2) QUANTUM MANY-BODY FORMALISM

2 2.2) Second Quantization (Name historic)

In principle we could work out ~~all~~ most of many-body QM using (anti-) symmetrized wavefunctions such as Eq. (1.12).

We could generalize it to more particles using the

(Anti-) symmetrisation operator

$$\hat{P}_{\left\{ {B \atop F} \right\}} \psi(\vec{x}_1, \dots \vec{x}_N) = \frac{1}{N!} \sum_P \varphi^P \psi(\vec{x}_{P(1)}, \dots \vec{x}_{P(N)}) \quad (2.13)$$

$\varphi = -1$ Fermions
$= +1$ Bosons

$P =$ Permutation of $\{1, 2, 3, \dots N\}$ (e.g. $\{1, 3, 2, 4, \dots, N\}$)

$\varphi^P \leftarrow \varphi$ to the power of parity of permutation

In practice, such a formalism gets cumbersome quickly. Discouraging example: Write the bosonic states for three-particles in three states A, B, C.

The only meaningful information in (2.13). is, how many particles are in which single-particle basis states φ_n (not "which")

We thus introduce:

~~Number~~ (Occupation) number representation

$$|\vec{N}\rangle = |N_0 \, N_1 \, N_2 \dots \rangle \;\hat{=}\; \begin{array}{ll} N_0 \text{ particles in state} & |\varphi_0\rangle \\ N_1 \quad \text{-"-} & |\varphi_1\rangle \\ \text{etc.} & \end{array} \quad (2.14)$$

capital!

The space of all $\{|N_0, \dots\rangle\}$ is called Fock space (see Negele/Orland p. 12)

- Correct (anti-) symmetrisation is automatically implied in these states

- Example (Bosons) $|2\,1\,0\,0\dots\rangle = \frac{1}{\sqrt{3}}\Big[\varphi_0(\vec{x}_1)\varphi_0(\vec{x}_2)\varphi_1(\vec{x}_3) + \varphi_0(\vec{x}_1)\varphi_0(\vec{x}_3)\varphi_1(\vec{x}_2) + \varphi_0(\vec{x}_2)\varphi_0(\vec{x}_3)\varphi_1(\vec{x}_1)\Big]$

Define one special number state

Vacuum $|0\rangle = |0 \ldots 0\rangle$ (2.15)

Now define

Creation operator for Bosons $\hat{a}_n^+ |N_0 N_1 \ldots\rangle = \sqrt{N_n+1}\, |N_0 N_1 \ldots (N_n+1) \ldots\rangle$

Annihilation — " — $\hat{a}_n |N_0 N_1 \ldots\rangle = \sqrt{N_n}\, |N_0 N_1 \ldots \underset{\uparrow \text{ slot } n}{(N_n-1)} \ldots\rangle$

Creation operator for Fermions $\hat{a}_n^+ |N_0 N_1 \ldots\rangle = \begin{cases} |N_0 N_1 \ldots \underset{n}{1} \ldots\rangle & \text{if } N_n = 0 \\ 0 & \text{if } N_n = 1 \end{cases}$

Annihilation — " — all $N_i \in \{0,1\}$ only

$\hat{a}_n |N_0 N_1 \ldots\rangle = \begin{cases} 0 & \text{if } N_n = 0 \\ |N_0 N_1 \ldots 0 \ldots\rangle & \text{if } N_n = 1 \end{cases}$

(2.16)

From these definitions, we can show

Commutation relations $[\hat{a}_i, \hat{a}_j] = 0$, $[\hat{a}_i^+, \hat{a}_j^+] = 0$

$$[\hat{a}_i, \hat{a}_j^+] = \delta_{ij} \quad \text{Bosons}$$

$$\{\hat{a}_i, \hat{a}_j\} = 0 \quad \{\hat{a}_i^+, \hat{a}_j^+\} = 0 \quad \{\hat{a}_i, \hat{a}_j^+\} = \delta_{ij} \quad \text{Fermions} \qquad (2.17)$$

$\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$ (anti-commutator)

- Proof: Apply $[\hat{a}_i, \hat{a}_j^+]$ to a "test-state" $|\vec{N}\rangle$
- This is all inspired by the S.H.O. ladder operators (1.4), for Bosons they share the commutator algebra with many-body creation operators.
- Factors $\sqrt{N_n}$, $\sqrt{N_n+1}$ take care of combinatorial factors that would arise from wavefunction symmetrisation (exercise)
- Using operators $\hat{a}^+$, we can span the entire Fock-space:

$$|N_0\, N_1\, N_2 \ldots\rangle = \frac{(\hat{a}_0^+)^{N_0} (\hat{a}_1^+)^{N_1} (\hat{a}_2^+)^{N_2} \ldots}{\sqrt{N_0!\, N_1!\, N_2! \ldots}} |0\rangle \qquad (2.18)$$

- Fock-states obey orthonormality

$$\langle N_0' N_1' N_2' \ldots | N_0\, N_1\, N_2 \ldots\rangle = \delta_{N_0 N_0'} \delta_{N_1 N_1'} \delta_{N_2 N_2'} \ldots$$

2.2.1) N-Body Operators

Consider a generic 2-body Hamiltonian (in first quantised form), e.g.

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\vec{\nabla}_{x_1}^2 + \vec{\nabla}_{x_2}^2\right) + V(\vec{x}_1) + V(\vec{x}_2) + U(\vec{x}_1, \vec{x}_2) \quad (2.19)$$

. where $\sim\vec{\nabla}_{x_1}$ $\sim\vec{\nabla}_{x_2}$ are kinetic energies of particle 1, 2

$V(x_1)$, $V(x_2)$ are some external potentials (e.g harmonic trap, gravity)

and $U(\vec{x}_1, \vec{x}_2)$ is an interaction potential

We can distinguish here:

Single-body operators (e.g kinetic energy, potential energy), that are a sum of identical replica acting on each particle.

and a $\hat{O}_1 = \sum_k \hat{O}^{(k)}$ where $\hat{O}^{(k)}$ acts only on particle k. (2.20)

two-body operator (Interaction potential), contains both $\hat{x}_1$, and $\hat{x}_2$ $\hat{O}_2 = \sum_{kl} \hat{O}^{(kl)}$ (in principle N-Body operators)

It is possible to express any first quantized Hamiltonian such as (2.19) in second quantized form, i.e using $\hat{a}$, $\hat{a}^\dagger$.

Operators $\hat{O}$ are maps in Hilbertspace $\Rightarrow$ they are identical if all matrix-elements such as $\langle \phi_A | \hat{O} | \phi_B \rangle$ are the same.

Let us do this conversion now

2.2.2 Second quantized Hamiltonian

Let us assume $\hat{H} = \hat{A} + \hat{B}$, where $\hat{A} = \sum_k \hat{A}^{(k)}$ is a single-body and $\hat{B} = \sum_{kl} B^{(kl)}$ a two-body operator, This results in

Second-quantized Hamiltonian:

$$\hat{H} = \sum_{nm} A_{nm}\, \hat{a}_n^\dagger \hat{a}_m + \sum_{\substack{nm \\ lk}} B_{nm,lk}\, \hat{a}_n^\dagger \hat{a}_m^\dagger \hat{a}_l \hat{a}_k \quad (2.21)$$

with

single-body matrix-elements $A_{nm} = \langle \varphi_n | \hat{A} | \varphi_m \rangle$ (2.22)

and two-body matrix-elements $B_{nm,\ell k} = \langle \varphi_n \varphi_m | \hat{B} | \varphi_\ell \varphi_k \rangle$

Example: Consider N identical ~~bosons~~ particles in a 1D harmonic trap, interacting with $U(\vec{x}_1, \vec{x}_2) = U_0 \exp\left(-\frac{|\vec{x}_1 - \vec{x}_2|^2}{2\sigma^2}\right)$

First quantized Hamiltonian:

$$\hat{H} = \sum_{k=1}^{N} \left(-\frac{\hbar^2}{2m} \nabla_{k}^2 + V(x_k) \right) + \frac{1}{2} \sum_{k,\ell=1}^{N} U(\vec{x}_k, \vec{x}_\ell) \qquad (2.23)$$

$$V(x_k) = \frac{1}{2} m \omega^2 x_k^2$$

We want to use the harmonic oscillator basis (1.2) to define our $\hat{a}, \hat{a}^\dagger$.

In the Notation used for (2.22): $\hat{A} = -\frac{\hbar^2}{2m} \vec{\nabla}_x^2 + V(\hat{x}) = \hat{H}_{0,osc}$

$\hat{B} = U(\hat{x}, \hat{y})$

Thus $A_{nm} = \langle \varphi_n | \hat{H}_{0,osc} | \varphi_m \rangle = E_m \langle \varphi_n | \varphi_m \rangle = \delta_{nm} E_m$ (E_m see (1.3))

$B_{nm,\ell k} = \langle \varphi_n \varphi_m | \hat{B} | \varphi_\ell \varphi_k \rangle$

$= \int d^3x \int d^3y \, \varphi_n^*(\vec{x}) \varphi_m^*(\vec{y}) \frac{U(\vec{x}, \vec{y})}{2} \varphi_\ell(\vec{x}) \varphi_k(\vec{y})$ (since U messy, let's not try to simplify more... (Try for me?))

Hence (10)

$$\hat{H} = \sum_n \underbrace{\hbar\omega\left(n + \tfrac{1}{2}\right)}_{E_n} \hat{a}_n^\dagger \hat{a}_n + \sum_{\substack{nm \\ \ell k}} B_{nm,\ell k} \, \hat{a}_n^\dagger \hat{a}_m^\dagger \hat{a}_\ell \hat{a}_k . \qquad (2.24)$$

Exercise:

- for $N=3$, explicitly confirm that the matrix-elements of operators (2.23) and (2.24) are the same between a few pairs of Fock-states (2.14)

2.2.3. Basis changes

We can always change the single particle basis underlying our second quantization with a unitary transformation

$$|\varphi_l\rangle = \sum_m U_{lm} \, |w_m\rangle \qquad U_{lm} = \langle w_m | \varphi_l \rangle \quad (2.25)$$

Define one set of operators for each, e.g.

$$\langle x | \hat{a}_n^+ | 0 \rangle' = \varphi_n(x) \qquad \langle x | \hat{c}_n^+ | 0 \rangle = w_n(x) \qquad // \text{sospad}$$

We can show the following

basis-transformation for second quantized operators

$$\hat{a}_l^+ = \sum_m U_{lm} \, \hat{c}_m^+ \qquad (2.26)$$

$$\Rightarrow \hat{a}_l = \sum_m U_{lm}^* \, \hat{c}_m$$

Example: Let us rewrite the Hamiltonian (2.24) in the previous example (p.13) in the momentum basis. Hence we have a continuous form of the transformation (2.25):

$$(m \to k) \quad \varphi_l(x) = \int U_l(k) \, e^{ikx} \, dk$$

Momentum space oscillator eigenstate

$$\langle x | w(k) \rangle = e^{ikx} \qquad U_l(k) = \frac{1}{2\pi} \int e^{-ikx} \, \varphi_l(x) \, dx = \tilde{\varphi}_l(k)$$

i.e.: $U_{lm} \to U_l(k)$ [m-index became continuous momentum "k" and $\sum_m \to \int dk$]

Hence we have $\hat{a}_l^+ = \int U_l(k) \, \hat{c}^+(k) \, dk$

Single-body term of (2.24) becomes

$$\sum_n \underbrace{\left(\hbar\omega\left(n+\tfrac{1}{2}\right)\right)}_{\equiv E_n} \hat{a}_n^+ \hat{a}_n = \sum_n E_n \int dk \int dk' \, U_n(k) \, U_n^*(k') \, \hat{c}^+(k) \, \hat{c}(k')$$

$$= \int dk \int dk' \, h(k,k') \, \hat{c}^+(k) \, \hat{c}(k')$$

with $h(k,k') = \sum_n E_n \, U_n(k) \, U_n^*(k')$

This term describes transitions between different momenta, as expected since momentum states are not eigenstates of the single particle Hamiltonian $\hat{H}_{0,osc}$

2.2.4. Application: Fermi blocking vs Bose-enhancement

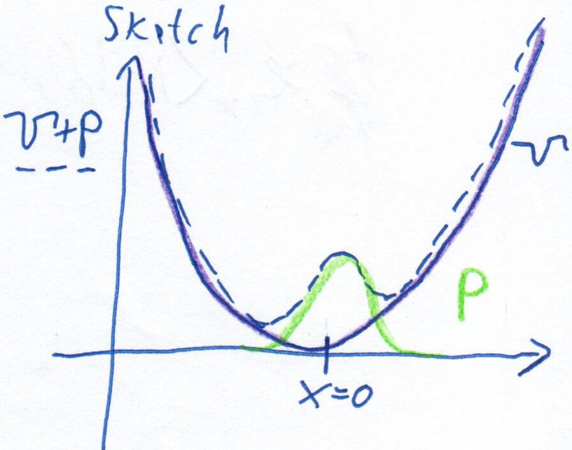
Again N atoms in harmonic trap, ignore interactions but add a small perturbing potential $\boxed{P(x)} = P_0 \exp\left(-\frac{x^2}{2\eta^2}\right)$

So (2.23) becomes

$$\hat{H} = \sum_{k=1}^{N}\left(-\frac{\hbar^2}{2m}\nabla^2_{x_k} + \boxed{V(x_k)} + P(x_k)\right) \qquad (2.24)$$

We can seperarately determine the contribution of $P(x)$ to the single-body operators and find

Sketch



$$\hat{H} = \left[\sum_n E_n \hat{a}_n^\dagger \hat{a}_n + \sum_{nm} \varkappa_{nm} \hat{a}_n^\dagger \hat{a}_m\right]$$

$$\varkappa_{nm} = \int dx\, \varphi_n^*(x)\, P(x)\, \varphi_m(x) \qquad (2.25)$$

In general $\varkappa_{nm}$ may be non-zero for $n \neq m$ $\Rightarrow$ Perturbation induces transitions between oscillator states n, m

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Fermi-blocking: What is the transition ~~rate~~ amplitude from $|A\rangle = |1, 1, 0, 0, ..\rangle \rightarrow |B\rangle = |2, 0, 0, 0 ...\rangle$ for Fermions?

should'nt write this for Fermions.
? What happens if we do?

$$\langle B|\hat{H}|A\rangle = \langle 0|\underbrace{\hat{a}_0 \hat{a}_0}\left(\sum_{nm} \varkappa_{nm} \hat{a}_n^\dagger \hat{a}_m\right)\hat{a}_0^\dagger \hat{a}_1^\dagger|0\rangle = 0$$

(i) $= 0$ from $\{\hat{a}_i, \hat{a}_j\} = 0$ in (2.17)

(ii) (or $= \langle 1|\hat{a}_0 = [\hat{a}_0^\dagger|1\rangle]^* = 0$ from (2.16.)

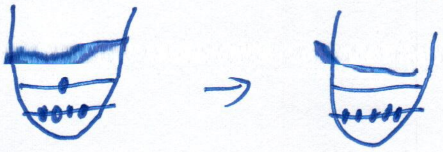
(iii) (or we say $\langle 2, 0, 0, ..|$ for Fermions didn't make sense to begin with.

Either way:

> Fermionic particles cannot make a transition into a state already occupied with another particle. (Fermi-blocking)

(Point: Algebra of operators preserves $\vec{N} \in$ binary for Fermions.)

Bose-enhancement: What is the transition amplitude from $|A'\rangle = |N,1,0,0,\dots\rangle \to |B'\rangle = |N+1,0,0,0,\dots\rangle$ for Bosons?



$$\langle B'|\hat{H}|A'\rangle = \langle N+1,0,0,\dots| \underbrace{\sum_{nm} \mathcal{H}_{nm}\, \hat{a}_n^{\dagger}\, \hat{a}_m}_{\text{Only term that will contribute is } \mathcal{H}_{01}\hat{a}_0^{\dagger}\hat{a}_1} |N,1,0,\dots\rangle$$

alternative/explicit (*)

$$= \langle N+1,0,0,\dots|\, \mathcal{H}_{01} \underbrace{\sqrt{N+1}\cdot 1}_{\text{see (2.16)}} \,|N+1,0,0,\dots\rangle = \sqrt{N+1}\,\mathcal{H}_{01} \quad \square$$

Bose-enhancement: The quantum transition amplitude of a Boson into a single-body state already occupied by N other identical Bosons is enhanced by a factor $\sqrt{N+1}$

(compared to if the state was empty)