\}$

We can always write $\hat{H}^{(1)}_\alpha$ as:

$$\hat{H}^{(1)}_\alpha = \sum_{k_\alpha=1}^{\infty} E_{k_\alpha} \hat{n}_{k_\alpha} + \text{const.}$$

where $\hat{n}_{k_\alpha}$ is projector to k_α-th eigenstate.

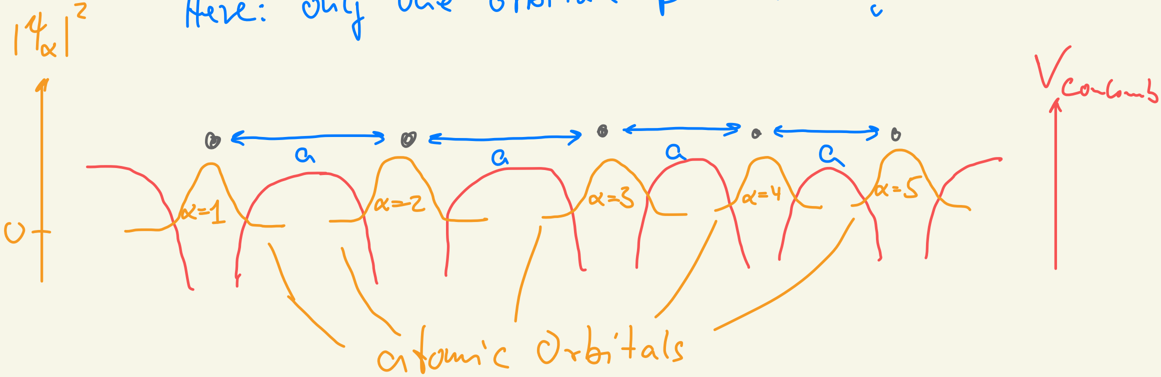
Then we can form tensor product states

$$\underbrace{|n_{k_1=0}\rangle |n_{k_1=1}\rangle \cdots}_{\text{subsystem } \alpha=1} \underbrace{|n_{k_2=0}\rangle |n_{k_2=1}\rangle}_{\text{subsystem } \alpha=2} \cdots \underbrace{|n_{k_N=0}\rangle |n_{k_N=1}\rangle}_{\text{subsystem } \alpha=N} \cdots$$

Example: Crystal composed of N atoms

Consider only the outermost orbital of each atom as subsystem α & assume the wave-functions are known (e.g. H-atom orbitals):

Here: only one orbital per atom!



If orbitals α & β are occupied & their wave-functions have finite overlap $\Rightarrow \langle \psi_\alpha | \frac{q}{|r_\alpha - r_\beta|} | \psi_\beta \rangle \neq 0$!

$\Rightarrow$ Coulomb interaction $\hat{V}$!

Tensor-product wave function of N electrons in L orbitals:

$$|\underline{n}\rangle = |n_1 \dots n_L\rangle \quad \text{with} \quad \sum_{\alpha=1}^{L} n_\alpha = N.$$

Expand operators in that basis:

- single site operator:

$$\hat{O}_\alpha = \sum_{n_\alpha, n_\alpha'} \langle n_\alpha | \hat{O}_\alpha | n_\alpha' \rangle |n_\alpha\rangle\langle n_\alpha'| \prod_{n_{\beta\neq\alpha}} |n_\beta\rangle\langle n_\beta|$$

- two site operators:

$$\hat{O}_{\alpha\beta} = \sum_{n_\alpha, n_\alpha'} \sum_{n_\beta, n_\beta'} \langle n_\alpha n_\beta | \hat{O}_{\alpha\beta} | n_\alpha' n_\beta' \rangle \prod_{n_{\gamma\neq\alpha,\beta}} |n_\gamma\rangle\langle n_\gamma|$$

$\vdots$

We introduce creation/annihilation operators for convenience:

$\hat{c}_\alpha^\dagger$: map $|n_\alpha\rangle \mapsto c\,|n_\alpha+1\rangle$

$\hat{c}_\alpha$: map $|n_\alpha\rangle \mapsto \bar{c}\,|n_\alpha-1\rangle$

choose $c \in \mathbb{R}$ such that $\hat{c}_\alpha^\dagger \hat{c}_\alpha = \hat{n}_\alpha$.

$$\langle n_\alpha | \hat{c}_\alpha^\dagger \hat{c}_\alpha | n_\alpha\rangle = |c|^2 \langle n_\alpha | n_\alpha\rangle \overset{!}{=} n_\alpha \langle n_\alpha | n_\alpha \rangle$$

$$\Rightarrow \quad \hat{c}_\alpha^\dagger = \sum_{n_\alpha} \sqrt{n_\alpha+1}\; |n_\alpha+1\rangle\langle n_\alpha|$$

$$\hat{c}_\alpha = \sum_{n_\alpha} \sqrt{n_\alpha}\; |n_\alpha-1\rangle\langle n_\alpha|$$

This simplifies operators in many-body systems. We can now construct operators on many-body Hilbert space by taking tensor products.

E.g.: • single particle operator with

$$\langle n_\alpha | \hat{O} | n_\alpha' \rangle = \delta_{n_\alpha, n_\alpha'} + \delta_{n_\alpha, n_\alpha' \pm 1}$$

$$\Rightarrow \hat{O}_\alpha = \underbrace{\mathbb{1}}_{\text{orbital } 1} \otimes \cdots \otimes \underbrace{\mathbb{1}}_{\text{orbital } \alpha-1} \otimes \underbrace{\left(O_\alpha^0 \hat{n}_\alpha + \hat{c}_\alpha^\dagger + \hat{c}_\alpha \right)}_{\text{orbital } \alpha} \otimes \underbrace{\mathbb{1} \otimes \cdots \otimes \mathbb{1}}_{\cdots}$$

• two-particle operator with

$$\langle n_\alpha n_\beta | \hat{O} | n_\alpha' n_\beta' \rangle = \delta_{n_\alpha, n_\alpha' + 1} \, \delta_{n_\beta, n_\beta' - 1}$$

$$\hat{O}_{\alpha\beta} = \underbrace{\mathbb{1}}_{\text{orbital } 1} \otimes \cdots \otimes \mathbb{1} \otimes \underbrace{\hat{c}^\dagger}_{\text{orbital } \alpha} \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes \underbrace{\hat{c}}_{\text{orbital } \beta} \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}$$

But be careful: This is valid only if excanging two particles does not change the state! ⇒ Bosons!

For Fermions the $\hat{c}_\alpha^{(\dagger)}$ must obey anti commutation relations: $\hat{c}_\alpha^\dagger \hat{c}_\beta = - \hat{c}_\beta \hat{c}_\alpha^\dagger$!

Proof: Consider $|\underline{n}\rangle = |n_1 \ldots n_L\rangle$ with $n_\alpha \in \{0,1\}$

Now add particle in unoccupied orbital

α: $\hat{c}_\alpha^\dagger |\underline{n}\rangle = \hat{c}_\alpha^\dagger \left[\hat{c}_1^\dagger\right]^{n_1} \left[\hat{c}_2^\dagger\right]^{n_2} \cdots \left[\hat{c}_L^\dagger\right]^{n_L} |\emptyset\rangle$

For each $n_\beta = 1$ the orbital β is occupied. We must thus exchange $\hat{c}_\alpha^\dagger$ with all those orbitals:

$$\hat{c}_\alpha^\dagger |\underline{n}\rangle = \underbrace{(1 - 2\hat{n}_1)}_{\text{change sign of state if } n_1 = 1} \left[\hat{c}_1^\dagger\right]^{n_1} \hat{c}_\alpha^\dagger \left[\hat{c}_2^\dagger\right]^{n_2} \cdots \left[\hat{c}_L^\dagger\right]^{n_L} |\emptyset\rangle$$

$$\vdots$$

$$= \underbrace{\prod_{\beta<\alpha} \underbrace{(1 - 2\hat{n}_\beta)}_{e^{i\pi\hat{n}_\beta}}}_{\text{Jordan-Wigner strings!}} |n_1 \ldots n_\alpha + 1 \ldots n_L\rangle$$

Using these Jordan-Wigner strings, we can calculate for fermionic operators $\hat{f}_\alpha^{(\dagger)}$:

$$\left\{\hat{f}_\alpha, \hat{f}_\beta^\dagger\right\} = \prod_{\gamma<\alpha} e^{i\pi\hat{n}_\gamma} \hat{c}_\alpha \prod_{\delta<\beta} e^{i\pi\hat{n}_\delta} \hat{c}_\beta^\dagger + \prod_{\gamma<\beta} e^{i\pi\hat{n}_\gamma} \hat{c}_\beta^\dagger \prod_{\delta<\alpha} e^{i\pi\hat{n}_\alpha} \hat{c}_\alpha$$

now since $\hat{c}_\alpha |n_\alpha = 0\rangle = 0$ & $\hat{c}_\alpha^\dagger |n_\alpha = 1\rangle = 0$

it follows with $\alpha \leq \beta$:

$$\hat{c}_\alpha \prod_{\delta<\beta} e^{i\pi \hat{n}_\delta} = \prod_{\substack{\delta<\beta \\ \delta\neq\alpha}} e^{i\pi\hat{n}_\delta}\, \hat{c}_\alpha e^{i\pi\hat{n}_\alpha} = -\prod_{\substack{\delta<\beta \\ \delta\neq\alpha}} \hat{c}_\alpha$$

$$\Rightarrow \{\hat{f}_\alpha, \hat{f}_\beta^\dagger\} = \prod_{\gamma<\alpha} e^{i\pi\hat{n}_\gamma} \prod_{\substack{\delta<\beta \\ \delta\neq\alpha}} e^{i\pi\hat{n}_\delta} \left(-\hat{c}_\alpha \hat{c}_\beta^\dagger\right)$$

$$+ \prod_{\gamma<\beta} e^{i\pi\hat{n}_\gamma} \prod_{\delta<\alpha} e^{i\pi\hat{n}_\delta} \left(\hat{c}_\beta^\dagger \hat{c}_\alpha\right)$$

$$= \prod_{\alpha\leq\gamma<\beta} e^{i\pi\hat{n}_\gamma} \underbrace{\left(\hat{c}_\beta^\dagger \hat{c}_\alpha - \hat{c}_\alpha \hat{c}_\beta^\dagger\right)}_{\delta_{\alpha\beta}\,(1-2\hat{n}_\alpha)}$$

$$\Rightarrow \{\hat{f}_\alpha, \hat{f}_\beta^\dagger\} = \delta_{\alpha\beta}$$

Important consequence:

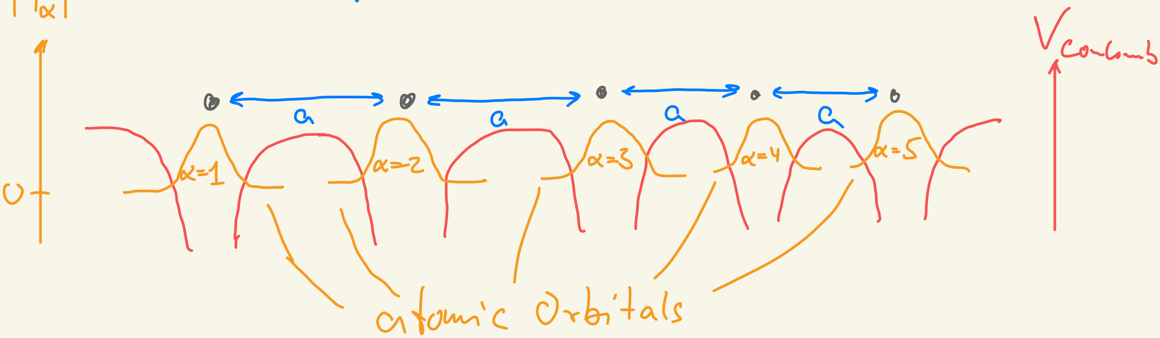
(i) Local bosonic operators $\hat{c}_\alpha^{(\dagger)}$ can be represented as simple tensor product: $\mathbb{1} \otimes \cdots \otimes \mathbb{1} \otimes \hat{c}^{(\dagger)} \otimes \mathbb{1} \otimes \cdots$

(ii) Local fermionic operators cannot be represented as simple tensor product, instead one must use Jordan-Wigner strings:

$$\hat f_\alpha^{(+)} = e^{i\pi \hat n} \otimes \cdots \otimes e^{i\pi \hat n} \otimes \hat c^{(+)} \otimes \mathbb{1} \otimes \cdots \otimes \mathbb{1}$$

Back to our example:

Here: only one orbital per atom!



We need $\hat H = \hat H^{(1)} + \hat V$ in second quantization!

Coulomb-potential.

$$\hat V = \sum_{\alpha\neq\beta}{}' \hat n_\alpha \hat n_\beta \frac{e^2}{|r_\alpha - r_\beta|}$$

Local problems: $\hat H_\alpha^{(1)} = \sum_\alpha{}' \frac{\hat p_\alpha^2}{2m} - \frac{e^2 Z}{|r_\alpha - R_\alpha|}$, R_α coord of atom

what are the overlaps $\langle n_\alpha | \hat f_\beta^{(1)} | n_\beta \rangle$?

Evaluate:

$$\int d^3 r_\alpha \, d^3 r_\beta \, \overline{\psi_{n_\alpha}(r_\alpha)} \left(-\frac{\nabla_\beta^2}{2m}\right) \psi_{n_\beta}(r_\beta) = S_{\alpha\beta}$$

with $S_{\alpha\beta}$ the overlap between orbitals.

Tight-binding approximation:

Only nearest neighbors have non-vanishing overlaps: $S_{\alpha\beta} \equiv -t\,\delta_{|\alpha-\beta|,1}$ (here isotropic)

But this yields a very simple form of the local Hamiltonians:

$$\hat{H}^{(1)} = -t \underbrace{\sum_{\langle\alpha,\beta\rangle}}_{\substack{\text{nearest neighbors} \\ \text{(or maybe even more)}}} \left(\hat{f}_\alpha^\dagger \hat{f}_\beta + \hat{f}_\beta^\dagger \hat{f}_\alpha\right) + \underbrace{\sum_\alpha \mu_\alpha \hat{n}_\alpha}_{\text{on-site potential energies}}$$

$\Rightarrow$ "hopping"

Now in solids the Coulomb potential is usually screened $\Rightarrow$ approx $V_{\alpha\beta} \simeq U\,\delta_{\alpha\beta}$.

This is the famous Hubbard model:

$$\hat{H} = -t \sum_{\langle\alpha,\beta\rangle} \sum_\sigma \left(\hat{f}_{\alpha,\sigma}^\dagger \hat{f}_{\beta,\sigma} + h.c.\right) + U \sum_\alpha \hat{n}_{\alpha,\uparrow} \hat{n}_{\alpha,\downarrow} + \mu \hat{N}$$

(adding the Spin σ as extra degree of freedom)