Ultracold Atoms and Quantum Simulators

Problem 2

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1 Heat capacity

The Bose–Einstein condensation is a genuine **phase transition**. Beyond the appearance of the condensed fraction, it manifests itself by a **non-analyticity of the heat capacity at the critical point in the thermodynamic limit**. The non-analyticity can either be a discontinuity of the heat capacity itself, or of its first derivative. The heat capacity is usually defined as the derivative of the total energy with respect to temperature at constant volume and partical number:

$$C_V \equiv \frac{1}{k_{\rm B}} \left.\frac{\partial E}{\partial T}\right|_{V,N}$$

We consider a gas of **free indistinguishable bosons confined in a cubic box of size** L. We describe the gas within the **grand-canonical ensemble** with a temperature T and a chemical potential μ. For convenience we define the inverse temperature $\beta = 1/k_{\rm B}T$ and the fugacity $z = e^{\beta(\mu-\varepsilon_0)}$, where ε_0 is the ground-state energy. We also consider the **continuous limit** where the momentum and energy are regarded as continuous functions instead of discrete numbers:

$$\mathbf{p} = \hbar\mathbf{k} \in \mathbb{R}^3 \quad \text{and} \quad \varepsilon_\lambda = \varepsilon(\mathbf{p}) = \mathbf{p}^2/2m \; .$$

In this limit, any sum over the eigenstates λ should be replaced by an integral over the available phase-space:

$$\sum_\lambda \to \int \frac{\mathrm{d}^3\mathbf{r}\,\mathrm{d}^3\mathbf{p}}{(2\pi\hbar)^3} \; .$$

1. Knowing that the total energy of the boson gas is given by

$$\langle E \rangle = \frac{3}{2}\, g_{5/2}(z) V (2\pi m)^{3/2} (k_{\rm B}T)^{5/2} \; ,$$

express the heat capacity as a function of the temperature, the fugacity and the partial derivative of the fugacity with respect to temperature, $\frac{1}{k_{\rm B}} \left.\frac{\partial z}{\partial T}\right|_\mu$.

2. We will now distinguish two cases: $T < T_{\rm c}$ (condensed phase) and $T > T_{\rm c}$ (non-condensed phase). What are the values of the fugacity and its derivative in the condensed phase? Give the corresponding expression for the heat capacity.

3. Calculating the derivative of the fugacity in the non-condensed phase is less obvious. To proceed we can remember that, since we work at fixed average particle number, the derivative of the fugacity with respect to temperature has to fulfil the implicit equation:

$$\left.\frac{\partial \langle N(z,T)\rangle}{\partial T}\right|_N = 0 \; .$$

Give the expression of $\langle N \rangle$ as a function of z and T in the non-condensed phase and calculate $\frac{1}{k_{\rm B}} \left.\frac{\partial z}{\partial T}\right|_N$.

4. Use the above result to express the heat capacity as a function of z and T only.

5. Comment on the behaviour of the heat capacity per particle at the critical point, $T = T_{\rm c}$.

2 Time-of-flight dynamics of a weakly-interacting BEC

We now turn to the time-of-flight dynamics of a BEC, corresponding to its **free-space expansion** once the external confining potential has been switched off (time $t = 0$). We will forget about the vertical acceleration caused by gravity because it affects only the centre-of-mass position of the density profile. Our study will be based on the **time-dependent Gross–Pitaevskii equation**:

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left[-\frac{\hbar^2}{2m}\Delta + U(\mathbf{r},t) + g|\Psi(\mathbf{r},t)|^2\right]\Psi(\mathbf{r},t)\ ,$$

where $U(\mathbf{r}, t \geq 0) = 0$. In the following we assume that the gas is initially in the **Thomas–Fermi regime**.

6. Under which form (kinetic, potential, interaction) is the energy stored in the trapped condensate? Under which form is it stored in the limit $t \to +\infty$ after the trap has been switched off?
7. Describe in a short sentence what happens to the condensate density profile during the time of flight.

In order to solve the time-dependent equation, we will have to 'guess' the form of the condensate wave function Ψ. As is often the case, our inspiration will come from the study of the classical analogue of the problem. We thus introduce here a model of a classical gas in which each particle initially experiences the force

$$\mathbf{F}(\mathbf{r}) = -\boldsymbol{\nabla}\left[U(\mathbf{r}) + g\, n_{\rm cl}(\mathbf{r})\right]\ , \tag{1}$$

where $n_{\rm cl}$ is the density profile of the classical gas. At $t = 0$, the equilibrium condition $\mathbf{F} = \mathbf{0}$ gives $n_{\rm cl}(\mathbf{r}) = \frac{1}{g}(\mu - U(\mathbf{r}))$, where μ is a constant that we identify with the chemical potential. In other words, the classical solution of the steady-state equation coincides with the quantum solution in the Thomas–Fermi limit. At $t > 0$, the classical gas expands in such a way that the distribution of atoms can be divided into infinitesimally small volumes, each moving along a trajectory

$$R_j(t) = \lambda_j(t)\, R_j(t=0)\ , \quad j = x, y, z\ , \tag{2}$$

where $\lambda_j(t)$ are scaling functions to be determined. The classical density profile at time $t > 0$ can therefore be written as:

$$n_{\rm cl}(\mathbf{r},t) = \frac{1}{\lambda_x(t)\,\lambda_y(t)\,\lambda_z(t)} \times n_{\rm cl}\left(\left\{\frac{r_j}{\lambda_j(t)}\right\}, t=0\right)\ . \tag{3}$$

8. Justify the form of the classical density profile given above for $t > 0$. What role does the prefactor play?
9. By applying Newton's second law to the classical gas, show that the functions $\lambda_j(t)$ verify the coupled system of differential equations:

$$\ddot{\lambda}_j(t) = \frac{\omega_j^2}{\lambda_j(t)\,\lambda_x(t)\,\lambda_y(t)\,\lambda_z(t)}\ .$$

10. Which are the initial conditions for these equations?

We now focus our attention to the case of an elongated trap where $\omega_x = \omega_y = \omega_\perp \gg \omega_z$. We introduce the dimensionless parameters $\varepsilon = \omega_z/\omega_\perp \ll 1$ and $\tau = \omega_\perp t$. The solutions of the set of equations satisfied by the scaling functions $\lambda_j(t)$ read in this case:

$$\lambda_\perp(\tau) = \sqrt{1+\tau^2} + \mathcal{O}(\varepsilon^2)$$
$$\lambda_z(\tau) = 1 + \varepsilon^2\big(\tau\,\mathrm{atan}\,\tau - \ln\sqrt{1+\tau^2}\big) + \mathcal{O}(\varepsilon^4)\ .$$

11. Give the expression of the width of the BEC in the transverse ($\perp$) and longitudinal (z) directions as a function of τ and ε.

12. The ellipticity of the condensate is defined as the ratio between the widths in the transverse and longitudinal directions: $\sigma_\perp/\sigma_z$. Compare the value of the ellipticity when $t = 0$ and $t \to +\infty$. Relate this result to the initial distribution of energy in the condensate along each direction of space.

To conclude this problem we will compare the expansion of the Bose–Einstein condensate with that of a classical thermal gas. We consider the same gas in the same trap but at a temperature $k_B T \gg \hbar\omega_\perp \gg \hbar\omega_z$. At such high temperature, the interaction energy is much lower than the kinetic and potential energies so we can model the system as a classical ideal gas.

13. Which known statistical distribution describes the classical phase-space density of the thermal gas?
14. How can we define the width of the system along the transverse ($\perp$) and longitudinal (z) directions?
15. At $t = 0$, the trap is switched off and the ideal gas expands. How does the width along each direction vary as a function of the dimensionless parameters $\tau = \omega_\perp t$. What happens to the ellipticity of the gas?
16. In the light of the results established here, explain briefly how it is possible to distinguish a Bose–Einstein condensate from a thermal gas in an ultracold atom experiment.