612 Midterm 2 review

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Integral formular

- Gaussian integral

$$\int e^{-ax^2}dx = \sqrt{\frac{\pi}{a}}$$

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$$\int \frac{k^2 dk}{\exp\left(ak^2\right)-1} = \frac{\sqrt{\pi}}{2a^{3/2}}\cdot\zeta\left(\frac{3}{2}\right)$$

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Quantum Mechanics of identical particles

- Hilbert space of a two particle system is generated by tensor product of 1-particle states

$$|a,\ b\rangle = |a\rangle_1 \otimes |b\rangle_2$$

here $|a\rangle$ and $|b\rangle$ include space coordinates and other inner d.o.f like spin.

- P_{ij} is the operator of swapping i^{th} and j^{th} particle in the state, then in QM of identical particles, we have $P_{ij}|\psi\rangle = e^{i\phi}|\psi\rangle$, which means the same state up to a possible phase.

- In 1-D or 3-D space, $\phi = 0\ or\ \pi$. Fermions have $P_{ij}|\psi\rangle = -|\psi\rangle$ and Bosons have $P_{ij}|\psi\rangle = +|\psi\rangle$.

- In 2-D, this is possible "anyons"(Wilczek). 2-D is special because there are two ways to swap two identical particles: rotate in clockwise direction or rotate in counterclockwise direction, which are not distinguishable in 1-D or 3-D space.

- Spin and statistics theorem: Unitary and causality in QFT requires
  - All particles with integer spins are bosons
  - All particles with half-integer spins are fermions
  - Even without interactions, statistics of identical particles can have dramatic effects like bosons like to get together while fermions hate

- Slator determinant: describe anti-symmetric many body states in terms of single particle levels
  - For two particles, $|\psi\rangle = \frac{1}{\sqrt{2}}\left(|a\rangle^1 \otimes |b\rangle^2 - |b\rangle^1 \otimes |a\rangle^2\right)$
  - For n particles, $|\psi\rangle = \frac{1}{\sqrt{N!}}\begin{vmatrix} |a\rangle^1 & |b\rangle^1 & \dots & |N\rangle^1 \\ |a\rangle^2 & |b\rangle^2 & & |N\rangle^2 \\ \dots & \dots & & \dots \\ |a\rangle^N & |b\rangle^N & \dots & |N\rangle^N \end{vmatrix}$

Degeneracy Pressure

- Suppose you have a rectangular box sides of length L_x, L_y, L_z with the periodic boundary condition

- Non-interacting particle with $H = \frac{1}{2m}\left(\vec{p}_x^{\,2} + \vec{p}_y^{\,2} + \vec{p}_z^{\,2}\right)$
- Because of the B.C., $\psi(x,y,z) = \psi(x+L_x,y,z) = \psi(x,y+L_y,z) = \psi(x,y,z+L_z)$, so

$$\psi = \eta \cdot \exp(i(k_x x + k_y y + k_z z))$$

- The number of particles with $E < E_0$ is

$$N(E_0) = d\sum_{n_x,n_y,n_z} \theta\left(E_0 - \frac{1}{2m}\left(\left(\frac{2\pi}{L_x}n_x\right)^2 + \left(\frac{2\pi}{L_y}n_y\right)^2 + \left(\frac{2\pi}{L_z}n_z\right)^2\right)\right)$$

where d is the spin degeneracy. With $\Delta n_x = \frac{L_x}{2\pi}\Delta k_x$, we have

$$N(E_0) \approx dL^3 \int \frac{dk_x}{2\pi}\cdot\frac{dk_x}{2\pi}\cdot\frac{dk_x}{2\pi}\cdot\theta\left(E_0 - \frac{|\vec{k}|^2}{2m}\right)$$

$$= dV_0 \int \frac{d^3\vec{k}}{(2\pi)^3}\theta\left(E_0 - \frac{|\vec{k}|^2}{2m}\right)$$

$$= dV_0 \int_0^{k_{max}} \frac{dk}{2\pi^2}k^2 = dV_0 \frac{k_{max}^3}{6\pi^2} \qquad \left[k_{max} = \sqrt{2mE_0}\right]$$

- Fill all energy levels up to E_F
  - $N(E_F) = dV_0\frac{k_F^3}{6\pi^2} = nV_0$, in which $n = \frac{k_F^3 d}{6\pi^2}$, so $k_F^2 = \left(\frac{6\pi^2 N}{dV_0}\right)^{2/3}$.
  - $\langle E\rangle = dV_0\int_0^{k_F}\frac{dk}{2\pi^2}k^2\cdot\frac{k^2}{2m} = \frac{N}{2m}\cdot\frac{\int_0^{k_F}k^4dk}{\int_0^{k_F}k^2dk} = \frac{3}{5}NE_F$, in which $E_F = \frac{k_F^2}{2m}$.
  - $\langle E\rangle = \frac{3}{5}N\cdot\frac{1}{2m}\cdot\left(\frac{6\pi^2N}{dV_0}\right)^{2/3}$, so the pressure is

$$P = -\left.\frac{\partial E}{\partial V}\right|_N = \frac{2}{5}N\cdot\frac{1}{2m}\cdot\left(\frac{6\pi^2N}{d}\right)^{2/3}V^{-5/3} = \frac{2}{5}\frac{N}{V}E_F$$

<u>**Von Neumann Entropy**</u>: $S = -Tr[\hat{\rho}\log\hat{\rho}]$, where $\hat{\rho}$ is density matrix.

- Pure state has $S = 0$.
- If the system is constructed by 2 uncorrelated systems, then $S = S_1 + S_2$.

<u>Find the density matrix so that the entropy maximized with fixed energy.</u>

- With Lagrange multiplier,

$$\delta[\ Tr[\hat{\rho}\log\hat{\rho}] + \beta Tr[\widehat{\rho H}] - \alpha\hat{\rho}\ ] = 0$$

- We got $\hat{\rho}_0 = Z^{-1}e^{-\beta\hat{H}}$, where z is a constant, to preserve $Tr[\hat{\rho}] = 1$, we have $Z = Tr\left[e^{-\beta\hat{H}}\right]$.

- $\beta = \dfrac{1}{k_B T} = \dfrac{1}{T}$ and Z is the partition function.
- $\widehat{\rho}_{eq}(\beta) = \dfrac{\exp(-\beta\widehat{H})}{Tr[\exp(-\beta\widehat{H})]}$ is called canonical thermal distribution or Boltzmann distribution.

With this distribution,

$$\langle E \rangle = \frac{Tr[H\exp(-\beta H)]}{Tr[\exp(-\beta H)]} = -\frac{\partial}{\partial\beta}(\log(Z))$$

$$S_{max} = -Tr[\rho_{eq}\log(\rho_{eq})] = -Tr[\rho_{eq}(-\beta H - \log Z)] = \beta E + \log Z$$

$$\frac{\partial S}{\partial E} = \beta$$

Define $Z = \exp(-\beta F)$, then we have $S = \beta(E - F)$ and $F = E - TS$.
If all N states within $[E, E + \Delta E]$ have the same probability, we have the entropy

$$S = -Tr\left[\frac{1}{N}\log\left(\frac{1}{N}\right)\right] = \log(N)$$

<u>Thermodynamics collection</u>

<u>Most important one is</u> $dU = TdS - PdV$

$$F = U - TS$$
$$H = U + PV$$
$$G = H - TS = U + PV - TS$$
$$\Phi_G = F - \mu N$$

From the partition function

$$U = -\frac{\partial(\log Z)}{\partial\beta}$$
$$F = -T\log Z$$
$$\Phi_G = -T\log Z_G$$
$$U - \mu N = -\frac{\partial(\log Z_G)}{\partial\beta}$$
$$N_i = T\frac{\partial\log Z_i}{\partial\mu}$$

Three kinds of ensembles:

- Micro canonical ensemble: fix N, V, E
- Canonical ensemble: fix N, V, T
- Grant canonical ensemble: fix μ, V, T

At thermal limit $N \to \infty,\ V \to \infty,\ \dfrac{N}{V}$ fixed, three kinds of ensembles can get the same result.

Ideal gas: classical

- No interaction
- Classical means $k \sim \sqrt{mT}$ and $L \gg \lambda \sim \frac{1}{k}$, so $\sqrt{mT} \cdot L \gg 1$.
- Canonical partition function

$$Z = \frac{1}{h^3}\int d^3q d^3p \exp\left(-\beta\frac{p^2}{2m}\right) = \frac{V}{h^3}(2\pi mT)^{3/2}$$

$$Z_N = Z^N = \frac{V^N}{h^{3N}}(2\pi mT)^{3N/2},\ [N\ \textit{distinguishable particles}]$$

$$Z_N = \frac{Z^N}{N!},\ [N\ \textit{indistinguishable particles}]$$

$$\log N! \approx N\log N - N$$

- Inner energy

$$U = -\frac{\partial(\log Z)}{\partial\beta} = \frac{3}{2}NT$$

- Maxwell velocity distribution

$$\rho(v) = 4\pi\left(\frac{m}{2\pi T}\right)^{3/2} v^2 \cdot \exp\left(-\frac{mv^2}{2T}\right)$$

- S-T equation

$$f = -\frac{T}{V}\log Z = nT\left(\log\left(\frac{nh^3}{(2\pi mT)^{3/2}}\right) - 1\right)$$

$$s = \frac{u-f}{T} = n\left(\frac{5}{2} - \log\left(\frac{nh^3}{(2\pi mT)^{3/2}}\right)\right)$$

- Equipartition Theorem
  - For each d.o.f. with only quadratic term of p or q, contributes equal energy

- Gibbs paradox
  - solution: make particles indistinguishable, so $Z_N = \frac{Z^N}{N!}$

Ideal gas: Bose

- No interaction, assume μ is general for all modes
- Grant partition function

$$Z_i = Tr_i[\exp(-\beta(H_i - \mu N_i))] = \sum_{N_i}\exp(-\beta(\epsilon_i - \mu)N_i) = \frac{1}{1-e^{-\beta(\epsilon_i-\mu)}}$$

$$Z_G = \exp\left(\sum_i \log(Z_i)\right)$$

- Particle number

$$\langle N_i \rangle = \sum_i N_i \rho_i = \frac{\sum_i N_i \exp(-\beta(\epsilon_i - \mu) N_i)}{1 - \exp(-\beta(\epsilon_i - \mu))} = \frac{1}{\beta} \frac{\partial \log Z_i}{\partial \mu} = \frac{1}{\exp(\beta(\epsilon_i - \mu)) - 1}$$

$$n = \frac{\langle N \rangle}{V} = \int \frac{dk}{2\pi^2} k^2 \cdot \frac{1}{\exp\left(\beta\left(\frac{k^2}{2m} - \mu\right)\right) - 1}$$

$$\langle N_i \rangle = \frac{1}{\beta} \frac{\partial \log Z_i}{\partial \mu} = \frac{1}{\exp(\beta(\epsilon_i - \mu)) - 1}$$

with the expression of $\langle N_i \rangle \geqslant 0$ when $\epsilon_i = 0$, we have $\mu < 0$ for all Bose gas.

- B-E condensate
  - Fixed T: $n_{critical} = n_{max}$
  - Fixed n: $T_{critical} = \frac{2\pi}{m} \cdot \left(\frac{n}{\zeta\left(\frac{3}{2}\right)} \right)^{2/3}$

$$n_{max} = \int \frac{dk}{2\pi^2} k^2 \cdot \frac{1}{\exp\left(\frac{k^2}{2mT}\right) - 1} = \left(\frac{mT}{2\pi}\right)^{3/2} \cdot \zeta\left(\frac{3}{2}\right), \textit{ except for g.s.}$$

- Classical limit
  - $T \to +\infty$ and $\beta\mu \to -\infty$
  - $\langle N_i \rangle \approx \exp(-\beta(\epsilon_i - \mu)) \ll 1$
  - $n \approx \int \frac{dk}{2\pi^2} k^2 \cdot \exp(-\beta(\epsilon_i - \mu)) = \exp(\beta\mu) \cdot 2\left(\frac{mT}{2\pi}\right)^{3/2}$
  - $u \approx \int \frac{dk}{2\pi^2} k^2 \cdot \frac{k^2}{2m} \cdot \exp(-\beta(\epsilon_i - \mu)) = -\frac{\partial n}{\partial \beta} + \mu n = \frac{3}{2} nT$

Ideal gas: photon

- No chemical potential, $\mu = 0$
- 2 polarization directions
- Dispersion relation, $\epsilon = |k|$
- For one mode

$$Z_i = \sum_{N_i} \exp(-\beta \epsilon_i N_i) = \frac{1}{1 - \exp(-\beta \epsilon_i)}$$

$$\langle N_i \rangle = \frac{1}{\exp(\beta |k_i|) - 1}$$

- Inner energy

$$u(T) = \frac{U}{V} = 2 \int \frac{dk}{2\pi^2} k^2 \cdot \frac{k}{\exp(\beta k) - 1} = \frac{\pi^2}{15} T^4$$

$$u(\omega, T) = \frac{\omega^3}{\pi^2(\exp(\beta\omega) - 1)}$$

- Classical limit: $T \to \infty$ corresponding to ω

$$u(\omega, T) \approx \frac{\omega^3}{\pi^2\beta\omega} = \frac{\omega^2}{\pi^2\beta}$$

$$u(T) = \int_0^\infty d\omega\, u(\omega, T) = \infty$$

but here ω is the integral variable and T is fixed, so the classical limit is not satisfied when $\omega \to \infty$.

Phonons

- Each of modes(ω_i) is basically a harmonic oscillator
- For one mode

$$Z_i = \sum_n \exp\left(-\beta\omega_i\left(n + \frac{1}{2}\right)\right) = \exp\left(-\frac{\beta\omega_i}{2}\right)\frac{1}{1 - \exp(-\beta\omega_i)}$$

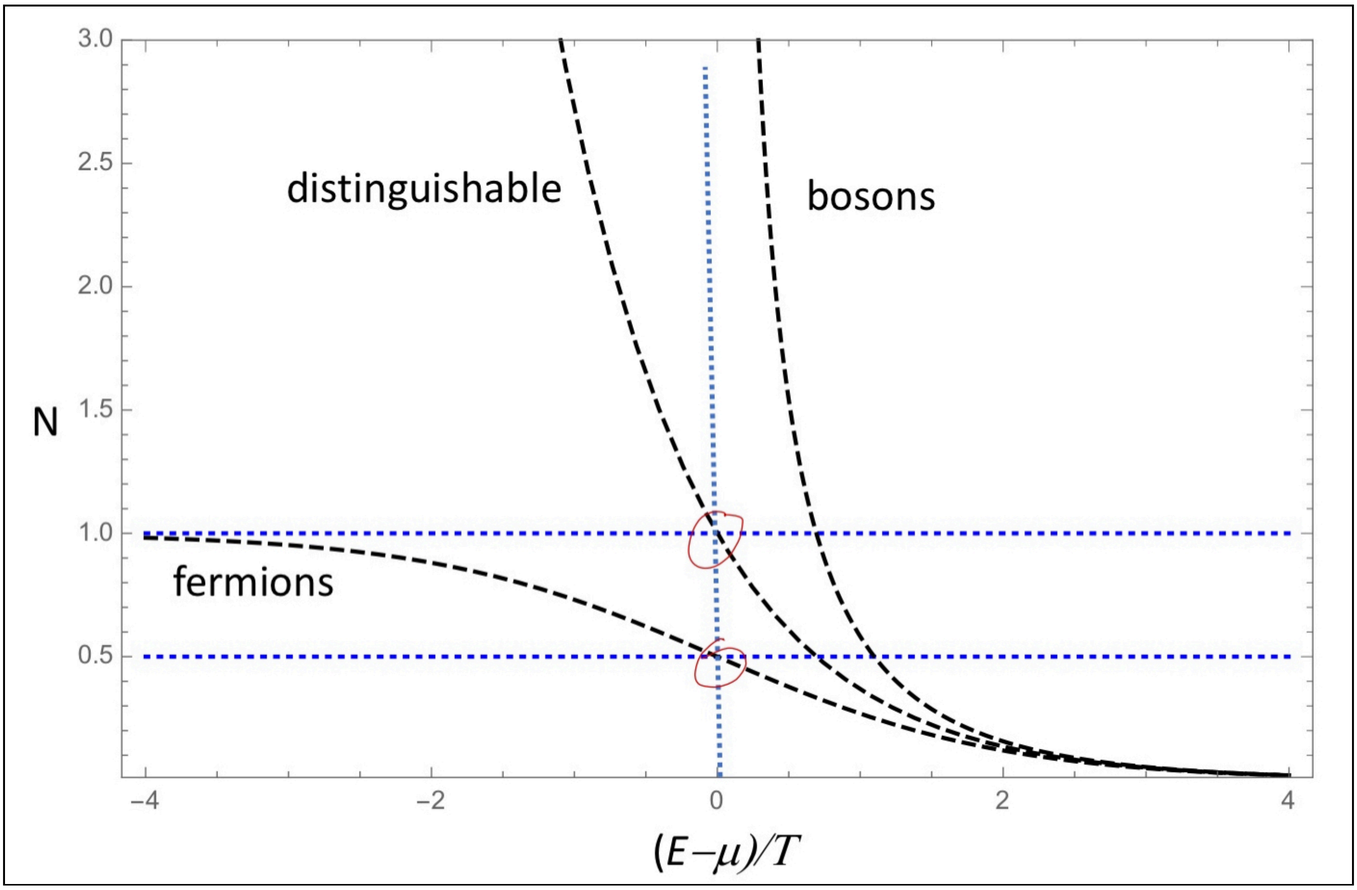
$$\langle E_i \rangle = \frac{-\partial \log Z_i}{\partial\beta} = \frac{\omega_i}{2} + \frac{\omega_i}{\exp(\beta\omega_i) - 1}; \quad u(\omega, T) = \frac{\omega^3}{2|v_s|^2\pi^2(\exp(\beta\omega_i) - 1)}$$

Ideal gas: Fermi

- For one mode (include spin)

$$Z_i = Tr_i[\exp(-\beta(H_i - \mu N_i))] = 1 + \exp(-\beta(\epsilon_i - \mu))$$

$$\langle N_i \rangle = \frac{1}{\beta}\frac{\partial \log Z_i}{\partial\mu} = \frac{1}{\exp(\beta(\epsilon_i - \mu)) + 1}$$



3.0
2.5
2.0
1.5
1.0
0.5
N
distinguishable
bosons
fermions
−4
−2
0
2
4
(E−μ)/T