Hamiltonian

- Many-body system's Hamiltonian is often of the form:

stands for x_i

$$\mathcal{H} \equiv \underbrace{\sum_i \left(-\frac{\hbar^2}{2m} \partial_i^2 + w(x_i) \right)}_{\sum_i \mathcal{H}_1(x_i)} + \sum_{(ij)} u(x_i\, x_j) \quad \text{— ①}$$

- In the 2nd quantization representation,

$$\hat{\mathcal{H}} = \int dx\, \hat{\psi}^{+}(x) \left(-\frac{\hbar^2}{2m} \partial^2 + w(x) \right) \hat{\psi}(x) + \frac{1}{2} \int dx dy\, \hat{\psi}^{+}(x) \hat{\psi}^{+}(y)\, u(x,y)\, \hat{\psi}(y)\, \hat{\psi}(x) \quad \text{— ②}$$

- Then, for an arbitrary N-particle state, Ψ and Ψ'
$|\Psi\rangle \equiv \int' d\mathbb{x}\, \Psi(\mathbb{x}) |\mathbb{x}\rangle$, we can prove,

$$\langle \Psi' | \hat{\mathcal{H}} | \Psi \rangle = \int' d\mathbb{x}\, \Psi'^{*}(\mathbb{x})\, \mathcal{H}\, \Psi(\mathbb{x}) \quad \text{— ③}$$

- In the following, we'll prove ③ for any fixed-N states.

One-Body Operators

- For an arbitrary function $w(x)$, we define

$$\hat{w}(x) \equiv \hat{\psi}^{+}(x)\, w(x)\, \psi(x)$$

and its integration over the real space

$$\hat{K} \equiv \int dx\, \hat{w}(x)$$

(the prime implies the prefactor $1/N!$ or the ordered $\mathbb{X}$) $\int'$

Then, for $|\Psi\rangle \equiv \int d\mathbb{X}\, \Psi(\mathbb{X})\, |\mathbb{X}\rangle$

$$\langle \Psi' | \hat{K} | \Psi \rangle = \int' d\mathbb{X}\, \Psi'^{*}(\mathbb{X}) \Big(\sum_i w(x_i) \Big) \Psi(\mathbb{X}) \quad ①$$

- Example: $w(x) = 1$ $\quad \hat{w}(x) \equiv \hat{n}(x) \equiv \hat{\psi}^{+}(x)\psi(x)$

$$\hat{N} = \int dx\, \hat{\psi}^{+}(x)\hat{\psi}(x)$$

$$\langle \Psi' | \hat{N} | \Psi \rangle = \int' d\mathbb{X}\, \Psi'^{*}(\mathbb{X}) \Big(\sum_i 1 \Big) \Psi(\mathbb{X})$$

$$= \int' d\mathbb{X}\, \Psi'^{*}(\mathbb{X})\; N\; \Psi(\mathbb{X})$$

$$= N$$

(have assumed that Ψ and Ψ' are both fixed-N states)

(We here assume the function $\Psi(\mathbb{X})$ satisfies the normalization $\int' d\mathbb{X}\, \Psi^{*}(\mathbb{X})\Psi(\mathbb{X}) = 1$.)

∘ Proof of ①

Using $\hat{\varphi}(x)\,|\mathbb{X}\rangle = \left(\sum_i \delta(x - x_i)\right)|\mathbb{X}^{[i]}\rangle$

where $|\mathbb{X}^{[i]}\rangle \equiv |(x_1\ x_2 \cdots x_{i-1}\ x_{i+1} \cdots x_N)\rangle$

$$\langle\Psi|\hat{K}|\Psi\rangle = \int' d\mathbb{X}' \int d\mathbb{X} \int dx\ \langle \mathbb{X}'|\,\Psi'^{+}(\mathbb{X}')\,\hat{\varphi}^{+}(x)\,w(x) \times \hat{\varphi}(x)\,\Psi(\mathbb{X})\,|\mathbb{X}\rangle$$

$$= \int' d\mathbb{X}' \int' d\mathbb{X} \int dx \left(\sum_j \delta(x - x'_j)\,\langle \mathbb{X}'^{[j]}|\right) \times \Psi'^{+}(\mathbb{X}')\,w(x)\,\Psi(\mathbb{X}) \left(\sum_i \delta(x - x_i)\,|\mathbb{X}^{[i]}\rangle\right)$$

$$= \sum_{ij} \int' d\mathbb{X}' \int' d\mathbb{X} \left(\delta(x_i - x'_j) \times \Psi'^{+}(\mathbb{X}')\,w(x_i)\,\Psi(\mathbb{X})\,\langle \mathbb{X}'^{[j]}|\mathbb{X}^{[i]}\rangle\right)$$

※

$$= \sum_i \int' d\mathbb{X}' \int' d\mathbb{X}\ \Psi'^{+}(\mathbb{X}')\,w(x_i)\,\Psi(\mathbb{X})\,\delta(\mathbb{X}' - \mathbb{X})$$

$$= \int' d\mathbb{X}\ \Psi'^{+}(\mathbb{X})\left(\sum_i w(x_i)\right)\Psi(\mathbb{X})$$

(※) If $i \neq j$ and both $\mathbb{X}$ and $\mathbb{X}'$ are ordered,
$\delta(x_i - x'_j)\,\langle \mathbb{X}'^{[j]}|\mathbb{X}^{[i]}\rangle = 0.$

If $i = j$, and $\mathbb{X}$ and $\mathbb{X}'$ are ordered,
$\delta(x_i - x'_j)\,\langle \mathbb{X}'^{[j]}|\mathbb{X}^{[i]}\rangle = \delta(\mathbb{X}' - \mathbb{X})$

Two-Body Operators

- For an arbitrary function $u(x, x')$, we define

$$\hat{u}(x, y) \equiv \hat{\psi}^{+}(x)\,\hat{\psi}^{+}(y)\,u(x, y)\,\hat{\psi}(y)\,\hat{\psi}(x)$$

and its integration over the real space

$$\hat{U} \equiv \int' dx\,dy\ \hat{u}(x, y) = \frac{1}{2}\int dx\,dy\ \hat{u}(x, y).$$

Then, for $|\Psi\rangle \equiv \int' d\mathbb{X}\ \Psi(\mathbb{X})\,|\mathbb{X}\rangle$

$$\langle \Psi' | \hat{U} | \Psi \rangle = \int' d\mathbb{X}\ \Psi'^{*}(\mathbb{X}) \Big(\sum_{(ij)} u(x_i, x_j) \Big) \Psi(\mathbb{X}) \qquad ①$$

$$\Big(\sum_{(ij)} \equiv \frac{1}{2} \sum_{i} \sum_{\substack{j \\ (i \neq j)}} \Big)$$

○ Proof of ①

$$\langle \Psi' | \hat{U} | \Psi \rangle = \frac{1}{2} \int' d\mathbb{x}' \int' d\mathbb{x} \int dx \int dy$$

$$\times \langle \mathbb{x}' | \Psi'^{*}(\mathbb{x}') \left(\frac{1}{2} \psi^{+}(x) \psi^{+}(y) u(x, y) \right.$$

$$\left. \times \ \psi(y) \psi(x) \right) \Psi(\mathbb{x}) | \mathbb{x} \rangle$$

$$\psi(y) \psi(x) | \mathbb{x} \rangle \doteq \sum_{\substack{i, j \\ (i \neq j)}} \delta(x_i - x) \delta(x_j - y) | \mathbb{x}^{[i, j]} \rangle$$

$$= \sum_{\substack{i, j \\ (i \neq j)}} \delta(x_i - x) \delta(x_j - y) | \mathbb{x}^{[i, j]} \rangle$$

$$\therefore \langle \Psi | \hat{U} | \Psi \rangle = \frac{1}{2} \sum_{\substack{i \neq j \\ i' \neq j'}} \int' d\mathbb{x}' \int d\mathbb{x} \int dx \int dy \ \Psi'^{*}(\mathbb{x}') \Psi(\mathbb{x})$$

$$\times \delta(x_i - x) \delta(x_j - y) \delta(x'_{i'} - x) \delta(x'_{j'} - y)$$

$$\times \langle \mathbb{x}'^{[i' j']} | \mathbb{x}^{[i j]} \rangle \times u(x, y)$$

$$= \frac{1}{2} \sum_{\substack{i \neq j \\ i' \neq j'}} \int' d\mathbb{x}' \int' d\mathbb{x} \quad u(x_i ; x_j) \Psi'^{*}(\mathbb{x}') \Psi(\mathbb{x})$$

$$\times \ \delta(x_i - x_{i'}) \delta(x_j - x_{j'})$$

$$\times \ \delta(\mathbb{x}'^{[i' j']} - \mathbb{x}^{[i j]})$$

$$= \frac{1}{2} \sum_{i \neq j} \int' d\mathbb{x}' \int' d\mathbb{x} \quad u(x_i \, x_j) \delta(\mathbb{x}' - \mathbb{x}) \Psi'^{*}(\mathbb{x}') \Psi(\mathbb{x})$$

$$= \int' d\mathbb{x} \ \Psi'^{*}(\mathbb{x}) \left(\sum_{(i j)} u(x_i \, x_j) \right) \Psi(\mathbb{x})$$

Differentiation Operator

- For $\hat{\Delta}_m \equiv \int dx\ \hat{\psi}^{\dagger}(x)\left(\frac{\partial}{\partial x}\right)^m \hat{\psi}(x)$, we can show

$$\langle \Psi' | \Delta_m | \Psi \rangle = \int' dX\ \Psi'^{*}(X)\left(\sum_i \left(\frac{\partial}{\partial x_i}\right)^m\right)\Psi(X) \quad (1)$$

$$\partial \equiv \frac{\partial}{\partial x}$$

∘ Proof of 1

$$\langle \Psi | \Delta_m | \Psi \rangle = \int' dX' \int' dX \int dx \, \underbrace{\langle X' | \hat{\psi}^{\dagger}(x) \, \partial^m \hat{\psi}(x) | X \rangle}_{\Psi'^{*}(X')\,\Psi(X)}$$

$$= \sum_{i,j} \int' dX' \int' dX \int dx \, \Psi'^{*}(X') \Psi(X) \langle X'^{[j]} | \delta(x - x'_j) \, \partial^m \delta(x - x_i) | X^{[i]} \rangle$$

$$= \sum_{i,j} \int' dX' \int' dX \int dx \, \Psi'^{*}(X') \Psi(X) \langle X'^{[j]} | \delta(x - x'_j) (-\partial_i)^m \delta(x - x_i) | X^{[i]} \rangle$$

$$\left(\partial_i \equiv \frac{\partial}{\partial x_i} \right)$$

$$= \sum_{i,j} \int' dX' \int' dX \int dx \, \Psi'^{*}(X') \, \partial_i^m \Psi(X) \, \delta(x - x'_j) \, \delta(x - x_i) \times \langle X'^{[j]} | X^{[i]} \rangle$$

$$= \sum_{i,j} \int' dX' \int' dX \, \Psi'^{*}(X') \, \partial_i^m \Psi(X) \, \delta_{ij} \, \delta(X' - X)$$

$$= \int' dX \, \Psi'^{*}(X) \left(\sum_i \partial_i^m \right) \Psi(X)$$

Non-Interacting Bosons

- When there is no interaction $\left(\begin{array}{c} u = 0 \\ \mathcal{H} = K(x) \equiv -\frac{\hbar^2}{2m}\partial^2 + w \end{array} \right)$

$$\hat{\mathcal{H}} = \hat{K} = \int dx \; \hat{\psi}^+(x) K(x) \hat{\psi}(x)$$

$$= \sum_{\kappa\kappa'} \int dx \; \phi^*_{\kappa'}(x) b^+_{\kappa'} K(x) \phi_\kappa(x) b_\kappa$$

$$= \sum_{\kappa\kappa'} K_{\kappa'\kappa} b^+_{\kappa'} b_\kappa$$

$$K_{\kappa'\kappa} \equiv \int dx \; \phi^*_{\kappa'}(x) K(x) \phi_\kappa(x)$$

- Example : If we take $\phi_\kappa(x)$ to be a plane wave $\phi_{\mathbb{k}}(x) = e^{i\mathbb{k}x}$ $(\kappa = \mathbb{k})$ $H^{(1)}_{\kappa'\kappa}$ is simply the Fourier transformation of $H^{(1)}$. The 1-body Hamiltonian.

- When we take $\phi_\kappa(x)$ to be the one with which $\hat{K}$ is diagonal, $\mathcal{H}$ becomes simple.

$$\hat{\mathcal{H}} = \sum_\kappa \epsilon_\kappa b^+_\kappa b_\kappa \qquad (K_{\kappa'\kappa} = \epsilon_\kappa \delta_{\kappa'\kappa})$$

- Example : If we consider particles confined in a cube with periodic boundary condition, and $u=0$, the plane waves diagonalize $H^{(1)}$:

$$\hat{\mathcal{H}} = \sum_{\mathbb{k}} \epsilon_{\mathbb{k}} b^+_{\mathbb{k}} b_{\mathbb{k}}$$

$$\epsilon_{\mathbb{k}} = \frac{\hbar^2 \mathbb{k}^2}{2m} \qquad \mathbb{k} = \frac{2\pi}{L} \times (\text{integer vector})$$

L : the system size

Finite-Temperature — Density Operator

- The thermodynamic properties can be derived from the density operator, the natural generalization of the classical Boltzmann distribution.

$$\hat{\rho} \equiv Z^{-1} e^{-\beta(\hat{\mathcal{H}} - \mu \hat{N})} \quad \left(Z \equiv \mathrm{Tr}\, e^{-\beta(\hat{\mathcal{H}} - \mu \hat{N})} \right) \quad \text{—— (1)}$$

(N : the total number of the particles.
Tr : the trace over the Fock space.)

- The expectation value of an arbitrary quatity Q :

$$\langle \hat{Q} \rangle = \mathrm{Tr}(\hat{\rho} \hat{Q})$$

Ex: The energy: $E = \langle \hat{\mathcal{H}} \rangle = \mathrm{Tr}(\hat{\rho} \hat{\mathcal{H}})$

- (1) is the only generalization that satisfies
  - (i) agrees with the classical Boltzmann distribution when the basis is chosen so that the Hamiltonian is diagonal
  - (ii) yields the same expectation value regardless of the choice of the basis.

Bose Distribution Function.

- For the non-interacting bosons, the density operator can be simply expressed as

$$\hat{\rho} = Z^{-1} \prod_{\kappa} e^{-\beta(\epsilon_\kappa - \mu) b_\kappa^+ b_\kappa}$$

- The expectation value of $\hat{n}_\kappa \equiv b_\kappa^+ b_\kappa$, since all the operators are diagonal in the basis where $\hat{n}_\kappa$ is diagonal, is

$$\langle n_\kappa \rangle = \mathrm{Tr}\left(\hat{\rho}\, b_\kappa^+ b_\kappa\right)$$

$$= \sum_{n_\kappa=0}^{\infty} e^{-\beta(\epsilon_\kappa - \mu) n_\kappa} n_\kappa \Big/ \sum_{n_\kappa=0}^{\infty} e^{-\beta(\epsilon_\kappa - \mu) n_\kappa}$$

$$= \frac{1}{e^{\beta(\epsilon_\kappa - \mu)} - 1} \equiv f_\kappa$$

This is called the Bose distribution function.

- Bose-Einstein condensation

As the temperature decreases, because of the exponential nature of the distribution function, a large portion of the population may take a relatively few number of states. This change may take place in a singular fashion, which is called Bose-Einstein condensation (BEC).

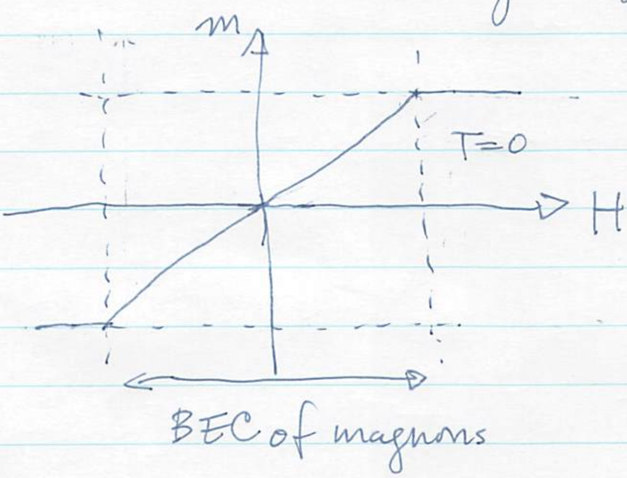
Most text books illustrate the BEC by the free bosons. While the concept of "condensation" is common to all BEC, the effect of interation may change the nature of the transition qualitatively.

ex 1 condensation of free Bosons
(the example found most frequently in the under-graduate text books)

ex 2 more realistic interaction with repulsive (hard core) interaction

$$u(x-y) = \infty \quad (\text{if } |x-y| \leq d)$$

ex 3 (spontaneous) transverse magnetization in magnets.



$D \geq 2$ AFH at $T=0$

ex 4 KT phase in 2 (or 1+1) dim. easy-plane magnets.