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BOSE-EINSTEIN CONDENSATION -
- a math-phys perspective

Plan

1. Quantum statistical mechanics
2. BEC in ideal gas
3. Scaling regimes
4. BEC in mean-field systems
5. Bogoliubov theory: heuristics and results

1. Quantum Statistical Mechanics

- framework / physical theory that allows to derive macroscopic properties of systems starting from first (quantum) principle

many particles

1.1 Many-body quantum mechanics

- Quantum system: $\mathcal{H}$, H → Hamiltonian

  separable Hilbert space

e.g.

one-body problem $\quad H = -\Delta + V(x)$, $\quad \mathcal{H} = L^2(\mathbb{R}^3)$, $\psi \equiv \psi(x)$

- What if there are many particles? (N - number of particles)

$$\mathcal{H}^N = \mathcal{H} \otimes \mathcal{H} \otimes \mathcal{H} \ldots \otimes \mathcal{H} \quad \text{- N-fold tensor product}$$

$\psi_N = \psi_N(x_1, x_2, \ldots, x_N)$ $\quad x_i \in \mathbb{R}^3$ $\quad \mathcal{H}^N = L^2(\mathbb{R}^3) \otimes \cdots \otimes L^2(\mathbb{R}^3) \simeq L^2(\mathbb{R}^{3N})$

How does the Hamiltonian look like?

$$H_N = \sum_{i=1}^{N} \left(-\Delta_{x_i} + V(x_i)\right) \quad \text{— non-interacting}$$

what is $-\Delta_{x_i} := \mathbb{1} \otimes \mathbb{1} \otimes \cdots \otimes \underbrace{-\Delta}_{i\text{-th variable}} \otimes \mathbb{1} \cdots \otimes \mathbb{1}$

- if there are many particles one can and should add interactions.

$$H_N = \sum_{i=1}^{N} \left(-\Delta_{x_i} + V(x_i) \right) + \sum_{i<j} \underbrace{w(x_i - x_j)}_{\text{two-body interaction}}$$

from now on: $w \geq 0$, $\hat{w} \geq 0$, w - smooth, decaying / compactly supported
NICE

- many particles $\longrightarrow$ statistics bosons / fermions
we deal with BOSONS!

$\hookrightarrow$ symmetric wave function

$$\psi_N(x_1, \ldots, x_i, \ldots, x_j, \ldots x_N) = \psi_N(x_1, \ldots, x_{i-1}, x_j, x_{i+1}, \ldots, x_i, \ldots x_N)$$
$$\forall i,j$$

in particular $L^2_{sym}(\mathbb{R}^{3N}) = L^2(\mathbb{R}^3) \otimes_{sym} L^2(\mathbb{R}^3) \otimes_{sym} \cdots \otimes_{sym} L^2(\mathbb{R}^3)$
(via $P_+ = (N!)^{-1} \sum_{\sigma \in S_N} U_\sigma$ acting on pure tensors.)

<u>Fact</u> / exercise

Assume $H = \sum_{i=1}^{N} T_i$ (ideal gas), bosons

If E_0 is the ground state energy $\left(E_0 = \inf_{\|\psi\|=1} \langle \psi, H\psi \rangle \right)$ of T (one-body), the NE_0 is the ground state energy of H. Moreover, if u is the ground state, then $u^{\otimes N} = u(x_1) \ldots u(x_N)$ is the ground state of H.

1.2 Quantum statistical mechanics

In general

- states of quantum systems are described (in general) by mixed states, i.e. positive, trace class operators with trace $= 1$.

- One special class of states are equilibrium states at positive temperatures: $T > 0$.

↳ canonical ensemble (fixed number of particles)

$$G(\beta, N) = \frac{e^{-\beta H_N}}{\mathrm{Tr}_{\mathcal{H}^N} e^{-\beta H_N}}, \quad \beta = 1/T.$$

$$\langle A \rangle = \mathrm{Tr}\,(A\, G(\beta, N))$$

↳ knowing the Gibbs state allows to compute the free energy

$$F(\beta, N) = -\frac{1}{\beta} \ln \mathrm{Tr}\, e^{-\beta H_N}$$

from which one can compute thermodynamical properties of the system ($S = -\left(\frac{\partial F}{\partial T}\right)_{V,N}$, $p = -\frac{\partial F}{\partial V}$ ...) in particular phase transitions (which occur when there is a discontinuity in the derivative of the free energy).

↳ grand canonical ensemble - non-fixed N

$$G^{gc}(\beta, \mu) = \frac{e^{-\beta(H - \mu N)}}{\mathrm{Tr}\, e^{-\beta(H - \mu N)}}$$

Hilbert space now has to include a non-fixed number of particles → Fock space (bosonic)

$$\mathcal{F}(\mathcal{H}) = \bigoplus_{N=0}^{\infty} \mathcal{H}^N \qquad (\underbrace{\mathcal{H}^0 \equiv \mathbb{C}}_{\text{vacuum}})$$

given $\Phi = \{\Phi^{(n)}\}_{n \geq 0} \in \mathcal{F}$, $\Psi = \{\Psi^{(n)}\}$ inner product

$$\langle \Phi, \Psi \rangle_{\mathcal{F}} = \sum_{n \geq 0} \langle \Phi^{(n)}, \Psi^{(n)} \rangle_{\mathcal{H}^n}$$

- number operator $(\mathcal{N}\Psi)^{(n)} = n\Psi^{(n)}$ (for any Ψ: $\sum n^2 \|\psi^{(n)}\|_{\mathcal{H}^n} < \infty$)

- How to lift operators to the Fock space?

1.3. Second quantization

given a one-particle operator O, let us define as before $O^{(n)} = \sum_{j=1}^{n} O_j^{(n)}$ $O_j \rightsquigarrow$ j-th position

Df Second quantization of O:

$$(d\Gamma(O)\Psi)^{(n)} = O^{(n)}\Psi^{(n)}$$

$$d\Gamma(O) = \bigoplus_{N=1}^{\infty} \sum_{j=1}^{N} O_j$$

Useful representation of operators lifted to $\mathcal{F}$ via creation/annihilation operators: $\Psi = \{\psi^{(n)}\}_{n\geq 0}$

$$(a^*(f)\Psi)^{(n)}(x_1, \dots, x_n) = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} f(x_j)\,\psi^{(n-1)}(x_1, \dots, \cancel{x_j}, x_{j+1}, \dots, x_n)$$

$\psi^{(n)} \in L^2_s(\Omega^n)$, $f \in L^2_s(\Omega)$

creation operator: creates/adds a particle

$$a^*(f) : \mathcal{H}^{N-1} \to \mathcal{H}^N$$

$$(a(f)\psi^{(n)})(x_1, \dots, x_n) = \sqrt{n+1}\int dx\, \overline{f(x)}\, \psi^{(n+1)}(x_1, \dots, x_n, x)$$

annihilation operator: $a(f) : \mathcal{H}^N \to \mathcal{H}^{N-1}$

They satisfy canonical commutation relations:

$$[a(f), a^*(g)] = \langle f, g\rangle_{\mathcal{H}} \qquad [a(f), a(g)] = 0$$

$[A,B] = AB - BA$

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Fact / exercise

Let $\{u_n\}_{n\geq 1}$ be an ONB for $\mathcal{H}$ and denote $a_n = a(u_n)$ / $a_n^* = a^*(u_n)$. Then

$$d\Gamma(h) = \sum_{m,n\geq 1} \langle u_m, h u_n \rangle a_m^* a_n \quad \text{for } h\text{-self-adjoint}$$

Similarly, the second quantization of a self-adjoint two-body operator w_{ij}, i.e.

$$\bigoplus_{n=0}^{\infty} \Big(\sum_{1\leq i<j\leq n} w_{ij} \Big) = 0 \oplus 0 \oplus w \oplus (w_{12} + w_{23} + w_{13}) \oplus \dots$$

is given by $\frac{1}{2} \sum_{m,n,p,q\geq 1} \langle u_m \otimes u_n, w\, u_p \otimes u_q \rangle_{\mathcal{H}^2} a_m^* a_n^* a_p a_q$ ⊠

Examples

a) $\mathcal{H} = L^2(\Lambda)$ $\quad \Lambda = [0,L]^3$ p.b.c. $\quad u_k(x) = \frac{1}{\sqrt{|\Lambda|}} e^{-ikx}$, $k \in \frac{2\pi}{L}\mathbb{Z}^3$

then $\sum_{i=1}^{N} -\Delta_{x_i} \rightsquigarrow \sum_{p\in\frac{2\pi}{L}\mathbb{Z}^3} p^2 a_p^* a_p$

$\mathcal{N} = \sum_p a_p^* a_p$

interaction:

$$\sum_{i<j} w_{ij} \rightsquigarrow \frac{1}{2} \sum_{p,k,q} \hat{w}(p)\, a_{k+p}^* a_{q-p}^* a_k a_q$$

$$H = \sum_p p^2 a_p^* a_p + \frac{1}{2} \sum_{p,k,q} \hat{w}(p)\, a_{k+p}^* a_{q-p}^* a_k a_q$$

(second quantization of a many-body Hamiltonian with two-body interactions)

1.4. Reduced densities

- Gibbs state — full knowledge but difficult
- access to average behaviour of single particle via one-body reduced density matrix:

$$\gamma_G^{(1)} = N \,\mathrm{Tr}_{2 \to N}\, G(\beta, N) \qquad \text{(positive, trace class operator on } \mathcal{H}\text{)}$$

$\downarrow$

integral kernel $\quad \gamma_G^{(1)}(x,y) = \mathrm{Tr}\,[a_x^* a_y G]$

for vector/pure states:

$$\gamma_{\Psi_N}^{(1)}(x,y) = N \int dx_2 \ldots dx_N \, \Psi_N(x, x_2 \ldots x_N) \overline{\Psi_N}(y, x_2, \ldots x_N)$$

In particular, for one-body observables

$$\langle A \rangle = \mathrm{Tr}\,(A \,\gamma_{\Psi_N}^{(1)})$$

Finally:

$$\hat{\gamma}_G^{(1)}(p) = \mathrm{Tr}\,[a_p^* a_p G]$$

expected number of particles with momentum p