Statmech II HW2

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1 Problem 5.1

We use the suggested unitary transformation:

$$U = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \tag{1.1}$$

Applying the transform to σ_x we find:

$$\sigma_x^t = U \sigma_x U^{-1} \tag{1.2}$$

$$\sigma_x^t = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \tag{1.3}$$

$$\sigma_x^t = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \tag{1.4}$$

So this has transformed us to the basis where σ_x is diagonal.
To calculate $\langle \sigma_z \rangle$ in this representation we will need to transform both σ_z and ρ. The transformed σ_z calculated as above is $\begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}$. Transforming ρ we find:

$$\rho = \frac{1}{e^{\beta \mu_b B} + e^{-\beta \mu_b B}} \begin{bmatrix} e^{\beta \mu_b B} & 0 \\ 0 & e^{-\beta \mu_b B} \end{bmatrix} \tag{1.5}$$

$$\rho^t = \frac{1}{2} \frac{1}{e^{\beta \mu_b B} + e^{-\beta \mu_b B}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} e^{\beta \mu_b B} & 0 \\ 0 & e^{-\beta \mu_b B} \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \tag{1.6}$$

Using the substitution $\kappa \equiv \beta \mu_b B$ we can write ρ^t as:

$$\rho^t = \frac{1}{2} \frac{1}{e^{\kappa} + e^{-\kappa}} \begin{bmatrix} e^{\kappa} + e^{-\kappa} & -e^{\kappa} + e^{-\kappa} \\ -e^{\kappa} + e^{-\kappa} & e^{\kappa} + e^{-\kappa} \end{bmatrix} \tag{1.7}$$

We can now find $\langle \sigma_z \rangle$:

$$\langle \sigma_z \rangle = Tr(\rho \sigma_z) \tag{1.8}$$

$$\langle \sigma_z \rangle = Tr(\frac{1}{2} \frac{1}{e^{\kappa} + e^{-\kappa}} \begin{bmatrix} e^{\kappa} + e^{-\kappa} & -e^{\kappa} + e^{-\kappa} \\ -e^{\kappa} + e^{-\kappa} & e^{\kappa} + e^{-\kappa} \end{bmatrix} \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix} \tag{1.9}$$

$$\langle \sigma_z \rangle = \frac{1}{2} \frac{2(e^{\kappa} - e^{-\kappa})}{e^{\kappa} + e^{-\kappa}} = \tanh \kappa \tag{1.10}$$

2 Problem 5.2

The Schrodinger equation in the q representation is:

$$H(-i\hbar\frac{\partial}{\partial q}, q)\psi(q) = E_q\psi(q) \tag{2.1}$$

Using the series definition of e:

$$e^{-\beta H}\psi(q) = \left(1 + (\beta H) + \frac{1}{2!}(\beta H)^2 + ...\right)\psi(q) \tag{2.2}$$

$$e^{-\beta H}\psi(q) = e^{-\beta E_q}\psi(q) \tag{2.3}$$

$$\langle q'| e^{-\beta H} |q\rangle = e^{-\beta E_q}\psi(q')\psi(q) \tag{2.4}$$

$$\langle q'| e^{-\beta H} |q\rangle = e^{-\beta H}\delta(q' - q) \tag{2.5}$$

The Hamiltonian for the free particle is $H = \frac{\hbar^2}{2m}\nabla^2$. Using $\delta(x_0) = \frac{1}{2\pi}\int e^{ik(q-q_0)}dk$ the density matrix in this representation is:

$$\rho = \frac{1}{Tr(e^{-\beta H})}\left(\frac{1}{2\pi}\right)^3 \int_{-\infty}^{\infty} e^{-\beta\frac{\hbar^2}{2m}\nabla^2} e^{ik(q-q_0)}d^3k \tag{2.6}$$

$$\rho = \frac{1}{Tr(e^{-\beta H})}\left(\frac{1}{2\pi}\right)^3 \int_{-\infty}^{\infty} e^{-\beta\frac{\hbar^2}{2m}k^2} e^{ik(q-q_0)}d^3k \tag{2.7}$$

So we have reproduced the result from class without converting a sum of energy states into an integral. Completing the square in the integral we find the numerator is:

$$\left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2} e^{-\frac{m}{2\beta\hbar^2}(q-q_0)^2} \tag{2.8}$$

As in class, we use this result to calculate the trace (the integral of the expression over all space).

$$Tr(e^{-\beta H}) = \int\left(\left(\frac{1}{2\pi}\right)^3 \int_{-\infty}^{\infty} e^{-\beta\frac{\hbar^2}{2m}k^2} e^{ik(q-q_0)}d^3k\right)d^3q \tag{2.9}$$

$$Tr(e^{-\beta H}) = \int\left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2} e^{-\frac{m}{2\beta\hbar^2}(q-q_0)^2} d^3q \tag{2.10}$$

$$Tr(e^{-\beta H}) = \left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2} \int e^{-\frac{m}{2\beta\hbar^2}(q-q_0)^2} d^3q \ (q = q_0) \tag{2.11}$$

$$Tr(e^{-\beta H}) = V\left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2} \tag{2.12}$$

So the density operator is:

$$\rho = \frac{1}{V} e^{-\frac{m}{2\beta\hbar^2}(q-q_0)^2} \tag{2.13}$$

The Hamiltonian for the simple harmonic oscillator is:

$$H = \frac{\hbar^2}{2m}\frac{\partial^2}{\partial q^2} + \frac{1}{2}\hbar\omega^2 q^2 \tag{2.14}$$

Using relation 2.5 and the integral representation of the delta function:

$$\langle q'| e^{-\beta H} |q\rangle = \left(\frac{1}{2\pi}\right)^3 \int e^{-\beta\frac{\hbar^2}{2m}(k^2+ik(q-q'))} e^{-\frac{\beta}{2}\hbar\omega^2 q^2 ik(q-q')} d^3k \tag{2.15}$$

$$\langle q'| e^{-\beta H} |q\rangle = \left(\frac{1}{2\pi}\right)^3 e^{-\beta\frac{\hbar}{2}} \int e^{\left(\frac{\hbar}{m}k^2+(\frac{\hbar}{m}+\omega^2 q^2)ik(q-q'\right)} d^3k \tag{2.16}$$

$$\tag{2.17}$$

3 Problem 5.4

We insert the Boltzmann wavefunctions into Pathria equation 11 and follow the same approach:

$$\langle 1...N| e^{-\beta H} |1'...N'\rangle = \sum_K e^{\frac{-\beta\hbar^2}{2m}K^2} \prod (u_{k1}(1)...u_{kN}(N)) \prod \left(u_{k1}(1')...u_{kN}(N'\right) \tag{3.1}$$

$$\langle 1...N| e^{-\beta H} |1'...N'\rangle = \sum_{k_1...k_N} e^{\frac{-\beta\hbar^2}{2m}(k_1^2+...+k_N^2)} \prod \left(u_{k1}(1)u^*_{k1}(1')...u_{kN}(N)u^*_{kN}(N')\right) \tag{3.2}$$

$$\langle 1...N| e^{-\beta H} |1'...N'\rangle = \frac{1}{(2\pi)^{3N}} \int e^{\frac{-\beta\hbar^2}{2m}k_1^2+ik_1(1-1')} d^3k_1 ... \int e^{\frac{-\beta\hbar^2}{2m}k_N^2+ik_N(N-N')} d^3k_N \tag{3.3}$$

$$\langle 1...N| e^{-\beta H} |1'...N'\rangle = \left(\frac{m}{2\pi\beta\hbar^2}\right)^{\frac{3N}{2}} \prod e^{-\frac{m}{2\beta\hbar^2}(i-i')^2} \tag{3.4}$$

We see that the Gibbs correction is not present in this result. The diagonal element ($i = i'$) are all equal to $\left(\frac{m}{2\pi\beta\hbar^2}\right)^{3N/2}$, so there is no correlation between particles either.

4 Problem 5.5

The classical partition function with $\sum_p = 1$ (zero-order) is $\frac{1}{N!}\left(\frac{V}{\lambda^3}\right)^N$. We rearrange v_s:

$$v_s = -kT\ln\left(1 \pm e^{-\frac{\pi}{\lambda^2}r^2}\right) \tag{4.1}$$

$$e^{-\beta v_s} = 1 \pm e^{-\frac{\pi}{\lambda^2}r^2} \tag{4.2}$$

The first-order to correction to $\sum_P$ is $\pm\sum f_i f_j$. To find the correction term we solve:

$$\int 1 + \sum_{i<j} f_i f_j \ d^{3N}r = \int 1 \pm \sum_{i<j} e^{-\frac{\pi}{\lambda^2}r_{ij}^2} \ d^{3N}r \tag{4.3}$$

$$\tag{4.4}$$

We therefore see that the first-order correction for Z_N is indeed $\int e^{-\beta v_s} \ d^{3N}r$. We now work on the integral. We arrange it into a product of terms of the form:

$$\int\int e^{\frac{-\pi}{\lambda^2}(r_i - r_j)^2} \ dr_i \ dr_j \tag{4.5}$$

$$\lambda \int dr_j \tag{4.6}$$

With N particles taking the sum over $i < j$, we have $\frac{N(N-1)}{2}$ of these terms.

$$Q_N = \frac{1}{N!}\frac{1}{\lambda^{3N}}\left(V^N \pm \lambda^{\frac{N(N-1)}{2}} V^{\frac{N(N-1)}{6}}\right) \tag{4.7}$$

We now calculate the equation of state for the first-order correction.

$$A = -kT\ln Q_N \tag{4.8}$$

$$A = -kT\left[N\ln V + \ln\left(1 \pm \lambda^{\frac{N(N-1)}{2}} V^{N^2/6 - \frac{7}{6}N}\right)\right] - kT\ln\left(N!\lambda^{3N}\right) \tag{4.9}$$

$$P = \frac{\partial A}{\partial V} = -\frac{NkT}{V} + \left(\pm\left(\frac{N^2}{6} - \frac{7}{6}N\right)\lambda^{\frac{N(N-1)}{2}} V^{N^2/6 - \frac{7}{6}N - 1}\right)\left(1 \pm \lambda^{\frac{N(N-1)}{2}} V^{N^2/6 - \frac{7}{6}N}\right)^{-1} \tag{4.10}$$