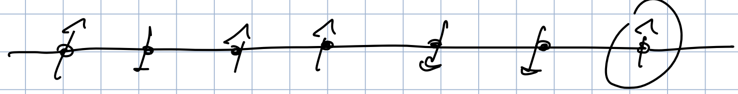
Computational Quantum Physics

Two classes of quantum many-body systems

1) localized (distinguishable) degrees of freedom

Ex. a lattice of quantum spins



N spins

quantum spin $\hat{\vec{S}} = (\hat{S}^x, \hat{S}^y, \hat{S}^z)$

$$\hat{\vec{S}}^2 = \hbar^2 S(S+1) \qquad (\hbar = 1)$$

Hilbert space $D = (2S+1)^N$

Reference state $|\Psi\rangle = |-S, -S, \ldots, -S\rangle$ $\qquad \hat{S}^z|m\rangle = m|m\rangle$

generate all the other basis states $|m_1, m_2, \ldots, m_N\rangle$

by applying S_i^+ operators

$$S^+|m\rangle = \sqrt{S(S+1) - m(m+1)}\,|m+1\rangle$$

2) Itinerant degrees of freedom

→ groups of identical particles

ex. electron gas in a metal

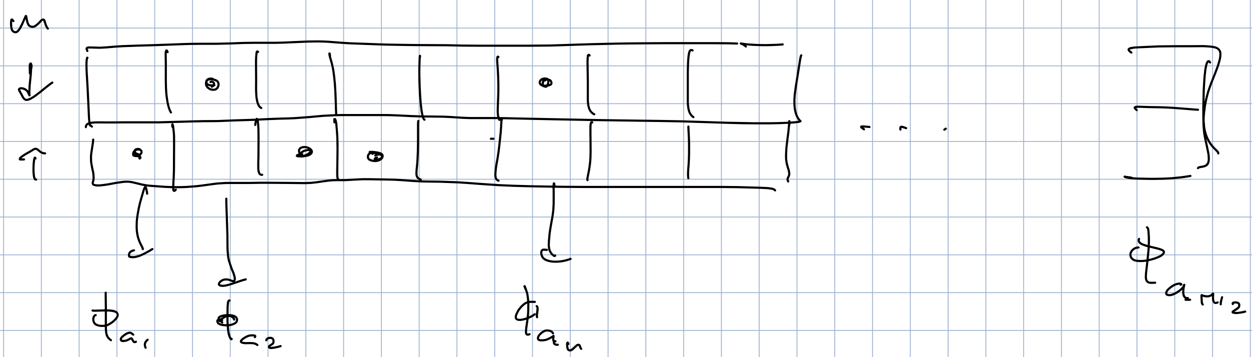
e cloud in atoms / molecules

identical in QM = indistinguishable

Only meaningful description of N identical particles in terms of the occupation of single-particle states

basis of Hilbert space for a single particle ex $\phi_a(\vec{x})\ |m\rangle$ orbital + spin state for an electron

$\vec{x} = (x_1, \dots, x_d)$



$\alpha = (a, m)$ label of the $\underbrace{\text{single-particle quantum state}}$

state of well-defined occupation of the = Fock state

$|n_1, n_2, \dots, n_\alpha, \dots, n_M\rangle$ → states / modes for a single particle

n_α ?

FERMIONS : $n_\alpha = 0, 1$

BOSONS : $n_\alpha = 0, \dots, \infty$

Most important Fock state : Vacuum

Reference $|0\rangle = |0, 0, 0, \dots, 0\rangle$

Out of $|0\rangle$ I can create all Fock states via creation operators

$$\hat{c}^+_\alpha |0, 0, \dots 0_\alpha, \dots\rangle = |0, 0, \dots, \underset{\alpha}{1}, \dots 0\rangle$$

FERMIONS

Pauli exclusion principle $\qquad \hat{c}_\alpha^+ \hat{c}_\alpha^+ = (\hat{c}_\alpha^+)^2 = 0$

Anti-symmetry of fermionic states

$\alpha \neq \beta \qquad \hat{c}_\alpha^+ \hat{c}_\beta^+ |0\rangle = - c_\beta^+ c_\alpha^+ |0\rangle$

? $\qquad$?

$$c_\alpha^+ c_\beta^+ = - c_\beta^+ c_\alpha^+$$

$$\{ c_\alpha^+, c_\beta^+ \} = 0$$

$$|0, 0, \ldots, 1_\alpha, \ldots, 1_\beta, \ldots, 0\rangle$$

Choice : order the single-particle states

$$\alpha = 1, 2, \ldots, M$$

Convention :

$$|n_1, n_2, \ldots n_\alpha, \ldots n_M\rangle$$

$$= (c_1^+)^{n_1} (c_2^+)^{n_2} \cdots (c_\alpha^+)^{n_\alpha} \cdots (c_M^+)^{n_M} |0\rangle$$

ordering

$$c_\alpha^+ \; |n_1, n_2 \ldots n_\alpha \ldots n_M\rangle$$

$$= c_\alpha^+ \; (c_1^+)^{n_1} (c_2^+)^{n_2} \cdots (c_\alpha^+)^{n_\alpha} \cdots (c_M^+)^{n_M} |0\rangle$$

$$= (-1)^{\sum_{\beta<\alpha} n_\beta} (c_\alpha^+)^{n_\alpha+1} \ldots (c_M^+)^{n_M} |0\rangle$$

$$= \begin{cases} (-1)^{\sum_{\beta<\alpha} n_\beta} \; |n_1, n_2, \ldots, n_\alpha+1, \ldots n_M\rangle & n_\alpha = 0 \\ 0 & n_\alpha = 1 \end{cases}$$

Destruction operator

$$\left(\langle n_1 n_2 \ldots n_\alpha, \ldots n_M | c_\alpha\right) | n_1, n_2, \ldots, n_\alpha + 1, \ldots n_M \rangle$$

$$= (-1)^{\sum_{\beta<\alpha} n_\beta}$$

$$c_\alpha | n_1 n_2 \ldots n_\alpha \ldots n_M \rangle = \begin{cases} (-1)^{\sum_{\beta<\alpha} n_\beta} | n_1 n_2 \ldots n_{\alpha-1} \ldots n_M \rangle & n_\alpha = 1 \\ 0 & n_\alpha = 0 \end{cases}$$

$$\underbrace{\hat{c}_\alpha^+ \hat{c}_\alpha}_{\hat{n}_\alpha} | n_1 n_2 \ldots n_\alpha \ldots n_M \rangle = n_\alpha | n_1 n_2 \ldots n_\alpha \ldots n_M \rangle$$

exercise

number operator

$$\hat{c}_\alpha \hat{c}_\alpha^+ | n_1 \ldots n_M \rangle = \begin{cases} 0 & n_\alpha = 1 \\ 1 & n_\alpha = 0 \end{cases}$$

$$= (1 - n_\alpha) | n_1 n_2 \ldots n_M \rangle$$

$$\hat{c}_\alpha \hat{c}_\alpha^+ = 1 - \hat{c}_\alpha^+ \hat{c}_\alpha$$

$$\{\hat{c}_\alpha, \hat{c}_\alpha^+\} = 1$$

$\hookrightarrow$ generalize this to

$$\boxed{\begin{aligned} \{c_\alpha, c_\beta^+\} &= \delta_{\alpha\beta} \\ \{c_\alpha, c_\beta\} &= \{c_\alpha^+, c_\beta^+\} = 0 \end{aligned}}$$

$\boxed{\text{BOSONS}}$ $c_\alpha, c_\alpha^\dagger$ operators: same as destruction / creation operators for a harmonic oscillator

$$\begin{cases} c_\alpha^\dagger \,|n_1 \dots n_\alpha \dots n_M\rangle = \sqrt{n_\alpha+1}\;|n_1 \dots (n_\alpha+1) \dots n_M\rangle \\ c_\alpha \,|n_1 \dots n_\alpha \dots n_M\rangle = \sqrt{n_\alpha}\;|n_1 \dots (n_\alpha-1) \dots n_M\rangle \end{cases}$$

$$c_\alpha^\dagger c_\alpha \,|n_1 \dots n_M\rangle = n_\alpha |n_1 \dots n_M\rangle$$

$$c_\alpha c_\alpha^\dagger \,|\quad\rangle = (n_\alpha+1)\,|n_1 \dots n_M\rangle$$

$$[c_\alpha, c_\alpha^\dagger] = 1 \qquad\qquad c_\alpha c_\alpha^\dagger = 1 + c_\alpha^\dagger c_\alpha$$

$$\boxed{[c_\alpha, c_\beta^\dagger] = \delta_{\alpha\beta}}$$

$$c_\alpha^\dagger c_\beta^\dagger = c_\beta^\dagger c_\alpha^\dagger \qquad\qquad \boxed{[c_\alpha^\dagger, c_\beta^\dagger] = [c_\alpha, c_\beta] = 0}$$

Quantum states in second quantization

for identical particles

Basis for Hilbert space (Fock space)

$$|n_1\, n_2 \dots n_\alpha \dots n_M\rangle$$

$$\langle n_1\, n_2 \dots n_M | n_1'\, n_2' \dots n_M'\rangle = \delta_{n_1 n_1'}\,\delta_{n_2 n_2'} \dots \delta_{n_M n_M'}$$

generic state for N particles

$$|\Psi\rangle = \sum_{\{n_\alpha\}:\, \sum_\alpha n_\alpha = N} \psi(n_1, n_2 \dots n_M)\,|n_1\, n_2 \dots n_M\rangle$$

$$\sim O(\exp(N, M))$$

# of dimensions D of Fock space for N particles on M modes/states

FERMIONS $M \geq N$

$$D = \binom{M}{N} = \frac{M!}{N!\,(M-N)!} \simeq \exp\left[N \ln\left(\frac{M}{N}\right) + \dots \right]$$

$M \gg N \gg 1$

BOSONS

$$D = \frac{(MN)!}{N!\,(MN-N)!\,N!}$$

more generally: if you allow for up to n_{max} particles per mode (fermions $n_{max} = 1$; bosons $n_{max} = N$)

$$D = \frac{(M n_{max})!}{N!\, n_{max}!\, (M n_{max} - N)!}$$

Non-generic state "Hartree-Fock state"

$$|\Psi_{HF}\rangle \sim \prod_{i=1}^{N} \underbrace{\left(\sum_{\alpha=1}^{M} \Phi^{(i)}_\alpha \, c^+_\alpha \right)}_{} |0\rangle$$

creates a particle in the state $\sum_\alpha \Phi^{(i)}_\alpha \,|\alpha\rangle$

$(|\alpha\rangle \to \phi_a(\vec{x})\,|m\rangle$ example$)$

Fermions : $\Phi_\alpha^{(i)}$ are orthogonal

$$\sum_\alpha \left(\Phi_\alpha^{(i)}\right)^* \Phi_\alpha^{(j)} = \delta_{ij}$$

Bosons : no restriction

$$|\Psi_{HF}\rangle = \Psi_{HF}\left(\{\Phi_\alpha^{(i)}\}\right)$$

$N \times M$ complex coefficients

as opposed to $D \sim o(\exp(N, M))$

$$\left(\psi(n_1 n_2 \dots n_M) \overset{HF}{\cancel{=}} \psi_1(n_1)\, \psi_2(n_2) \dots \psi_M(n_M) \right)$$

Normalization of Fock states

$$|n_1 n_2 \dots n_M\rangle = \frac{(c_1^\dagger)^{n_1}}{\sqrt{n_1!}} \frac{(c_2^\dagger)^{n_2}}{\sqrt{n_2!}} \dots \frac{(c_M^\dagger)^{n_M}}{\sqrt{n_M!}} |0\rangle$$

Operators in second quantization

Basis change formula

$|\alpha\rangle$ for a single particle

$|\gamma\rangle$ another basis

$$|\gamma\rangle = \sum_\alpha \langle\alpha|\gamma\rangle\, |\alpha\rangle \qquad |\alpha\rangle = \sum_\gamma \langle\gamma|\alpha\rangle\, |\gamma\rangle$$

$$\boxed{\begin{cases} c_\alpha^\dagger = \sum_\gamma \langle \gamma | \alpha \rangle \; c_\gamma^\dagger \\ c_\alpha = \sum_\gamma \langle \alpha | \gamma \rangle \; c_\gamma \end{cases}}$$

Observables in terms of c, $c^\dagger$ operators

one-body observables : $\hat{A} = \sum_{i=1}^{N} \hat{A}_i^{(1)}$

ex. kinetic energy $\hat{A}_i = \frac{\hat{\vec{p}}_i^{\,2}}{2m}$

$\hat{A}^{(1)} | a_\alpha \rangle = a_\alpha | a_\alpha \rangle$ eigenstates of $\hat{A}^{(1)}$ for a single particle

$$\hat{A} = \sum_\alpha a_\alpha \; c_\alpha^\dagger c_\alpha$$

any basis

$$= \sum_{\mu\nu} \sum_\alpha a_\alpha \; \langle \mu | \alpha \rangle \langle \alpha | \nu \rangle \; c_\mu^\dagger c_\nu$$

$$= \sum_{\mu\nu} \langle \mu | \underbrace{\Big(\sum_\alpha a_\alpha | \alpha \rangle \langle \alpha | \Big)}_{\hat{A}^{(1)}} | \nu \rangle \; c_\mu^\dagger c_\nu$$

$$\boxed{\hat{A} = \sum_{\mu\nu} \langle \mu | \hat{A}^{(1)} | \nu \rangle \; c_\mu^\dagger c_\nu}$$

Two - body operators

$$\hat{V} = \frac{1}{2} \sum_{i \neq j} \hat{v}^{(2)}(\hat{A}^{(1)}_i, \hat{A}^{(1)}_j)$$

$\hat{A}^{(1)}_i \to \hat{\vec{r}}_i$, $\hat{A}^{(1)}_j \to \vec{r}_j$

ex. interaction potential $\hat{v}^{(2)}(\vec{r}_i, \vec{r}_j)$

$$= \frac{1}{2} \left(\sum_{ij} v^{(2)}(\hat{A}^{(1)}_i, \hat{A}^{(1)}_j) - \underbrace{\sum_i v^{(2)}(\hat{A}^{(1)}_i, \hat{A}^{(1)}_i)} \right)$$

↪ second quantization

$$\hat{v}^{(2)}(\hat{A}^{(1)}_1, \hat{A}^{(1)}_2) |a_{\alpha_1} a_{\alpha_2}\rangle = v^{(2)}(a_{\alpha_1}, a_{\alpha_2}) |a_{\alpha_1}, a_{\alpha_2}\rangle$$

$$\hat{V} = \frac{1}{2} \left[\sum_{\alpha\beta} v^{(2)}(a_\alpha, a_\beta) \, c^\dagger_\alpha c_\alpha c^\dagger_\beta c_\beta - \sum_\alpha v^{(2)}(a_\alpha, a_\alpha) \, c^\dagger_\alpha c_\alpha \right]$$

exercise : for both bosons and fermions

$$= \frac{1}{2} \sum_{\alpha\beta} v^{(2)}(a_\alpha, a_\beta) \, c^\dagger_\alpha c^\dagger_\beta c_\beta c_\alpha$$

ex. { basis change to a generic basis

$$\boxed{\hat{V} = \frac{1}{2} \sum_{\mu\nu\rho\lambda} \langle \mu\nu | v^{(2)}(\hat{A}^{(1)}, \hat{A}^{(1)}) | \rho\lambda \rangle \, c^\dagger_\mu c^\dagger_\nu c_\lambda c_\rho}$$