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),

$$\sum_i \dot{w}_i = \sum_i \sum_j (P_{ij} w_j - P_{ij} w_i) = 0. \tag{2}$$

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. We will provide an example to prove that the equation is not time reversible.

Consider a two-state system with states $|1\rangle$ and $|2\rangle$, which has

$$P = \begin{bmatrix} 1/2 & 1/2 \\ 1/2 & 1/2 \end{bmatrix}.$$

Let $|\psi(t)\rangle$ be the state of the system. Suppose that at $t = 0$, $w_1 = 1$ and $w_2 = 0$; that is, $|\psi(0)\rangle = |1\rangle$. At this instant,

$$\dot{w}_1(0) = [P_{11} w_1(0) - P_{11} w_1(0)] + [P_{12} w_2(0) - P_{21} w_1(0)] = -\frac{1}{2},$$
$$\dot{w}_2(0) = [P_{21} w_1(0) - P_{12} w_2(0)] + [P_{22} w_2(0) - P_{22} w_2(0)] = \frac{1}{2}.$$

At some later time t^*, the system may be in the state $|\psi(t^*)\rangle = (|1\rangle + |2\rangle)/2$. At this instant, $w_1 = w_2 = 1/2$, and

$$\dot{w}_1(t^*) = [P_{11} w_1(t^*) - P_{11} w_1(t^*)] + [P_{12} w_2(t^*) - P_{21} w_1(t^*)] = 0,$$
$$\dot{w}_2(t^*) = [P_{21} w_1(t^*) - P_{12} w_2(t^*)] + [P_{22} w_2(t^*) - P_{22} w_2(t^*)] = 0.$$

It is now impossible for a transition to occur, so the system cannot return to its initial state $|\psi(0)\rangle$. Therefore, Eq. (1) is not reversible. □

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

Solution. 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 w_i represent probabilities, $0 \leq w_i \leq 1$ for all i, which implies $\ln w_i \leq 0$. As shown in Eq. (2), $\sum_i \dot{w}_i = 0$. Thus, $\dot{S} \geq 0$ 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).

Solution. Firstly,

$$S_\alpha = \lim_{\alpha \to 1} \frac{1}{1-\alpha} \ln \sum_i w_i^\alpha.$$

Note that

$$\lim_{\alpha \to 1} \ln \sum_i w_i^\alpha = \ln \sum_i w_i = \ln(1) = 0, \qquad \lim_{\alpha \to 1}(1-\alpha) = 0,$$

where we have used the result of Prob. 1.1(a). Applying L'Hôpital's rule, we find

$$\lim_{\alpha \to 1} S_\alpha = \lim_{\alpha \to 1} \frac{d(\ln \sum_i w_i^\alpha)/d\alpha}{d(1-\alpha)/d\alpha} = \lim_{\alpha \to 1} -\frac{d(\sum_i w_i^\alpha)/d\alpha}{\sum_i w_i^\alpha} = \lim_{\alpha \to 1} -\sum_i w_i^\alpha \ln w_i = -\sum_i w_i \ln w_i,$$

where we have used $d(a^x)/dx = (\ln a)a^x$ [**?**]. This is the Shannon entropy, as desired. □

1.2(b) Show that Rényi entropy doesn't decrease: $\dot{S}_\alpha \geq 0$.

Solution. We note that

$$\dot{S}_\alpha = \frac{d}{dt}\left(\frac{1}{1-\alpha} \ln \sum_i w_i^\alpha\right) = \frac{1}{1-\alpha} \ln \sum_i \frac{d(w_i^\alpha)}{dt} = \frac{1}{1-\alpha} \ln \sum_i \dot{w}_i \frac{d(w_i^\alpha)}{dw_i} = \frac{\alpha}{1-\alpha} \ln \sum_i \dot{w}_i\, w_i^{\alpha-1}.$$

As noted in Prob. 1.1(b), $0 \leq w_i \leq 1$ and $\sum_i \dot{w}_i = 0$. Thus, $\dot{S} \geq 0$ as desired. □

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]

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

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 $\langle(\Delta E)^2\rangle = \left\langle(E - \langle E\rangle)^2\right\rangle$ and the number fluctuation $\langle(\Delta N)^2\rangle = \left\langle(N - \langle N\rangle)^2\right\rangle$ 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

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

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,

$$\begin{aligned}p &\propto \exp\left\{\frac{1}{2T}\left[\left(\frac{\partial P}{\partial T}\right)_V \Delta T\,\Delta V + \left(\frac{\partial P}{\partial V}\right)_t (\Delta V)^2 - \frac{\partial C_v}{\partial T}^2 - \left(\frac{\partial P}{\partial T}\right)_V \Delta V\,\Delta T\right]\right\} \\ &= \exp\left[\left(\frac{1}{2T}\frac{\partial P}{\partial V}\right)_t (\Delta V)^2 - \frac{C_v}{2T^2}(\Delta T)\right] = \exp\left[\left(\frac{1}{2T}\frac{\partial P}{\partial V}\right)_t (\Delta V)^2\right]\exp\left[-\frac{C_v}{2T^2}(\Delta T)\right]. \qquad (3)\end{aligned}$$

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

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

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

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

where Li is the polylogarithm [**?**], we have

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

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

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

So the fluctuations are

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

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.