

PHYSICS 210A : STATISTICAL PHYSICS
HW ASSIGNMENT #2 SOLUTIONS

(1) Consider a d -dimensional ideal gas with dispersion $\varepsilon(\mathbf{p}) = A|\mathbf{p}|^\alpha$, with $\alpha > 0$. Find the density of states $D(E)$, the statistical entropy $S(E)$, the equation of state $p = p(N, V, T)$, the heat capacity at constant volume $C_V(N, V, T)$, and the heat capacity at constant pressure $C_p(N, V, T)$.

Solution:

The density of states is

$$D(E, V, N) = \frac{V^N}{N!} \int \frac{d^d p_1}{h^d} \dots \int \frac{d^d p_N}{h^d} \delta(E - Ap_1^\alpha - \dots - Ap_N^\alpha) .$$

The Laplace transform is

$$\begin{aligned} \widehat{D}(\beta, V, N) &= \frac{V^N}{N!} \left(\int \frac{d^d p}{h^d} e^{-\beta Ap^\alpha} \right)^N \\ &= \frac{V^N}{N!} \left(\frac{\Omega_d}{h^d} \int_0^\infty dp p^{d-1} e^{-\beta Ap^\alpha} \right)^N \\ &= \frac{V^N}{N!} \left(\frac{\Omega_d \Gamma(d/\alpha)}{\alpha h^d A^{d/\alpha}} \right)^N \beta^{-Nd/\alpha} . \end{aligned}$$

Now we inverse transform, recalling

$$K(E) = \frac{E^{t-1}}{\Gamma(t)} \iff \widehat{K}(\beta) = \beta^{-t} .$$

We then conclude

$$D(E, V, N) = \frac{V^N}{N!} \left(\frac{\Omega_d \Gamma(d/\alpha)}{\alpha h^d A^{d/\alpha}} \right)^N \frac{E^{\frac{Nd}{\alpha}-1}}{\Gamma(Nd/\alpha)}$$

and

$$\begin{aligned} S(E, V, N) &= k_B \ln D(E, V, N) \\ &= Nk_B \ln \left(\frac{V}{N} \right) + \frac{d}{\alpha} Nk_B \ln \left(\frac{E}{N} \right) + Na_0 , \end{aligned}$$

where a_0 is a constant, and we take the thermodynamic limit $N \rightarrow \infty$ with V/N and E/N fixed. From this we obtain the differential relation

$$\begin{aligned} dS &= \frac{Nk_B}{V} dV + \frac{d}{\alpha} \frac{Nk_B}{E} dE + s_0 dN \\ &= \frac{p}{T} dV + \frac{1}{T} dE - \frac{\mu}{T} dN , \end{aligned}$$

where s_0 is a constant. From the coefficients of dV and dE , we conclude

$$pV = Nk_B T$$

$$E = \frac{d}{\alpha} Nk_B T .$$

Setting $dN = 0$, we have

$$\begin{aligned} dQ &= dE + p dV \\ &= \frac{d}{\alpha} Nk_B dT + p dV \\ &= \frac{d}{\alpha} Nk_B dT + p d\left(\frac{Nk_B T}{p}\right) . \end{aligned}$$

Thus,

$$C_V = \left. \frac{dQ}{dT} \right|_V = \frac{d}{\alpha} Nk_B \quad , \quad C_p = \left. \frac{dQ}{dT} \right|_p = \left(1 + \frac{d}{\alpha}\right) Nk_B .$$

(2) Find the velocity distribution $f(v)$ for the particles in problem (1). Compute the most probable speed, mean speed, and root-mean-square velocity.

Solution:

The momentum distribution is

$$g(\mathbf{p}) = C e^{-\beta A p^\alpha} ,$$

where C is a normalization constant, defined so that $\int d^d p g(\mathbf{p}) = 1$. Changing variables to $t \equiv \beta A p^\alpha$, we find

$$C = \frac{\alpha (\beta A)^{\frac{d}{\alpha}}}{\Omega_d \Gamma\left(\frac{d}{\alpha}\right)} .$$

The velocity \mathbf{v} is given by

$$\mathbf{v} = \frac{\partial \varepsilon}{\partial \mathbf{p}} = \alpha A p^{\alpha-1} \hat{\mathbf{p}} .$$

Thus, the speed distribution is given by

$$f(v) = C \int d^d p e^{-\beta A p^\alpha} \delta(v - \alpha A p^{\alpha-1}) .$$

Thus,

$$\langle v^r \rangle = C \int d^d p e^{-\beta A p^\alpha} (\alpha A p^{\alpha-1})^r ,$$

and

$$\|v\|_r = \langle v^r \rangle^{1/r} = \alpha A^{\alpha-1} (k_B T)^{1-\alpha-1} \left(\frac{\Gamma\left(\frac{d-r}{\alpha} + r\right)}{\Gamma\left(\frac{d}{\alpha}\right)} \right)^{1/\alpha} .$$

To find the most probable speed, we extremize $f(v)$. We write

$$\delta(v - \alpha A p^{\alpha-1}) = \frac{\delta(p - (v/\alpha A)^{1/(\alpha-1)})}{\alpha(\alpha-1)A p^{\alpha-2}}.$$

We then find

$$f(v) = \frac{C}{\alpha(\alpha-1)A} p^{d-\alpha+1} e^{-\beta A p^\alpha} \Big|_{p=(v/\alpha A)^{1/(\alpha-1)}}.$$

Extremizing, we obtain

$$\beta A p^\alpha = \frac{d - \alpha + 1}{\alpha},$$

which means

$$v = \alpha A \left(\frac{d - \alpha + 1}{\alpha \beta A} \right)^{1-\alpha^{-1}} = (\alpha A)^{\alpha^{-1}} (d - \alpha + 1)^{1-\alpha^{-1}} (k_B T)^{1-\alpha^{-1}}.$$

(3) A spin-1 Ising magnet is described by the noninteracting Hamiltonian

$$H = -\mu_0 H \sum_{i=1}^N \sigma_i,$$

where $\sigma_i = -1, 0, +1$.

(a) Find the entropy $S(H, T, N)$.

(b) Suppose the system starts off at a temperature $T = 10$ mK and a field $H = 20$ T. The field is then lowered adiabatically to $H = 1$ T. What is the final temperature of the system?

Solution:

The partition function for a single spin is

$$\zeta = 1 + 2 \cosh(\beta \mu_0 H).$$

The free energy is therefore

$$F = -N k_B T \ln \left(1 + 2 \cosh(\mu_0 H / k_B T) \right).$$

The entropy is

$$S = - \left(\frac{\partial F}{\partial T} \right)_{VN} = N k_B \ln \left(1 + 2 \cosh(\mu_0 H / k_B T) \right) - N \frac{\mu_0 H}{T} \frac{2 \sinh(\mu_0 H / k_B T)}{1 + 2 \cosh(\mu_0 H / k_B T)}$$

Note that $S = N s(H/T)$. Thus, an adiabatic process is one which takes place at constant H/T . If H is lowered by a factor of 20, then T is lowered by a factor of 20. For this problem, then, the final temperature is 0.5 mK.

(4) Consider an adsorption model where each of N sites on a surface can accommodate either one or two adsorbate molecules. For a single molecule the energy is $\varepsilon = -\Delta$, but when two are present the energy is $\varepsilon = -2\Delta + U$, where U models the local interaction of two adsorbate molecules at the same site. You should think of there being two possible binding locations within each adsorption site, so there are four possible states per site: unoccupied (1 possibility), singly occupied (2 possibilities), and doubly occupied (1 possibility). The surface is in equilibrium with a gas at temperature T and number density n .

(a) Find the surface partition function.

(b) Find the fraction f_j which contain j adsorbate molecules, where $j = 0, 1, 2$.

Solution:

The surface partition function is

$$\Xi = \left(1 + 2 e^{\beta(\mu+\Delta)} + e^{2\beta(\mu+\Delta)} e^{-\beta U} \right)^N,$$

hence

$$\Omega = -Nk_B T \ln \left(1 + 2 e^{(\mu+\Delta)/k_B T} + e^{2(\mu+\Delta)/k_B T} e^{-U/k_B T} \right).$$

In the gas, we have $e^{\mu/k_B T} = n\lambda_T^3$. Therefore

$$\begin{aligned} f_0 &= \frac{1}{1 + 2n\lambda_T^3 e^{\Delta/k_B T} + n^2 \lambda_T^6 e^{2\Delta/k_B T} e^{-U/k_B T}} \\ f_1 &= \frac{2n\lambda_T^3 e^{\Delta/k_B T}}{1 + 2n\lambda_T^3 e^{\Delta/k_B T} + n^2 \lambda_T^6 e^{2\Delta/k_B T} e^{-U/k_B T}} \\ f_2 &= \frac{(n\lambda_T^3)^2 e^{2\Delta/k_B T} e^{-U/k_B T}}{1 + 2n\lambda_T^3 e^{\Delta/k_B T} + n^2 \lambda_T^6 e^{2\Delta/k_B T} e^{-U/k_B T}}. \end{aligned}$$

(5) Consider a system of dipoles with the Hamiltonian

$$H = \sum_{i<j} J_{ij}^{\alpha\beta} n_i^\alpha n_j^\beta - \mu_0 \sum_i H_i^\alpha n_i^\alpha,$$

where

$$J_{ij}^{\alpha\beta} = \frac{J}{R_{ij}^3} (\delta^{\alpha\beta} - 3 \hat{R}_{ij}^\alpha \hat{R}_{ij}^\beta).$$

Here \mathbf{R}_i is the spatial position of the dipole \mathbf{m}_i , and $\mathbf{R}_{ij} = \mathbf{R}_i - \mathbf{R}_j$ with $\hat{R}_{ij}^\alpha \equiv R_{ij}^\alpha / R_{ij}$ the unit direction vector from j to i . The dipole vectors \mathbf{m}_i^α are three-dimensional unit vectors. H_i^α is the local magnetic field.

(a) Find an expression for the free energy $F(T, \{\vec{H}_i\})$ valid to order β^2 , where $\beta = 1/k_B T$.

(b) Obtain an expression for the uniform field magnetic susceptibility tensor $\chi_{\alpha\beta}$.

(c) An experimentalist plots the quantity $T\chi_{\alpha\beta}$ versus T^{-1} for large temperatures. What should the data resemble if the dipoles are arranged in a cubic lattice structure? How about if they are arranged in a square lattice in the (x, y) plane? (You'll need to separately consider the various cases for the indices α and β . You will also need to numerically evaluate certain lattice sums.)

Solution:

Since $Z = e^{-\beta F}$, we will need to expand Z to order β^3 in order to obtain F to order β^2 . We have

$$\begin{aligned} Z &= \text{Tr} e^{-\beta H} \\ &= \text{Tr} 1 - \beta \text{Tr} H + \frac{1}{2}\beta^2 \text{Tr} H^2 - \frac{1}{6}\beta^3 \text{Tr} H^3 + \mathcal{O}(\beta^4). \end{aligned}$$

Taking the logarithm, and recalling $\ln(1 + \varepsilon) = \sum_{k=1}^{\infty} (-1)^{k-1} \varepsilon^k / k$, we have

$$F = \text{Tr} H - \frac{1}{2}\beta \left[\text{Tr} (H^2) - (\text{Tr} H)^2 \right] + \frac{1}{6}\beta^2 \left[\text{Tr} (H^3) - 3 \text{Tr} (H^2) (\text{Tr} H) + 2 (\text{Tr} H)^3 \right] + \mathcal{O}(\beta^3).$$

We define the trace as

$$\text{Tr} F(\hat{\mathbf{n}}_1, \dots, \hat{\mathbf{n}}_N) = \int \prod_{j=1}^N \frac{d\hat{\mathbf{n}}_j}{4\pi} F(\hat{\mathbf{n}}_1, \dots, \hat{\mathbf{n}}_N),$$

so that $\text{Tr} 1 = 1$. Thus,

$$\text{Tr} (n_i^\mu n_j^\nu) = \frac{1}{3} \delta_{ij} \delta^{\mu\nu}.$$

Clearly the trace of any product of an odd number of terms n_i^μ with the same i , no matter what the choices of the $O(3)$ indices (e.g. μ), must vanish, since the trace itself is invariant under $\hat{\mathbf{n}}_i \rightarrow -\hat{\mathbf{n}}_i$. It isn't so easy to compute traces of higher order even products, since the unit vector constraint on $\hat{\mathbf{n}}_i$ invalidates the application of Wick's theorem, which can be invoked when computing the averages of Gaussianly distributed variables. For example, one finds $\text{Tr} (n^x n^x n^y n^y) = \frac{2}{3}$ while $\text{Tr} (n^x n^x n^x n^x) = \frac{1}{5}$. No matter; we shall only need $\text{Tr} (n_i^\mu n_j^\nu)$, computed above.

We now write $H = H_0 + H_1$, where $H_0 = \sum_{i < j} J_{ij}^{\alpha\beta} n_i^\alpha n_j^\beta$ and $H_1 = -\mu_0 \sum_i H_i^\alpha n_i^\alpha$. Eliminating the odd terms whose traces vanish, we have

$$\begin{aligned} \text{Tr} H &= \text{Tr}(H_0 + H_1) = 0 \\ \text{Tr} (H^2) &= \text{Tr} (H_0^2 + 2 H_0 H_1 + H_1^2) = \text{Tr} (H_0^2) + \text{Tr} (H_1^2) \\ \text{Tr} (H^3) &= \text{Tr} (H_0^3 + 3 H_0^2 H_1 + 3 H_0 H_1^2 + H_1^3) = \text{Tr} (H_0^3) + 3 \text{Tr} (H_0 H_1^2), \end{aligned}$$

so the free energy is

$$F = -\frac{1}{2}\beta \text{Tr} (H_0^2) - \frac{1}{2}\beta \text{Tr} (H_1^2) + \frac{1}{6}\beta^2 \text{Tr} (H_0^3) + \frac{1}{2}\beta^2 \text{Tr} (H_0 H_1^2)$$

Note that $\text{Tr } H_0 = 0$ since i and j are distinct in the sum. We may now compute

$$\begin{aligned}\text{Tr}(H_0^2) &= \sum_{i<j} \sum_{k<l} J_{ij}^{\mu\nu} J_{ij}^{\alpha\beta} \text{Tr}(n_i^\mu n_j^\nu n_k^\alpha n_l^\beta) = \frac{1}{9} \sum_{i<j} J_{ij}^{\mu\nu} J_{ij}^{\mu\nu} \\ \text{Tr}(H_1^2) &= \mu_0^2 \sum_i \sum_j H_i^\alpha H_j^\beta \text{Tr}(n_i^\alpha n_j^\beta) = \frac{1}{3} \mu_0^2 \sum_i H_i^\alpha H_i^\alpha \\ \text{Tr}(H_0^3) &= \sum_{i<j} \sum_{k<l} \sum_{m<n} J_{ij}^{\mu\nu} J_{kl}^{\alpha\beta} J_{rs}^{\sigma\tau} \text{Tr}(n_i^\mu n_j^\nu n_k^\alpha n_l^\beta n_r^\sigma n_s^\tau) = \frac{2}{9} \sum_{l<m<n} J_{lm}^{\mu\nu} J_{ln}^{\mu\sigma} J_{mn}^{\nu\sigma} \\ \text{Tr}(H_0 H_1^2) &= \mu_0^2 \sum_{i<j} \sum_k \sum_l J_{ij}^{\mu\nu} H_k^\alpha H_l^\beta \text{Tr}(n_i^\mu n_j^\nu n_k^\alpha n_l^\beta) = \frac{2}{9} \mu_0^2 \sum_{i<j} J_{ij}^{\mu\nu} H_i^\mu H_j^\nu.\end{aligned}$$

Note that $J_{ij}^{\mu\nu}$ is separately symmetric under interchange of the (ij) and/or $(\mu\nu)$ indices. Next we must contract the $O(3)$ indices. We find

$$\begin{aligned}J_{ij}^{\mu\nu} J_{ij}^{\mu\nu} &= \frac{6J^2}{R_{ij}^6} \\ J_{ij}^{\mu\nu} J_{jk}^{\nu\lambda} J_{ki}^{\lambda\mu} &= \left[-6 + 9(\hat{R}_{ij} \cdot \hat{R}_{jk})^2 + 9(\hat{R}_{jk} \cdot \hat{R}_{ki})^2 + 9(\hat{R}_{ki} \cdot \hat{R}_{ij})^2 \right. \\ &\quad \left. - 27(\hat{R}_{ij} \cdot \hat{R}_{jk})(\hat{R}_{jk} \cdot \hat{R}_{ki})(\hat{R}_{ki} \cdot \hat{R}_{ij}) \right] \cdot \frac{J^3}{R_{ij}^3 R_{jk}^3 R_{ki}^3}.\end{aligned}$$

(a) Thus, the free energy is

$$\begin{aligned}F &= -\frac{J^2}{3k_B T} \sum_{i<j} \frac{1}{R_{ij}^6} - \frac{\mu_0^2}{6k_B T} \sum_i H_i^\mu H_i^\mu + \frac{\mu_0^2 J}{9(k_B T)^2} \sum_{i<j} \left(\frac{\delta^{\mu\nu} - 3\hat{R}_{ij}^\mu \hat{R}_{ij}^\nu}{R_{ij}^3} \right) H_i^\mu H_j^\nu \\ &\quad + \frac{2J^3}{9(k_B T)^2} \sum_{i<j<k} \frac{-2 + 3\hat{R}_{ij} \cdot \hat{R}_{jk} + 3\hat{R}_{jk} \cdot \hat{R}_{ki} + 3\hat{R}_{ki} \cdot \hat{R}_{ij} - 9(\hat{R}_{ij} \cdot \hat{R}_{jk})(\hat{R}_{jk} \cdot \hat{R}_{ki})(\hat{R}_{ki} \cdot \hat{R}_{ij})}{R_{ij}^3 R_{jk}^3 R_{ki}^3}\end{aligned}$$

to order β^2 .

(b) We have

$$\begin{aligned}\chi_{ij}^{\mu\nu} &= \frac{\partial \langle \mu_0 n_i^\mu \rangle}{\partial H_j^\nu} = -\frac{\partial^2 F}{\partial H_i^\mu \partial H_j^\nu} \\ &= \frac{\mu_0^2}{3k_B T} \delta^{\mu\nu} \delta_{ij} - \frac{2\mu_0^2 J}{9(k_B T)^2} \left(\frac{\delta^{\mu\nu} - 3\hat{R}_{ij}^\mu \hat{R}_{ij}^\nu}{R_{ij}^3} \right) (1 - \delta_{ij}) + \mathcal{O}(T^{-3}).\end{aligned}$$

The second term is here multiplied by $(1 - \delta_{ij})$ since i and j must be distinct in the corresponding term from the free energy. $\chi_{ij}^{\mu\nu}$ tells us how the moment at site i changes in response to a change in the magnetic field at site j . To get the uniform magnetic susceptibility, we differentiate the total moment $M^\mu = \mu_0 \sum_i \langle n_i^\mu \rangle$ with respect to a uniform field H^ν , and we then divide by the system volume. Thus,

$$\chi^{\mu\nu} = \frac{1}{V} \sum_{i,j} \chi_{ij}^{\mu\nu} = \frac{N}{V} \cdot \frac{\mu_0^2}{3k_B T} \delta^{\mu\nu} - \frac{2\mu_0^2 J}{9(k_B T)^2} \cdot \frac{1}{V} \sum_{i \neq j} \left(\frac{\delta^{\mu\nu} - 3\hat{R}_{ij}^\mu \hat{R}_{ij}^\nu}{R_{ij}^3} \right) + \mathcal{O}(T^{-3}).$$

The above expression is valid for any spatial arrangement of the dipoles. They don't have to be in a regular lattice, for example.

(c) If the dipoles are located at the sites of a Bravais lattice, then we may write

$$\chi^{\mu\nu} = \frac{1}{V} \sum_{i,j} \chi_{ij}^{\mu\nu} = \frac{N}{V} \cdot \frac{\mu_0^2}{3k_B T} \delta^{\mu\nu} - \frac{N}{V} \cdot \frac{2\mu_0^2 J}{9(k_B T)^2} \sum_{\mathbf{R} \neq 0} \left(\frac{\delta^{\mu\nu} - 3\hat{R}^\mu \hat{R}^\nu}{R^3} \right) + \mathcal{O}(T^{-3}),$$

where the sum is over all Bravais lattice vectors (*i.e.* all lattice points) other than $\mathbf{R} = 0$. Now let's do the lattice sum in the second term for the case of a cubic lattice. We write $\mathbf{R} = (l\hat{x} + m\hat{y} + n\hat{z})a$, where a is the lattice constant and (l, m, n) are integers. We sum over all triples of integers (l, m, n) other than $(0, 0, 0)$. We then have

$$R = (l^2 + m^2 + n^2)^{1/2} a, \quad \hat{R} = \frac{\mathbf{R}}{R} = \frac{l\hat{x} + m\hat{y} + n\hat{z}}{(l^2 + m^2 + n^2)^{1/2}}.$$

It is clear that the off-diagonal terms in $\chi^{\mu\nu}$ must vanish due to the cubic symmetry. For example, when $\mu = x$ and $\nu = y$ we have to compute

$$\sum'_{l,m,n} \frac{lm}{(l^2 + m^2 + n^2)^{5/2}} = 0,$$

since the summand is odd separately in both l and m . The prime on the sum indicates that the term $(0, 0, 0)$ is to be excluded.

Next, consider the diagonal elements. For a cubic lattice, we must have $\chi^{xx} = \chi^{yy} = \chi^{zz}$, so we need only compute the xx term:

$$\sum_{\mathbf{R} \neq 0} \left(\frac{1 - 3\hat{R}^x \hat{R}^x}{R^3} \right) = \frac{1}{a^3} \sum'_{l,m,n} \frac{m^2 + n^2 - 2l^2}{(l^2 + m^2 + n^2)^{5/2}} = 0.$$

To see why this term vanishes, note that any permutation of the triple (l, m, n) is also a Bravais lattice site. Summing over all permutations, we see that the above sum must vanish. We therefore conclude that all components of the $\mathcal{O}(T^{-2})$ term in the susceptibility vanish for a cubic lattice. In fact, it is clear from the outset that

$$\text{Tr}(\delta^{\mu\nu} - 3\hat{R}^\mu \hat{R}^\nu) = 0,$$

so this result coupled with the cubic symmetry immediately tells us that the $\mathcal{O}(T^{-2})$ must vanish for all components.

For a square lattice, we set $n = 0$. The off-diagonal component χ^{xy} still vanishes due to the square symmetry, but now we have $\chi^{xx} = \chi^{yy} = -\frac{1}{2}\chi^{zz}$. The lattice sum for the xx term is

$$-\sum'_{l,m} \frac{m^2 - 2l^2}{(l^2 + m^2)^{5/2}} = \sum'_{l,m} \frac{l^2}{(l^2 + m^2)^{5/2}} = \frac{1}{2} \sum'_{l,m} \frac{1}{(l^2 + m^2)^{3/2}} = 1.7302,$$

where the numerical value is obtained by numerical summation. Thus,

$$\chi^{\mu\nu}(\text{SC}) = \frac{N}{V} \cdot \frac{\mu_0^2}{3k_B T} \delta^{\mu\nu} + \mathcal{O}(T^{-3})$$

$$\chi^{\mu\nu}(\text{SQ}) = \frac{N}{V} \cdot \frac{\mu_0^2}{3k_B T} \delta^{\mu\nu} + \frac{N}{V} \cdot \frac{2\mu_0^2 J}{9(k_B T)^2} \cdot \frac{1.7302}{a^3} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix} + \mathcal{O}(T^{-3})$$

for simple cubic and square lattices, respectively. Thus, if we plot $T\chi^{\mu\nu}$ versus T^{-1} at high temperatures, we should observe a straight line with intercept $n\mu_0^2/3k_B$, with $n = N/V$. The slope of the line is zero for the case of a cubic lattice, but for a square lattice, we should observe a positive slope of $0.3845 n\mu_0^2 J/k_B^2$ for χ^{xx} and χ^{yy} and a negative slope of twice this magnitude for χ^{zz} .

(6) The general form of the kinetic energy for a rotating body is

$$T = \frac{1}{2}I_1(\dot{\phi} \sin \theta \sin \psi + \dot{\theta} \cos \psi)^2 + \frac{1}{2}I_2(\dot{\phi} \sin \theta \cos \psi - \dot{\theta} \sin \psi)^2 + \frac{1}{2}I_3(\dot{\phi} \cos \theta + \dot{\psi})^2,$$

where (ϕ, θ, ψ) are the Euler angles.

(a) Find the Hamiltonian $H(p_\phi, p_\theta, p_\psi)$ for a free asymmetric rigid body.

(b) Compute the rotational partition function,

$$\xi_{\text{rot}}(T) = \frac{1}{h^3} \int_{-\infty}^{\infty} dp_\phi \int_{-\infty}^{\infty} dp_\theta \int_{-\infty}^{\infty} dp_\psi \int_0^{2\pi} d\phi \int_0^\pi d\theta \int_0^{2\pi} d\psi e^{-H(p_\phi, p_\theta, p_\psi)/k_B T}$$

and show that you recover the result in §4.10.4 of the notes.

Solution:

We define generalized coordinates (ϕ, θ, ψ) , in which case we may write $T = \frac{1}{2}T_{ij} \dot{q}_i \dot{q}_j$, with

$$T_{ij} = \begin{pmatrix} (I_1 \sin^2 \psi + I_2 \cos^2 \psi) \sin^2 \theta + I_3 \cos^2 \theta & (I_1 - I_2) \sin \theta \sin \psi \cos \psi & I_3 \cos \theta \\ (I_1 - I_2) \sin \theta \sin \psi \cos \psi & I_1 \cos^2 \psi + I_2 \sin^2 \psi & 0 \\ I_3 \cos \theta & 0 & I_3 \end{pmatrix}$$

The generalized momenta are $p_i = \partial T / \partial \dot{q}_i = T_{ij} \dot{q}_j$, and the Hamiltonian is

$$H = \frac{1}{2}T_{ij}^{-1} p_i p_j.$$

Recall the general formula for a matrix inverse: $M_{ij}^{-1} = (-1)^{i+j} \Delta_{ji} / \det M$, where the *minor* Δ_{ij} is the determinant of the square matrix formed from M by eliminating the i^{th} row and the j^{th} column. The matrix T is of the form

$$T = \begin{pmatrix} a & d & e \\ d & b & 0 \\ e & 0 & c \end{pmatrix},$$

hence the determinant is $\det T = abc - cd^2 - be^2$ and the inverse is

$$T^{-1} = \frac{1}{abc - cd^2 - be^2} \begin{pmatrix} bc & -cd & -be \\ -cd & ac - e^2 & de \\ -be & de & ab - d^2 \end{pmatrix}.$$

Taking the determinant of T is straightforward, and one finds $\det T = I_1 I_2 I_3 \sin^2 \theta$. The rotational partition function is then given by the multidimensional integral

$$\begin{aligned} \xi_{\text{rot}}(T) &= \frac{1}{h^3} \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \int_0^{2\pi} d\psi \int_{-\infty}^{\infty} dp_{\phi} \int_{-\infty}^{\infty} dp_{\theta} \int_{-\infty}^{\infty} dp_{\psi} e^{-T_{ij}^{-1} p_i p_j / 2k_B T} \\ &= \frac{1}{h^3} \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \int_0^{2\pi} d\psi (2\pi k_B T)^{3/2} \sqrt{\det T} \\ &= \left(\frac{2k_B T}{h^2} \right)^{3/2} \sqrt{\pi I_1 I_2 I_3}, \end{aligned}$$

as in §4.10.4 of the notes.