“Condensed Matter Physics” course (part 2): Problem set 1

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I. IDEAL BOSE GAS IN A 3D BOX (NUMERICAL)

Consider an ideal Bose gas of N (non-interacting) bosons in a three-dimensional (3D) cubic box with periodic boundary conditions. The gas is at thermal equilibrium at a temperature T.

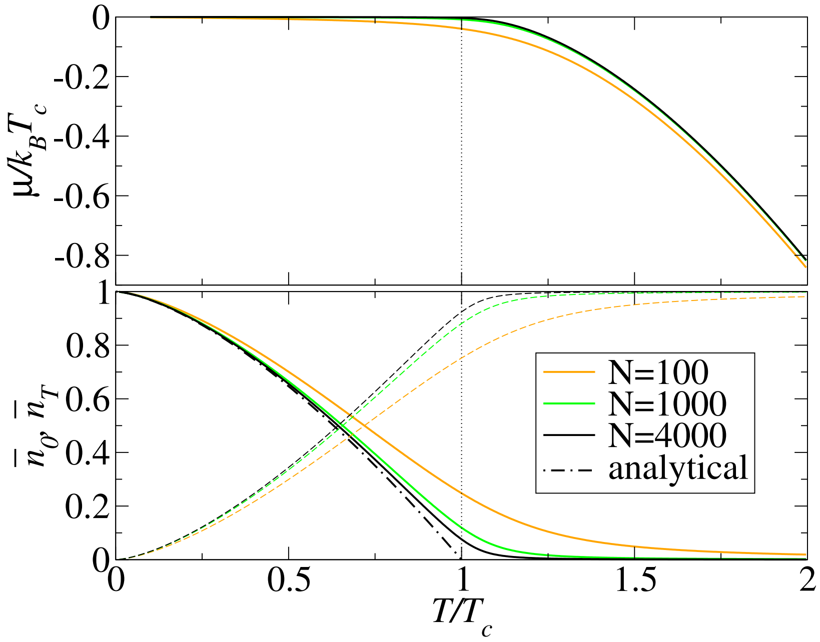
1. Invert numerically the equation which fixes the total number of particles N,

$$N = \frac{1}{e^{-\beta\mu} - 1} + N \left(\frac{T}{T_c}\right)^{3/2} \frac{g_{3/2}(e^{\beta\mu})}{g_{3/2}(1)} \qquad\qquad g_{3/2}(e^{\beta\mu}) = \frac{1}{\Gamma(\alpha)} \int_0^\infty dx \frac{\sqrt{x}}{e^{-\beta\mu} e^x - 1} \, , \tag{1}$$

   in order to obtain the rescaled chemical potential $\mu/(k_B T_c)$ as a function of N and the rescaled temperature T/T_c, where T_c is the critical temperature for BEC.

2. Plot $\mu/(k_B T_c)$ as a function of T/T_c for different values of the total number of particles N and comment the results you get.

3. Plot the condensate fraction $\bar{n}_0 = N_0(N, T/T_c)/N$ and the thermal fraction $\bar{n}_T = N_T(N, T/T_c)/N$ as a function of T/T_c for different values of the total number of particles N and compare the numerical results with the analytical formula valid in the thermodynamic limit. Compare your results with those of the following picture.



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II. IDEAL BOSE GAS IN 2D

4. Show that, for a free gas in a box of dimension $d = 1, 2, 3$ and volume $V = L^d$, the DoS is given by

$$\mathcal{N}(\epsilon) = \frac{dG(\epsilon)}{d\epsilon} = \frac{\Omega_d}{2}\frac{V}{(2\pi)^d}\left(\frac{2m}{\hbar^2}\right)^{d/2}\epsilon^{d/2-1} \qquad\qquad G(\epsilon) = \sum_{\mathbf{p}}^{\epsilon_{\mathbf{p}}<\epsilon} , \tag{2}$$

   where $\Omega_d = 4\pi (d = 3), 2\pi (d = 2), 1 (d = 1)$.

5. Evaluate the condition determining the critical temperature of an ideal gas in a 2D box (with boundary conditions) and comment why the condition $N_T(\mu \to 0^-, T) \leq N$ can never be satisfied at finite temperature. Does a critical temperature for BEC T_c exists in 2D for an ideal gas?

III. ISOTHERMAL PRESSURE CURVES (NUMERICAL)

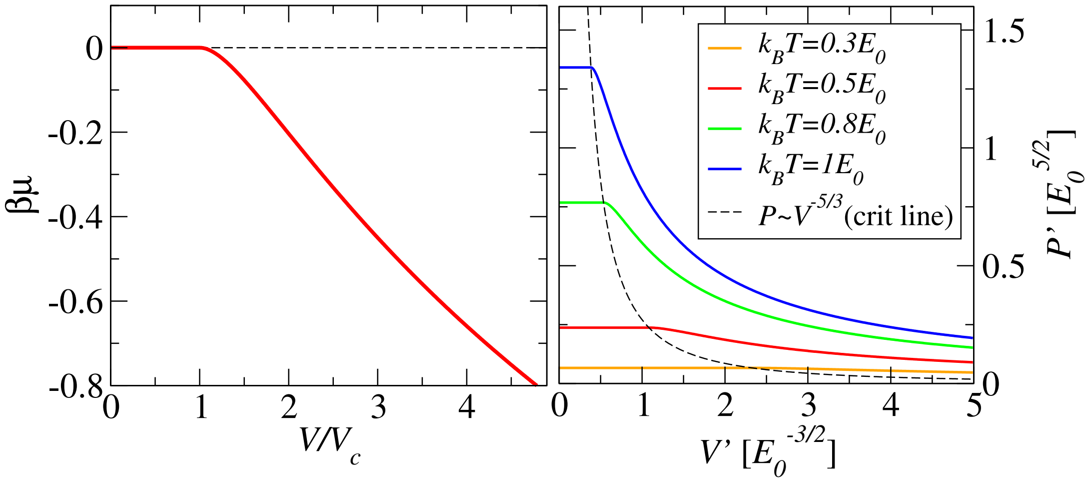
Numerically invert the equation

$$1 = \frac{V}{V_c}\frac{g_{3/2}(e^{\beta\mu})}{g_{3/2}(1)} \qquad\qquad V > V_c\ . \tag{3}$$

in order to obtain the rescaled chemical potential $\beta\mu$ as a function of the rescaled volume V/V_c for $V > V_c$ (compare your result with the left panel of the figure below). Use this result for plotting, at a given fixed temperature, the Bose gas isothermal curves of pressure,

$$P = \frac{2}{3}\frac{E}{V} = \frac{2}{3}\frac{1}{V}\sum_{\mathbf{p}}\frac{\epsilon_{\mathbf{p}}}{e^{\beta(\epsilon_{\mathbf{p}}-\mu)}-1} = \left(\frac{m}{2\pi\hbar^2}\right)^{3/2}(k_BT)^{5/2}g_{5/2}(e^{\beta\mu})\ . \tag{4}$$

as a function of the volume V — remember that $\mu \to 0$ in the BEC phase $V < V_c$. Change temperature and find the BEC critical line in the $P-V$ plane; add it to the plot. Compare your results with the right panel of the figure below. Note that there we have used rescaled variables such as pressure $P' = P/(m/2\pi\hbar^2)^{3/2}$ (measured in units of $E_0^{5/2}$, where $E_0 = k_BT_0$ is a reference energy scale), and volume $V' = V/(2\pi\hbar^2/m)^{3/2}$ (measured in units of $E_0^{-3/2}$). When one recovers the $P_{cl} = k_BT/V$ expression for a classical gas?



IV. HARMONICALLY TRAPPED SYSTEMS

Consider an ideal gas of bosons in a 3D harmonic trap:

$$V_{ext}(\mathbf{r}) = \frac{1}{2}m\boldsymbol{\omega}^2 \cdot \mathbf{r}^2 = \frac{1}{2}m\left(\omega_1^2x^2 + \omega_2^2y^2 + \omega_3^2z^2\right)\ . \tag{5}$$

6. Evaluate the system DoS and show that is given by

$$\mathcal{N}(\epsilon) = \frac{G(\epsilon)}{d\epsilon} = C_\alpha \epsilon^{\alpha-1} \qquad\qquad C_3 = \frac{1}{2\hbar^3\bar{\omega}^3} \ . \tag{6}$$

7. Repeat the same calculations for 2D and 1D harmonic traps and evaluate the corresponding critical temperature for BEC.

V. SECOND QUANTISATION

Consider the definitions of creation and annihilation operators for bosons (occupation $N_i = 0, 1, 2, \dots$)

$$\hat{a}_j^\dagger |N_0, N_1, \dots N_j, \dots\rangle = \sqrt{N_j + 1} |N_0, N_1, \dots, N_j + 1, \dots\rangle \tag{7}$$

$$\hat{a}_j |N_0, N_1, \dots N_j, \dots\rangle = \sqrt{N_j} |N_0, N_1, \dots N_j - 1, \dots\rangle \ , \tag{8}$$

and for fermions (occupation $N_i = 0, 1$):

$$\hat{c}_j^\dagger |N_0, N_1, \dots N_j, \dots\rangle = (-1)^{\mathcal{P}} (1 - N_j) |N_0, N_1, \dots, N_j + 1, \dots\rangle \tag{9}$$

$$\hat{c}_j |N_0, N_1, \dots N_j, \dots\rangle = (-1)^{\mathcal{P}} N_j |N_0, N_1, \dots N_j - 1, \dots\rangle \ , \tag{10}$$

where $\mathcal{P} = N_0 + N_1 + \dots + N_{i-1}$ and where we indicate with $i = 0, 1, \dots$ the energy levels of the single-particle problem $\widehat{\mathcal{H}}|\epsilon_i\rangle = \epsilon_i|\epsilon_i\rangle$ and with N_i the occupation number of each such a state.

8. Derive the canonical commutation and anticommuation relations

$$[\hat{a}_i, \hat{a}_j^\dagger] = \delta_{ij} \qquad\qquad [\hat{a}_i, \hat{a}_j] = 0 = [\hat{a}_i^\dagger, \hat{a}_j^\dagger] \ , \tag{11}$$

and

$$\{\hat{c}_i, \hat{c}_j^\dagger\} = \delta_{ij} \qquad\qquad \{\hat{c}_i, \hat{c}_j\} = 0 = \{\hat{c}_i^\dagger, \hat{c}_j^\dagger\} \ . \tag{12}$$

For bosons show that in general one has that

$$[a_i, \hat{a}_j^\dagger \hat{a}_k] = \delta_{1j} a_k \qquad\qquad [a_i^\dagger, \hat{a}_j^\dagger \hat{a}_k] = -\delta_{ik} a_j^\dagger \ . \tag{13}$$

9. Consider the following two-state Hamiltonian

$$\hat{H} = \epsilon \left(\hat{a}_1^\dagger \hat{a}_1 + \hat{a}_2^\dagger \hat{a}_2 \right) + \Delta \left(\hat{a}_1^\dagger \hat{a}_2^\dagger + \hat{a}_2 \hat{a}_1 \right) \ , \tag{14}$$

for two boson fields (all operators commute except $[\hat{a}_1, \hat{a}_1^\dagger] = 1 = [\hat{a}_2, \hat{a}_2^\dagger]$) — note that this Hamiltonian does not conserve the number of particles. Show that you can rewrite the Hamiltonian in the form

$$\hat{H} = \begin{pmatrix} \hat{a}_1^\dagger & \hat{a}_2 \end{pmatrix} \begin{pmatrix} \epsilon & \Delta \\ \Delta & \epsilon \end{pmatrix} \begin{pmatrix} \hat{a}_1 \\ \hat{a}_2^\dagger \end{pmatrix} - \epsilon \ . \tag{15}$$

Find a general transformation to a new set of operators

$$\begin{pmatrix} \hat{\gamma}_1 \\ \hat{\gamma}_2^\dagger \end{pmatrix} = O \begin{pmatrix} \hat{a}_1 \\ \hat{a}_2^\dagger \end{pmatrix} \tag{16}$$

where O is a 2×2 matrix, such that the bosonic canonical transformation relations are preserved for $\hat{\gamma}_i$. Choose the parameters of this transformation O such that now the Hamiltonian expressed in terms of these new operators is diagonal, i.e., of the form

$$\hat{H} = E_1 \hat{\gamma}_1^\dagger \hat{\gamma}_1 + E_2 \hat{\gamma}_2^\dagger \hat{\gamma}_2 \ . \tag{17}$$