Statistical Mechanics

Worksheet 10

June 22nd, 2023

1 Thermal de Broglie wavelength

The thermal de Broglie wavelength (λ_{th}, sometimes written also as Λ) is roughly the average of the de Broglie wavelength for a free ideal gas in equilibrium at a specific temperature T. It is a way to estimate whether a gas should be treated as classical or quantum. Consider we take the average inter-particle spacing in a gas to be $(V/N)^{1/3}$, with V the volume and N the number of particles of the gas. When the thermal de Broglie wavelength, λ_{th} is much smaller than the inter-particle distance, the gas can be considered to be a classical or a so called, Maxwell–Boltzmann gas. Instead, in the case of the thermal de Broglie wavelength being on the order of, or larger than, the inter-particle distance, quantum effects will dominate and the gas must be treated as a Fermi gas or a Bose gas, depending on the nature of the gas particles.

1. The thermal de Broglie wavelength is defined as,

$$\lambda_{\mathrm{th}} = \sqrt{\frac{2\pi\hbar^2}{mk_BT}} = \frac{h}{\sqrt{2\pi m k_B T}}, \tag{1}$$

   where h is the Planck constant, k_B the Boltzmann constant and m the mass of the particle.

   Compute the thermal de Broglie wavelength, and estimate the temperature where we can consider the particles as classic, for

   (a) Electrons
   (b) Protons
   (c) Neutrons

   Discuss the differences.

2. As this definition is done based on the momenta of the particles rather than their masses, λ_{th} can also be defined for massless particles as,

$$\lambda_{\mathrm{th}} = \frac{hc}{2\pi^{1/3}k_{\mathrm{B}}T} = \frac{\pi^{2/3}\hbar c}{k_{\mathrm{B}}T}, \tag{2}$$

   where c is the speed of light.

   Compute the thermal de Broglie wavelength for photons. What does it mean to treat light as classical or quantum?

2 Does entropy increase in quantum systems?

Using the evolution law

$$\frac{\partial \rho}{\partial t} = \frac{1}{i\hbar}[\mathcal{H}, \rho] \tag{3}$$

prove that the entropy $S = \mathrm{Tr}(\rho \ln \rho)$ is time independent, where ρ is any density matrix.

Hint: There are two approaches. Use just one of the following:

1. Go to an orthonormal basis ψ_i that diagonalizes ρ. Show that $\psi_i(t)$ is also orthonormal, and take the trace in that basis.

2. Let $U(t) = \exp(-i\mathcal{H}t/\hbar)$ be the unitary operator that time evolves the wave function $\psi(t)$.

   (a) Show that $\rho(t) = U(t)\rho(0)U^\dagger(t)$.

   (b) Write a general function $F(\rho)$ as a formal power series[1] in $\rho(t)$.

   (c) Show, term-by-term in the series, that $F(t) = U(t)F(0)U^\dagger(t)$. Then use the cyclic invariance of the trace.

Give an explanation on why the entropy does not increase in this case.

3 Density matrix of polarized light

Find the density matrix for a partially polarized incident beam of electrons in a scattering experiment, in which a fraction f of the electrons are polarized along the z direction and fraction $1-f$ in the opposite direction.

4 Electron spin

The Hamiltonian for an electron in a magnetic field $\vec{B}$ is

$$\mathcal{H} = -\mu_B \vec{\sigma} \cdot \vec{B} \tag{4}$$

where $\vec{\sigma}$ is the Pauli spin operator vector, defined as,

$$\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z) \quad \text{with} \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{5}$$

and μ_B is the Bohr magneton.

1. In the quantum canonical ensemble evaluate the density matrix if $\vec{B}$ is along the z direction.

2. Repeat the calculation assuming that $\vec{B}$ points along the x direction.

3. Calculate the average energy in each of the above cases.

[1]One must note that $S(\rho) = -k_B \rho \ln \rho$ is singular as $\rho \to 0$ and does not have a series expansion.

5 Quantum harmonic oscillator

Consider a single harmonic oscillator with the Hamiltonian

$$\mathcal{H} = \frac{p^2}{2m} + \frac{m\omega^2 q^2}{2}, \qquad \text{with} \qquad p = \frac{\hbar}{i}\frac{d}{dq} \tag{6}$$

1. Find the partition function Z, at a temperature T, and calculate the energy $\langle \mathcal{H} \rangle$.

2. Write down the formal expression for the canonical density matrix ρ in terms of the eigenstates ($\{|n\rangle\}$), and energy levels ($\{\epsilon_n\}$) of $\mathcal{H}$.

3. Show that for a general operator $A(x)$

$$\frac{\partial}{\partial x}\exp\left[A(x)\right] \neq \frac{\partial A}{\partial x}\exp\left[A(x)\right], \qquad \text{unless} \qquad \left[A, \frac{\partial A}{\partial x}\right] = 0 \tag{7}$$

   while in all cases

$$\frac{\partial}{\partial x}\operatorname{Tr}\left\{\exp\left[A(x)\right]\right\} = \operatorname{Tr}\left\{\frac{\partial A}{\partial x}\exp\left[A(x)\right]\right\} \tag{8}$$

4. Note that the partition function calculated in part (1) does not depend on the mass m, that is, $\partial Z/\partial m = 0$. Use this information, along with the result in part (3), to show that

$$\left\langle \frac{p^2}{2m} \right\rangle = \left\langle \frac{mw^2 q^2}{2} \right\rangle. \tag{9}$$

5. In a coordinate representation, calculate $\langle q'|\rho|q\rangle$ in the high-temperature limit.

   Hint: One approach is to use the result

$$\exp(\beta A)\exp(\beta B) = \exp\left[\beta(A+B) + \beta^2[A,B]/2 + \mathcal{O}(\beta^3)\right]. \tag{10}$$

6. At low temperatures, ρ is dominated by low-energy states. Use the ground state wave function to evaluate the limiting behavior of $\langle q'|\rho|q\rangle$ as $T \to 0$.

7. Calculate the exact expression for $\langle q'|\rho|q\rangle$.

6 Quantum rotor

Consider a rotor in two dimensions with

$$\mathcal{H} = -\frac{\hbar^2}{2I}\frac{d^2}{d\theta^2}, \qquad \text{and} \qquad 0 \leq \theta \leq 2\pi \tag{11}$$

1. Find the eigenstates and energy levels of the system.

2. Write the expression for the density matrix $\langle \theta'|\rho|\theta\rangle$ in a canonical ensemble of temperature T, and evaluate its low- and high-temperature limits.