Review of some basic concepts for enjoying and getting most out of B6

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1 Mathematical tools

1.1 Analysis

- basic definitions: relation, map, function, operator, functional, domain, range, maximum, minimum, limit
- derivative and primitive function (knowing the derivatives of simple analytical functions - polynomials, exponential, trigonometric functions)
- definite integral (limit of a sum)
- differentiation of products of functions, functions of functions (chain rule)
- linearisation and Taylor expansion
- gradient
- integration by parts, variable substitution
- coordinate transformation
- 2D integration

1.2 Numerical computation

- least squares
- interpolation of data (Lagrange polynomial, spline)
- numerical differentiation and integration

- finding the roots of systems of algebraic equations (linear and non-linear)
- unconstrained optimisation
- matrix diagonalisation, condition number
- initial value problem (Euler propagator)

1.3 Statistics

- random variable, probability density, distribution
- discrete vs continuous distribution
- characteristic values of distributions - mean value, median, standard deviation
- binomial, poisson, uniform, exponential, normal, log-normal distributions
- independence and correlation
- central limit theorem

1.4 Miscellaneous

- geometric series, infinite sums
- binomial formula
- constrained optimisation - Lagrange multipliers
- Stirling formula
- Laplace (Gaussian) integral
- dimensional analysis
- scalar, vector field
- Gauss law

1.5 Software proficiency

- something for analytical derivations (Mathematica / Maple / Maxima)
- something for numerical work (MATLAB / Octave / FORTRAN / C / C++ / python)

2 Physics and physical chemistry

2.1 Classical mechanics

- classical equations of motion
  - Newton
  - Hamiltonian
  - Lagrange
- harmonic oscillator, normal modes
- rigid rotator
- moment of inertia, angular momentum

2.2 Phenomenological thermodynamics

- state function, intensive, extensive quantity
- heat and work
- Laws of thermodynamics
- Legendre transformation and the 4 potentials
- Maxwell relations
- Equation of state (EOS), corresponding state theorem
- EOS for gases, solids, liquids
- condition for equilibrium
- irreversible processes - phenomenological description
- chemical potential
- ideal solution
- phase diagram, Gibbs phase law

2.3 Molecular forces

- Coulombic interaction (interaction between point charges and/or multipoles)
- Madelung constant
- Born equation
- dispersion forces
- Pauli exclusion principle
- Buckingham potential, Lennard-Jones potential
- Baeyer, Pitzer, van der Waals strain

2.4 Physical kinetics

- Maxwell-Boltzmann distribution
- virial theorem
- thermodynamic temperature, pressure
- equipartition principle
- continuity equation, Fick's law
- rate equations for chemical reactions