Week 5

PHY 635 Many-body Quantum Mechanics of Degenerate Gases
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3 Bose-Einstein Condensates

3.1 Quantum statistical physics

For large systems, we cannot know all microscopic detail $\implies$ describe with density-matrix (see 1.3.2).

All essential postulates take a very similar form to classical statistical physics.

Quantum statistical ensembles:

Microcanonical ensemble (fixed N,V,E)

$$\hat{\rho} = \frac{1}{\Gamma(E)} \sum_{\substack{k \\ E_k \approx E}} |\,\psi_k\,\rangle\langle\,\psi_k\,| \tag{3.1}$$

- the sum runs over all many-body states k with energy in energy range $E \leq E_k \leq E + \Delta E$, for a small ΔE. See Eq. (1.23) for the definition of $|\,\psi_k\,\rangle$, E_k, i.e., they are generic many-body states.

Canonical ensemble (fixed N,V,T)

$$\hat{\rho} = \frac{1}{Z} e^{-\beta \hat{H}}, \tag{3.2}$$

where $\beta = (k_B T)^{-1}$ and Z is the partition function, $Z = \mathrm{Tr}[e^{-\beta \hat{H}}]$.

- Z normalizes $\hat{\rho}$ to fulfill $\mathrm{Tr}[\hat{\rho}] = 1$.
- The exponential of an operator is defined via the power series of exp.

- In eigenbasis of $\hat{H}$, $\langle\, \psi_k \,|$, we can write

$$\hat{\rho} = \frac{1}{Z} \sum_k e^{-\beta E_k} |\, \psi_k \,\rangle\langle\, \psi_k \,|. \tag{3.3}$$

- (3.3) is however more general. We may not know the eigenbasis, since finding it is hard for interacting many-body systems.

Grand-canonical ensemble (fixed μ,V,T)

$$\hat{\rho} = \frac{1}{Z_G} e^{-\beta(\hat{H}-\mu\hat{N})}, \tag{3.4}$$

where μ is the chemical potential (operationally defined later), $\hat{N}$ the total number operator for the system and $Z_G = Tr[e^{-\beta(\hat{H}-\mu\hat{N})}]$ the grand-canonical partition function.

- In eigenbasis of $\hat{H}$ and $\hat{N}$, $\langle\, \psi_k \,|$, we can write:

$$\hat{\rho} = \frac{1}{Z_G} \sum_k e^{-\beta(E_k-\mu N_k)} |\, \psi_k \,\rangle\langle\, \psi_k \,|, \tag{3.5}$$

where N_k is the number of particles in the state $|\, \psi_k \,\rangle$.

We focus on the latter example, and explore the
Consequences for Indistinguishable particles:

Consider single particle basis $H_0 |\, \varphi_m \,\rangle = \varepsilon_m |\, \varphi_m \,\rangle$ and non-interacting many-body Hamiltonian

$$\hat{H} = \sum_m \varepsilon_m \hat{a}_m^\dagger \hat{a}_m. \tag{3.6}$$

- Convince yourself that Fock states $|\, \mathbf{N} \,\rangle = |\, N_1 N_2 N_3 \cdots \rangle$ in (2.2) are eigenstates of $\hat{H} |\, \mathbf{N} \,\rangle = E_{\mathbf{N}} |\, \mathbf{N} \,\rangle$ with $E_{\mathbf{N}} = \sum_m N_m \varepsilon_m$.
- From (3.5)

$$\hat{\rho} = \sum_{\mathbf{N}} P_{\mathbf{N}} |\, \mathbf{N} \,\rangle\langle\, \mathbf{N} \,|$$

with (define $N_{\mathbf{N}} = \sum_m N_m$)

$$P_{\mathbf{N}} = \frac{e^{-\beta(E_{\mathbf{N}}-\mu N_{\mathbf{N}})}}{\sum_{\mathbf{N}} e^{-\beta(E_{\mathbf{N}}-\mu N_{\mathbf{N}})}} = \frac{\exp\left[-\beta\left(\sum_m N_m \varepsilon_m\right) + \beta\mu\left(\sum_m N_m\right)\right]}{\sum_{N_1,N_2,N_3,\ldots} \exp\left[-\beta\left(\sum_m N_m \varepsilon_m\right) + \beta\mu\left(\sum_m N_m\right)\right]} \tag{3.7}$$

$$= \frac{\prod_m \exp[\beta N_m(\mu - \varepsilon_m)]}{\prod_l \left[\sum_{N_l} \exp[\beta N_l(\mu - \varepsilon_l)]\right]} = \prod_m P_m(N_m) \tag{3.8}$$

with

$$P_m(N_m) = \frac{\exp[\beta N_m(\mu - \varepsilon_m)]}{\sum_{N_l} \exp[\beta N_l(\mu - \varepsilon_l)]}, \tag{3.9}$$

the probability to have N_m particles in mode number m. To see the latter statement more rigorously, define this probability as $P_m(N_m) = \bar{\sum}_{\mathbf{N}'} P_{\mathbf{N}'}$ with $\bar{\sum}$ running *only* over all $\bar{\mathbf{N}}'$ that fulfill $N'_m = N_m$. Starting from (3.7) you then reach (3.9) (excercise).

Now: What is the mean number of particles in state $|\,\psi_b\,\rangle$, with energy ε_b?

$$\begin{aligned}\bar{m}_b = \langle \underset{\substack{\downarrow \\ = \hat{a}_b^\dagger \hat{a}_b}}{\hat{N}_b} \rangle = \mathrm{Tr}[\hat{\rho}\hat{N}_b] &= \sum_{\mathbf{N}} P_{\mathbf{N}} \mathrm{Tr}\left(N_b |\,\mathbf{N}\,\rangle\langle\,\mathbf{N}\,|\right) \\ &= \sum_{\mathbf{N}} P_{\mathbf{N}} N_b \overset{\text{as}\circledast}{=} \sum_{N_b} P_b(N_b) N_b\end{aligned} \tag{3.10}$$

So far, our discussion was valid for both, Bosons and Fermions. Now we have to specifiy.

Fermions: Allowed values of $N_b = 0, 1$

$$\Longrightarrow \; \bar{m}_b = 0 + P_b(1) \times 1 = \frac{\exp(\beta(\mu - \varepsilon_b))}{1 + \exp(\beta(\mu - \varepsilon_b))} \; \Longrightarrow$$

Fermi-Dirac distribution Mean number of indistinguishable Fermions in a given state b with energy ε_b:

$$\bar{m}_b = \frac{1}{\exp(\beta(\varepsilon_b - \mu)) + 1}. \tag{3.11}$$

Bosons: All values of $N_b = 0, 1, 2, ..., \infty$ are allowed

- Define $a = \exp[\beta(\mu - \varepsilon_b)]$ and note that we can then write

$$\bar{m}_b = \sum_{N_b} P_b(N_b) N_b = \frac{a \frac{d}{da}\left(\sum_{N_b} a^{N_b}\right)}{\sum_{N_b} a^{N_b}}$$

- Use geometric series $\sum_n a^n = 1/(1-a)$ to reach[2]

Bose-Einstein distribution Mean number of indistinguishable Bosons in a given state b with energy ε_b:

$$\bar{m}_b = \frac{1}{\exp(\beta(\varepsilon_b - \mu)) - 1}. \tag{3.12}$$

[2] Using this expression requires $a < 1$, which is the case since $\mu < 0$, as we shall see shortly.

- The classical limit $\bar{m}_b \ll 1$ is reached when the occupation of each state is very small. $\implies \exp \gg 1$

$$\implies \bar{m}_b = \exp(-\beta(\varepsilon_b - \mu)),$$

so we recover the Boltzmann-distribution from classical physics.

- For given system (i.e. fixed ε_k and temperature), the chemical potential controls the mean total particle number via $N = \sum_k \bar{m}_k$.

3.2 Bose-Einstein condensation

Consider non-interacting Bosonic atoms in a harmonic trap, with

$$\varepsilon_{\mathbf{n}} = \hbar\omega(n_x + n_y + n_z + \frac{3}{2}).$$

⚠ In section **??**, n_x, n_y, n_z label oscillator states not occupation numbers. For those we use capital N as before

The mean total atom number now is

$$N = \sum_{n_x n_y n_z} \bar{m}_{n_x n_y n_z} \overset{(3.12)}{=} \sum_{n_x n_y n_z} \frac{1}{\exp[\beta(\hbar\omega(n_x + n_y + n_z + \frac{3}{2}) - \mu)] - 1}$$

- Define $\tilde{\mu} = \mu - \frac{3}{2}\hbar\omega$. We need $\tilde{\mu} < 0$ for reasonable results, which means positive mean occupation, $\bar{m}_{\mathbf{n}} > 0$.

- We see that, for a given state $\mathbf{n} = (n_x, n_y, n_z)$, if we lower the temperature (T↓) then all mean occupations go down ($\bar{m}_{\mathbf{n}} \downarrow$). On the other hand, for a given state $\mathbf{n}$ and T, if we increase the adjusted chemical potential ($\tilde{\mu} \uparrow$) then all mean occupations go up ($\bar{m}_{\mathbf{n}} \uparrow$).

- Thus, if we would want to keep the total particle numbers N fixed as we lower the temperature T, we need to simultaneously increase μ.

- But in that we are limited by the requirement $\tilde{\mu} < 0$, so the question is what happens when we reach $\tilde{\mu} = 0$? In that case we see for the groundstate occupation: $\underset{\text{Ground-state occupation}}{\underset{\downarrow}{\bar{m}_{000}}} = \frac{1}{e^{\beta . 0} - 1} \to \infty$, which is a problem, while for all other states the formula (3.12) could still be OK.

- The solution is to separately write the occupation of the ground-state as in:

$$N = N_0 + \sum_{\mathbf{n} \neq (000)} \bar{m}_{\mathbf{n}} \tag{3.13}$$

Let us find the lowest temperature T_c where $N_0 \approx 0$ is still possible. In other words, what is the lowest temperature for which we are still able to distribute "enough" atoms among all the excited states, using the B.E. distribution function (3.12). This will correspond to $\tilde{\mu} = 0$. Hence:

$$N = \sum_{\mathbf{n} \neq (000)} \frac{1}{\exp[\beta_c(\hbar\omega(n_x + n_y + n_z)) - \underset{=0}{\underset{\downarrow}{\tilde{\mu}}}] - 1} \qquad \beta_c = \frac{1}{k_B T_c}$$

$$\approx \int dn_x dn_y dn_z \frac{1}{\exp[\beta_c(\hbar\omega(n_x + n_y + n_z))] - 1} \qquad \text{Let } n'_{x/y/z} = \hbar\omega n_{x/y/z}$$

$$\approx \left(\frac{k_B T_c}{\hbar\omega}\right)^3 \int_0^\infty dn'_x dn'_y dn'_z \frac{1}{e^{n'_x + n'_y + n'_z} - 1} = \left(\frac{k_B T_c}{\hbar\omega}\right)^3 \sum_{p=1}^\infty \int d^3\mathbf{n} e^{-p(n'_x + n'_y + n'_z)} \qquad \underbrace{\left[\because \sum_{p=1}^\infty e^{-p\alpha} = \frac{1}{e^\alpha - 1}\right]}_{\text{geometric series}}$$

$$= \left(\frac{k_B T_c}{\hbar\omega}\right)^3 \sum_{p=1}^\infty \underbrace{\left(\int_0^\infty dn'_x e^{-pn'_x}\right)}_{=1/p} \left(\int_0^\infty dn'_y e^{-pn'_y}\right) \left(\int_0^\infty dn'_z e^{-pn'_z}\right)$$

$$= \left(\frac{k_B T_c}{\hbar\omega}\right)^3 \sum_{p=1}^\infty \frac{1}{p^3} = \left(\frac{k_B T_c}{\hbar\omega}\right)^3 \zeta(3)$$

where $\zeta(s) = \sum_{p=1}^\infty \frac{1}{p^s}$ is the Riemann-Zeta function. Below T_C, we have to allow $N_0 > 0$ in (3.13) in order to allocate all our N atoms into a quantum state. We thus derived the

Critical temperature for Bose-Einstein condensation in a 3D isotropic harmonic trap

$$k_B T_c = \hbar\omega N^{1/3} \zeta(3)^{-1/3} = 0.94 N^{1/3} \hbar\omega \qquad (3.14)$$

- depends on the dimension and trap details.
- numerical estimate: $N = 10000, \omega = (2\pi)100\text{Hz} \implies T_c = 97$ nK (nano-Kelvin)

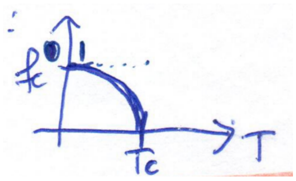
Now let $T < T_c$. From (3.13) $\implies$

$$N = N_0(T) + \sum_{\mathbf{n} \neq (000)} \bar{m}_\mathbf{n} \underset{\text{as before}}{\underset{\downarrow}{=}} N_0(T) + \int dn_x dn_y dn_z \frac{1}{\exp[\underset{\beta = 1/k_B T \text{ (not } T_c \text{ now)}}{\underset{\downarrow}{\beta}}(\hbar\omega(n_x + n_y + n_z))] - 1}$$

$$= N_0(T) + \left(\frac{k_B T}{\hbar\omega}\right)^3 \zeta(3) = N_0(T) + \left(\frac{k_B T}{k_B T_c}\right)^3 N \implies$$

Fraction of Bose condensed atoms:

$$f_c = \frac{N_0(T)}{N} = \left[1 - \left(\frac{T}{T_c}\right)^3\right] \qquad (3.15)$$



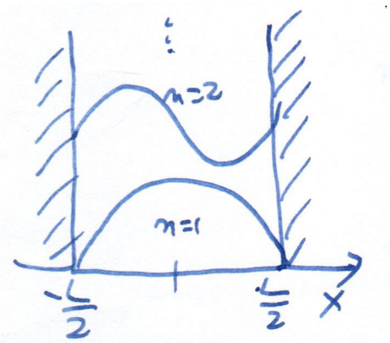
- Bose Einstein condensation has the properties of a second order phase transition.
- Unlike most of those, it does not require interactions (except indirectly, for thermalization).
- At $T = 0$, the system is in the state of $N_0 = N$, with

$$\hat{\rho} = |\, N000... \rangle\langle\, N000... \,| \longleftrightarrow |\, \psi_0 \,\rangle = |\, \underset{\downarrow}{N}000... \,\rangle \tag{3.16}$$

Fock-state with all N atoms in the ground state

3.2.1 De-Broglie Wave overlap

To work out one more aspect of condensation, let us redo the derivation in 3.2 for Bosons in a 3D infinite square (cubic) well (of volume $L^3 = V$).



$$E_{\mathbf{n}} = \frac{\pi^2\hbar^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2) \qquad\qquad \mathbf{k} = \frac{\mathbf{n}\pi}{L}$$

Using a similar calculations as in 3.2 (bit harder due to $E \sim n^2$) one can show:

$$T_c \approx \frac{\hbar^2}{2m\pi k_b}\left(\frac{N}{2.6V}\right)^{2/3}$$. Let us define the

Thermal de-Broglie Wavelength

$$\lambda_T = \frac{\hbar}{\sqrt{mk_BT}}. \tag{3.17}$$

as the wavelength of a particle with kinetic energy $E_{\text{kin}} \approx k_BT$. Mean nearest neighbour distance of randomly distributed atoms at density $\rho = N/V$ is $\bar{d} = \frac{1}{3}\left(\frac{3}{4\pi\rho}\right)^{1/3}\Gamma(1/3) \approx 0.5\rho^{-1/3}$. Thus

$$\lambda_{T_c} = \hbar\sqrt{\frac{1}{mk_B}\left(\frac{2\pi mk_B}{\hbar^2}\left(\frac{2.6V}{N}\right)^{2/3}\right)} = \frac{\sqrt{2\pi(2.6)^{2/3}}}{\rho^{1/3}} \approx 3\rho^{-1/3}$$

Thus around T_c, the atomic de-Broglie waves begin to overlap: