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5 Task Theoretical Physics VI - Statistics

5.1 (Distinguishable vs. indistinguishable particles)

(a)

Using canonical ensemble:

$$
\begin{aligned}
Z_{\text{red}}\Big|_N &= \frac{1}{h^{3N}N!}\int d^{3N}q\int d^{3N}p\exp\left(-\beta\sum_{i=1}^{N}\frac{\vec{p_i}^2}{2m}\right)\\
&= \frac{1}{h^{3N}N!}\int d^{3N}q\left[\int dp\exp\left(-\beta\frac{\vec{p}^2}{2m}\right)\right]^{3N}\\
&= \frac{1}{h^{3N}N!}V^N\left[\sqrt{\frac{2m\pi}{\beta}}\right]^{3N}\\
&= \frac{V^N}{\lambda_T^{3N}N!}
\end{aligned}
$$

with $\lambda_T = \frac{h}{\sqrt{2\pi m k_B T}}$, same for blue and green. Therefore we get (red, blue and green distinguishable):

$$
Z_{\text{red,blue,green}} = \Pi_{i=1}^3 Z_i = Z_{\text{red}}\cdot Z_{\text{blue}}\cdot Z_{\text{green}} = Z_{\text{red}}^3 = \left(\frac{V^N}{\lambda_T^{3N}N!}\right)^3
$$

free energy:

$$
\begin{aligned}
F_{\text{red,blue,green}} &= -\frac{1}{\beta}\ln Z\\
&= -\frac{1}{\beta}\ln\left[\left(\frac{V^N}{\lambda_T^{3N}N!}\right)^3\right]\\
&= -3k_BT\left[N\cdot\ln V-\ln N!-3N\cdot\ln\lambda_T\right]\\
&= -3k_BT\left[N\cdot\ln V-\ln N!+\frac{3}{2}N\cdot\ln\left(\frac{2\pi m k_B}{h^2}T\right)\right]
\end{aligned}
$$

entropy:

$$
\begin{aligned}
S_{\text{red,blue,green}} &= -\frac{\partial F}{\partial T}\\
&= 3k_B\left[N\cdot\ln V-\ln N!+\frac{3}{2}N\cdot\ln\left(\frac{2\pi m k_B}{h^2}T\right)\right]\\
&+ 3k_BT\frac{3}{2}N\cdot\frac{1}{T}\\
&= 3k_B\left[N\cdot\ln V+\frac{3}{2}N\cdot\left[1+\ln\left(\frac{2\pi m k_B}{h^2}T\right)\right]-\ln N!\right]
\end{aligned}
$$

(b)

For $3N$ red atoms (all indistinguishable):

$$Z_{\text{red}}\Big|_{3N} = \frac{1}{\left(h^{3N}\right)^3 (3N)!}\left[\int d^{3N}q \int d^{3N}p \exp\left(-\beta\sum_{i=1}^{N}\frac{\vec{p_i}^2}{2m}\right)\right]^3$$
$$= \left(\frac{V^N}{\lambda_T^{3N}\left((3N)!\right)^{\frac{1}{3}}}\right)^3$$

this leads to:

$$F_{3\text{red}} = -3k_BT\left[N\cdot\ln V - \frac{1}{3}\ln(3N)! + \frac{3}{2}N\cdot\ln\left(\frac{2\pi mk_B}{h^2}T\right)\right]$$

and the entropy is:

$$S_{3\text{red}} = 3k_B\left[N\cdot\ln V + \frac{3}{2}N\cdot\left[1+\ln\left(\frac{2\pi mk_B}{h^2}T\right)\right] - \frac{1}{3}\ln(3N)!\right]$$

Therefore the difference is (using Stirling formula $\ln N! \approx N\ln N - N$):

$$\left|S_{\text{red,blue,green}} - S_{3\text{red}}\right| = \left|3k_B\left[-\ln N! + \frac{1}{3}\ln(3N)!\right]\right|$$
$$\approx \left|3k_B\left[-N\cdot\ln N + N + N\cdot\ln(3N) - N\right]\right|$$
$$= \left|3k_B\left[N\cdot\ln 3\right]\right|$$
$$= 3Nk_B\ln 3$$

5.2 (Simplified model for adsorption on a surface)

We first define the density of states at one site functions:

$$D_0(E) = \delta(E-0)$$
$$D_1(E) = \delta(E-\epsilon_1)$$
$$D_2(E) = \delta(E-\epsilon_2)$$

(a)

definition of grand partition function:

$$Z_G(T,V,\mu) = \sum_{N=0}^{\infty}\int_{-\infty}^{\infty} dE\, D_N(E)\, e^{-\beta(E-\mu N)}$$

with defined $D_N(E)$, for one site and the condition, that there are only three possible states $0,1,2$:

$$Z_{1,G} = \int_{-\infty}^{\infty} dE\left(\delta(E-0)\,e^{-\beta E} + \delta(E-\epsilon_1)\,e^{-\beta(E-\mu)} + \delta(E-\epsilon_2)\,e^{-\beta(E-2\mu)}\right)$$
$$= \left(1 + e^{-\beta(\epsilon_1-\mu)} + e^{-\beta(\epsilon_2-2\mu)}\right)$$

for non-interacting particles $Z_{M,G} = Z_{1,G}^M$, this therefore leads to:

$$Z_{M,G} = \left(1 + e^{-\beta(\epsilon_1-\mu)} + e^{-\beta(\epsilon_2-2\mu)}\right)^M$$

(b)

definition of grand potential:

$$\Phi(T,V,\mu) = -k_B T \ln Z_G(T,V,\mu) = -k_B T M \ln\left(1 + e^{-\beta(\epsilon_1-\mu)} + e^{-\beta(\epsilon_2-2\mu)}\right)$$

definition of average number of particles:

$$\begin{aligned}
\langle N\rangle &= \frac{1}{\beta}\frac{\partial}{\partial\mu}\ln Z_G(T,V,\mu)\Big|_{T,V} \\
&= \frac{M}{\beta}\frac{\partial}{\partial\mu}\ln\left(1 + e^{-\beta(\epsilon_1-\mu)} + e^{-\beta(\epsilon_2-2\mu)}\right) \\
&= \frac{M}{\beta}\left(1 + e^{-\beta(\epsilon_1-\mu)} + e^{-\beta(\epsilon_2-2\mu)}\right)^{-1}\left[e^{-\beta(\epsilon_1-\mu)}\beta + e^{-\beta(\epsilon_2-2\mu)}2\beta\right] \\
&= \frac{M\left[e^{-\beta(\epsilon_1-\mu)} + 2e^{-\beta(\epsilon_2-2\mu)}\right]}{1 + e^{-\beta(\epsilon_1-\mu)} + e^{-\beta(\epsilon_2-2\mu)}}
\end{aligned}$$

definition of the mean energy:

$$\begin{aligned}
\langle E\rangle &= -\frac{\partial}{\partial\beta}\ln Z_G + \mu\langle N\rangle \\
&= -\frac{\partial}{\partial\beta}\ln\left(1 + e^{-\beta(\epsilon_1-\mu)} + e^{-\beta(\epsilon_2-2\mu)}\right)^M + \mu\langle N\rangle \\
&= -M\frac{\left(-(\epsilon_1-\mu)e^{-\beta(\epsilon_1-\mu)} - (\epsilon_2-2\mu)e^{-\beta(\epsilon_2-2\mu)}\right)}{1 + e^{-\beta(\epsilon_1-\mu)} + e^{-\beta(\epsilon_2-2\mu)}} + \mu\langle N\rangle \\
&= M\frac{(\epsilon_1-\mu)e^{-\beta(\epsilon_1-\mu)} + (\epsilon_2-2\mu)e^{-\beta(\epsilon_2-2\mu)}}{1 + e^{-\beta(\epsilon_1-\mu)} + e^{-\beta(\epsilon_2-2\mu)}} - \mu\frac{M\left[e^{-\beta(\epsilon_1-\mu)} + 2e^{-\beta(\epsilon_2-2\mu)}\right]}{1 + e^{-\beta(\epsilon_1-\mu)} + e^{-\beta(\epsilon_2-2\mu)}} \\
&= M\frac{(\epsilon_1-\mu-\mu)e^{-\beta(\epsilon_1-\mu)} + (\epsilon_2-2\mu-2\mu)e^{-\beta(\epsilon_2-2\mu)}}{1 + e^{-\beta(\epsilon_1-\mu)} + e^{-\beta(\epsilon_2-2\mu)}} \\
&= M\frac{\epsilon_1 e^{-\beta(\epsilon_1-\mu)} + \epsilon_2 e^{-\beta(\epsilon_2-2\mu)}}{1 + e^{-\beta(\epsilon_1-\mu)} + e^{-\beta(\epsilon_2-2\mu)}}
\end{aligned}$$

(c)

definition of pressure using Sackur-Tetrode-equation for S:

$$\begin{aligned}
p &= T\left\langle\frac{\partial S}{\partial V}\right\rangle\Big|_{N=N_g} \\
&= T\left\langle\frac{\partial}{\partial V}\left(N_g k_B\left[\ln\frac{V}{N_g} + \frac{3}{2}\ln\left(\frac{4\pi m E}{3Nh^2}\right) + \frac{5}{2}\right]\right)\right\rangle \\
&= T\left\langle\left(N_g k_B\frac{1}{V}\right)\right\rangle \\
&= k_B T\frac{\langle N_g\rangle}{V}
\end{aligned}$$

Therefore:

$$\langle N_g \rangle = \frac{pV}{k_B T}$$

Using the equation for $\langle N \rangle$ from **b)** and the μ of an ideal gas (N_g is the number of particles in the gas, which acts as the particle reservoir):

$$\mu = -k_B T \ln\left(\frac{V}{\langle N_g \rangle \lambda_T^3}\right) = k_B T \ln\left(\frac{\langle N_g \rangle \lambda_T^3}{V}\right)$$

we get:

$$\begin{aligned}
\langle N \rangle &= \frac{M\left[e^{-\beta(\epsilon_1-\mu)} + 2e^{-\beta(\epsilon_2-2\mu)}\right]}{1+e^{-\beta(\epsilon_1-\mu)}+e^{-\beta(\epsilon_2-2\mu)}} \\
&= \frac{M\left[e^{-\beta\epsilon_1+\ln\left(\frac{\langle N_g\rangle \lambda_T^3}{V}\right)} + 2e^{-\beta\epsilon_2+2\ln\left(\frac{\langle N_g\rangle \lambda_T^3}{V}\right)}\right]}{1+e^{-\beta\epsilon_1+\ln\left(\frac{\langle N_g\rangle \lambda_T^3}{V}\right)}+e^{-\beta\epsilon_2+2\ln\left(\frac{\langle N_g\rangle \lambda_T^3}{V}\right)}} \\
&= \frac{M\left[\left(\frac{\langle N_g\rangle \lambda_T^3}{V}\right)e^{-\beta\epsilon_1} + 2\left(\frac{\langle N_g\rangle \lambda_T^3}{V}\right)^2 e^{-\beta\epsilon_2}\right]}{1+\left(\frac{\langle N_g\rangle \lambda_T^3}{V}\right)e^{-\beta\epsilon_1}+\left(\frac{\langle N_g\rangle \lambda_T^3}{V}\right)^2 e^{-\beta\epsilon_2}}
\end{aligned}$$

with $\lambda_T = \frac{h\sqrt{\beta}}{\sqrt{2\pi m}}$ and $\langle N_g \rangle = \frac{pV}{k_B T}$ this leads to:

$$\langle N \rangle = \frac{M\left[p\beta^{\frac{5}{2}}\left(h^2(2\pi m)^{-1}\right)^{\frac{3}{2}} e^{-\beta\epsilon_1} + 2p^2\beta^5\left(h^2(2\pi m)^{-1}\right)^3 e^{-\beta\epsilon_2}\right]}{1+p\beta^{\frac{5}{2}}\left(h^2(2\pi m)^{-1}\right)^{\frac{3}{2}} e^{-\beta\epsilon_1}+p^2\beta^5\left(h^2(2\pi m)^{-1}\right)^3 e^{-\beta\epsilon_2}}$$

assuming $\epsilon_1, \epsilon_2 < 0$ we observe the special cases of high and low temperature, first starting with high temperature ($\beta \to 0$):

$$\langle N \rangle = \lim_{\beta\to 0} \frac{M\left[\alpha\beta^{\frac{5}{2}}e^{-\beta\epsilon_1} + 2\alpha^2\beta^5 e^{-\beta\epsilon_2}\right]}{1+\alpha\beta^{\frac{5}{2}}e^{-\beta\epsilon_1}+\alpha^2\beta^5 e^{-\beta\epsilon_2}} = \frac{0}{1}\cdot M = 0$$

with $\alpha = p\left(h^2(2\pi m)^{-1}\right)^{\frac{3}{2}}$. The interpretation of this situation is, that there will be no occupied states, since the temperature is very high, the particles won't be adsorbed by a surface. The particles become free since the kinetic energy is bigger then the binding energy.

Special case of low temperature $\beta \to \infty$, the 1 in the denominator can be neglected while the exponentials will become big, since $\epsilon_1, \epsilon_2 < 0$:

$$\langle N \rangle = \lim_{\beta\to\infty} \frac{M\left[\alpha\beta^{\frac{5}{2}}e^{-\beta\epsilon_1} + 2\alpha^2\beta^5 e^{-\beta\epsilon_2}\right]}{1+\alpha\beta^{\frac{5}{2}}e^{-\beta\epsilon_1}+\alpha^2\beta^5 e^{-\beta\epsilon_2}} = \lim_{\beta\to\infty} \frac{M\left[\alpha\beta^{\frac{5}{2}}e^{-\beta\epsilon_1} + 2\alpha^2\beta^5 e^{-\beta\epsilon_2}\right]}{\left[\alpha\beta^{\frac{5}{2}}e^{-\beta\epsilon_1}+\alpha^2\beta^5 e^{-\beta\epsilon_2}\right]}$$

We now can have a look at the case of $|\epsilon_1| > |\epsilon_2|$:

$$\langle N\rangle = \lim_{\beta\to\infty} \frac{M\alpha\beta^{\frac{5}{2}}e^{-\beta\epsilon_1}}{\alpha\beta^{\frac{5}{2}}e^{-\beta\epsilon_1}} = M$$

which perfectly fits the expectation, that every site will be occupied with 1 particle of ϵ_1 being dominating. The second and more likely case (because two particles will have a higher binding energy then one) $|\epsilon_2| > |\epsilon_1|$ leads to:

$$\langle N\rangle = \lim_{\beta\to\infty} \frac{M2\alpha^2\beta^5 e^{-\beta\epsilon_2}}{\alpha^2\beta^5 e^{-\beta\epsilon_2}} = 2M$$

This is also the maximum, because now two particles are adsorbed on each site. This seems to be the most likely result.

5.3 (Atoms in a lattice)

There are $2N$ lattices sites, N normal and N interstitial. N of them are occupied, while M interstitial and $N-M$ normal sites could be occupied. Therefore we can use the binomial $\left(\begin{array}{c} N \\ M \end{array}\right)$ for the probability of an interstitial site to be occupied and the binomial $\left(\begin{array}{c} N \\ N-M \end{array}\right) = \frac{N!}{(N-M)!(N-M-N)!} = \frac{N!}{(N-M)!M!} = \left(\begin{array}{c} N \\ M \end{array}\right)$ for an normal site to be occupied. We can therefore define W:

$$W = \left(\begin{array}{c} N \\ M \end{array}\right)^2$$

which we can use to define the entropy:

$$S = k_B \ln W = 2k_B \ln W'$$

with $W' = \left(\begin{array}{c} N \\ M \end{array}\right)$. We can get the internal energy from here with:

$$dU = TdS$$

but first we rewrite S using Stirling's formula ($\ln N! = N\ln N - N$):

$$\begin{aligned}
S &= 2k_B \ln W_0 \\
&= 2k_B \ln \frac{N!}{M!\,(N-M)!} \\
&= 2k_B \left(\ln N! - \ln M! - \ln (N-M)!\right) \\
&= 2k_B \left(N\ln N - N - M\ln M + M - (N-M)\ln (N-M) + (N-M)\right) \\
&= 2k_B \left(N\left(\ln N - \ln (N-M)\right) - M\left(\ln M - \ln (N-M)\right)\right) \\
&= 2k_B \left(N\left(\ln \frac{N}{N-M}\right) - M\left(\ln \frac{M}{N-M}\right)\right)
\end{aligned}$$

using $N \gg M$ and $U = M\epsilon$ we can rewrite:

$$
\begin{aligned}
S &= 2k_B \left(N \left(\ln \frac{N}{N} \right) - M \left(\ln \frac{M}{N} \right) \right) \\
&= -2k_B \frac{U}{\epsilon} \ln \left(\frac{U}{N\epsilon} \right)
\end{aligned}
$$

Now we can use:

$$
\frac{1}{T} = \left(\frac{\partial U}{\partial S} \right)_N^{-1} = \left(\frac{\partial S}{\partial U} \right)_N
$$

therefore we can write:

$$
\begin{aligned}
-\frac{\epsilon}{2k_B T} &= \frac{\partial}{\partial U} \left(U \ln \left(\frac{U}{N\epsilon} \right) \right) \\
-\frac{\epsilon}{2k_B T} &= \ln \left(\frac{U}{N\epsilon} \right) + U \frac{1}{U}
\end{aligned}
$$

This can be rewritten to:

$$
U = N\epsilon \exp \left(- \left(\frac{\epsilon}{2k_B T} + 1 \right) \right)
$$

now using $\frac{\epsilon}{2k_B T} \gg 1$ we can simplify our result to:

$$
U = N\epsilon e^{-\frac{\epsilon}{2k_B T}}
$$

definition of heat capacity:

$$
C_v (T) = \frac{\partial U}{\partial T}
$$

with this we get:

$$
\begin{aligned}
C_v (T) &= \frac{\partial}{\partial T} \left(N\epsilon e^{-\frac{\epsilon}{2k_B T}} \right) \\
&= N\epsilon e^{-\frac{\epsilon}{2k_B T}} \left(\frac{\epsilon}{2k_B T^2} \right) \\
&= 2Nk_B \left(\frac{\epsilon}{2k_B T} \right)^2 e^{-\frac{\epsilon}{2k_B T}}
\end{aligned}
$$

5.4 (Density operator)

Matrix representation of density operator in basis $\{|m_i\rangle\}$:

$$
\langle m_j|\hat{\rho}|m_i\rangle = \frac{1}{4} \begin{pmatrix} 2 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}
$$

Eigenvalues of operator $\hat{\mathbf{J}}_{\mathbf{z}}$: $\lambda_1 = -1$, $\lambda_2 = 0$, $\lambda_3 = 1$:

$$\left\langle m_j|\hat{J}_z|m_i\right\rangle = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

with eigenvectors (using $\left(\left\langle m_j|\hat{J}_z|m_i\right\rangle - \lambda E\right) \cdot \vec{x} = 0$):

$$\begin{aligned} |-1\rangle &= \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \\ |0\rangle &= \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \\ |1\rangle &= \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \end{aligned}$$

(a)

hermicity:

$$\hat{\rho} = \hat{\rho}^\dagger$$

using complexconjugation on the matrix and transposing it leads to:

$$\left\langle m_j|\hat{\rho}^\dagger|m_i\right\rangle = \frac{1}{4}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

while all elements are real and the matrix is symmetric.

Before checking positive semi-definiteness, we calculate the eigenvalues and eigenvectors:

$$\begin{aligned} |\langle m_j|\hat{\rho}|m_i\rangle - \lambda E| &= 0 \\ \left[(2-4\lambda)(1-4\lambda)^2 - (1-4\lambda) - (1-4\lambda)\right] &= 0 \\ (1-4\lambda)\left[2 - 8\lambda - 4\lambda + 16\lambda^2 - 2\right] &= 0 \\ \left(\lambda - \frac{3}{4}\right)\left(\frac{1}{4} - \lambda\right)\lambda &= 0 \end{aligned}$$

this leads to the eigenvalues:

$$\begin{aligned} \lambda_1 &= 0 \\ \lambda_2 &= \frac{1}{4} \\ \lambda_3 &= \frac{3}{4} \end{aligned}$$

for the eigenvectors we get:

$$\begin{pmatrix} 2-4\lambda_i & 1 & 1 \\ 1 & 1-4\lambda_i & 0 \\ 1 & 0 & 1-4\lambda_i \end{pmatrix} \cdot \vec{x} = 0$$

this leads to:

$$\begin{aligned} \begin{pmatrix} 2 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \cdot \vec{x}_1 &= 0 \\ \vec{x}_1 &= a \cdot \begin{pmatrix} 1 \\ -1 \\ -1 \end{pmatrix} \end{aligned}$$

$$\begin{aligned} \begin{pmatrix} 1 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \cdot \vec{x}_2 &= 0 \\ \vec{x}_2 &= b \cdot \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} \end{aligned}$$

$$\begin{aligned} \begin{pmatrix} -1 & 1 & 1 \\ 1 & -2 & 0 \\ 1 & 0 & -2 \end{pmatrix} \cdot \vec{x}_3 &= 0 \\ \vec{x}_3 &= c \cdot \begin{pmatrix} 2 \\ 1 \\ 1 \end{pmatrix} \end{aligned}$$

normalising the eigenvectors leads to:

$$\begin{aligned} \vec{x}_1 &= \frac{1}{\sqrt{3}} \cdot \begin{pmatrix} 1 \\ -1 \\ -1 \end{pmatrix} \\ \vec{x}_2 &= \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix} \\ \vec{x}_3 &= \frac{1}{\sqrt{6}} \cdot \begin{pmatrix} 2 \\ 1 \\ 1 \end{pmatrix} \end{aligned}$$

The eigenvectors form a ONB, therefore every vector can be constructed with them $\vec{x} = a_1\vec{x}_1 + a_2\vec{x}_2 + a_3\vec{x}_3$.

positive semi-definiteness:

$$\vec{x}^T \langle m_j|\hat{\rho}|m_i\rangle \vec{x} =\geq 0$$

for all vectors $\vec{x} = (x_1, x_2, x_3) \neq \vec{0}$. We can prove that:

$$\begin{aligned}
\vec{x}^T \langle m_j|\hat{\rho}|m_i\rangle \vec{x} &= \sum_{i,j} \alpha_j \vec{x}_j^T \langle m_j|\hat{\rho}|m_i\rangle \alpha_i \vec{x}_i \\
&= \sum_{i,j} \alpha_j \lambda_i \alpha_i \vec{x}_j^T \cdot \vec{x}_i \\
&= \sum_{i,j} \alpha_j \lambda_i \alpha_i \delta_{ij} \\
&= \sum_{i} \alpha_i^2 \lambda_i \\
&\geq 0
\end{aligned}$$

while we calculated λ_i, which are either positive or 0 and α_i^2 will always be positive.

Calculation of the trace:

$$Tr\left(\hat{\rho}\right) = \frac{1}{4}\sum_{i=1}^{3} \langle m_i|\hat{\rho}|m_i\rangle = \frac{1}{4}\left(2+1+1\right) = 1$$

So all requirements for a density operator are fullfilled.

(b)

We can use, that we will only have a pure state for $Tr\left(\hat{\rho}^2\right) = 1$:

$$\begin{aligned}
Tr\left(\hat{\rho}^2\right) &= Tr\left(\frac{1}{16}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 2 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}\right) \\
&= \frac{1}{16} Tr\left(\begin{pmatrix} 6 & 3 & 3 \\ 3 & 2 & 1 \\ 3 & 1 & 2 \end{pmatrix}\right) \\
&= \frac{10}{16}
\end{aligned}$$

Therefore this is not a pure state, that means it is a mixed state.

(c)

mean:

$$\left\langle \hat{\mathbf{J}}_{\mathbf{z}} \right\rangle = Tr\left(\hat{\rho}\hat{\mathbf{J}}_{\mathbf{z}}\right)$$

this is:

$$\left\langle \hat{\mathbf{J}}_{\mathbf{z}} \right\rangle = Tr\left(\frac{1}{4}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right)$$

$$\begin{aligned}
&= \frac{1}{4} Tr\left(\begin{pmatrix} -2 & 0 & 1 \\ -1 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix}\right) \\
&= \frac{1}{4}
\end{aligned}$$

variance $\Delta\mathbf{\hat{J}_z^2} = \left\langle \mathbf{\hat{J}_z^2} \right\rangle - \left\langle \mathbf{\hat{J}_z} \right\rangle^{\mathbf{2}}$, with:

$$\begin{aligned}
\left\langle \mathbf{\hat{J}_z^2} \right\rangle &= Tr\left(\hat{\rho}\mathbf{\hat{J}_z^2}\right) \\
&= Tr\left(\frac{1}{4}\begin{pmatrix} 2 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}\right) \\
&= \frac{1}{4} Tr\left(\begin{pmatrix} 2 & 0 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix}\right) \\
&= \frac{3}{4}
\end{aligned}$$

The variance therefore is:

$$\Delta\mathbf{\hat{J}_z^2} = \left\langle \mathbf{\hat{J}_z^2} \right\rangle - \left\langle \mathbf{\hat{J}_z} \right\rangle^{\mathbf{2}} = \frac{3}{4} - \frac{1}{16} = \frac{11}{16}$$

5.5 (Purity)

To show:

$$Tr\left(\hat{\rho}^2\right) \leq 1, \text{ in general} \quad \text{and} \quad Tr\left(\hat{\rho}^2\right) = 1 \text{ for a pure state}$$

in general (with $\hat{\rho} = \sum_m p_m |m\rangle\langle m|$):

$$\begin{aligned}
Tr\left(\hat{\rho}^2\right) &= \sum_k \langle k|\hat{\rho}^2|k\rangle \\
&= \sum_{n,m,k} \langle k|p_n|n\rangle\langle n|p_m|m\rangle\langle m|k\rangle \\
&= \sum_{n,m,k} p_n p_m \langle k|n\rangle\langle n|m\rangle\langle m|k\rangle \\
&= \sum_{n,m,k} p_n p_m \langle k|n\rangle\delta_{nm}\langle m|k\rangle \\
&= \sum_{m,k} p_m^2 \left|\delta_{mk}\right|^2 \\
&\leq 1
\end{aligned}$$

using $0 \leq p_m \leq 1$ and $\sum_m p_m = 1$. For a pure state $\hat{\rho}^2 = |n\rangle \underbrace{\langle n|n\rangle}_{=1} \langle n| = |n\rangle\langle n| = \hat{\rho}$, where $|n\rangle$ is the only occuring state in the ensemble meaning $p_n = 1 \Leftrightarrow p_m = \delta_{nm}$:

$$
\begin{aligned}
Tr\left(\hat{\rho}^2\right) &= \sum_m \langle m|n\rangle \delta_{nm} \langle n|m\rangle \\
&= 1
\end{aligned}
$$