Problem 1. *H*-theorem and Pauli kinetic balance equation The Pauli balance equation 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. $\square$

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

Solution. We will first provide an example and then give a more general treatment. We assume the probabilities are properly normalized, so $\sum_i P_{ij} = \sum_j P_{ij} = 1$.

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

$$P = \begin{bmatrix} 1-\mu & \mu \\ \mu & 1-\mu \end{bmatrix},$$

where $0 \leq \mu \leq 1$. Applying Eq. (1), we obtain the system of differential equations

$$\begin{aligned} \dot{w}_1 &= (P_{11} w_1 - P_{11} w_1) + (P_{12} w_2 - P_{21} w_1) = \mu(w_2 - w_1), \\ \dot{w}_2 &= (P_{21} w_1 - P_{12} w_2) + (P_{22} w_2 - P_{22} w_2) = \mu(w_1 - w_2). \end{aligned}$$

This system can be written as the matrix equation

$$\frac{d}{dt} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} = \mu \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \end{bmatrix} \equiv A \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}, \tag{3}$$

where we have defined the matrix A. A has eigenvalues λ given by

$$0 = \begin{vmatrix} -(\mu+\lambda) & \mu \\ \mu & -(\mu+\lambda) \end{vmatrix} = (\mu+\lambda)^2 - \mu^2 \quad \Longrightarrow \quad (\mu+\lambda)^2 = \mu^2 \quad \Longrightarrow \quad \lambda = -2\mu, 0.$$

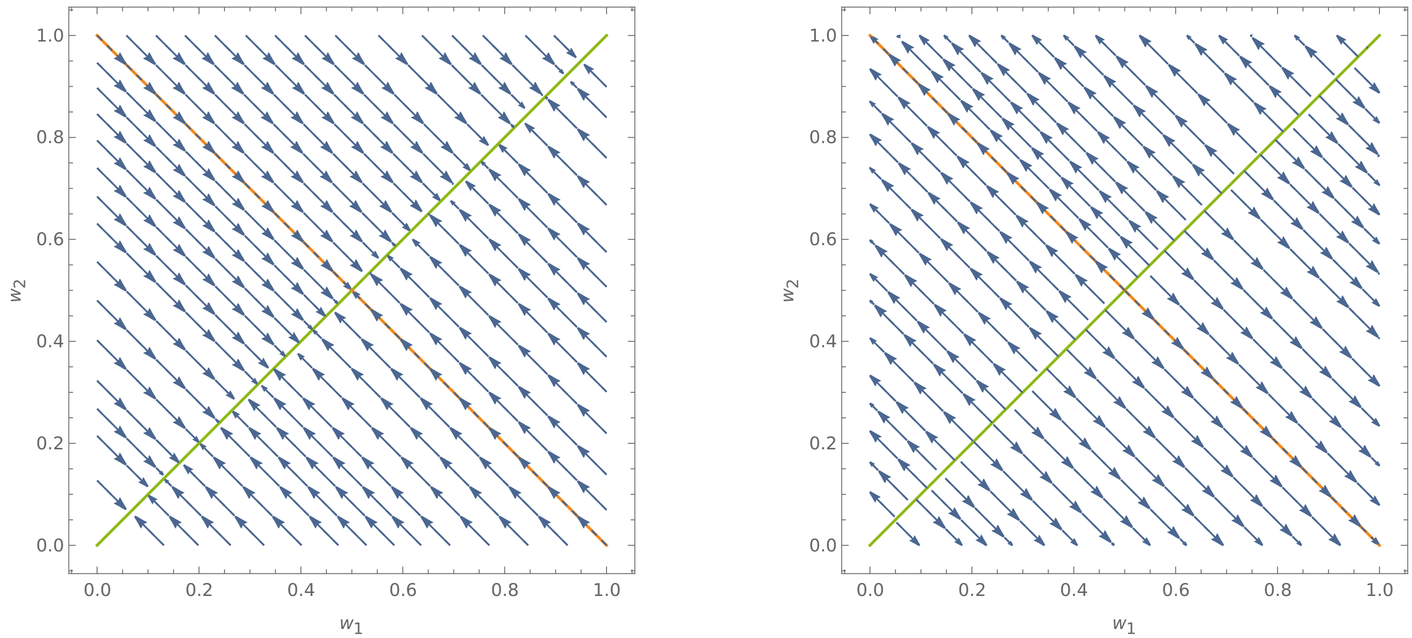

Figure 1: Plot of the (w_1, w_2) phase plane indicating trajectories for (left) the nominal system and (right) the system with $t \to -t$. The normalization $\sum_i w_i = 1$ confines the system to the orange line. The green line represents the equilibrium, which is stable for the nominal system and unstable for the time-reversed system.

The respective eigenvectors u, v can be found by

$$\mu \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = -2\mu \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \quad \Longrightarrow \quad -u_1 + u_2 = -2\mu u_1 \quad \Longrightarrow \quad u_1 = 1, u_2 = -1,$$
$$\mu \begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = 0 \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} \quad \Longrightarrow \quad -v_1 + v_2 = 0 \quad \Longrightarrow \quad v_1 = v_2 = 1.$$

We can analyze the behavior of the system using stability analysis methods which are well known in applied mathematics, but which we will not prove here [1, pp. 127–130]. Since one of the eigenvalues is 0, there is a line of fixed points along the direction of the corresponding eigenvector, $\mathbf{v} = (1, 1)$. Since the other eigenvalue is negative, these fixed points are stable; all trajectories are along $\mathbf{u} = (-1, 1)$ and point toward the fixed points.

In practice, however, the normalization condition $\sum_i w_i = 1$ restricts the system to a line. The blue arrows in Fig. 1 (left) shows trajectories in the (w_1, w_2) phase plane. The green line indicates the line of stable fixed points. The orange line indicates the allowed values of w_1, w_2 under the normalization condition. For any initial condition along the line, the system will tend toward the point $w_1 = w_2 = 1/2$.

Under time reversal $t \to -t$, the directions of the trajectories change. This scenario is shown in Fig. 1 (right). Clearly the equilibrium has switched stability under this transformation. Thus, the system evolves in the opposite direction for any initial condition (unless the systems starts out at equilibrium, in which case it will not evolve in either case). So this system is time irreversible.

Now we will generalize the argument to an N-state system. From Eq. (1), note that

$$\dot{w}_i = P_{ii}(w_i - w_i) + \sum j \neq i^N P_{ij}(w_j - w_i) = \sum j \neq i^N P_{ij} w_j - \left(\sum j = 1^N P_{ij} - P_{ii} \right) w_i$$
$$= \sum j \neq i^N P_{ij} w_j + (P_{ii} - 1) w_i.$$

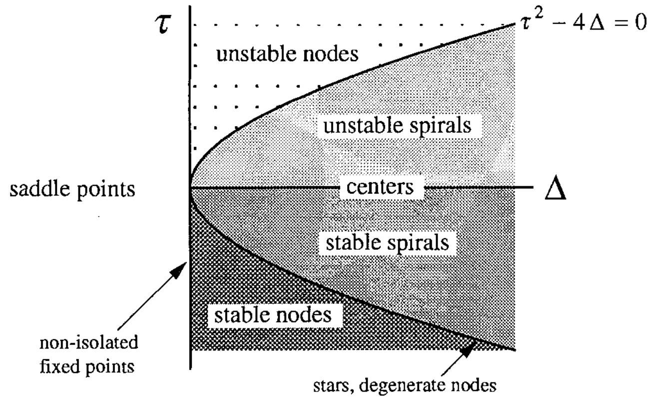

Figure 2: Fixed point classification scheme using $\tau = \mathrm{Tr}(A)$ and $\Delta = \det(A)$ [1, p. 137]

Then A is an $N \times N$ matrix,

$$A = \begin{bmatrix} P_{11}-1 & P_{12} & P_{13} & \cdots & P_{1N} \\ P_{21} & P_{22}-1 & P_{23} & \cdots & P_{2N} \\ P_{31} & P_{32} & 1-P_{33} & \cdots & P_{3N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ P_{N1} & P_{N2} & P_{N3} & \dots & 1-P_{NN} \end{bmatrix}, \tag{4}$$

and the generalization of Eq. (3) is

$$\frac{d}{dt}\begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_N \end{bmatrix} = \begin{bmatrix} P_{11}-1 & P_{12} & P_{13} & \cdots & P_{1N} \\ P_{21} & P_{22}-1 & P_{23} & \cdots & P_{2N} \\ P_{31} & P_{32} & 1-P_{33} & \cdots & P_{3N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ P_{N1} & P_{N2} & P_{N3} & \dots & 1-P_{NN} \end{bmatrix}\begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ \vdots \\ w_N \end{bmatrix}.$$

Another method of analyzing stability in applied mathematics is by analyzing the signs of the trace and determinant of A [1, pp. 136–137]. Let $\tau = \mathrm{Tr}(A)$ and $\Delta = \det(A)$. Referring to Eq. (4), clearly τ is negative (unless it is precisely 0, which would not be very interesting). For Δ, we note that the columns of A sum to the zero vector and therefore are *not* linearly independent, meaning A is not invertible [2]. Thus, it is a singular matrix with zero determinant [3].

The stability and type of fixed point(s) of the system can be determined using Fig. 2 [1, p. 137]. For $\tau < 0$ and $\Delta = 0$, the system has a stable non-isolated fixed point, which manifested as a line of stable fixed point in the two-state example. Due to the normalization condition, the system is confined to a $N-1$ dimensional region of the N dimensional phase space. The equilibrium is a generalization of a stable node, so all trajectories in the N-dimensional phase space end on the allowed equilibrium point. Under $t \to -t$, then, the trajectories change direction as in the two-state example. (This is in contrast to, say, a stable "center" whose trajectories are orbits that would change direction under time reversal, but remain stable.) In other words, the stable equilibrium becomes an unstable one, so the system described by Eq. (1) is time irreversible. □

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). We now apply Eq. (1):

$$\dot{S} = -\sum_i \sum_j (P_{ij}w_j - P_{ji}w_i)\ln w_i = -\frac{1}{2}\left(\sum_i \sum_j (P_{ij}w_j - P_{ji}w_i)\ln w_i + \sum_j \sum_i (P_{ji}w_i - P_{ij}w_j)\ln w_j\right),$$

where we have split the sum in half and swapped indices for the second half. Then, using the symmetry of P,

$$\begin{aligned}\dot{S} &= -\frac{1}{2}\sum_i \sum_j P_{ij}[(w_j - w_i)\ln w_i + (w_i - w_j)\ln w_j] = \frac{1}{2}\sum_i \sum_j P_{ij}[(w_i - w_j)\ln w_i - (w_i - w_j)\ln w_j] \\ &= \frac{1}{2}\sum_i \sum_j P_{ij}(w_i - w_j)(\ln w_i - \ln w_j).\end{aligned}$$

Since w_i represent probabilities, $0 \leq w_i \leq 1$ for all i, which implies $\ln w_i \leq 0$. If $w_i > w_j$, $\ln w_j$ is more negative than $\ln w_i$. That is,

$$\begin{aligned} w_i \geq w_j \quad &\Longrightarrow \quad \ln w_i - \ln w_j \geq 0 \quad \text{and} \quad w_i - w_j \geq 0, \\ w_i \leq w_j \quad &\Longrightarrow \quad \ln w_i - \ln w_j \leq 0 \quad \text{and} \quad w_i - w_j \leq 0. \end{aligned}$$

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 Shannon entropy.

Solution. Firstly,

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

Note that

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

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 $d(a^x)/dx = (\ln a)a^x$ [4]. 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

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

Applying Eq. (1) and the same trick as in Prob. 1.1(c),

$$\begin{aligned}
\dot{S}_\alpha &= \frac{\alpha}{1-\alpha}\frac{1}{\sum_i w_i^\alpha}\sum_i w_i^{\alpha-1}\sum_j (P_{ij}w_j - P_{ji}w_i) \\
&= \frac{\alpha}{1-\alpha}\frac{1}{2\sum_i w_i^\alpha}\left(\sum_i w_i^{\alpha-1}\sum_j (P_{ij}w_j - P_{ji}w_i) + \sum_j w_j^{\alpha-1}\sum_i (P_{ji}w_i - P_{ij}w_j)\right) \\
&= \frac{\alpha}{1-\alpha}\frac{1}{2\sum_i w_i^\alpha}\sum_i\sum_j P_{ij}[w_i^{\alpha-1}(w_j - w_i) + w_j^{\alpha-1}(w_i - w_j)] \\
&= \frac{\alpha}{1-\alpha}\frac{1}{2\sum_i w_i^\alpha}\sum_i\sum_j P_{ij}[(w_i^{\alpha-1} - w_j^{\alpha-1})(w_j - w_i)].
\end{aligned}$$

Keeping in mind that $0 \leq w_i \leq 1$, this result is non-negative in all possible regimes:

$$\begin{aligned}
w_j \geq w_i \quad &\text{and} \quad \alpha < 1 \quad \Longrightarrow \quad \frac{\alpha}{1-\alpha} > 0 \quad \text{and} \quad w_i^{\alpha-1} - w_j^{\alpha-1} \geq 0 \quad \text{and} \quad w_j - w_i \geq 0, \\
w_j \geq w_i \quad &\text{and} \quad \alpha > 1 \quad \Longrightarrow \quad \frac{\alpha}{1-\alpha} < 0 \quad \text{and} \quad w_i^{\alpha-1} - w_j^{\alpha-1} \leq 0 \quad \text{and} \quad w_j - w_i \geq 0, \\
w_j \leq w_i \quad &\text{and} \quad \alpha < 1 \quad \Longrightarrow \quad \frac{\alpha}{1-\alpha} > 0 \quad \text{and} \quad w_i^{\alpha-1} - w_j^{\alpha-1} \leq 0 \quad \text{and} \quad w_j - w_i \leq 0, \\
w_j \leq w_i \quad &\text{and} \quad \alpha > 1 \quad \Longrightarrow \quad \frac{\alpha}{1-\alpha} < 0 \quad \text{and} \quad w_i^{\alpha-1} - w_j^{\alpha-1} \geq 0 \quad \text{and} \quad w_j - w_i \leq 0.
\end{aligned}$$

Of course $\sum_i w_i^\alpha > 0$ in any case. Thus, $\dot{S}_\alpha \geq 0$ 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. The atoms gain additional spin energy in the presence of a magnetic field $\mathbf{B} = B\,\hat{\mathbf{z}}$. In the spin-1/2 case, the thermodynamic potential becomes

$$\Omega(\mu) = \frac{\Omega_0(\mu + \mu_B B)}{2} + \frac{\Omega_0(\mu - \mu_B B)}{2}, \tag{5}$$

where Ω_0 is the thermodynamic potential when no magnetic field is present and $\mu_B = e\hbar/2mc$ is the Bohr magneton. This formulation is due to each particle's picking up extra energy $\pm\mu_B B$ from the component of its spin in the direction of the field. Since the thermodynamic potential depends on $\epsilon - \mu$, we can equivalently make the substitution $\mu \to \mu \mp \mu_B B$ [5, p. 172].

For an atom of arbitrary spin s, there are $g = 2s+1$ possible z components of the spin. They are described by the matrix S_z. Note that

$$S_z = \frac{\hbar}{2}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \hbar \begin{bmatrix} s & 0 \\ 0 & -s \end{bmatrix} \quad (s = 1/2), \qquad S_z = \hbar \begin{bmatrix} s & 0 & 0 & \cdots & 0 \\ 0 & s-1 & 0 & \cdots & 0 \\ 0 & 0 & s-2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & -s \end{bmatrix} \quad (s \text{ arbitrary}).$$

Let $\mu_R = |q|\hbar/2mc$, where q and m are the charge and mass of the atom, respectively. Then, by analogy with Eq. (5), for arbitrary s

$$\Omega(\mu) = \frac{1}{g}\sum_{j=0}^{s-1/2} \Omega_0[\mu + 2(s-j)\mu_R B] \equiv \frac{1}{g}\sum_{j=0}^{s-1/2} \Omega_0(\mu_j), \tag{6}$$

where we have defined $\mu_j = \mu + 2(s-j)\mu_R B$.

Since B is small, we can Taylor expand Eq. (6) about $\mu_R B = 0$ [5, p. 172]:

$$\Omega(\mu) \approx \Big[\Omega(\mu)\Big]_{\mu_R B=0} + \mu_R B \left[\frac{\partial\Omega(\mu)}{\partial(\mu_R B)}\right]_{\mu_R B=0} + \frac{\mu_R^2 B^2}{2}\left[\frac{\partial^2\Omega(\mu)}{\partial(\mu_R B)^2}\right]_{\mu_R B=0}.$$

Note that

$$\frac{\partial\Omega}{\partial(\mu_R B)} = \frac{1}{g}\sum_{j=0}^{2s}\frac{\partial\Omega_0(\mu)}{\partial\mu_j}\frac{\partial\mu_j}{\partial(\mu_R B)} = \frac{1}{g}\sum_{j=0}^{2s} 2(s-j)\frac{\partial\Omega_0(\mu)}{\partial\mu_j},$$

$$\frac{\partial^2\Omega}{\partial(\mu_R B)^2} = \frac{1}{g}\sum_{j=0}^{2s} 2(s-j)\frac{\partial^2\Omega_0(\mu)}{\partial\mu_j^2}\frac{\partial\mu_j}{\partial(\mu_R B)} = \frac{1}{g}\sum_{j=0}^{2s} 4(s-j)^2\frac{\partial^2\Omega_0(\mu)}{\partial\mu_j^2},$$

so

$$\left[\frac{\partial\Omega}{\partial(\mu_R B)}\right]_{\mu_R B=0} = \frac{1}{g}\sum_{j=0}^{2s} 2(s-j)\left[\frac{\partial\Omega_0(\mu)}{\partial\mu_j}\right]_{\mu_R B=0} = \frac{1}{g}\sum_{j=0}^{s-1/2} 2(s-j)\frac{\partial\Omega_0(\mu)}{\partial\mu} = 0,$$

$$\left[\frac{\partial^2\Omega}{\partial(\mu_R B)^2}\right]_{\mu_R B=0} = \frac{1}{g}\sum_{j=0}^{2s} 4(s-j)^2\left[\frac{\partial^2\Omega_0(\mu)}{\partial\mu_j^2}\right]_{\mu_R B=0} = \frac{1}{g}\sum_{j=0}^{2s} 4(s-j)^2\frac{\partial^2\Omega_0(\mu)}{\partial\mu^2} = \frac{8}{g}\frac{\partial^2\Omega_0(\mu)}{\partial\mu^2}\sum_{j=0}^{s-1/2}(s-j)^2,$$

where we have used the fact that s is an integer multiple of $1/2$ for a fermion. So we have

$$\Omega(\mu) \approx \Omega_0(\mu) + \frac{4\mu_R^2 B^2}{g}\frac{\partial^2\Omega_0(\mu)}{\partial\mu^2}\sum_{j=0}^{s-1/2}(s-j)^2.$$

The magnetic moment of the gas is $M = -(\partial\Omega/\partial B)_{T,V,\mu}$ [5, p. 172]. Here,

$$M = -\frac{8\mu_R^2 B}{g}\frac{\partial^2\Omega_0(\mu)}{\partial\mu^2}\sum_{j=0}^{s-1/2}(s-j)^2.$$

According to p. 2 of lecture 12, the paramagnetic susceptibility is defined $\chi_{\text{para}} = (\partial M/\partial B)/V$. Then

$$\chi_{\text{para}} = -\frac{8\mu_R^2}{gV}\frac{\partial^2\Omega_0(\mu)}{\partial\mu^2}\sum_{j=0}^{s-1/2}(s-j)^2 = \frac{8\mu_R^2}{gV}\left(\frac{\partial N}{\partial\mu}\right)_{T,V}\sum_{j=0}^{s-1/2}(s-j)^2,$$

where we have used $\partial\Omega_0/\partial\mu = -N$ [5, p. 172]. The number of particles in a degenerate Fermi gas is [6, p. 152] [5, p. 173]

$$N = \frac{gV}{6\pi^2\hbar^3}(2m\mu)^{3/2}.$$

So

$$\chi_{\text{para}} = \frac{8\mu_R^2}{gV}\frac{\partial}{\partial\mu}\left(\frac{gV}{6\pi^2\hbar^3}(2m\mu)^{3/2}\right)\sum_{j=0}^{s-1/2}(s-j)^2 = \frac{3}{2}\frac{8q^2\hbar^2}{4m^2c^2gV}\frac{gV}{6\pi^2\hbar^3}\sqrt{2^3m^3\mu}\sum_{j=0}^{s-1/2}(s-j)^2$$
$$= \frac{q^2}{c^2\pi^2\hbar}\sqrt{\frac{2\mu}{m}}\sum_{j=0}^{s-1/2}(s-j)^2.$$

Problem 3. Landau diamagnetism

3.1 Compute the Landau diamagnetic susceptibility for an ultra-relativistic Fermi gas in a weak field.

Solution. We will assume an electron gas. The energy levels ϵ for a relativistic electron in magnetic field $\mathbf{B} = B\,\hat{\mathbf{z}}$ are given by

$$\epsilon^2 - m^2 - p_z^2 = eB(2n+1) + eB\sigma,$$

where $\sigma = \pm 1$ are the eigenvalues of σ_z and $n = 0, 1, 2, \ldots$ [7, p. 101]. Then

$$\epsilon^2 = eB(2n+1+\sigma) + m^2 + p_z^2.$$

In order to take σ into account, we renumber the states such that $\epsilon^2 = 2neB + p_z^2$, where nth state has degeneracy 2 for $n > 0$, and the 0th state is not degenerate. Then

$$\epsilon = \pm c\sqrt{2neB + m^2c^2 + p_z^2},$$

which has no degeneracy, since the $\pm$ sign splits the degenerate levels, and we have inserted factors of c. In practice, however, we need only consider the positive energy levels, since the negative ones have exponentially suppressed contributions at small T.

The number of states in the interval dp_z for a given ϵ is the same as in the nonrelativistic case [5, p. 173]:

$$\frac{2eVB}{(2\pi\hbar)^2c}\,dp_z\,, \tag{7}$$

where $2 = g$ for the electron.

The relevant thermodynamic potential for a nonrelativistic electron gas, for which $\epsilon = p_z^2/2m + (2n+1)\mu_B B$, is [5, p. 173]

$$\Omega = 2\mu_B B\sum_{n=0}^{\infty} f[\mu - (2n+1)\mu_B B], \qquad \text{where} \quad f(\mu) = -\frac{TmV}{2\pi^2\hbar^3}\int_{-\infty}^{\infty}\ln\left[1+\exp\left(\frac{\mu}{T} - \frac{p_z^2}{2mT}\right)\right]dp_z\,. \tag{8}$$

For the ultra-relativistic gas, then,

$$\Omega = -\frac{\mu_B BTmV}{\pi^2\hbar^3}\sum_{n=0}^{\infty}\int_{-\infty}^{\infty}\ln\left[1+\exp\left(\frac{\mu - c\sqrt{2neB+m^2c^2+p_z^2}}{T}\right)\right]dp_z$$
$$= -\frac{\mu_B BTmV}{\pi^2\hbar^3}\sum_{n=0}^{\infty}\int_{0}^{\infty}\ln\left[1+\exp\left(\frac{\mu - c\sqrt{2neB+m^2c^2+p_z^2}}{T}\right)\right]dp_z\,, \tag{9}$$

where we have used that fact that $p_z^2 = (-p_z)^2$.

The Euler-Maclaurin formula is [5, p. 173]

$$\frac{1}{2}F(a) + \sum_{n=1}^{\infty} F(a+n) \approx \int_a^\infty F(x)\,dx - \frac{1}{12}F'(a).$$

In our case $a = 0$, so

$$\sum_{n=0}^{\infty} F(n) \approx \int_0^\infty F(x)\,dx + \frac{1}{2}F(0) - \frac{1}{12}F'(0), \tag{10}$$

where we have added $F(0)/2$ to both sides. From Eq. (9), note that

$$F(0) = -\frac{2\mu_B BTmV}{\pi^2\hbar^3}\int_0^\infty \ln\left[1+\exp\left(\frac{\mu - c\sqrt{m^2c^2+p_z^2}}{T}\right)\right] dp_z\,,$$

$$\begin{aligned}
F'(0) &= -\frac{2\mu_B BTmV}{\pi^2\hbar^3}\left[\frac{d}{dn}\int_0^\infty \ln\left\{1+\exp\left(\frac{\mu - c\sqrt{2neB+m^2c^2+p_z^2}}{T}\right)\right\} dp_z\right]_{n=0} \\
&= -\frac{2\mu_B BTmV}{\pi^2\hbar^3}\left[-\int_0^\infty \frac{ceB}{T\sqrt{2neB+m^2c^2+p_z^2}}\left\{\exp\left(\frac{c\sqrt{2neB+m^2c^2+p_z^2}-\mu}{T}\right)+1\right\}^{-1} dp_z\right]_{n=0} \\
&= \frac{2\mu_B BTmV}{\pi^2\hbar^3}\frac{ceB}{T}\int_0^\infty \frac{dp_z}{\sqrt{m^2c^2+p_z^2}\,(e^{c(\sqrt{m^2c^2+p_z^2}-\mu)/T}+1)} \\
&= \frac{4m^2c^2\mu_B^2B^2V}{\pi^2\hbar^4}\int_0^\infty \frac{dp_z}{\sqrt{m^2c^2+p_z^2}\,(e^{c(\sqrt{m^2c^2+p_z^2}-\mu)/T}+1)}.
\end{aligned}$$

Then

$$\begin{aligned}
\Omega = -\frac{2\mu_B BTmV}{\pi^2\hbar^3}&\int_0^\infty\int_0^\infty \ln\left[1+\exp\left(\frac{\mu - c\sqrt{2eBx+m^2c^2+p_z^2}}{T}\right)\right] dp_z\,dx \\
&- \frac{\mu_B BTmV}{\pi^2\hbar^3}\int_0^\infty \ln\left[1+\exp\left(\frac{\mu - c\sqrt{m^2c^2+p_z^2}}{T}\right)\right] dp_z \\
&+ \frac{m^2c^2\mu_B^2B^2V}{3\pi^2\hbar^4}\int_0^\infty \frac{dp_z}{\sqrt{m^2c^2+p_z^2}\,(e^{c(\sqrt{m^2c^2+p_z^2}-\mu)/T}+1)}.
\end{aligned}$$

The magnetic moment of the gas is $M = -(\partial\Omega/\partial B)_{T,V,\mu}$ [6, p. 172], so

$$\begin{aligned}
M = \frac{2\mu_B TmV}{\pi^2\hbar^3}&\int_0^\infty\int_0^\infty \ln\left[1+\exp\left(\frac{\mu - c\sqrt{2eBx+m^2c^2+p_z^2}}{T}\right)\right] dp_z\,dx \\
&+ \frac{\mu_B TmV}{\pi^2\hbar^3}\int_0^\infty \ln\left[1+\exp\left(\frac{\mu - c\sqrt{m^2c^2+p_z^2}}{T}\right)\right] dp_z \\
&- \frac{2m^2c^2\mu_B^2BV}{3\pi^2\hbar^4}\int_0^\infty \frac{dp_z}{\sqrt{m^2c^2+p_z^2}\,(e^{c(\sqrt{m^2c^2+p_z^2}-\mu)/T}+1)},
\end{aligned}$$

and the diamagnetic susceptibility is $\chi_{\text{dia}} = (\partial M/\partial B)/V$, so

$$\chi_{\text{dia}} = -\frac{2m^2c^2\mu_B^2V}{3\pi^2\hbar^4}\int_0^\infty \frac{dp_z}{\sqrt{m^2c^2+p_z^2}\,(e^{c(\sqrt{m^2c^2+p_z^2}-\mu)/T}+1)}.$$

At the limit $T = 0$, the gas is completely degenerate and the occupation number $\langle n \rangle = 1$ for $p_z < p_0$, $\langle n \rangle = 0$ for $p_z > p_0$ where p_0 is the Fermi momentum [5, p. 357]. In this limit, then,

$$\chi_{\text{dia}} \approx -\frac{2m^2c^2\mu_B^2 V}{3\pi^2\hbar^4}\int_0^{p_0}\frac{dp_z}{\sqrt{m^2c^2+p_z^2}} = -\frac{2m^2c^2\mu_B^2 V}{3\pi^2\hbar^4}\tanh^{-1}\left(\frac{p_0}{\sqrt{m^2c^2+p_0^2}}\right).$$

In the non-relativistic limit $m \to \infty$, the leading asymptotic is

$$\chi_{\text{dia}} \approx -\frac{2m^2c^2\mu_B^2 V}{3\pi^2\hbar^4}\frac{p_0}{mc} = -\frac{2mc\mu_B^2 p_0 V}{3\pi^2\hbar^4} = -\frac{2c}{3\hbar}\chi_{\text{para}}^{\text{nonrel}} = -\frac{2}{3}\chi_{\text{para}}^{\text{nonrel}},$$

where the final equality is true if we take natural units.

In the ultra-relativistic limit, $m \to 0$. Then, taking the Taylor series expansion for small m using Mathematica, we have

$$\chi_{\text{dia}} \approx -\frac{2m^2c^2\mu_B^2 V}{3\pi^2\hbar^4}\left[\tanh^{-1}\left(\frac{1}{p_0}\right) + \frac{m^2c^2}{4p_0^2}\right].$$

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 $\mu_B B$.

Solution. Once again, we will consider an electron gas. For this geometry, the energy levels are

$$\epsilon = \hbar\omega(n+1/2) + \frac{2\pi^2\hbar^2 n'^2}{mL_z^2},$$

where $\omega = eB/mc$ is the cyclotron frequency, $n = 0, 1, 2, \ldots$, and $n' = 0, \pm1, \pm2, \ldots$ [9, pp. 3–4]. In terms of the quantities used in Probs. 4 and 5.1,

$$\epsilon = \mu_B B(2n+1) + \left(\frac{2\pi\hbar}{L_z}\right)^2\frac{n'^2}{2m}. \tag{11}$$

The degeneracy of a state with a given n is $L_xL_y eB/2\pi\hbar c$, which is the same as in the textbook case [10, p. 243]. In notation similar to that of Eq. (8), we have

$$L_xL_y\frac{eB}{2\pi\hbar c} = L_xL_y\frac{2mc\mu_B B}{2\pi\hbar^2 c} = L_zL_y\frac{mT}{\pi\hbar^2}.$$

So the analogue of Eq. (8) in this case is

$$\Omega = 2\mu_B B\sum_{n=0}^{\infty} f[\mu-(2n+1)\mu_B B], \tag{12}$$

$$\text{where}\quad f(\mu) = -2L_xL_y\frac{mT}{\pi\hbar^2}\sum_{n'=0}^{\infty}\ln\left[1+\exp\left(\frac{\mu}{T}-\left(\frac{2\pi\hbar}{L_z}\right)^2\frac{n'^2}{2mT}\right)\right],$$

where in the second expression we written the sum over $n' \in (-\infty, \infty)$ as twice the sum over $n' \in (0, \infty)$, since the expression depends only on n'^2.

In the case where the energy spacing is much smaller than the cyclotron energy, it is sufficient to replace the sum in $f(\mu)$ by an integral. In this limit,

$$f(\mu) \approx -L_xL_y\frac{mT}{\pi\hbar^2}\int_{-\infty}^{\infty}\ln\left[1+\exp\left(\frac{\mu}{T}-\left(\frac{2\pi\hbar}{L_z}\right)^2\frac{n'^2}{2mT}\right)\right]dn' = -\frac{TmV}{2\pi^2\hbar^3}\int_{-\infty}^{\infty}\ln\left[1+\exp\left(\frac{\mu}{T}-\frac{p_z^2}{2mT}\right)\right]dp_z\,,$$

where we defined $p_z = 2\pi\hbar n'/L_z$ and $V = L_x L_y L_z$. This is exactly the same as the expression for the textbook case in which does not impose the restriction $L_z \ll L_x, L_y$, so the diamagnetic susceptibility is [5, pp. 173–174]

$$\chi_{\text{dia}} = -\frac{\mu_B^2 p_0 m}{3\pi^2\hbar^3} = -\frac{\chi_{\text{para}}}{3}$$

when the energy spacing is much smaller than the cyclotron energy.

In the case where the energy spacing is much larger than the cyclotron energy, we can replace the expression of Ω in Eq. (12) with an integral and use the Euler-Maclaurin formula to handle the sum in $F(\mu)$. Applying Eq. (10) to $f(\mu)$, note that

$$\begin{aligned}
F'(0) &= \left[\frac{\partial}{\partial n'}\ln\left\{1+\exp\left(\frac{\mu}{T}-\left(\frac{2\pi\hbar}{L_z}\right)^2\frac{n'^2}{2mT}\right)\right\}\right]_{n'=0} \\
&= \left[\left(\frac{2\pi\hbar}{L_z}\right)^2\frac{n'}{2mT}\left\{1+\exp\left(\frac{4\pi^2\hbar^2}{L_z^2}\frac{n'^2}{2mT}-\frac{\mu}{T}\right)\right\}^{-1}\right]_{n'=0} = 0, \\
F(0) &= \ln\left(1+e^{\mu/T}\right).
\end{aligned}$$

Then we have

$$\Omega = -4L_x L_y \frac{mT}{\pi\hbar^2}\mu_B B\int_0^\infty \left\{\int_0^\infty \ln\left[1+\exp\left(\frac{\mu}{T}-(2x+1)\frac{\mu_B B}{T}-\left(\frac{2\pi\hbar}{L_z}\right)^2\frac{n'^2}{2mT}\right)\right]dn' + \ln\left(1+e^{\mu/T-(2x+1)\mu_B B}\right)\right\}dx\,,$$

so

$$\chi_{\text{dia}} = \frac{1}{V}\frac{\partial M}{\partial B} = -\frac{1}{V}\frac{\partial^2\Omega}{\partial B^2} = 0$$

when the energy spacing is much larger than the cyclotron energy.

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.

Solution. Planck's distribution, which gives the occupation number for state k of a blackbody, is [6, p. 163]

$$\langle n_k\rangle = \frac{1}{e^{\hbar\omega_k/T}-1}.$$

This is a special case of the Bose distribution with $\mu = 0$ and $\epsilon_k = \hbar\omega_k$. The Bose distribution is [6, p. 146]

$$\langle n_k\rangle = \frac{1}{e^{(\epsilon_k-\mu)/T}-1}.$$

Applying $\langle(\Delta N)^2\rangle = T\,\partial\langle N\rangle/\partial\mu$, which is derived in Prob. 4.2, we find [6, p. 355]

$$\begin{aligned}
\langle(\Delta n_k)^2\rangle &= T\frac{\partial\langle n_k\rangle}{\partial\mu} = T\frac{\partial}{\partial\mu}\left(\frac{1}{e^{(\epsilon_k-\mu)/T}-1}\right) = T\frac{e^{(\epsilon_k-\mu)/T}}{T(e^{(\epsilon_k-\mu)/T}-1)^2} = \frac{e^{(\epsilon_k-\mu)/T}-1+1}{(e^{(\epsilon_k-\mu)/T}-1)^2} \\
&= \frac{1}{e^{(\epsilon_k-\mu)/T}-1} + \frac{1}{(e^{(\epsilon_k-\mu)/T}-1)^2} = \langle n_k\rangle\,(1+\langle n_k\rangle).
\end{aligned}$$

The number of photons in the frequency interval $d\omega$ is [6, p. 163]

$$dN_\omega = \frac{V}{\pi^2 c^3} \frac{\omega^2}{e^{\hbar\omega/T} - 1}\, d\omega = \frac{V}{\pi^2 c^3} \omega^2 \langle n_k \rangle \, d\omega \,,$$

where $\langle n_k \rangle = 1/(e^{\hbar\omega/T} - 1)$ is the Planck distribution. By analogy,

$$\left\langle (\Delta\, dN_\omega)^2 \right\rangle = \frac{V}{\pi^2 c^3} \omega^2 \left\langle (\Delta n_k)^2 \right\rangle d\omega = \frac{V}{\pi^2 c^3} \omega^2 \langle n_k \rangle (1 + \langle n_k \rangle)\, d\omega = dN_\omega + \langle n_k \rangle \, dN_\omega \,.$$

For the total number of particles, we integrate over $\omega \in (0, \infty)$ [6, p. 165]:

$$\begin{aligned} \langle (\Delta N)^2 \rangle &= \int_0^\infty \left\langle (\Delta\, dN_\omega)^2 \right\rangle = \int_0^\infty (dN_\omega + \langle n_k \rangle \, dN_\omega) = N + \frac{V}{\pi^2 c^3} \int_0^\infty \frac{\omega^2}{(e^{\hbar\omega/T} - 1)^2}\, d\omega \\ &= N + \frac{VT^3}{\pi^2 c^3 \hbar^3} \int_0^\infty \frac{x^2}{(e^x - 1)^2}\, dx = \frac{VT^3}{\hbar^3 c^3} \frac{2\,\zeta(3)}{\pi^2} + \frac{VT^3}{\pi^2 c^3 \hbar^3} \left(\frac{\pi^2}{3} - 2\,\zeta(3) \right) = \frac{VT^3}{3c^3\hbar^3}, \end{aligned}$$

where N is given in the book, and we have evaluated the second integral using Mathematica.

Likewise, the radiation energy in the interval $d\omega$ is $dE_\omega = \hbar\omega\, dN_\omega$. So we need to multiply $\left\langle (\Delta\, dN_\omega)^2 \right\rangle$ by $(\hbar\omega)^2$ [6, p. 346]:

$$\begin{aligned} \langle (\Delta E)^2 \rangle &= \hbar^2 \int_0^\infty \omega^2 \left\langle (\Delta\, dN_\omega)^2 \right\rangle = \hbar^2 \int_0^\infty \omega^2 (dN_\omega + \langle n_k \rangle \, dN_\omega) \\ &= \frac{\hbar^2 V}{\pi^2 c^3} \left(\int_0^\infty \frac{\omega^4}{e^{\hbar\omega/T} - 1}\, d\omega + \int_0^\infty \frac{\omega^4}{(e^{\hbar\omega/T} - 1)^2}\, d\omega \right) = \frac{\hbar^2 V}{\pi^2 c^3} \left[\frac{24\,\zeta(5)\, T^5}{\hbar^5} + \left(\frac{4\pi^4 T^5}{15\hbar^5} - \frac{24\,\zeta(5)\, T^5}{\hbar^5} \right) \right] \\ &= \frac{\hbar^2 V}{\pi^2 c^3} \frac{4\pi^4 T^5}{15\hbar^5} = \frac{4\pi^2 V T^5}{15 c^3 \hbar^3}. \end{aligned}$$

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 [6, 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 [6, 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 [6, 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 $\partial E/\partial V = -P$ [6, 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 $C_v = T(\partial S/\partial T)_V$ [6, pp. 45, 50, 349]. Making these substitutions,

$$\begin{aligned} p \propto \exp\left\{\frac{1}{2T}\left[\left(\frac{\partial P}{\partial T}\right)_V \Delta T\,\Delta V + \left(\frac{\partial P}{\partial V}\right)_t (\Delta V)^2 - \frac{\partial C_v}{\partial T}^2 - \left(\frac{\partial P}{\partial T}\right)_V \Delta V\,\Delta T\right]\right\} \\ = \exp\left[\left(\frac{1}{2T}\frac{\partial P}{\partial V}\right)_t (\Delta V)^2 - \frac{C_v}{2T^2}(\Delta T)\right] = \exp\left[\left(\frac{1}{2T}\frac{\partial P}{\partial V}\right)_t (\Delta V)^2\right]\exp\left[-\frac{C_v}{2T^2}(\Delta T)\right]. \end{aligned} \tag{13}$$

Thus, the expression is separable and fluctuations in V and in T can be regarded as independent [6, p. 349].

We will focus on fluctuations in volume, and assume their probability to be Gaussian distributed. The Gaussian distribution is given by [6, 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. (13), we find that [6, p. 350]

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

Dividing both sides by N^2 [6, p. 351],

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

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 $N/V = (\partial P/\partial\mu)_T$ [6, pp. 351–352]. Since we associated all quantities with those at equilibrium, we have shown that

$$\langle(\Delta N)^2\rangle = T\frac{\partial\langle N\rangle}{\partial\mu} \tag{14}$$

as desired. □

For a classical Boltzmann gas, the number of particles in a interval d^3p is [6, pp. 108–109]

$$dN_{\mathbf{p}} = \frac{V}{(2\pi mT)^{3/2}}\exp\left(\frac{\mu}{T} - \frac{\mathbf{p}^2}{2mT}\right)d^3p\,,$$

so the total number of particles is

$$N = \frac{V}{(2\pi mT)^{3/2}} \int \exp\left(\frac{\mu}{T} - \frac{\mathbf{p}^2}{2mT}\right) d^3p\,.$$

To apply Eq. (14), note that

$$\begin{aligned} T\frac{\partial\langle N\rangle}{\partial\mu} &= T\frac{\partial}{\partial\mu}\left(\frac{V}{(2\pi mT)^{3/2}} \int \exp\left(\frac{\mu}{T} - \frac{\mathbf{p}^2}{2mT}\right) d^3p\right) = T\frac{V}{(2\pi mT)^{3/2}} \int \frac{d}{dT}\left(e^{\mu/T} e^{-\mathbf{p}^2/(2mT)}\, d^3p\right) \\ &= \frac{T}{T}\frac{\partial}{\partial\mu}\left(\frac{V}{(2\pi mT)^{3/2}} \int \exp\left(\frac{\mu}{T} - \frac{\mathbf{p}^2}{2mT}\right) d^3p\right) = N. \end{aligned}$$

Thus, for the Boltzmann gas,

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

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 $z = \epsilon/T$ [6, pp. 149, 354]. Evaluating the integrals using

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

where Li is the polylogarithm [8], 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 $d\mathrm{Li}_n(x)/dx = \mathrm{Li}_{n-1}(x)/x$ [8], we find

$$T\frac{\partial}{\partial\mu}[\mathrm{Li}_{3/2}(\mp e^{\mu/T})] = \mp T\frac{\partial}{\partial\mu}\left(\mp e^{\mu/T}\right)\frac{\mathrm{Li}_{1/2}(\mp e^{\mu/T})}{e^{\mu/T}} = T\frac{\mathrm{Li}_{1/2}(\mp e^{\mu/T})}{T} = \mathrm{Li}_{1/2}(\mp e^{\mu/T}).$$

So the fluctuations are

$$\begin{aligned} \langle(\Delta N)^2\rangle &= \mp\frac{gV}{\pi^2\hbar^2}\left(\frac{mT}{2}\right)^{3/2}\mathrm{Li}_{1/2}(\mp e^{\mu/T}) \\ &= \mp\frac{gV}{\pi^2\hbar^2}\left(\frac{mT}{2}\right)^{3/2}\frac{1}{\mp\Gamma(1/2)}\int_0^\infty \frac{dz}{\sqrt{z}(e^{z-\mu/T} \pm 1)} = \frac{gVT}{\hbar^2}\sqrt{\frac{m^3}{2^3\pi^5}}\int_0^\infty \frac{d\epsilon}{\sqrt{\epsilon}(e^{(\epsilon-\mu)/T} \pm 1)} \begin{cases} \text{Fermi,} \\ \text{Bose.} \end{cases} \end{aligned}$$

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 2D. Discuss various distance regimes.

Solution. The spatial correlation of the density fluctuations in a 2D Fermi gas is given by

$$\langle \Delta n_1\, \Delta n_2\rangle = \frac{1}{A^2} {\sum_{\sigma,\mathbf{p},\mathbf{p}'}}' (1 - \langle n_{\mathbf{p}'\sigma}\rangle)\, \langle n_{\mathbf{p}\sigma}\rangle\, e^{i(\mathbf{p}-\mathbf{p}')(\mathbf{r}_2-\mathbf{r}_1)/\hbar},$$

where n is an occupation number, $\mathbf{p}$ and $\mathbf{p}'$ are momenta, and σ is a spin component [5, p. 356]. We can approximate the sum by an integral using the momentum elements $A\, d^2p\,/(2\pi\hbar)^2$ and $A\, d^2p'\,/(2\pi\hbar)^2$:

$$\langle \Delta n_1\, \Delta n_2\rangle = \frac{1}{(2\pi\hbar)^4} \sum_\sigma \iint (1 - \langle n_{\mathbf{p}'\sigma}\rangle)\, \langle n_{\mathbf{p}\sigma}\rangle\, e^{i(\mathbf{p}-\mathbf{p}')(\mathbf{r}_2-\mathbf{r}_1)/\hbar}\, d^2p\, d^2p'\,. \tag{15}$$

For the first term [5, p. 356],

$$\begin{aligned}
\iint \langle n_{\mathbf{p}\sigma}\rangle\, e^{i(\mathbf{p}-\mathbf{p}')(\mathbf{r}_2-\mathbf{r}_1)/\hbar}\, d^2p\, d^2p' &= \sum_\sigma \int \langle n_{\mathbf{p}\sigma}\rangle\, e^{i\mathbf{p}(\mathbf{r}_2-\mathbf{r}_1)/\hbar}\, d^3p \int e^{-i\mathbf{p}'(\mathbf{r}_2-\mathbf{r}_1)/\hbar}\, d^2p' \\
&= \sum_\sigma \int \langle n_{\mathbf{p}\sigma}\rangle\, \delta(\mathbf{r}_2-\mathbf{r}_1)\, e^{i\mathbf{p}(\mathbf{r}_2-\mathbf{r}_1)/\hbar}\, d^2p \\
&= \delta(\mathbf{r}_2-\mathbf{r}_1) \sum_\sigma \int \langle n_{\mathbf{p}\sigma}\rangle\, d^2p = \langle n\rangle\, \delta(\mathbf{r}_2-\mathbf{r}_1).
\end{aligned}$$

This is the first term in the definition of the spatial correlation, which is

$$C(r_1, r_2) = \langle \Delta n_1\, \Delta n_2\rangle = \langle n\rangle\, \delta(\mathbf{r}_2-\mathbf{r}_1) + \langle n\rangle\, \nu(r), \tag{16}$$

meaning we can associate $\nu(r)$ with the second term in Eq. (18) [5, pp. 351, 356]. So the correlation function is

$$\nu(r) = -\frac{1}{(2\pi\hbar)^4\, \langle n\rangle} \sum_\sigma \left| \int e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}\, \langle n_{\mathbf{p}\sigma}\rangle\, d^2p \right|^2.$$

For a Fermi gas, $\langle n_{\mathbf{p}\sigma}\rangle = \langle n_{\mathbf{p}}\rangle = 1/(e^{(\epsilon-\mu)/T}+1)$, which does not depend on σ. Then [5, p. 356]

$$\begin{aligned}
\nu(r) &= -\frac{g}{\langle n\rangle\, (2\pi\hbar)^4} \left| \int \frac{e^{i\mathbf{p}\cdot\mathbf{r}/\hbar}}{e^{(\epsilon-\mu)/T}+1}\, d^2p \right|^2 = -\frac{g}{\langle n\rangle\, (2\pi\hbar)^2} \left| \int_0^{2\pi} \int_0^\infty \frac{p\, e^{ipr\cos\theta/\hbar}}{e^{(\epsilon-\mu)/T}+1}\, dp\, d\theta \right|^2 \qquad (17) \\
&= \frac{(2\pi)^2 g}{\langle n\rangle\, (2\pi\hbar)^4} \left(\int_0^\infty \frac{p\, J_0(pr/\hbar)}{e^{(\epsilon-\mu)/T}+1}\, dp \right)^2 \equiv \frac{g}{4\pi^2\hbar^4\, \langle n\rangle} I^2, \qquad (18)
\end{aligned}$$

where $J_0(x)$ is a Bessel function of the first kind, and we have defined I.

For $T \ll E_F = p_0^2/2m$ where p_0 is the Fermi momentum, the integral has contributions from only $p \in (0, p_0)$. Thus $\langle n\rangle$ is approximately a step function in the $T = 0$ limit, with $\langle n\rangle = 1$ for $p < p_0$ [6, p. 357]. This gives us

$$I \approx \int_0^{p_0} p\, J_0\!\left(\frac{pr}{\hbar}\right) dp = \left[\frac{\hbar p}{r} J_1\!\left(\frac{pr}{\hbar}\right) \right]_0^{p_0} = \frac{\hbar p_0}{r} J_1\!\left(\frac{p_0 r}{\hbar}\right),$$

where we have used the identity $d[x^m J_m(x)]/dx = x^m J_{m-1}(x)$ [11]. Substituting into Eq. (18),

$$\nu(r) = \frac{g p_0^2}{4\pi^2\hbar^2 r^2\, \langle n\rangle} J_1^2\!\left(\frac{p_0 r}{\hbar}\right),$$

and feeding this into Eq. (16), we find

$$C(r) = \langle n \rangle\, \delta(r) + \frac{g p_0^2}{4\pi^2\hbar^2 r^2} J_1^2\Big(\frac{p_0 r}{\hbar}\Big).$$

For $r \ll \hbar/p_0$, the argument of J_0 is small everywhere. This follows because for a degenerate gas, only the range $p \in (0, p_0)$ contributes to the integral. Then we can use the asymptotic approximation $J_m(z) \approx z^m/[2^m\,\Gamma(m+1)]$ [11]. In this limit,

$$C(r) \approx \langle n \rangle\, \delta(r) + \frac{g p_0^2}{4\pi^2\hbar^2 r^2}\left(\frac{1}{2}\frac{p_0 r}{\hbar}\right)^2 = \langle n \rangle\, \delta(r) + \frac{g p_0^4}{16\pi^2\hbar^4},$$

which is independent of r.

For $r \gg \hbar/p_0$, the argument of J_1 is large everywhere. This means we can use the asymptotic approximation [11]

$$J_m(z) \approx \sqrt{\frac{2}{\pi z}} \cos\Big(z - \frac{m\pi}{2} - \frac{\pi}{4}\Big).$$

The integral then becomes

$$\begin{aligned}
I &\approx \sqrt{\frac{2\hbar}{\pi r}} \int_0^{p_0} \sqrt{p}\cos\Big(\frac{pr}{\hbar} - \frac{\pi}{4}\Big)\, dp = \sqrt{\frac{2\hbar^3}{\pi r^3}} \frac{\partial}{\partial r} \int_0^{p_0} \frac{\sin(pr/\hbar - \pi/4)}{\sqrt{p}}\, dp \\
&= \sqrt{\frac{2\hbar^3}{\pi r^3}} \frac{\partial}{\partial r}\left\{\sqrt{\frac{\pi\hbar}{r}}\left[S\left(\sqrt{\frac{2p_0 r}{\pi\hbar}}\right) - C\left(\sqrt{\frac{2p_0 r}{\pi\hbar}}\right)\right]\right\} \approx -\sqrt{\frac{2\hbar^3}{\pi r^3}} \frac{\partial}{\partial r}\left\{\sqrt{\frac{\pi\hbar}{r}}\sqrt{\frac{\hbar}{2\pi p_0 r}}\left[\sin\Big(\frac{p_0 r}{\hbar}\Big) + \cos\Big(\frac{p_0 r}{\hbar}\Big)\right]\right\} \\
&= -\sqrt{\frac{2\hbar^5}{\pi p_0 r^3}} \frac{\partial}{\partial r}\left(\frac{\sin(p_0 r/\hbar + \pi/4)}{r}\right) = -\sqrt{\frac{4\hbar^5}{\pi p_0 r^3}}\left(\frac{p_0\cos(p_0 r/\hbar + \pi/4)}{\hbar r} - \frac{\sin(p_0 r/\hbar + \pi/4)}{r^2}\right) \\
&\approx -\sqrt{\frac{4\hbar^3 p_0}{\pi r^5}} \cos\Big(\frac{p_0 r}{\hbar} + \frac{\pi}{4}\Big) \approx -\sqrt{\frac{4\hbar^3 p_0}{\pi r^5}} \cos\Big(\frac{p_0 r}{\hbar}\Big),
\end{aligned}$$

where S and C are the Fresnel integrals, and we have used the asymptotic expansions

$$C(u) \approx \frac{1}{2} + \frac{\sin(\pi u^2/2)}{\pi u}, \qquad S(u) \approx \frac{1}{2} - \frac{\cos(\pi u^2/2)}{\pi u},$$

which are valid for $u \gg 1$ [12]. In going to the final line, we have retained only the term in the lowest power of $1/r$ [6, p. 357]. So we have

$$C(r) \approx \langle n \rangle\, \delta(r) + \frac{g p_0}{\pi^3 \hbar r^5}\cos^2\Big(\frac{p_0 r}{\hbar}\Big).$$

For small but nonzero temperatures, $\mu \approx \epsilon_0 = p_0^2/2m$, where ϵ_0 and p_0 are the Fermi energy and momentum, respectively. Let $x = (\epsilon - \epsilon_0)/T = p_0(p - p_0)/mT$, where $\lambda = mT/\hbar p_0$ [5, p. 358]. Making this substitution and integrating by parts [6, p. 358],

$$I = \int_0^\infty \frac{p\, J_0(pr/\hbar)}{e^x + 1}\, dp = \left[\frac{\hbar p\, J_1(pr/\hbar)}{r(e^x+1)}\right]_0^\infty + \frac{\hbar p_0}{mTr}\int_0^\infty \frac{p\, J_1(pr/\hbar)\, e^x}{(e^x+1)^2}\, dp = \frac{\hbar p_0}{mTr}\int_0^\infty \frac{p\, J_1(pr/\hbar)}{(e^x+1)(e^{-x}+1)}\, dp$$

where we have used $d[x^m J_m(x)]/dx = x^m J_{m-1}(x)$ and the fact that $J_1(0) = 0$ [11]. Once again applying the large-argument asymptotic limit, Let $z = p_0 r/\hbar + \lambda r x$. Then

$$\begin{aligned}
I &\approx \frac{\hbar p_0}{mTr}\sqrt{\frac{2}{\pi}} \int_0^\infty (\hbar\lambda x + p_0)\frac{\cos(z - 3\pi/4)}{\sqrt{z}(e^x+1)(e^{-x}+1)}\, dp = \frac{\hbar p_0}{mTr}\sqrt{\frac{2}{\pi}}\int_0^\infty \frac{\hbar z}{r}\frac{\cos(z - 3\pi/4)}{\sqrt{z}(e^x+1)(e^{-x}+1)}\, dp \\
&= -\frac{\hbar^2 p_0}{mTr^2}\sqrt{\frac{2}{\pi}}\frac{\partial}{\partial r}\left(\frac{\hbar}{r}\int_0^\infty \frac{\sin(z - 3\pi/4)}{\sqrt{z}(e^x+1)(e^{-x}+1)}\, dp\right) \approx -\frac{\hbar^3 p_0}{mTr^2}\sqrt{\frac{2}{\pi}}\frac{\partial}{\partial r}\left(\frac{1}{r}\int_{-\infty}^\infty \frac{\sin(p_0 r/\hbar + \lambda r x - 3\pi/4)}{(e^x+1)(e^{-x}+1)}\, dp\right),
\end{aligned}$$

where the final approximation follows since $\sqrt{z}$ varies slowly. Then, using the calculations on p. 358 of Ref. [5],

$$I = -\frac{\hbar^3 p_0}{mTr^2}\frac{\partial}{\partial r}\left[\frac{\pi\lambda}{\sinh(\pi\lambda r)}\sin\left(\frac{p_0 r}{\hbar}\right)\right] = -\frac{\hbar^3 p_0}{mTr^2}\left[\frac{\pi\lambda p_0\cos(p_0 r/\hbar)}{\hbar\sinh(\pi\lambda r)} - \frac{\pi^2\lambda^2\sin(p_0 r/\hbar)}{\tanh(\pi\lambda r)\sinh(\pi\lambda r)}\right],$$

which yields in the $r \gg \hbar/p_0$ limit, upon taking the average of $\cos^2$ [5, p. 358],

$$I^2 \approx \frac{\hbar^6 p_0^2}{m^2T^2r^4}\frac{\pi^2\lambda^2 p_0^2}{2\hbar^2\sinh^2(\pi\lambda r)} = \frac{\hbar^6 p_0^2}{m^2T^2r^4}\frac{\pi^2 m^2 T^2}{2\hbar^4\sinh^2(\pi mTr/\hbar p_0)} = \frac{\pi^2\hbar^2 p_0^2}{2r^4}\operatorname{csch}^2\left(\frac{\pi mTr}{\hbar p_0}\right).$$

Finally, we find the correlation function

$$C(r) \approx \langle n\rangle\,\delta(r) + \frac{gp_0^2}{8\hbar^2 r^4}\operatorname{csch}^2\left(\frac{\pi mTr}{\hbar p_0}\right).$$

In the limit that $p_0 r/\hbar$ is also large compared to ϵ_0/T [5, p. 358],

$$C(r) \approx \langle n\rangle\,\delta(r) + \frac{gp_0^2}{2\hbar^2 r^4}\exp\left(-\frac{2\pi mTr}{\hbar p_0}\right).$$

The general expression for the fluctuation of the occupation number for a Fermi gas is, in three dimensions [5, p. 356],

$$\langle|\Delta n_k|^2\rangle = \frac{g}{(2\pi\hbar)^3 V}\int \langle n_{\mathbf{p}}\rangle\left(1 - \langle n_{\mathbf{p}+\hbar\mathbf{k}}\rangle\right)d^3p\,.$$

The 2D analogue is then

$$\langle|\Delta n_k|^2\rangle = \frac{g}{(2\pi\hbar)^2 V}\int \langle n_{\mathbf{p}}\rangle\left(1 - \langle n_{\mathbf{p}+\hbar\mathbf{k}}\rangle\right)d^2p\,.$$

We will assume that we are interested in small wave numbers, $k \ll p_0/\hbar$. In the $T = 0$ limit, the integrand above is nonzero only for $\langle n_{\mathbf{p}}\rangle = 1$ and $\langle n_{\mathbf{p}+\hbar\mathbf{k}}\rangle = 0$; that is, points that are in a circle of radius p_0, with center at $p = 0$, but not in the circle of radius p_0 with center at $p = \hbar k$ [6, p. 357]. The area of the parts of these circles that *intersect* is [13]

$$A' = 2p_0^2\cos^{-1}\left(\frac{\hbar k}{2R}\right) - \frac{\hbar k}{2}\sqrt{4R^2 - (\hbar k)^2} = 2p_0^2\cos^{-1}\left(\frac{\hbar k}{2R}\right) - \frac{\hbar k p_0}{2}\sqrt{4 - \left(\frac{\hbar k}{R}\right)^2} \approx \pi p_0^2 - \hbar k p_0,$$

where we have approximated each term to zeroeth order in $\hbar k/p_0$. So the area we are interested in is $A = \pi p_0^2 - A' \approx \hbar k p_0$. This gives us

$$\langle|\Delta n_k|^2\rangle = \frac{g}{(2\pi\hbar)^2 V}\hbar k p_0 = \frac{g}{(2\pi\hbar)^2 V}\hbar k 2\hbar\sqrt{\frac{\pi\langle n\rangle}{g}} = \frac{k}{2\hbar V}\sqrt{\frac{g\langle n\rangle}{\pi^3}},$$

where we have used $p_0 = 2\hbar\sqrt{\pi\langle n\rangle/g}$ from the result of Homework 3, Prob. 3.1.

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

Solution. For a Bose gas, $\langle n_{\mathbf{p}\sigma}\rangle = \langle n_{\mathbf{p}}\rangle = 1/(e^{(\epsilon-\mu)/T} - 1)$, which does not depend on σ. Then the analogue of Eq. (17) is [5, p. 356]

$$\nu(r) = \frac{(2\pi)^2 g}{\langle n\rangle\,(2\pi\hbar)^4}\left(\int_0^\infty \frac{p\,J_0(pr/\hbar)}{e^{(\epsilon-\mu)/T}-1}\,dp\right)^2 \equiv \frac{g}{4\pi^2\hbar^4\,\langle n\rangle}I^2, \tag{19}$$

where we have defined I. Just above the condensation temperature T_0, the integral is dominated by small p, so $p^2/mT \sim |\mu|/T \ll 1$ [5, p. 358]. In this limit,

$$e^{(\epsilon-\mu)/T} = \exp\left(\frac{p^2}{2mT} - \frac{\mu}{T}\right) \approx 1 + \frac{p^2}{2mT} - \frac{\mu}{T},$$

where we have used $e^x \approx 1 + x$ for small x. Then

$$I \approx T\int_0^\infty \frac{p\,J_0(pr/\hbar)}{p^2/2m + |\mu|}\,dp = 2mTK_0\left(\frac{\sqrt{2m|\mu|}r}{\hbar}\right),$$

where we have evaluated the integral using Mathematica, and K_0 is the modified Bessel function of the second kind. From Eq. (19),

$$\nu(r) = \frac{g}{4\pi^2\hbar^4\,\langle n\rangle}\left[2mTK_0\left(\frac{\sqrt{2m|\mu|}r}{\hbar}\right)\right]^2 = \frac{gm^2T^2}{\pi^2\hbar^4\,\langle n\rangle}K_0^2\left(\frac{\sqrt{2m|\mu|}r}{\hbar}\right),$$

so from Eq. (16),

$$C(r) = \langle n\rangle\,\delta(r) + \frac{gm^2T^2}{\pi^2\hbar^4}K_0^2\left(\frac{\sqrt{2m|\mu|}r}{\hbar}\right),$$

which is valid for all distance regimes.

For $r \ll \hbar/\sqrt{2m|\mu|}$, we Taylor expand $K_0(z)$ about $z = 0$. Using Mathematica, $K(z) = \ln(2) - \gamma - \ln z + \mathcal{O}(z^2)$, where γ is Euler's constant. Feeding this into Eq. (19), we find

$$\nu(r) \approx \frac{g}{4\pi^2\hbar^4\,\langle n\rangle}\left[\ln(2) - \gamma - \ln\left(\frac{\sqrt{2m|\mu|}r}{\hbar}\right)\right]^2 = \frac{g}{4\pi^2\hbar^4\,\langle n\rangle}\left[-\gamma - \ln\left(\sqrt{\frac{m|\mu|}{2}}\frac{r}{\hbar}\right)\right]^2,$$

so, from Eq. (16),

$$C(r) = \langle n\rangle\,\delta(r) + \frac{g}{4\pi^2\hbar^4}\left[\gamma + \ln\left(\sqrt{\frac{m|\mu|}{2}}\frac{r}{\hbar}\right)\right]^2.$$

For $r \gg \hbar\sqrt{m/2|\mu|}$, we use the series expansion about $z \to \infty$, $K_\nu(z) \propto e^{-z}\sqrt{\pi/2z} + \mathcal{O}(1/z)$, also evaluated with Mathematica. Equation (19) becomes

$$\nu(r) \approx \frac{g}{4\pi^2\hbar^4\,\langle n\rangle}\left[\sqrt{\frac{\pi}{2}}\left(\frac{\hbar}{\sqrt{2m|\mu|}r}\right)^{1/2}\exp\left(-\frac{\sqrt{2m|\mu|}r}{\hbar}\right)\right]^2 = \frac{g}{8\pi\hbar^3\,\langle n\rangle}\frac{1}{\sqrt{2m|\mu|}r}\exp\left(-2\frac{\sqrt{2m|\mu|}r}{\hbar}\right),$$

so, from Eq. (16),

$$C(r) = \langle n\rangle\,\delta(r) + \frac{g}{8\pi\hbar^3 r}\frac{1}{\sqrt{2m|\mu|}}\exp\left(-2\frac{\sqrt{2m|\mu|}r}{\hbar}\right).$$

The general expression for the fluctuation of the occupation number for a Bose gas is, in three dimensions [5, p. 356],

$$\langle|\Delta n_k|^2\rangle = \frac{g}{(2\pi\hbar)^3 V}\int \langle n_{\mathbf{p}}\rangle\left(1+\langle n_{\mathbf{p}+\hbar\mathbf{k}}\rangle\right)d^3p\,.$$

The 2D analogue is then

$$\langle|\Delta n_k|^2\rangle = \frac{g}{(2\pi\hbar)^2 V}\int \langle n_{\mathbf{p}}\rangle\left(1+\langle n_{\mathbf{p}+\hbar\mathbf{k}}\rangle\right)d^2p\,,$$

and, assuming once more that we are interested in small wave numbers, the integrand above is nonzero only for $\langle n_{\mathbf{p}}\rangle = 1$ and $\langle n_{\mathbf{p}+\hbar\mathbf{k}}\rangle = 0$ [6, p. 357]. This yields the same result as in Prob. 5.1:

$$\langle|\Delta n_k|^2\rangle = \frac{g}{(2\pi\hbar)^2 V}\hbar k 2\hbar\sqrt{\frac{\pi\langle n\rangle}{g}} = \frac{k}{2\hbar V}\sqrt{\frac{g\langle n\rangle}{\pi^3}}.$$

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