Ultracold Atoms and Quantum Simulators

Problem 1

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marc.cheneau@institutoptique.fr

We consider a gas of **free indistinguishable bosons confined in a cubic box of size** L. The single-particle eigenstates $\{\lambda\}$ have wavefunctions of the form:

$$\psi_\lambda(x, y, z) \propto \sin(k_x x)\sin(k_y y)\sin(k_z z)$$

with $k_i = n_i\pi/L$ and $n_i \in \mathbb{N}_{\neq 0}$ $(i = x, y, z)$. The corresponding eigenenergies read:

$$\varepsilon_\lambda = \frac{\hbar^2\pi^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2) \ .$$

In the following 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 $\beta = 1/k_{\mathrm{B}}T$ and the fugacity $z = e^{\beta(\mu-\varepsilon_0)}$, where ε_0 is the ground-state energy.

We will also consider a **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 Equation of state of the ideal Bose gas

1. Write the total number of particles in the system, $\langle N\rangle$, as the sum of the occupation numbers, $\langle N_\lambda\rangle$, and give the expression of $\langle N_\lambda\rangle$ as a function of β, μ and ε_λ. In the continuous limit, this expression becomes:
$$\langle N\rangle = \int \frac{\mathrm{d}^3\mathbf{r}\,\mathrm{d}^3\mathbf{p}}{(2\pi\hbar)^3} \frac{1}{\exp[\beta(\varepsilon(\mathbf{p}) - \mu)] - 1} \ .$$
2. What is the value of the ground-state energy ε_0 in the continuous limit? Replace the chemical potential μ by the fugacity z in the equation above.
3. Using the equality $\frac{1}{1/(zu)-1} = \frac{zu}{1-zu}$ and the expansion of the function $\frac{1}{1-zu}$ in powers of zu, show that
$$\langle N\rangle = \sum_{j=1}^{+\infty} z^j \int \frac{\mathrm{d}^3\mathbf{r}\,\mathrm{d}^3\mathbf{p}}{(2\pi\hbar)^3} \exp[-j\beta\varepsilon(\mathbf{p})] \ .$$
4. Using the equality $\int_{-\infty}^{+\infty} \mathrm{d}v\, \exp(-v^2/2\sigma^2) = \sigma\sqrt{2\pi}$, and introducing the polygarithm function:
$$g_{3/2}(z) = \sum_{j=1}^{+\infty} \frac{z^j}{j^{3/2}} \ ,$$
calculate the total number of particles in terms of the volume $V = L^3$, the temperature T, the fugacity z and the mass m. The equation obtained is the **equation of state** of the ideal Bose gas.

5. Express the equation of state in terms of the particle density, $n = \langle N \rangle / V$ and introduce the de Broglie wavelength $\lambda_{\mathrm{T}} = \sqrt{2\pi\hbar^2/mk_{\mathrm{B}}T}$. Knowing that $g_{3/2}(z)$ is a number of order 1 for all values of z, comment on the possible values of the density in the ideal Bose gas. What do you think of this result?

2 Equipartition theorem

In classical statistical mechanics, one can show that each degree of freedom associated with a quadratic energy term —for instance the projection of the momentum p_x, which is associated with the kinetic energy $p_x^2/2m$— contributes to the total energy by an amount $k_{\mathrm{B}}T/2$. This is not necessarily the case in quantum statistical mechanics, as we will see now.

1. According to the classical equipartition theorem, what should the total energy per particle of our system be for a given temperature T?
2. Within quantum statistical mechanics, the proper way to calculate the total energy of the system is to write:
$$\langle E \rangle = \sum_{\lambda} \frac{\varepsilon_\lambda}{e^{\beta(\varepsilon_\lambda - \mu)} - 1} \, .$$
Using the continuous limit, show that the total energy can be written
$$\langle E \rangle = -g_{5/2}(z) V \frac{\partial}{\partial \beta} \left(\frac{2\pi m}{\beta} \right)^{3/2} = \frac{3}{2} g_{5/2}(z) V (2\pi m)^{3/2} (k_{\mathrm{B}}T)^{5/2} \, .$$
Here, $g_{5/2}(z) = \sum_{j=1}^{+\infty} z^j / j^{5/2}$ is the polylogarithm function of order $5/2$.
3. Using the expression of the total number of particles obtained in the previous section, express the total energy per particle, $\langle E \rangle / \langle N \rangle$, as a function of T and the ratio $g_{5/2}(z)/g_{3/2}(z)$.
4. Compare the expression obtained above to that predicted by classical statistical mechanics. Which of the two energies is the lowest? How can we qualitatively understand this result without going through the detailed calculation? Would the energy per particle in a gas of indistinguishable fermions be lower or larger than that of the equivalent classical gas?