

Equilibrium Statistical Mechanics Dictionary

UCI Chem 232B (Mandelsham)

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Chapter 2 – Canonical Ensemble

Ensemble: Collection of very large number of independent systems, each constructed to be a replica on a thermodynamic (macroscopic) level of particular thermodynamic system of interest. All members are identical from a thermodynamic point of view (not necessarily on molecular level). 36

Partition function: Describes statistical properties of a system in thermodynamic equilibrium. PFs are functions of thermodynamic state variables (e.g. T, V). Most thermodynamic properties can be expressed in terms of partition function or derivatives thereof. 44

Characteristic state function: thermodynamic function with the same natural variables of the particular ensemble. For some partition function Z, the characteristic state function is X from the form $Z = e^{-\beta X}$. 45, 55

Microcanonical: Ensemble with constant (fixed) N, V, E. The PF Ω is fundamental to all ensembles (Laplace transform). Characteristic state function is TS. Probabilities of all states equal (principle of equal a priori probabilities): $\bar{F} = \sum_j F_j$.

Canonical: Ensemble with constant N, V, T. Physical representation is mechanical system in thermal equilibrium with a heat bath at some fixed temperature. PF is Laplace transform of microcanonical ensemble over E. Characteristic state function is A. PF is:

$$Q = \sum_j e^{-\beta E_j}$$

Helmholtz free energy: Thermodynamic potential which is the characteristic state function (having the same natural variables) of canonical ensemble. 45

$$A = -k_B T \ln Q$$

Chapter 3 – Other Ensembles & Fluctuations

Grand canonical: ensemble with constant μ, V, T . Physical representation is mechanical system in thermal and chemical equilibrium with a reservoir. PF is Laplace transform of microcanonical ensemble over N and E. Characteristic state function is Ξ . PF is:

$$\Xi = \sum_N \sum_j e^{-\beta E_{Nj}} e^{\beta \mu N}$$

Isothermal-isobaric: ensemble with constant N, P, T. Laplace transform of microcanonical ensemble over E and V. Physical representation is mechanical system with constant temperature and pressure, especially relevant conditions for many chemical reactions. Characteristic state function is Gibbs free energy. 55 Partition function:

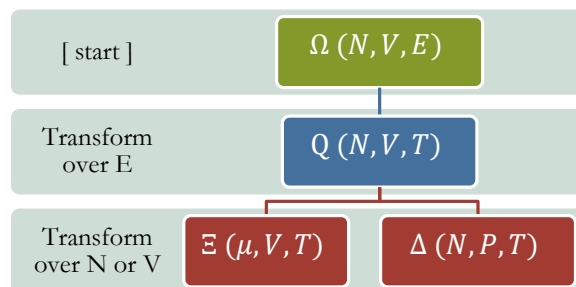
$$\Delta = \sum_V \sum_j e^{-\beta E_{Vj}} e^{-\beta p V}$$

Laplace transform: Connects different statistical ensembles together. To go from $f(x)$ to $F(y)$:

$$F(y) = L \{f(x)\} = \int_0^\infty f(x) e^{-xy} dx$$

For example, Laplace of transform to go from microcanonical to canonical:

$$Q = \int \Omega e^{-\beta E} dE$$



Chapter 4 – Boltzmann, FD, BE Statistics

Boltzmann statistics: statistical behavior exhibited by classical ideal particles as well as FD and BE particles in the classical limit (negligible quantum effects), when $\mu\beta \rightarrow 0$. Valid when the number of available molecular states is much greater than the number of particles in the system. Probability:

$$P = \frac{e^{-\beta E_j}}{Q}; \quad Q = \frac{q^N}{N!} \text{ (indisting.)}$$

Fermi-Dirac statistics: statistical behavior exhibited by fermions. Symmetry in wavefunction, in which ψ changes sign upon interchanging two particles. Reflects natural behavior following Pauli exclusion principle (no two particles can occupy same state). Partition function (grand):

$$\Xi_{\text{FD}} = \prod_k [1 + e^{-\beta(\epsilon_k - \mu)}]^{+1}$$

Bose-Einstein statistics: statistical behavior exhibited by bosons. Symmetry in wavefunction, in which ψ is unchanged upon interchanging two particles. Reflects natural behavior in which multiple particles can occupy same state. Partition function (grand):

$$\Xi_{\text{BE}} = \prod_k [1 - e^{-\beta(\epsilon_k - \mu)}]^{-1}$$

Chapter 5 – Ideal Monatomic Gas

Ideal gas of monatomic molecules: gas composed of monatomic particles; ideal meaning IMFs can be neglected; when $p < 1$ atm and $T >$ room temp. Equation of state is well represented by $pV = NkT$. Number of available quantum states far exceeds number of particles. Partition function:

$$Q = \frac{[q(V, T)]^N}{N!}$$

$$q = q_{\text{trans}} q_{\text{elec}} q_{\text{nuc}}$$

Classical configuration integral: $3N$ dimensional over spatial coordinates, with exponential of N -body potential. Arises in evaluation of canonical partition function. Not analytically soluble. 116

$$Z = \int e^{-\beta U(\vec{p}, \vec{q})} d\vec{q}$$

Chapter 6 – Ideal Diatomic Gas

Ideal gas of diatomic molecules: gas composed of diatomic molecules; ideal meaning IMFs can be neglected; when $p < 1$ atm and $T >$ room temp. Can be well approximated by RR-HO approximation. Partition function:

$$Q = \frac{[q(V, T)]^N}{N!}$$

$$q = q_{\text{trans}} q_{\text{rot}} q_{\text{vib}} q_{\text{elec}} q_{\text{nuc}}$$

Rigid rotor-harmonic oscillator approximation: Approximation to treat ideal gas of diatomic molecules to separate the Hamiltonian into respective degrees of freedom, esp. $H_{\text{vib-rot}} = H_{\text{vib}} + H_{\text{rot}}$, where H_{vib} is treated as a harmonic oscillator, and H_{rot} is treated as a rigid rotor. With the Hamiltonian being separable, the total partition function can be written as a product of individual partition functions.

Chapter 7 – Classical Statistical Mechanics

Partition function:

$$Q = \sum_j e^{-\beta \epsilon_j} \rightarrow$$

$$\frac{1}{N! h^{sN}} \int \dots \int e^{\beta H(p, q)} dp dq$$

Phase space: For molecules with sN dimensional degrees of freedom, phase space is a $2sN$ dimensional space ($6N$ for Cartesian) of coordinates and momenta. An ensemble can be represented as a cloud of points, with each individual point being a single system in phase space. Just as systems are independent in ensembles, phase space trajectories are independent.

Liouville equation: equation of motion for the distribution function f in phase space for a conservative Hamiltonian. 119

$$\frac{\partial f}{\partial t} = - \sum_{j=1}^{3N} \left(\frac{\partial H}{\partial p_j} \frac{\partial f}{\partial q_j} - \frac{\partial H}{\partial q_j} \frac{\partial f}{\partial p_j} \right)$$

Liouville theorem: $\frac{df}{dt} = 0$, The density of states is constant along every trajectory in phase space. Means that %s is conserved: phase space volume = number of systems in the ensemble. (e.g., Arnold's cat). Leads to ergodic hypothesis.

Ergodic hypothesis: consequence of Liouville theorem. Time average of one system = ensemble average at a particular time; over long periods of time, the time spent by a system in some region of the phase space of microstates with the same energy is proportional to the volume of this region; all accessible microstates are equiprobable over a long period of time.

Equipartition theorem: Each degree of freedom will contribute $\frac{Nk_B T}{2}$ to the average energy and $\frac{Nk_B}{2}$ to the heat capacity. For a Cartesian system, the contributions are (1) translational $\frac{3Nk_B T}{2}$, (2) rotational $\frac{3Nk_B T}{2}$, (3) vibrational $(3n - 6)k_B T$. Note that linear molecule as rotational $\frac{2Nk_B T}{2}$ or $3n-5$ for a linear molecule. (less rot but minus less)

Path integral formulation: method by which quantum mechanical contributions can be incorporated within a classical simulation using Feynman path integrals. Maps quantum problem to classical one. Each particle and its path can be interpreted as a polymer with strings connecting nearest neighbors in each chain (ring polymer). Moving a quantum particle is equivalent to evolving this polymer.

Path integral → Monte Carlo: To take quantum effects into account when calculating properties, a path integral formulation may be used. This approach leads to a multi-dimensional integral which can be calculated using Metropolis Monte Carlo, resulting in the path integral Monte Carlo method (PIMC). ([link](#), see p. 43)

Metropolis Monte Carlo: (see flowchart below) Direct sampling from some probability distribution

may be difficult (e.g. no analytical solutions). MMC generates sequence of random samples according to the desired statistical mechanics distribution. Equilibrium properties can be studied.

Algorithm goes by making a random move, then evaluating the Boltzmann probability of such a move and comparing the probability against a random number. If the Boltzmann probability of the move is larger than the random number, the move is accepted; otherwise the system is returned to its original configuration.

At the end, a set of configurations is obtained according to Boltzmann statistics and the expectation value of a property is obtained as a simple arithmetic average of property values from individual accepted configurations.

Chapter 8 – Ideal Polyatomic Gas

Ideal gas of polyatomic molecules: Extended using methods of diatomic molecules and classical stat mech. (1) Translational same, (2) Vibrational: normal coordinates, (3) Rotational: use classical instead of quantum, (4, 5) presumably electronic and nuclear are same.

Hindered rotation: rotation that is hindered due to atomic interactions, such as from hydrogens for C-C bond of ethane. Leads to sinusoidal potential energy due to rotation.

Chapter 9 – Chemical Equilibrium

Equilibrium constant: value of the reaction quotient when the reaction has reached equilibrium. Function of temperature only for an ideal system. 143

$$K_c = \frac{\rho_c^{v_c} \rho_D^{v_D}}{\rho_A^{v_A} \rho_B^{v_B}} = \frac{\rho_c^{v_c} \rho_D^{v_D}}{\rho_A^{v_A} \rho_B^{v_B}}$$

Chapter 10 – Quantum Statistics

Quantum degeneracy: weakly degenerate represents small deviations from classical behavior - high T and low density; strongly degenerate represents large deviations from classical behavior - low T and high density. 161

Virial coefficients: coefficients of virial expansion (in p or V); reflect deviations from ideality - intermolecular interactions. For $B_2(T)$ positive: fermions, repulsive, increase in pressure compared to ideal. For $B_2(T)$ negative: bosons, attractive. 163, 170

Strongly degenerate FD gas: ideal FD gas at low T and/or high density. Can be applied to free electron model of metals (metallic crystals), in which many of the physically observable properties are due to quantum statistical effects.

Fermi energy: μ_0 , at 0 K, the conduction electrons in the metal fill all the energy states up to this energy value; typically on the order of 1-5 eV. Distribution of energy is essentially step function, with value of 1 up until μ_0 , and 0 after.

Fermi temperature: μ_0/k_B , compared to this characteristic temperature, $T_F \gg T_{RT}$, so FD distribution is like a step function which goes from 1 to zero at ϵ . 166

ZPE of FD gas: temperature independent, implies no contribution of conduction electrons to heat capacity, which contrasts with equipartition value of $3k/2$ for each electron. Why? Since μ_0 is so large compared to kT , very few particles will be within kT near μ_0 , so only very few can contribute.

$$E_0 = \frac{3}{5} N \mu_0$$

Bose-Einstein condensation: the condensation of molecules into their ground states at $T \rightarrow T_0$ or as density goes down to some critical density. **FIRST order process**, although there is a uniform macroscopic density. Condensation occurs in momentum space, since particles are found in same region of momentum space (zero momentum). Occurs because of effective interaction through the

symmetry requirement of the N-body wavefunction.

Clapeyron equation: characterizes discontinuous phase transition:

$$\frac{dp}{dT} = \frac{\Delta H_{cond}}{T \Delta V}$$

By taking dp/dT of BE gas and comparing to this, the heat of transition between condensed (with volume 0) and dilute phases (with specific volume) can be derived.

Chapter 11 – Crystals

Distribution function $g(\nu)$: times $d\nu$, gives the number of normal frequencies between ν and $\nu+d\nu$. Difficult to calculate exactly. There are two useful and well-known approximations to $g(\nu)$, Einstein and Debye models. 197

Law of Dulong and Petit: if the N atoms of a crystalline solid behave as harmonic oscillators about their equilibrium positions, classical theory (equipartition) predicts that each atom would contribute R cal/deg-mole for each of its 3 vibrational degrees of freedom. Molar heat capacity at constant volume $C_V = 3Nk = 3R = 6$ cal/deg-mol. Good agreement with observed heat capacity of many crystals at high enough temp, but fails completely at low temperatures. 198

Note to self: don't confuse with Cartesian equipartition theorem with $3Nk/2$ translational

T^3 law: experimental observation that, as $T \rightarrow 0$, C_V falls rapidly to zero as T^3 . Successful theories should reproduce this law.

Einstein model: [1] each atom in crystal vibrates about equilibrium configuration as simple harmonic oscillator, so entire crystal is set of $3N$ independent HOs, each with frequency ν . [2] each atom of the crystal sees the same environment as any other, and so all N atoms could be treated as independent oscillators in the x, y, and z directions. [3] *Energy of each of these $3N$ independent oscillators was quantized according to the procedure developed by Planck (blackbody radiation theory).*

$$g(\nu) = 3N \delta(\nu - \nu_E)$$

Assessment: (a) upholds Dulong and Petit value of $3Nk$ as $T \rightarrow \infty$. (b) DOES NOT go as T^3 as T goes to zero. (c) IS consistent with law of corresponding states. 198

Einstein frequency, ν_E : single frequency assigned to all $3N$ independent oscillators of the crystal. Varies from substance to substance. Reflects the nature of interatomic interactions for the particular crystal. Einstein temperature is $h\nu/k$.

Law of corresponding states, part 1 of __: C_v is predicted to be the same function for *all* substances, when plotted against reduced temperature T/Θ_E . 200

Debye model: treats the long-wavelength frequencies of a crystal in an exact manner. [1] Normal modes whose wavelengths are long cf. atomic spacing do not depend on atomic character of solid and could be calculated by assuming that the crystal is a continuous elastic body. Approximates all normal frequencies with this.

$$g(\nu) d\nu = \frac{4\pi V \nu^2}{v^3} d\nu$$

Assessment: three criteria satisfied of (a) Dulong and Petit, (b) T -cubed law, (c) corresponding states. However, Debye temperature depends on temperature, unlike horizontal for exact theory.

Debye frequency: “artificial” maximum frequency introduced so that the integral of $g(\nu)d\nu$ from 0 to ν_D equals $3N$. 202

Dispersion curve: relation between the frequency ω and wave vector k representing wave of wavelength $2\pi/k$ and frequency ω traveling along chain. For frequency distribution for lattice dynamics. 208

Phonon: “quasi-particles,” essentially quanta of lattice vibrations, just as photons are quanta of EM vibrations. Can be thought of as quanta of sound waves, since lattice vibrations are closely related to sound waves passing through the crystals. 213

Brillouin scattering: inelastic scattering of phonons with photons, tangent: *neutron* scattering

can be used to determine vibrational frequency spectrum of crystal. 213

Chapter 12 – Imperfect Gases

Imperfect gas: Partition function is no longer of the form $f(T)V$ leading to the ideal gas equation of state. Imperfect gases are at lower T or higher P (higher density), so the intermolecular potential U becomes nonnegligible. Deviations are expressed as an infinite power series in the density ρ .

Second virial coefficient: can be calculated as function of T having intermolecular potential $u(r)$. Can be measured experimentally. 233

Law of corresponding states, part 2 of __: virial coefficients can be written in a reduced form as functions of only the reduced temperature. This function of T^* would be the same for *all* systems. 243

Lennard-Jones potential: $u(r)$, but can't analytically integrate $B_2(T)$

$$u(r) = 4\epsilon \left\{ \left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right\}$$

Hard sphere potential: simulates steep repulsive part of realistic potentials, but no attractive part:

$$u(r) = \begin{cases} \infty & r < \sigma \\ 0 & r > \sigma \end{cases}$$

Square well potential: extension of hard sphere potential that includes attractive term, can be handled analytically: Reduces to hard sphere result when $\lambda \rightarrow 1$ or $\epsilon \rightarrow 0$.

$$u(r) = \begin{cases} \infty & r < \sigma \\ -\epsilon & \sigma < r < \lambda\sigma \\ 0 & r > \lambda\sigma \end{cases}$$

Chapter 13 – Distribution Functions in Classical Monatomic Liquids

Broad picture: instead of considering 2-body, etc., here, consider constant interaction with a large number of neighbors in dense systems, e.g. liquids, to derive thermodynamic properties.

Probability distribution function $\rho^{(1)}(\mathbf{r}_1)$: probability that any one molecule will be found in $d\mathbf{r}_1$. Independent of \mathbf{r}_1 for a fluid in which all points within V are equivalent. $\rho^{(1)} = \rho$. 258

Correlation function $g^{(n)}(\mathbf{r}_1, \dots, \mathbf{r}_n)$: factor that relates ρ^n to $\rho^{(n)}$. It corrects for the “nonindependence” or, i.e., the correlation between the molecules. / $g^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = g(r)$ can be determined experimentally. In liquid of spherically symmetric molecules, it depends only on the relative distance r_{12} . 258

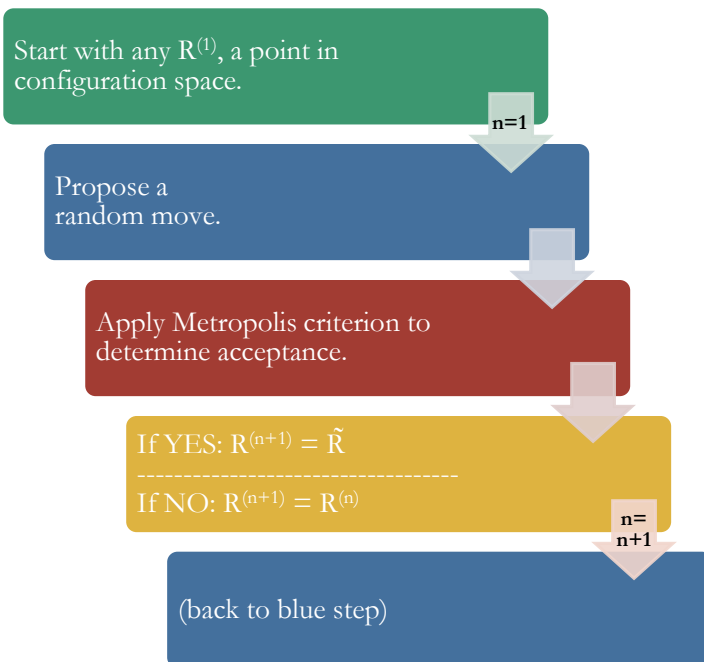
Radial distribution function $g(r)$: $\rho^*g(r)*4\pi r^2$ is the number of molecules between r and $r+dr$ about

a central molecule. $g(r)$ is the factor that multiplies the bulk density ρ to give a local density $\rho(r)$ about some fixed molecule. As $r \rightarrow 0$, $g \rightarrow 0$. As $r \rightarrow \infty$, $g \rightarrow 1$.

Importance: [1] if we assume that the total potential energy of the N-body system is pair-wise additive, then all the thermodynamic functions of the system can be written in terms of $g(r)$.

[2] The radial distribution function can be determined by X-ray diffraction studies on liquids, related by the scattering of EM radiation. 259

Metropolis Monte Carlo Algorithm



$$\tilde{R} = R^{(n)} + c \cdot \xi$$

ξ : random number, $[-1, 1]$
 c : constant to scale ξ

$$\text{if } \frac{P(\tilde{R})}{P(R^{(n)})} = e^{-\beta[U(\tilde{R}) - U(R^{(n)})]} > \eta$$

η : random number, $[0, 1]$

Derivations of Partition Functions

Isothermal-Isobaric Ensemble (μ, P, T)

Page 38-40, 52-54, 55/65

Note: This derivation can be followed analogously for (1) canonical partition function, easier since only two constraints for A and E, dealing with single sums; (2) grand-canonical partition function, constrain A, E, N; and (3) showing that β depends only on temperature, with two separate ensembles A, B in thermal contact.

V is index of particular volumes of individual system, since they vary. As usual, i is index of energy level.

1. Establish constraints for Lagrange multipliers.

- a. Total systems:

$$A = \sum \sum a_{Vi} \rightarrow \alpha (\sum \sum a_{Vi} - A) = 0$$

- b. Total energy:

$$\varepsilon = \sum \sum a_{Vi} E_{Vi} \rightarrow \beta (\sum \sum a_{Vi} E_{Vi} - \varepsilon) = 0$$

- c. Total volume:

$$\tilde{V} = \sum \sum a_{Vi} V_{Vi} \rightarrow \delta (\sum \sum a_{Vi} V_{Vi} - \tilde{V}) = 0$$

2. Write the formula for probability.

$$P = \frac{a^*}{A}, \text{ where } a^* \text{ is the most probable occupation.}$$

3. Consider number of possible rearrangements (W) to find most probable one (a^*). Basic min/max problem: differentiate and set equal to zero.

$$W(a) = \frac{A!}{\prod_V \prod_j a_{Vj}!}$$

- a. Here, we will use $\ln(W)$ to make the math easier, since we get to use Stirling's law in the limit of large W, where $\ln(M!) = M \ln M - M$.

$$\ln W(a) = \ln(A!) - \ln(\prod_V \prod_j a_{Vj}!)$$

$$= A \ln A - A - \prod_V \prod_j a_{Vj} \ln(\prod_V \prod_j a_{Vj}) + \prod_V \prod_j a_{Vj}$$

- b. Subtract in the three zeros from the constraints of step 1.
- c. Differentiate with respect to a. Rename this a^* in the expression since it is the sought var.
 - i. Note that all terms without little a automatically go to zero.
 - ii. Summation goes away, since only considering the specific a_i of maxing W.
 - iii. Solve for a, which should have exponentials to undo the log.

4. Now pass this back to expression for probability in step 2. The denominator is the partition function!

Note: alpha is eliminated from expression at the end:

1. Taking a^* expression with exponentials,
2. Summing over all k on both sides,
3. LHS goes to A,
4. RHS pull $e^{-\alpha}$ out of denominator, and solve for this.
5. Plug step 4 into probability, and the A terms should cancel top and bottom.

Monatomic Ideal Gas (translational)

Page 82

1. Start with energies for **particle in a 3D box**:

$$\varepsilon_{n_x n_y n_z} = \frac{h^2}{8ma^2} (n_x^2 + n_y^2 + n_z^2)$$

2. Insert into general form of canonical partition function:

$$\begin{aligned} q_{trans} &= \sum_{n_x, n_y, n_z=1}^{\infty} e^{-\beta \varepsilon_{n_x n_y n_z}} \\ &= \sum_{n_x=1}^{\infty} \exp\left(-\frac{\beta h^2 n_x^2}{8ma^2}\right) \sum_{n_y=1}^{\infty} \exp\left(-\frac{\beta h^2 n_y^2}{8ma^2}\right) \sum_{n_z=1}^{\infty} \exp\left(-\frac{\beta h^2 n_z^2}{8ma^2}\right) \end{aligned}$$

3. Apply box symmetry (cube the equation).

$$= \left[\sum_{n=1}^{\infty} \exp\left(-\frac{\beta h^2 n^2}{8ma^2}\right) \right]^3$$

4. Approximate with integral, since successive terms are very close to each other:

$$= \left[\int_0^{\infty} \exp\left(-\frac{\beta h^2 n^2}{8ma^2}\right) dn \right]^3$$

5. Use Gaussian integral property, and also replace $V=a^3$.

$$= \left(\frac{2\pi mkT}{h^2} \right)^{\frac{3}{2}} V$$

Diatomic Ideal Gas (vibrational)

Page 96

1. Start with energies for **harmonic oscillator**:

$$\varepsilon = \left(n + \frac{1}{2}\right) h\nu \quad n = 0, 1, 2, \dots$$

2. Insert into general form of canonical partition function:

$$q_{vib} = \sum_{n=0}^{\infty} e^{-\beta\varepsilon_n} = \sum_{n=0}^{\infty} e^{-\beta\left(n+\frac{1}{2}\right)h\nu}$$

3. Separate the $\frac{1}{2}$ term out.

$$= e^{-\beta\frac{1}{2}h\nu} \sum_{n=0}^{\infty} e^{-\beta nh\nu}$$

4. Recognize that the second term (summation) is a geometric series:

$$= \frac{e^{-\beta\frac{1}{2}h\nu}}{1 - e^{-\beta h\nu}}$$

5. (opt.) At very high temperatures, go from step 3, replace with integral, and use exponential integral:

$$= e^{-\frac{\beta h\nu}{2}} \int_0^{\infty} e^{-\beta nh\nu} dn = \frac{kT}{h\nu}$$

Diatomic Ideal Gas (rotational)

Page 99

1. Start with energies and degeneracies(!!) for **rigid rotor**:

$$\varepsilon = \frac{\hbar^2 J(J+1)}{2I} \quad J = 0, 1, 2, \dots$$

$$\omega = 2J + 1$$

2. Insert into general form of canonical partition function:
(don't forget to multiply each energy by its degeneracy!!)

$$q_{vib} = \sum_{J=0}^{\infty} (2J+1) e^{-\beta \frac{\hbar^2 J(J+1)}{2I}}$$

3. (opt.) Introduce rotational temperature: $\Theta_{rot} = \frac{\hbar^2}{2Ik}$

$$q_{vib} = \sum_{J=0}^{\infty} (2J+1) e^{-\Theta_{rot} J(J+1)/T}$$

4. (opt.) At very high temperatures, replace sum with integral, and use exponential integral.

Polyatomic Ideal Gas (rotational, symmetric top)

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Note: For a *spherical* top, follow the same algorithm: (1) get energy, (2) insert into partition function; don't forget to multiply by exponential, (3) convert to integral. Approximation for integral is to neglect 1 in comparison to J.

1. Start with energies and degeneracies(!!) for symmetric top (**rigid rotor**):

$$\varepsilon = \frac{\hbar^2}{2} \left\{ \frac{J(J+1)}{I_A} + K^2 \left(\frac{1}{I_c} - \frac{1}{I_A} \right) \right\} \quad J = 0, 1, 2, \dots \quad K = -J, \dots, J$$

$$\omega = 2J + 1$$

2. Insert into general form of canonical partition function:
(don't forget to multiply each energy by its degeneracy!!)

$$q_{vib} = \frac{1}{\sigma} \sum_{J=0}^{\infty} (2J+1) e^{-\alpha_A J(J+1)} \sum_{K=-J}^{+J} e^{-(\alpha_c - \alpha_A) K^2}$$

3. Convert sum to double integral over J and K.
4. Use high temperature approximation to neglect 1 in degeneracy and J term in exponential.
5. Switch order of integration from dK dJ to dJ dK. Don't forget to switch limits of integrand!
6. Use M-substitution, $M=J^2$, $dM = 2J dJ$.
7. Integrate the K part. Will need to break up into one term from 0 to inf, subtract term from 0 to K^2 .
8. Simplify (one part of K integral cancels the alpha-K). Integrate the J part.