Problem 1. H-theorem and Pauli kinetic balance equation The Pauli balance equation (a version of the Boltzmann kinetic equation more suitable for a quantum setting) reads

$$\dot{w}_i = \sum_j (P_{ij}w_j - P_{ji}w_i),\tag{1}$$

where w_i is the probability of a system to be in the state $|i\rangle$ and P_{ij} is a transition probability rate (i.e. the probability of a state $|i\rangle$ to transition to $|j\rangle$ during unit time). In addition, a detailed balance condition is imposed: $P_{ij} = P_{ji}$.

1.1(a) Show that the Pauli balance equation respects the normalization condition $\sum_i w_i = 1$.

Solution. Since $P_{ij} = P_{ji}$,

$$\sum_{i} \sum_{j} P_{ij} w_j = \sum_{i} \sum_{j} P_{ji} w_j.$$

Swapping indices on the right side.

$$\sum_{i} \sum_{j} P_{ij} w_j = \sum_{i} \sum_{j} P_{ij} w_i = \sum_{i} \sum_{j} P_{ji} w_i,$$

where we have once again applied $P_{ij} = P_{ji}$. Then, by Eq. (1),

$$\sum_{i} \dot{w}_{i} = \sum_{i} \sum_{j} (P_{ij}w_{j} - P_{ij}w_{i}) = 0.$$
(2)

This implies $\sum_i w_i = k$, where k is some constant. If $k \neq 1$, we may redefine $w_i \to w_i/k$ without affecting the validity of the proof. Thus, we have shown that Eq. (1) respects the normalization condition.

1.1(b) Show that the Pauli balance equation is time irreversible.

Solution. Under time reversal $t \to -t$, $d/dt \to -d/dt$. From Eq. (1),

$$-\dot{w}_i = \sum_j (P_{ji}w_i - P_{ij}w_j)$$

???

1.1(c) Show that the entropy $S = -\sum_i w_i \ln w_i$ is non-decreasing: $\dot{S} \geq 0$.

Solution. Firstly, note that

$$\dot{S} = -\sum_{i} \frac{d}{dt} (w_i \ln w_i) = -\sum_{i} \frac{dw_i}{dt} \frac{d}{dw_i} (w_i \ln w_i) = -\sum_{i} \dot{w}_i (\ln w_i + 1) = -\sum_{i} \dot{w}_i \ln w_i,$$

where we have applied Eq. (2). Since all $0 \le w_i \le 1$ for all i, $\ln w_i \le 0$. Since Eq. (1) is time irreversible, $\dot{w}_i > 0$ for all i. Thus, $\dot{S} \ge 0$ as desired.

- **1.2** Rényi entropy of the order α is defined by the formula $S_{\alpha} = 1/(1-\alpha) \ln \sum_{i} w_{i}^{\alpha}$.
- 1.2(a) Show that Rényi entropy of the order 1 is the Boltzmann entropy (in the context of information theory, Boltzmann entropy is called Shannon entropy).
- **1.2(b)** Show that Rényi entropy doesn't decrease: $\dot{S}_{\alpha} \geq 0$.

May 29, 2020

Problem 2. Pauli paramagnetism Cold atomic gases could be realized by atomic isotopes which are fermions (6 Li, 40 K, etc.). Such isotopes may have a large atomic spin. Assuming that the Fermi gas is degenerate and its constituents have a spin s > 1/2, compute the Pauli magnetic susceptibility.

Solution. According to p. 2 of Lecture 12, the magnetic susceptibility is defined

$$\chi = \frac{1}{V} \frac{\partial N}{\partial \mu},$$

where $N = \partial \Omega / \partial \mu$, and

$$\Omega(\mu, B) = \frac{1}{2}\Omega_0(\mu + B) + \frac{1}{2}\Omega_0(\mu - B) \approx \Omega_0(\mu) + \frac{B^2}{2}\frac{\partial^2 \Omega_0}{\partial \mu^2},$$

where B is the strength of the magnetic field and Ω_0 is the thermodynamic potential with no field present. but I think this doesn't work because it is only for spin 1/2

For a Fermi gas, the thermodynamic potential is [?, p. 145]

$$\Omega_0 = -T \sum_k \ln \left(1 + e^{(\mu - \epsilon_k)/T} \right).$$

Note that

$$\frac{\partial \Omega_0}{\partial \mu} =$$

Then the thermodynamic potential in the magnetic field is

$$\Omega =$$

Problem 3. Landau diamagnetism

3.1 Compute the Landau diamagnetic susceptibility for ultra-relativistic Fermi gas.

3.2 (*) Compute the Landau diamagnetic susceptibility for a Fermi gas confined to a box whose linear size in the z direction is $L_z \ll L_x, L_y$. The magnetic field is directed along the z direction. Consider two cases when the energy spacing $(2\pi\hbar/L_z)^2/2m$ is much larger/smaller than the cyclotron energy $\mu_B B$.

Problem 4. Fluctuations of thermodynamics

4.1 Find the energy fluctuation $\langle (\Delta E)^2 \rangle = \langle (E - \langle E \rangle)^2 \rangle$ and the number fluctuation $\langle (\Delta N)^2 \rangle = \langle (N - \langle N \rangle)^2 \rangle$ for photons in the black body radiation.

4.2 Show that the number of particles in a sub-volume of a gas fluctuates according the formula $\langle (\Delta N)^2 \rangle = T \partial \langle N \rangle / \partial \mu$. Furthermore, apply this formula to the Boltzmann, Fermi, and Bose ideal gases.

Solution. Let p(x) denote the probability of a fluctuation in x. Then $p(x) \propto e^{S(x)}$, where S(x) is the entropy of a closed system representing a sub-volume of a gas [?, pp. 343, 348]. It follows that $p(x) \propto e^{\Delta S(x)}$, where $\Delta S(x)$ is the change in the entropy due to the fluctuation [?, p. 348]. This change is equal to the difference between S(x) and its equilibrium value, which is given by

$$\Delta S(x) = -\frac{\Delta E - T \, \Delta S + P \, \Delta V}{T},$$

where T and P are the equilibrium values [?, pp. 60, 349]. Assuming small fluctuations and thus small ΔE , we can expand ΔE as

$$\begin{split} \Delta E &= \frac{\partial E}{\partial S} \Delta S + \frac{\partial E}{\partial V} \Delta V + \frac{1}{2} \left[\frac{\partial^2 E}{\partial S^2} + 2 \frac{\partial^2 E}{\partial S \partial V} \Delta S \, \Delta V + \frac{\partial E}{\partial V}^2 \right] \\ &= T \, \Delta S - P \, \Delta V + \frac{1}{2} \left[\left(\Delta \frac{\partial E}{\partial S} \right)_V \, \Delta S + \left(\Delta \frac{\partial E}{\partial V} \right)_S \, \Delta V \right] = T \, \Delta S - P \, \Delta V + \frac{\Delta S \, \Delta T - \Delta P \, \Delta V}{2}, \end{split}$$

where we have used $\partial E/\partial S=T$ and $\partial E/\partial V=-P$ [?, pp. 60, 349]. Then the fluctuation probability has the proportionality

$$p \propto e^{\Delta S(x)} = \exp\left(\frac{\Delta P \,\Delta V - \Delta S \,\Delta T}{2T}\right).$$

Expanding ΔS and ΔP in terms of V and T, we find

$$\Delta P = \left(\frac{\partial P}{\partial T}\right)_{V} \Delta T + \left(\frac{\partial P}{\partial V}\right)_{t} \Delta V, \qquad \Delta S = \left(\frac{\partial S}{\partial T}\right)_{V} \Delta T + \left(\frac{\partial S}{\partial V}\right)_{T} \Delta V = \frac{C_{v}}{T} \Delta T + \left(\frac{\partial P}{\partial T}\right)_{V} \Delta V,$$

where we have used $(\partial S/\partial V)_T = (\partial P/\partial T)_V$ and $C_v = T(\partial S/\partial T)_V$ [? , pp. 45, 50, 349]. Making these substitutions,

$$p \propto \exp\left\{\frac{1}{2T} \left[\left(\frac{\partial P}{\partial T}\right)_{V} \Delta T \Delta V + \left(\frac{\partial P}{\partial V}\right)_{t} (\Delta V)^{2} - \frac{\partial C_{v}^{2}}{\partial T} - \left(\frac{\partial P}{\partial T}\right)_{V} \Delta V \Delta T \right] \right\}$$

$$= \exp\left[\left(\frac{1}{2T} \frac{\partial P}{\partial V}\right)_{t} (\Delta V)^{2} - \frac{C_{v}}{2T^{2}} (\Delta T) \right] = \exp\left[\left(\frac{1}{2T} \frac{\partial P}{\partial V}\right)_{t} (\Delta V)^{2} \right] \exp\left[-\frac{C_{v}}{2T^{2}} (\Delta T) \right]. \tag{3}$$

Thus, the expression is separable and fluctuations in V and in T can be regarded as independent [? p. 349].

We will focus on fluctuations in volume, and assume their probability to be Gaussian distributed. The Gaussian distribution is given by [?, p. 345]

$$p(x) dx = \frac{1}{\sqrt{2\pi \langle x^2 \rangle}} \exp\left(-\frac{x^2}{2 \langle x^2 \rangle}\right) dx.$$

Comparing Eq. (3), we find that [?, p. 350]

$$\langle (\Delta V)^2 \rangle = -T \left(\frac{\partial V}{\partial P} \right)_T.$$

Dividing both sides by N^2 [?, p. 351],

$$\langle [\Delta(V/N)]^2 \rangle = -\frac{T}{N^2} \left(\frac{\partial V}{\partial P} \right)_T.$$

Now we fix V and consider fluctuations in N. Note that

$$\Delta(V/N) = V \, \Delta(1/N) = -\frac{V}{N^2} \, \Delta N,$$

so we have

$$\langle (\Delta N)^2 \rangle = -\frac{TN^2}{V^2} \left(\frac{\partial V}{\partial P} \right)_T.$$

Since N = V f(P, T), we can write

$$-\frac{N^2}{V^2}\left(\frac{\partial V}{\partial P}\right)_T = N\left[\frac{\partial}{\partial P}\left(\frac{N}{V}\right)\right]_{T,N} = N\left[\frac{\partial}{\partial P}\left(\frac{N}{V}\right)\right]_{T,v} = \frac{N}{V}\left(\frac{\partial N}{\partial P}\right)_{T,v} = \left(\frac{\partial P}{\partial \mu}\right)_{T,V}\left(\frac{\partial N}{\partial P}\right)_{T,V} = \left(\frac{\partial N}{\partial \mu}\right)_{T,V},$$

where we have used $N/V = (\partial P/\partial \mu)_T$ [? , pp. 351–352]. Since we associated all quantities with those at equilibrium, we have shown that

$$\langle (\Delta N)^2 \rangle = T \frac{\partial \langle N \rangle}{\partial \mu}$$

as desired.

Boltzmann $\langle (\Delta N)^2 \rangle = N$

For the Fermi and Bose gases, the number of particles is given by

$$N = \frac{gV}{\pi^2 \hbar^2} \sqrt{\frac{m^3 T^3}{2}} \int_0^\infty \frac{\sqrt{z}}{e^{z-\mu/T} \pm 1} dz \begin{cases} \text{Fermi,} \\ \text{Bose,} \end{cases}$$

where $z=\epsilon/T$ [? , pp. 149, 354]. Evaluating the integrals using

$$\int_0^\infty \frac{k^s}{e^{k-\mu} \pm 1} \, dk = -\Gamma(s+1) \operatorname{Li}_{1+s}(\mp e^{\mu}),$$

where Li is the polylogarithm [?], we have

$$N = \mp \frac{gV}{\pi^2 \hbar^2} \sqrt{\frac{m^3 T^3}{2}} \Gamma(3/2) \operatorname{Li}_{3/2}(\mp e^{\mu/T}) = \mp \frac{gV}{\pi^2 \hbar^2} \left(\frac{mT}{2}\right)^{3/2} \operatorname{Li}_{3/2}(\mp e^{\mu/T}).$$

Using the formula $d\text{Li}_n(x)/dx = \text{Li}_{n-1}(x)/x$ [?], we find

$$\frac{\partial}{\partial \mu}[\mathrm{Li}_{3/2}(\mp e^{\mu/T})] = \mp \frac{\partial}{\partial \mu} \Big(\mp e^{\mu/T}\Big) \frac{\mathrm{Li}_{3/2}(\mp e^{\mu/T})}{e^{\mu/T}} = \frac{\mathrm{Li}_{3/2}(\mp e^{\mu/T})}{T}.$$

So the fluctuations are

$$\langle (\Delta N)^2 \rangle = \mp \frac{gV}{\pi^2 \hbar^2} \left(\frac{mT}{2} \right)^{3/2} \frac{\text{Li}_{3/2}(\mp e^{\mu/T})}{T} \begin{cases} \text{Fermi,} \\ \text{Bose.} \end{cases}$$

Problem 5. Pair correlation function

5.1 Compute the pair correlation of density $C(r) = \langle \langle n(r)n(0) \rangle \rangle$ and the fluctuation of the occupation number $\langle |n_k|^2 \rangle$ of the degenerate Fermi gas $(T \ll E_F)$ in dimensions d = 1, 2, 3. Discuss various distance regimes.

5.2 Repeat the above for the Bose gas above the condensation temperature.