Topics in Quantum Many-Body Theory

Week I 2025.02.27

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P. Jakubczyk Thursdays $8^{15}-10^{00}$
K. Byczuk Tuesdays $11^{15}-13^{00}$
} Equivalent roles of lecturers/tutors

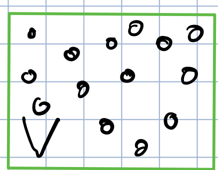
- Course assumes familiarity with QM I/II and Stat. Phys I.
- For the first part → book by Negele, Orland
  → book by Dupuis
  → book by Wegner
  → book by Zinn-Justin

Grading based on oral exam → Topics given before the exam
→ Homeworks

Intro: Many-body problem (in equilibrium)

$N \simeq 10^{23}$ particles at fixed (say) (T, V) $\qquad (N \gg 1 \longrightarrow N \to \infty)$

Microscopic description $\hat{H}(\{\hat{r}_i, \hat{p}_i\}_{i=1}^{N}) \longrightarrow$ Macroscopic description

T 

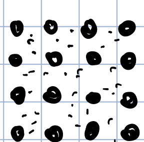
$p(T,V,N)$, $\vec{j}(T,V,N,\vec{E})$, ...

(thermodynamic and transport properties)

Example (prototype) many-body Hamiltonian

lattice of ions + electrons

e.g. metallic material



$$H_e = \sum_i \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i<j} V_{ee}(\vec{r}_i - \vec{r}_j)$$

$$H_i = \sum_I \frac{\vec{P}_I^{\,2}}{2M} + \sum_{I<J} V_{ii}(\vec{R}_J - \vec{R}_I)$$

$$H_{ei} = \sum_{i,I} V_{ei}(\vec{R}_I - \vec{r}_i)$$

$$H = H_e + H_i + H_{ei}$$

(certain elements, e.g. lattice structure put in "by hand").

- Not fully realistic (spin, impurities...)
- Valid only down to some length scale (e.g. does not resolve ions' structure)
- Valid only up to some energy scale (too high T → lattice melts...)

Non-interacting systems worked out in previous courses

Statistical physics problem : $Z = \mathrm{Tr}\, e^{-\beta H} \longrightarrow Z = \int \mathcal{D}\phi\, e^{-S[\phi]}$
(EQUILIBRIUM) (path integral formulation)

NOTATION SETTING

Notation/construction (standard) of many body states/operators (see previous semester, or Negele-Orland book)

$\mathcal{H}$ - space of one-particle states

$\{|\alpha\rangle\}$ - orthonormal basis of $\mathcal{H}$ $\quad ((\vec{k},\sigma)) \hookrightarrow \alpha$

$$\mathcal{H}_N := \underbrace{\mathcal{H}\otimes\mathcal{H}\otimes\ldots\otimes\mathcal{H}}_{N \text{ times}}$$

$|\alpha_1\ldots\alpha_N) := |\alpha_1\rangle\otimes|\alpha_2\rangle\otimes\ldots\otimes|\alpha_N\rangle$ - orthonormal basis of $\mathcal{H}_N$

Systems of identical particles - only totally symmetric or antisymmetric states observed in nature

$$\zeta := \begin{cases} +1 & \text{bosons} \\ -1 & \text{fermions}\end{cases} \qquad [A,B]_{-\zeta} := \begin{cases} AB - BA & \text{FOR BOSONS} \\ AB + BA & \text{FOR FERMIONS}\end{cases} = AB - \zeta BA$$

Symmetrization/antisymmetrization operator $P_{\{B\}\{F\}}$

$$|\alpha_1\ldots\alpha_N\} := \sqrt{N!}\, P_{\{B\}\{F\}}|\alpha_1\ldots\alpha_N) = \frac{1}{\sqrt{N!}}\sum_P \zeta^P |\alpha_{P_1}\rangle\otimes|\alpha_{P_2}\rangle\otimes\ldots\otimes|\alpha_{P_N}\rangle$$

$P_{\{B\}\{F\}}$ is a projection $\begin{cases} \mathcal{B}_N := P_B \mathcal{H}_N \\ \mathcal{F}_N := P_F \mathcal{H}_N \end{cases}$

"Occupation number" representation

Orthonormal basis of $\mathcal{B}_N/\mathcal{F}_N$: $|\alpha_1,\alpha_2\ldots\alpha_N\rangle = \frac{1}{\sqrt{\prod_\alpha n_\alpha!}}|\alpha_1\ldots\alpha_N\} = |n_1,n_2,\ldots\rangle$ - symmetrized, normalized state with n_1 particles in state 1 and so on.

$$= \frac{1}{\sqrt{N!\prod_\alpha n_\alpha!}}\sum_P \zeta^P |\alpha_{P_1}\rangle\otimes|\alpha_{P_2}\rangle\otimes\ldots\otimes|\alpha_{P_N}\rangle$$

Creation/annihilation operators: $\quad a^+_\alpha|\alpha_1\ldots\alpha_N\} := |\alpha\,\alpha_1\ldots\alpha_N\}$

$$a^+_\alpha|\alpha_1\ldots\alpha_N\rangle = \sqrt{n_\alpha+1}\,|\alpha\,\alpha_1\ldots\alpha_N\rangle$$

Fock space : $\mathcal{B} = \mathcal{B}_0\oplus\mathcal{B}_1\oplus\mathcal{B}_2\oplus\ldots = \bigoplus_{n=0}^{\infty}\mathcal{B}_n$

$\mathcal{F} = \mathcal{F}_0\oplus\mathcal{F}_1\oplus\mathcal{F}_2\oplus\ldots = \bigoplus_{n=0}^{\infty}\mathcal{F}_n$

vacuum state $\quad a^+_\alpha|0\rangle = |\alpha\rangle$

$|\lambda_1 \ldots \lambda_N\} = a^+_{\lambda_1} a^+_{\lambda_2} \ldots a^+_{\lambda_N} |0\rangle$

$|\lambda_1 \ldots \lambda_N\rangle = \frac{1}{\sqrt{\prod_\lambda n_\lambda!}} a^+_{\lambda_1} a^+_{\lambda_2} \ldots a^+_{\lambda_N} |0\rangle$

Creation operators generate the Fock space by repeated action on the vacuum.

Commutation relations: $[a_\lambda, a^+_\mu]_{-\zeta} = \delta_{\lambda\mu}$

One-body operators: $\hat{U} = \sum_{\alpha\alpha'} \langle\alpha|\hat{U}|\alpha'\rangle a^+_\alpha a_{\alpha'}$

Two-body operators: $\hat{V} = \frac{1}{2} \sum_{\alpha_1\alpha_2\alpha_3\alpha_4} (\alpha_1\alpha_2|\hat{V}|\alpha_4\alpha_3)\, a^+_{\alpha_1} a^+_{\alpha_2} a_{\alpha_3} a_{\alpha_4}$

COHERENT STATES

IN QMI POSITION AND MOMENTUM EIGENSTATES PLAY A DISTINCT ROLE (SINCE $H = H(\bar{r}, \bar{p})$)
IN PARTICULAR THE PATH-INTEGRAL REPRESENTATION REQUIRES $id = \sum |\bar{p}\rangle\langle\bar{p}|$ → SEE THE CLASS OF K.B.

IN OCCUPATION NUMBER REPRESENTATION OPERATORS ARE EXPRESSED BY COMBINATIONS OF PRODUCTS OF CREATION/ANNIHILATION OPERATORS

NATURAL QUESTION: CAN WE HAVE BASES OF FOCK SPACE CONSTRUCTED FROM EIGENSTATES OF CREATION/ANNIHILATION OPERATORS?

{ a_α, a^+_α ARE NOT SELF-ADJOINT }

COHERENT STATES ⟶ EIGENSTATES OF ANNIHILATION OPERATORS

{ Existence of eigenstates of creation op. and annihilation op.

$|\phi\rangle$ - general vector of the Fock space. Can be expanded as $|\phi\rangle = \sum_{N=0}^{\infty} \sum_{\alpha_1 \ldots \alpha_N} \phi_{\alpha_1 \ldots \alpha_N} |\alpha_1 \ldots \alpha_N\rangle$ must necessarily have a component with a minimum number of particles. If we apply any creation op. to $|\phi\rangle$ the minimum number of particles is increased by one – the resulting state cannot be a multiple of the original state ⟹ creation op. cannot have an eigenstate. Nothing a priori forbids the existence of eigenstates of annihilation op. }

Assuming we construct an eigenstate of the annihilation operators: $\forall_\alpha \; a_\alpha |\phi\rangle = \phi_\alpha |\phi\rangle$

Fundamental difference arises between fermions and bosons: $[a_\alpha, a_\beta]_{-\zeta} = 0$

$\Rightarrow [a_\alpha, a_\beta]_{-\zeta} |\phi\rangle = (\phi_\alpha \phi_\beta - \zeta \phi_\beta \phi_\alpha) |\phi\rangle = 0 \quad = \phi_\alpha \phi_\beta = \zeta \phi_\beta \phi_\alpha$

→ eigenvalues commute for bosons ($\mathbb{C}$-numbers ok) but anticommute for fermions!!

→ Grassman numbers – see later.

Treat the two cases separately – bosons first.

Coherent states for bosons

The eigenvalues may be real or complex numbers. $a_\alpha|\phi\rangle = \phi_\alpha|\phi\rangle$

Expand in occupation number representation : $|\phi\rangle = \sum_{n_{\alpha_1}, n_{\alpha_2}, \dots, n_{\alpha_p}, \dots} \phi_{n_{\alpha_1} n_{\alpha_2} \dots n_{\alpha_p} \dots} |n_{\alpha_1} n_{\alpha_2} \dots n_{\alpha_p} \dots\rangle$ (✱)

normalized, symmetrized state with n_{α_1} particles in $|\alpha_1\rangle$, n_{α_2} in $|\alpha_2\rangle$ and so on.

Now: explicit construction of $|\phi\rangle$ such that $a_\alpha|\phi\rangle = \phi_\alpha|\phi\rangle$ for any α and $\phi_\alpha \in \mathbb{C}$.

$$a_{\alpha_i}|\phi\rangle = \sum_{n_{\alpha_1} \dots n_{\alpha_i} \dots} \phi_{n_{\alpha_1} \dots n_{\alpha_i} \dots} \sqrt{n_{\alpha_i}}\, |n_{\alpha_1} n_{\alpha_2} \dots (n_{\alpha_i}-1) \dots\rangle = \phi_{\alpha_i} \sum_{n_{\alpha_1} \dots n_{\alpha_i} \dots} \phi_{n_{\alpha_1} \dots n_{\alpha_i} \dots} |n_{\alpha_1} n_{\alpha_2} \dots n_{\alpha_i} \dots\rangle$$

Equate coefficients in front of $|n_{\alpha_1} n_{\alpha_2} \dots (n_{\alpha_i}-1) \dots\rangle$

$$\phi_{n_{\alpha_1} \dots n_{\alpha_i} \dots} \sqrt{n_{\alpha_i}} = \phi_{\alpha_i} \phi_{n_{\alpha_1} \dots n_{\alpha_i}-1 \dots} \longrightarrow \phi_{n_{\alpha_1} \dots n_{\alpha_i} \dots} = \frac{1}{\sqrt{n_{\alpha_i}}} \phi_{\alpha_i} \phi_{n_{\alpha_1} \dots (n_{\alpha_i}-1) \dots} \quad (✱✱) \quad (\text{FOR ANY } \alpha_i)$$

Fix the coefficient for the vacuum state in (✱) to be 1. Use (✱✱) to relate each coefficient in (✱) to the vacuum state coefficient.

$$\rightarrow \phi_{n_{\alpha_1} n_{\alpha_2} \dots n_{\alpha_i} \dots} = \frac{\phi_{\alpha_1}^{n_{\alpha_1}}}{\sqrt{n_{\alpha_1}!}} \frac{\phi_{\alpha_2}^{n_{\alpha_2}}}{\sqrt{n_{\alpha_2}!}} \dots \frac{\phi_{\alpha_i}^{n_{\alpha_i}}}{\sqrt{n_{\alpha_i}!}} \dots$$

Substitute this into (✱), use the fact that $|n_{\alpha_1} n_{\alpha_2} \dots n_{\alpha_i} \dots\rangle = \frac{(a_{\alpha_1}^\dagger)^{n_{\alpha_1}}}{\sqrt{n_{\alpha_1}!}} \frac{(a_{\alpha_2}^\dagger)^{n_{\alpha_2}}}{\sqrt{n_{\alpha_2}!}} \dots \frac{(a_{\alpha_i}^\dagger)^{n_{\alpha_i}}}{\sqrt{n_{\alpha_i}!}} \dots |0\rangle$

$$\longrightarrow |\phi\rangle = \sum_{n_{\alpha_1} n_{\alpha_2} \dots} \frac{(\phi_{\alpha_1} a_{\alpha_1}^\dagger)^{n_{\alpha_1}}}{n_{\alpha_1}!} \frac{(\phi_{\alpha_2} a_{\alpha_2}^\dagger)^{n_{\alpha_2}}}{n_{\alpha_2}!} \dots |0\rangle \quad \left\{\text{EVERYBODY COMMUTES}\right\} \longrightarrow |\phi\rangle = e^{\sum_\alpha \phi_\alpha a_\alpha^\dagger} |0\rangle$$

(no restrictions on the eigenvalues $\phi_\alpha \in \mathbb{C}$)

Some properties:

- Action of $a_\alpha^\dagger$ on $|\phi\rangle$: $a_\alpha^\dagger|\phi\rangle = a_\alpha^\dagger e^{\sum_{\alpha'} \phi_{\alpha'} a_{\alpha'}^\dagger} |0\rangle = \frac{\partial}{\partial \phi_\alpha} e^{\sum_{\alpha'} \phi_{\alpha'} a_{\alpha'}^\dagger} |0\rangle = \frac{\partial}{\partial \phi_\alpha} |\phi\rangle$

- Overlap of two coherent states : $\langle\phi| = \langle 0| e^{\sum_\alpha \phi_\alpha^* a_\alpha}$

$$\langle\phi|\phi'\rangle = \sum_{n_{\alpha_1} n_{\alpha_2} \dots} \sum_{n'_{\alpha_1} n'_{\alpha_2} \dots} \left(\frac{(\phi_{\alpha_1}^*)^{n_{\alpha_1}}}{\sqrt{n_{\alpha_1}!}} \frac{(\phi_{\alpha_2}^*)^{n_{\alpha_2}}}{\sqrt{n_{\alpha_2}!}} \dots\right) \left(\frac{(\phi'_{\alpha_1})^{n'_{\alpha_1}}}{\sqrt{n'_{\alpha_1}!}} \frac{(\phi'_{\alpha_2})^{n'_{\alpha_2}}}{\sqrt{n'_{\alpha_2}!}} \dots\right) \underbrace{\langle n_{\alpha_1} n_{\alpha_2} \dots | n'_{\alpha_1} n'_{\alpha_2} \dots\rangle}_{= \delta_{n_{\alpha_1} n'_{\alpha_1}} \delta_{n_{\alpha_2} n'_{\alpha_2}} \dots} =$$

$$= \sum_{n_{\alpha_1} n_{\alpha_2} \dots} \frac{(\phi_{\alpha_1}^* \phi'_{\alpha_1})^{n_{\alpha_1}} (\phi_{\alpha_2}^* \phi'_{\alpha_2})^{n_{\alpha_2}} \dots}{n_{\alpha_1}!\ n_{\alpha_2}! \dots} = e^{\sum_\alpha \phi_\alpha^* \phi'_\alpha}$$

- Closure relation : $\int \prod_\alpha \left(\frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i}\right) e^{-\sum_\alpha \phi_\alpha^* \phi_\alpha} |\phi\rangle\langle\phi| = id$ ⟶ HOMEWORK — DEMONSTRATE THIS

UNITY OF Fock SPACE

$$\frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i} \equiv \frac{d(\mathrm{Re}\phi_\alpha)\, d(\mathrm{Im}\phi_\alpha)}{\pi}$$

- Useful expression for the trace (in Fock space) : $\mathrm{Tr}\,A = \sum_n \langle n|A|n\rangle =$ ($\{|n\rangle\}$ - BASIS OF FOCK SPACE)

$$= \int \prod_\alpha \frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i} e^{-\sum_\alpha \phi_\alpha^*\phi_\alpha} \sum_n \langle n|\phi\rangle\langle\phi|A|n\rangle = \int \prod_\alpha \frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i} e^{-\sum_\alpha \phi_\alpha^*\phi_\alpha} \langle\phi|A \underbrace{\sum_n |n\rangle\langle n|}_{=id}\phi\rangle =$$

$$= \int \prod_\alpha \frac{d\phi_\alpha^* d\phi_\alpha}{2\pi i} e^{-\sum_\alpha \phi_\alpha^*\phi_\alpha} \langle\phi|A|\phi\rangle$$

- Useful property: consider $A(a_\alpha^\dagger, a_\alpha)$ (normal ordered) $\longrightarrow \langle\phi|A(a_\alpha^\dagger, a_\alpha)|\phi'\rangle = A(\phi_\alpha^*, \phi_\alpha')\, e^{\sum_\alpha \phi_\alpha^*\phi_\alpha'}$

For example: 2-body interaction: $\langle\phi|V|\phi'\rangle = \frac{1}{2}\sum_{\lambda\mu\nu\xi} (\lambda\mu|V|\xi\nu)\langle\phi|a_\lambda^\dagger a_\mu^\dagger a_\nu a_\xi|\phi'\rangle =$

$$= \frac{1}{2}\sum_{\lambda\mu\nu\xi} (\lambda\mu|V|\xi\nu)\, \phi_\lambda^* \phi_\mu^* \phi_\nu' \phi_\xi'\, e^{\sum_\alpha \phi_\alpha^*\phi_\alpha'}$$

- Occupation number n_α (for each α) is Poisson distributed with mean value $|\phi_\alpha|^2$:

$$|\langle n_{\alpha_1} n_{\alpha_2} \ldots|\phi\rangle|^2 = \prod_\alpha \frac{|\phi_\alpha|^{2n_\alpha}}{n_\alpha!}$$

$$P(n) = e^{-\lambda}\frac{\lambda^n}{n!}$$

$\lambda \to |\phi_\alpha|^2$

- $\langle\hat{N}\rangle = \frac{\langle\phi|\hat{N}|\phi\rangle}{\langle\phi|\phi\rangle} = \frac{\sum_\alpha\langle\phi|a_\alpha^\dagger a_\alpha|\phi\rangle}{\langle\phi|\phi\rangle} = \sum_\alpha \phi_\alpha^*\phi_\alpha$

- $\langle\hat{N}^2\rangle - \langle\hat{N}\rangle^2 = (\bullet) = \langle\hat{N}\rangle$

In the thermodynamic limit $\langle\hat{N}\rangle \to \infty$

and $\frac{\sigma}{\langle\hat{N}\rangle} = \frac{1}{\sqrt{\langle\hat{N}\rangle}} \to$ sharply peaked around $\langle\hat{N}\rangle$.