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Fakultät 7 – Physik und Mechatronik

Fachrichtung 7.1 – Theoretische Physik
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Blatt 11 zur Theoretischen Physik IV, WS2023/2024

(Abgabe bis 26.01.2024, 8.30 Uhr)

Exercise 1 *Einstein and Debye model for phonons* [12 Points]

In the following, the contribution of phonons (bosonic quasiparticles of lattice vibrations) to the heat capacity of solids will be investigated. To do this, consider N atoms, each with three isotropic vibration modes. Each vibration mode should represent a harmonic oscillator with frequency ω_i. Analogous to photons, the chemical potential for phonons disappears.

a) Specify the mean internal energy as a function of the inverse temperature β and the discrete frequencies ω_i. For large N, these frequencies are very close, so that they can also be regarded as continuously distributed. What is the average internal energy?
Hint: Take the density of states $Z(\omega)$ (i.e. in the interval $[\omega, \omega + d\omega]$ there are $Z(\omega)\, d\omega$ possible frequencies) as given.

In the *Einstein model*, it is now assumed for the sake of simplicity that all oscillators oscillate at the same frequency ω_{E}.

b) Use this to explicitly calculate the mean value of the internal energy and the heat capacity. Examine the limiting cases $\beta \to 0$ and $\beta \to \infty$ and compare with the Dulong-Petit and Debye's T^3-law.

The *Debye model* provides an improved description. The possible frequencies are continuously distributed and limited upwards by a specified cut-off frequency ω_{D}. The density of states is taken to be

$$Z(\omega) = \alpha\omega^2\Theta(\omega_{\mathrm{D}} - \omega).$$

with $\alpha = \text{const}$ and Θ as a Heaviside function.

c) How must α be chosen so that the density of states is correctly normalized? Calculate the mean internal energy and the heat capacity again.
Hint: You do not need to solve the integrals for internal energy and heat capacity here.

d) Now introduce the *Debye temperature* $\Theta_{\mathrm{D}} = \frac{\hbar\omega_{\mathrm{D}}}{k_B}$ and calculate the heat capacity explicitly $T \gg \Theta_{\mathrm{D}}$ or $T \ll \Theta_{\mathrm{D}}$. Compare with the result from b.).
Hint: Develop the numerator and denominator of the integral for $T \gg \Theta_{\mathrm{D}}$ in leading order. Use the following identity for $T \ll \Theta_{\mathrm{D}}$:

$$\int_0^\infty \frac{x^4\, \mathrm{e}^x}{(\mathrm{e}^x - 1)^2}\, \mathrm{d}x = \frac{4\pi^4}{15}.$$

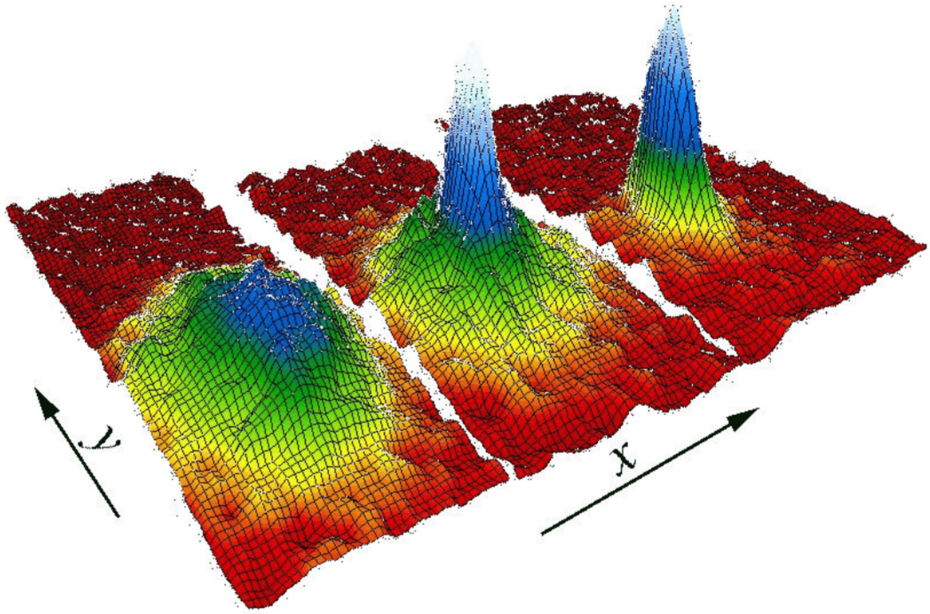

Figure 1: **Bose–Einstein condensation** at 400, 200, and 50 nano-Kelvin. The pictures are spatial distributions 60 ms after the potential is removed; the field of view of each image is $200\,\mu m \times 270\,\mu m$. The left picture is roughly spherically symmetric, and is taken before Bose condensation; the middle has an elliptical Bose condensate superimposed on the spherical thermal background; the right picture is nearly pure condensate. From Anderson, M. H., Ensher, J. R., Matthews, M. R., Wieman, C. E., and Cornell, E. A. (1995). Observation of Bose–Einstein condensation in a dilute atomic vapor. Science, 269, 198.

Exercise 2 *Bose condensation: the experiment* [12 Points]

Anderson, Ensher, Matthews, Wieman, and Cornell in 1995 were able to get a dilute gas of rubidium-87 atoms to Bose condense.

a) Is rubidium-87 (37 protons and electrons, 50 neutrons) a boson or a fermion?

b) At their quoted maximum number density of $2.5\times10^{12}/\text{cm}^3$, at what temperature T_c^{predict} do you expect the onset of Bose condensation in free space? They claim that they found Bose condensation starting at a temperature of $T_c^{\text{measured}} = 170$ nK. Is that above or below your estimate? (Useful constants: $h = 6.6262 \times 10^{-27}$ erg s, $m_n \sim m_p = 1.6726 \times 10^{-24}$ g, $k_B = 1.3807 \times 10^{-16}$ erg/K.)

The trap had an effective potential energy that was harmonic in the three directions, but anisotropic with cylindrical symmetry. The frequency along the cylindrical axis was $f_0 = 120$Hz so $\omega_0 \sim 750$Hz, and the two other frequencies were smaller by a factor of $\sqrt{8}$: $\omega_1 \sim 265$Hz. The Bose condensation was observed by abruptly removing the trap potential, and letting the gas atoms spread out; the spreading cloud was imaged 60 ms later by shining a laser on them and using a CCD to image the shadow.

For your convenience, the ground state of a particle of mass m in a one-dimensional harmonic oscillator with frequency ω is $\psi_0(x) = (\frac{m\omega}{\pi\hbar})^{1/4}\, e^{-m\omega x^2/2\hbar}$, and the momentum-space wavefunction is $\tilde{\psi}_0(p) = (\pi m\hbar\omega)^{-1/4}\, e^{-p^2/2m\hbar\omega}$. In this 3D problem the solution is a product of the corresponding Gaussians along the three axes.

c) Will the momentum distribution be broader along the high-frequency axis (ω_0) or one of the low-frequency axes (ω_1)?
Assume that you may ignore the small width in the initial position distribution, and that the positions in Fig. 1 thus reflect the velocity distribution times the time elapsed. Which axis, x or y in Fig. 1 , corresponds to the high-frequency cylinder axis? What anisotropy would one expect in the momentum distribution at high temperatures (classical statistical mechanics)? Does this high-temperature anisotropy agree with the experimental measurement in 1 ?

Their Bose condensation is not in free space; the atoms are in a harmonic oscillator potential. In the calculation in free space, we approximated the quantum states as a continuum density of states $g(E)$. That is only sensible if $k_B T$ is large compared to the level spacing near the ground state.

d) Compare $\hbar\omega$ to $k_B T$ at the Bose condensation point T_c measured in their experiment. ($\hbar = 1.05459 \times 10^{-27}$erg s; $k_B = 1.3807 \times 10^{-16}$erg/K.)

For bosons in a one-dimensional harmonic oscillator of frequency ω_0, it is clear that $g(E) = 1/(\hbar\omega_0)$; the number of states in a small range ΔE is the number of $\hbar\omega_0$ it contains.

e) Calculate the density of single-particle eigenstates

$$g(E) = \int_0^\infty \mathrm{d}\epsilon_1 \mathrm{d}\epsilon_2 \mathrm{d}\epsilon_3 \mathrm{g}_1(\epsilon_1)\mathrm{g}_2(\epsilon_2)\mathrm{g}_3(\epsilon_3) \times \delta(\mathrm{E} - (\epsilon_1 + \epsilon_2 + \epsilon_3))$$

for a three-dimensional harmonic oscillator, with one frequency ω_0 and two of frequency ω_1.
Hint: What is the shape of the energy shell in ϵ space?

Their experiment has $N = 2 \times 10^4$ atoms in the trap as it condenses.

f) By working in analogy with the calculation in free space and your density of states from part (e), find the maximum number of atoms that can occupy the three-dimensional harmonic oscillator potential (without Bose condensation) at temperature T.
Hint: $\int_0^\infty z^2/(e^z - 1)\mathrm{d}z = 2\zeta(3) = 2.40411$.
According to your calculation, at what temperature T_c^{H0} should the real experimental trap have Bose condensed?

Exercise 3 *One-dimensional XY-model* [12 Points]

Consider a 1D spin model, which is defined by the variables ϕ_i , each of which can take the values $-\pi$ and π and interact with their neighbors ϕ_{i+1} and ϕ_{i-1} such that the sum of states is given by

$$Z = \int_{-\pi}^{\pi} \prod_{l=1}^{N} \frac{\mathrm{d}\phi_l}{2\pi} e^{K\sum_{k=1}^{N-1}\cos(\phi_k - \phi_{k+1}) + K\cos(\phi_N - \phi_1)}.$$

a) Find the transfer matrix.

b) Calculate the sum of states in the limit $N \to \infty$.
Hint: The eigenvalue equation is an integral equation and the normalized eigenfunctions of the transfer matrix are $\frac{e^{in\phi}}{\sqrt{2\pi}}$ for $n = 0, \pm 1, \pm 2, \ldots$. For real a and integer n, you can use the modified Bessel function $I_n(a) = \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{a\cos\phi + in\phi}\,\mathrm{d}\phi$.

c) Determine the correlation length ξ in the limiting case $N \to \infty$.

Exercise 4 *Computational task: 2D Ising model of ferromagnetism* [4 Points]

Simulate the 2D Ising model of ferromagnetism, and calculate the magnetization of the system at different temperatures. Interpret the result. As a guide, there is a Python code in the exercise folder (blatt11_2D-Ising.py), you can complete it.