

Name: _____

Student Number: _____

PHY294 Quantum and Thermal Physics

University of Toronto

Faculty of Applied Science and Engineering

April 28, 2023

Duration: 150min

Number of pages: 22

Question	Maximum	Marks
1	20	
2	20	
3	10	
4	25	
5	25	
6	25	
7	25	
Total	150	

Answer all questions on the question paper in the space provided.

Write legibly with a pen or pencil.

Do not separate pages

Exam Type: B, Calculator Type: 2

No aids are allowed except for a non-programable and non-communicating calculator.

Questions 1-4 on pages 2-10 relate to the Quantum Physics half of the course.

Questions 5-7 on pages 11-16 relate to the Thermal Physics half of the course.

Pages 17 and 18 may be used if you run out of space for certain questions. If these are used you must indicate that you are continuing your answer somewhere else in the space left for each question.

Formula sheets for the Quantum and Thermal portions of the course can be found on pages 19-22.

1. (20 pts). Brief explanations.

a) (5 pts) What is the selection rule for the absorption of light for electronic transitions (exciting electrons to upper electronic levels) for multi-electron atoms with respect to symmetry and spin?

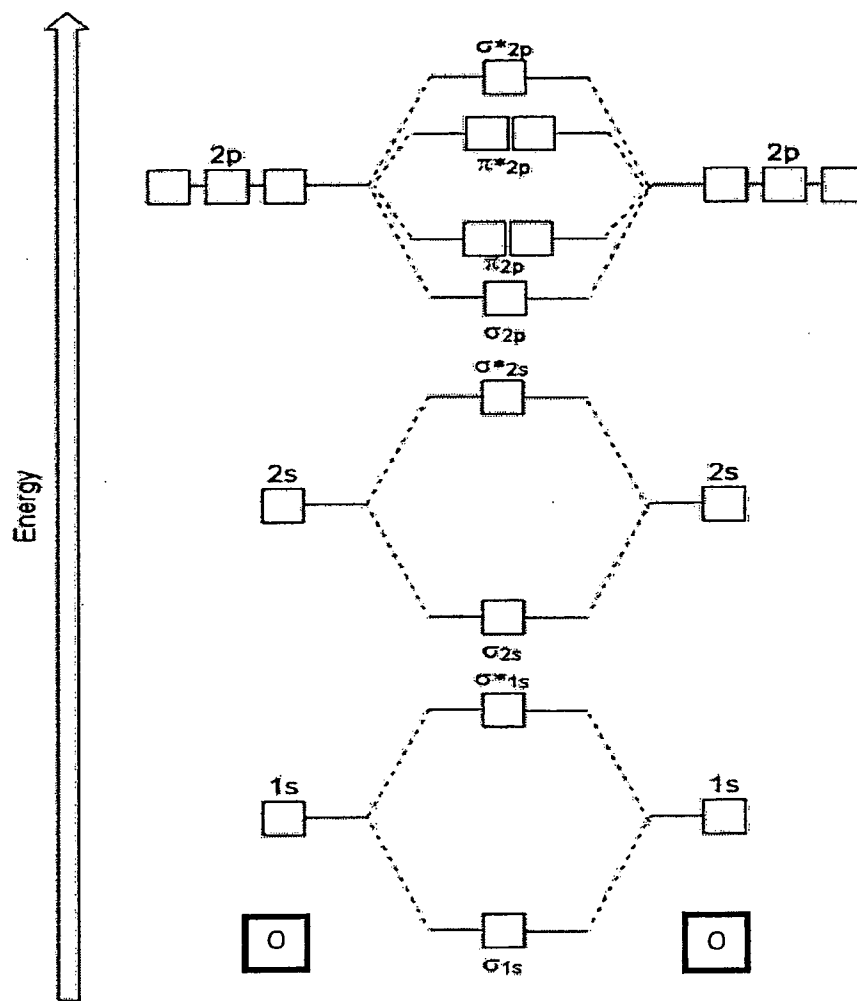
b) (5pts) Explain the Pauli Exclusion Principle and the need for antisymmetric wavefunctions to describe multielectron atoms or molecules.

c) (5 pts) Describe hydrogen bonding in water specifically discussing the structure of water (valence orbital hybridization) and number of hydrogen bonds in ice and liquid water.

d) (5pts) Franck-Condon Factors determine the transition probability for the absorption of light involving vibrational levels between different electronic states (eg. S_0 and S_1). Write down the equation for the transition probability including Franck-Condon factors. Briefly explain how the nuclear probability distribution weights the transition probability for the absorption of light.

2. (20 pts)

a) (5 pts) Using the molecular orbital diagram below (LCAO-MO) and the Pauli Exclusion Principle, assign electron configurations from valence orbitals to molecular orbitals for O_2 .



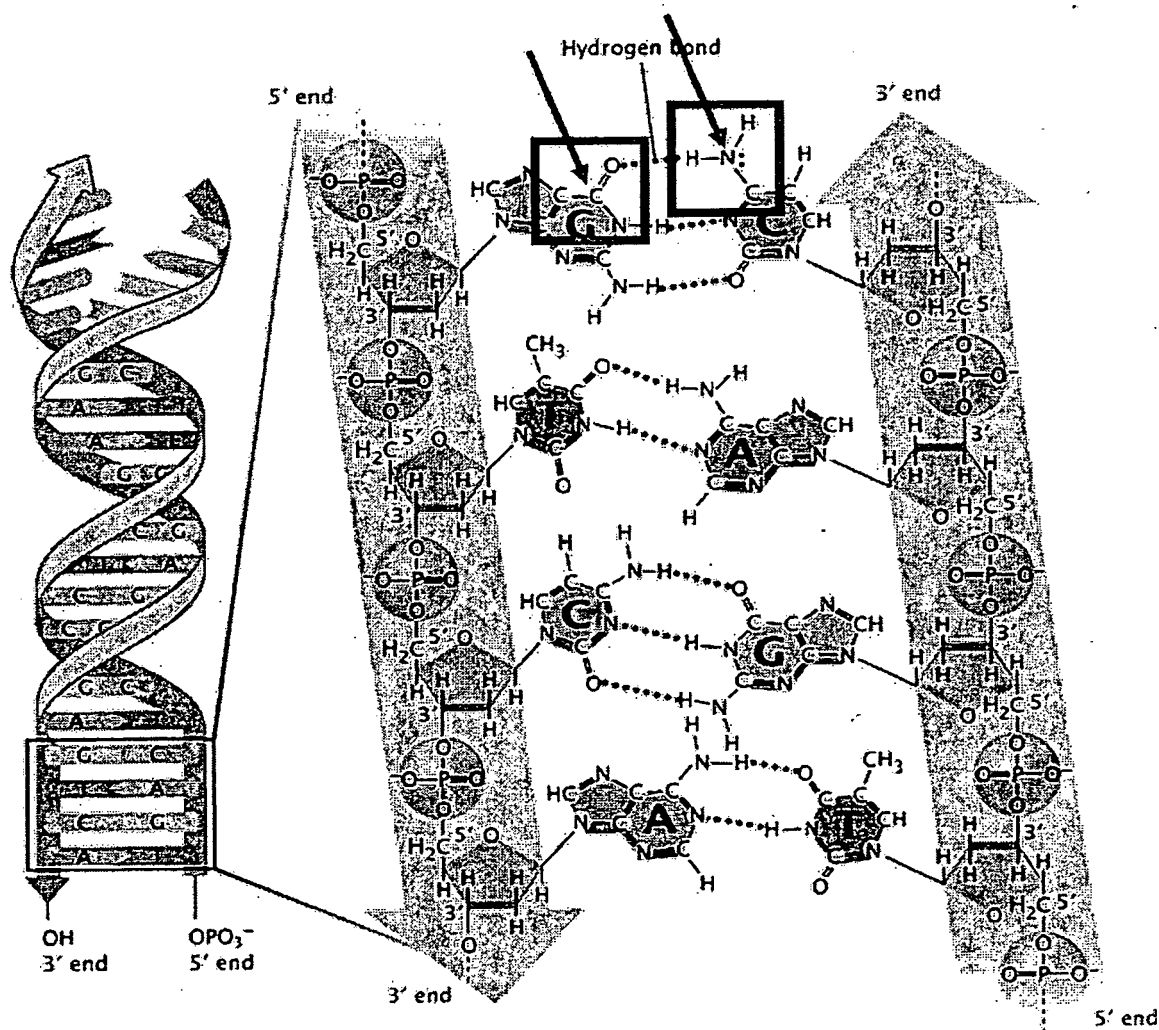
b) (5 pt) What is the bond order of O_2 and O_2^+ ? Which species is paramagnetic?

c) (5pts) The heteronuclear diatomic molecule NO is an important cardiovascular molecule that increases blood flow and is involved in cell signaling. Repeat the above assignment of electron configurations for the molecule NO. Redraw below the above molecular orbital energy level diagram (problem 2a), $n=2$ valence shell suffices. Show explicitly the relative energy ordering for valence orbitals for N relative to O in terms of contributions to the molecular orbitals.

d) (5 pts) Which molecules have IR active modes for O_2 , O_2^+ and NO? Brief explanation.

3. (10 pts)

a) (5 pts) Referring to the figure below for double stranded DNA, state the valence orbital hybridization and geometry (bond angles) around the C atom and N atom involved in the G=C hydrogen bonding. The central atoms in question are indicated by arrows in the figure below.



b) (5 pts) Levinthal's paradox refers to the enormous number of nuclear configurations associated with protein structure and search process to spontaneously find the active biological structure. The protein folding problem involves the collapse of a hydrophobic core to guide protein structure. DNA has even more nuclear degrees of freedom yet forms a double helix with virtually no error based on complementary nucleotide base sequences. It is so robust that it is possible to "program" DNA by base sequence to have the double helix twist and turn into specific shapes called DNA origami. Note, the interior of DNA is not completely hydrophobic. Discuss how DNA finds its double helix structure using the funnel model and identify the various forces that define the gradient directing the system to the double helix structure. (List all the forces involved in forming the DNA double helix.)

4. (25 pts)

a) (5pts) Write down the Schroedinger equation for the Harmonic Oscillator.

b) (5pts) What are the boundary conditions to solve this differential equation.

c) (5pts) The wavefunction solutions involve a series solution, i.e.,

$$\psi_n(x) = N_n e^{-\beta^2 x^2 / 2} H_n(\beta x), \quad n = 0, 1, 2, 3, \dots \quad \text{with } E = (n + \frac{1}{2})h\nu, \text{ where:}$$

$$H_0(y) = 1$$

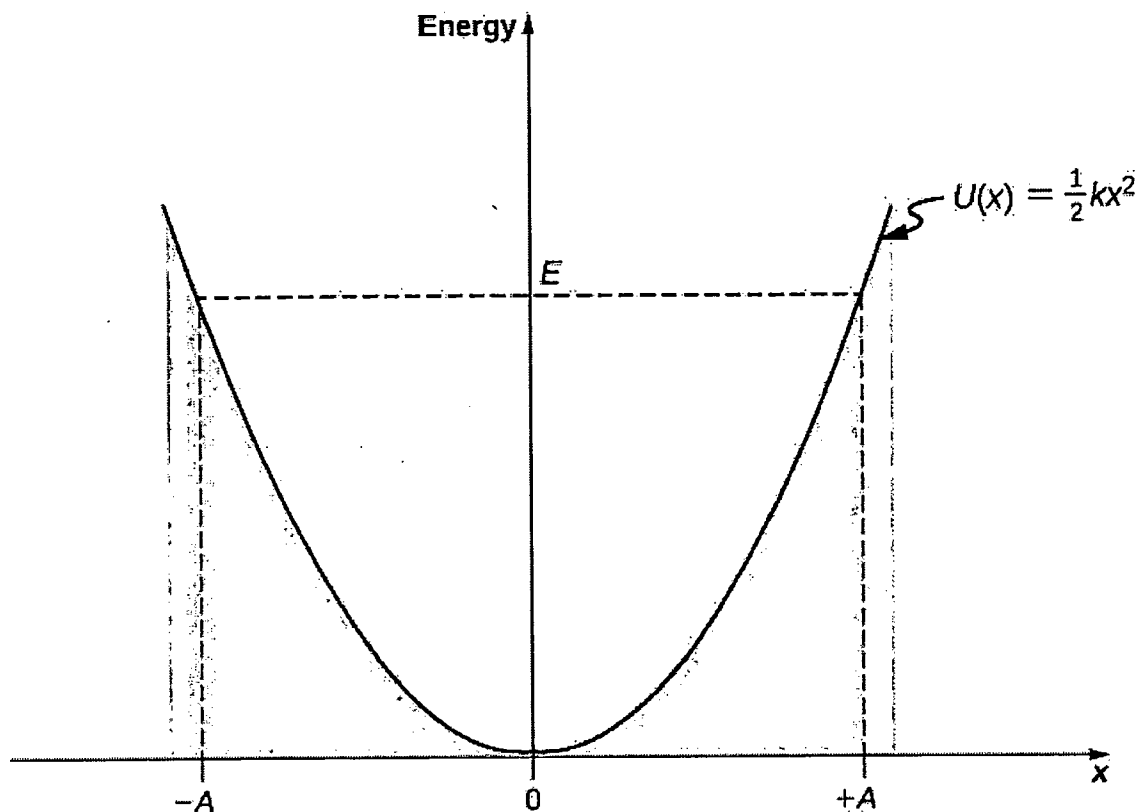
$$H_1(y) = 2y \quad \text{with } y = \beta x \text{ and } \beta = \left(\frac{mv}{h}\right)^{1/2}$$

$$H_2(y) = 4y^2 - 2$$

$$H_3(y) = 8y^3 - 12y.$$

Using the above functions, write the mathematical description of the probability distribution for the zero point energy solution.

d) (5pts) Draw the probability distributions for the first 4 vibrational levels in the potential below. Clearly show the region related to the tunneling probability for a given reduced mass (shade the relevant area).



e) (5pts) Derive an expression to determine the overall tunneling probability for a given reduced mass μ and force constant k . (Hint: Derive an expression for the classical turning points where the energy is all potential energy.) You do not have to evaluate the integrals, just show the proper limits.

4. e) cont.

5. (25 pts)

Answer the following questions qualitatively. (No long-winded expressions and derivations!)

a) (7 pts) Why don't we have to take into account the structure of the nucleus when considering the partition function (or, in general, the thermodynamics) at room temperature of, say, a hydrogen gas? How about the (supposed) string-like structure of the electrons, of the quarks inside the proton, etc.?

b) (4 pts) For a monatomic ideal gas of atoms of mass m , of number density $n = N/V$, at what temperature T_c do you expect the $C_V = \frac{3}{2}kN$ law (C_V is the constant-volume heat capacity) to break down? Answer the question parametrically, i.e. find the dependence of T_c on n , m , and on any fundamental constants that might be involved, neglecting numerical factors.

c) (8 pts) Does thermodynamic stability require that C_V be positive or negative? How about $\left(\frac{\partial p}{\partial V}\right)_{T,N}$, a quantity proportional to the “bulk modulus” (a measure of the material's stiffness)? Explain qualitatively why.

d) (6 pts) Much of the material of this class used the “Einstein solid,” a collection of N simple harmonic oscillators of frequency ω , as one of the toy models of statistical mechanics. One reason for this system's domination of the course is because it is fairly easy to study. Do you think the study of the thermodynamics of the Einstein solid is relevant for real physical systems? How about the study of several Einstein solids (say with different frequencies) in thermal equilibrium? Enumerate as many examples as you can possibly think of (only a qualitative discussion of their relevance is needed!).

6. (25 pts)

Consider a two-dimensional gas of point-like particles of mass m at temperature T (recall that a computer simulation of a two-dimensional gas of billiard balls, shown in the first and last thermal physics classes, was used to motivate much of the material in this course!). Here, you shall consider any one particle of the gas as the “system” coupled to the “thermal reservoir” of the rest of the particles of the gas.

a) (20 pts) Use the Boltzmann distribution to find the probability density $P(v)$, defined such that $P(v)dv$ is the probability that the particle’s speed is in the infinitesimal interval $(v, v + dv)$. What is the most likely speed of the particle? Normalize the probability distribution and use it to compute the average kinetic energy $\frac{mv^2}{2}$ of the particle. Did you find an answer you expect? Explain. (Various integrals you can use are given in the formula sheet.)

b) (5 pts) Apart from computer simulations (a numerical “experiment”), do you know of ways to measure the speed distributions of particles in a gas (in three dimensions) in a real experiment?

7. (25 pts)

Consider an Einstein solid of N oscillators of frequency ω . Recall that we take (setting the “zero-point” energy to zero) the energy levels of a single oscillator to equal $\hbar\omega$ times the number of quanta excited. We studied the Einstein solid using the canonical distribution and found the partition function of a single oscillator, $Z_1 = \frac{1}{1 - e^{-\beta\hbar\omega}}$, using $\beta = \frac{1}{kT}$. We also studied the Einstein solid using the microcanonical distribution, where we determined its multiplicity function $\Omega(N, q)$ (q is the total number of quanta excited in the entire solid). When N and q are both large, in the $q \gg N$ limit, the multiplicity function was found to be $\Omega_{high}(q, N) \approx \left(\frac{qe}{N}\right)^N$.

a) (12 pts) Use the single-oscillator partition function Z_1 to find the entropy of the gas as a function of the temperature, $S = S(T, N)$. The expression you find may look daunting at first, but don't despair: in what follows, it is sufficient to consider the expression for the entropy only in the high-temperature limit. Thus, you may want to simplify S assuming $kT \gg \hbar\omega$.

b) (7 pts) Now use the multiplicity function Ω_{high} to find the entropy as a function of the energy, i.e. $S(E, N)$, in the $q \gg N$ limit. Use the statistical definition of the temperature to express the entropy as a function of T in this limit.

c) (6 pts) Compare the result of part b. with the expression obtained from the partition function (part a. above). Are you surprised? Do you have a comment on the result? Do you find one calculation easier than the other?

Additional space for answers. If using this space clearly indicate which question your work corresponds to.

Additional space for answers. If using this space clearly indicate which question your work corresponds to.

Equations for Quantum Mechanics Part	Comment
$E = h\nu$	Photon energy
$E_n = -\frac{m_e Z^2 e^4}{8h^2 \epsilon_0^2} \frac{1}{n^2} = -Z^2 E_R / n^2$; $E_R = 13.6 \text{ eV}$	Energy of hydrogen ($Z=1$) and Hydrogen like atom with atomic number Z
$h\nu = \Phi + \frac{1}{2} m_e v^2$	Einstein Photoemission relation
$\Delta E = E_f - E_i = h\nu$	Photon transitions between quantized levels
$\psi_n(x) = N_n e^{-\beta^2 x^2 / 2} H_n(\beta x)$, $n = 0, 1, 2, 3, \dots$	QM Harmonic Oscillator wave functions
$E = \frac{1}{2} m v^2$	Kinetic energy
$U = \frac{1}{2} k x^2$	Potential energy for harmonic oscillator
$\Delta x \Delta p \geq \frac{h}{4\pi}$	Uncertainty Principle in momentum/position
$F(\nu) = (8\pi \nu^3 / c^3) h\nu / (e^{h\nu/kT} - 1)$	Blackbody emission/spectral density
$U = -Z_{\text{eff}} k e^2 / r$ where $Z_{\text{eff}} \rightarrow Z$ as $r \rightarrow 0$ and $Z_{\text{eff}} \rightarrow 1$ as $r \rightarrow \infty$	IPA potential, extrapolation of limits in Z_{eff} from Gauss's law
$E = (n + \frac{1}{2}) h\nu$; $n = 0, 1, 2, 3, \dots$ $\nu = \frac{1}{2\pi} \sqrt{\frac{k}{\mu_{AB}}}$ $\mu_{AB} = \frac{m_A m_B}{m_A + m_B}$	Quantum Harmonic Oscillator Energies, resonant frequency, and reduced mass
$\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} = \frac{2M}{\hbar^2} [U - E] \psi$	Three Dimensional Schroedinger equation for a single particle of mass M .
$\Delta E \Delta t \geq \frac{h}{4\pi}$	Uncertainty Relation for time/energy
$f = Ze^2 / 4\pi \epsilon_0 r^2 = ke^2 / r^2$; $U = -Zke^2 / r$	Coulomb force for charge Z protons and 1 e; Coulomb potential energy for Z protons and 1 electron
$\lambda = \frac{h}{mv} = \frac{h}{p}$	De Broglie relation
$\mu_{mn} = \{ \int \psi_m \mu \psi_n d\tau_e \} \{ \int \psi_m(v) \psi_n(v') d\tau_v \}$	Molecular Electronic Transition Probability weighted by Franck Condon Factors
$\mu_{mn} = \int \psi_n \mu \psi_m d\tau$;	Transition Probability for absorption of light.
$-(\hbar^2 / 8\pi^2 m) d^2/dx^2 (\psi) = E\psi$; $U(x) = 0$; $0 < x < L$; $U(x) = \infty$ for $x < 0$ or $x > L$	Schroedinger eq. for 1D Box
$\psi = (2/L)^{1/2} \sin(n\pi/L)x$; $E = n^2 \hbar^2 / 8mL^2$	Solutions to 1D Particle in the Box
$U = -Zke^2 / r$; $U = +ke^2 / r$	Attractive potential of nucleus; repulsive e-e
$\Delta E = m \mu_B B$; $m = 0, 1, \dots, \pm l$	Zeeman (mag. field B) effect re: Orbital angular momentum
$\Delta E = \pm \frac{e\hbar}{2m_e} B = \pm \mu_B B$	Zeeman effect (B) re: spin magnetic moment
$L = \sqrt{l(l+1)} \hbar$; $S = \sqrt{s(s+1)} \hbar$	Quantized orbital angular; spin momentum $l = 0, 1, 2, 3, \dots$; $m_s = \pm \frac{1}{2}$; $L_z = m \hbar$ and $S_z = m_s \hbar$
Bond order = (number of bonding e – Antibonding e)/2	Using Pauli Exclusion Principle to determine number of bonds from MO e configurations

Named Constants

Atomic mass unit:	$1u = \frac{1}{12} m(^{12}\text{C atom})$ $= 1.66 \times 10^{-27} \text{ kg}$ $= 931.5 \text{ MeV}/c^2$
Avogadro's constant:	$N_A = 6.02 \times 10^{23} \text{ particles/mole}$
Bohr magneton:	$\mu_B = e\hbar/(2m_e)$ $= 5.79 \times 10^{-5} \text{ eV/T}$ $= 9.27 \times 10^{-24} \text{ J/T (or A} \cdot \text{m}^2)$
Bohr radius:	$a_B = \hbar^2/(k e^2 m_e)$ $= 5.29 \times 10^{-11} \text{ m}$
Boltzmann's constant:	$k_B = 8.62 \times 10^{-5} \text{ eV/K}$ $= 1.38 \times 10^{-23} \text{ J/K}$
Coulomb force constant:	$k = 1/(4\pi\epsilon_0) = \mu_0 c^2/(4\pi)$ $= 8.99 \times 10^9 \text{ N} \cdot \text{m}^2/\text{C}^2$
Electron Compton wavelength:	$\lambda_c = h/(m_e c)$ $= 2.43 \times 10^{-12} \text{ m}$
Electron volt:	$1 \text{ eV} = 1.60 \times 10^{-19} \text{ J}$
Elementary charge:	$e = 1.60 \times 10^{-19} \text{ C}$
Fine-structure constant:	$\alpha = k e^2/(\hbar c)$ $= 7.30 \times 10^{-3} \approx 1/137$
Gas constant:	$R = 8.31 \text{ J/(mole} \cdot \text{K)}$ $= 0.0821 \text{ liter} \cdot \text{atm/(mole} \cdot \text{K)}$
Gravitational constant:	$G = 6.67 \times 10^{-11} \text{ N} \cdot \text{m}^2/\text{kg}^2$
Mass of electron:	$m_e = 5.49 \times 10^{-4} u$ $= 9.11 \times 10^{-31} \text{ kg}$ $= 0.511 \text{ MeV}/c^2$
Mass of proton:	$m_p = 1.007 u$ $= 1.673 \times 10^{-27} \text{ kg}$ $= 938.3 \text{ MeV}/c^2$
Mass of neutron:	$m_n = 1.009 u$ $= 1.675 \times 10^{-27} \text{ kg}$ $= 939.6 \text{ MeV}/c^2$
Nuclear magneton:	$\mu_N = e\hbar/(2m_p)$ $= 3.15 \times 10^{-8} \text{ eV/T}$ $= 5.05 \times 10^{-27} \text{ J/T}$
Permeability of space:	$\mu_0 = 4\pi \times 10^{-7} \text{ N/A}^2$ $= 1.26 \times 10^{-6} \text{ N/A}^2$
Permittivity of space:	$\epsilon_0 = 1/(\mu_0 c^2)$ $= 8.85 \times 10^{-12} \text{ C}^2/(\text{N} \cdot \text{m}^2)$

Planck's constants:	$h = 6.63 \times 10^{-34} \text{ J} \cdot \text{s}$ $= 4.14 \times 10^{-15} \text{ eV} \cdot \text{s}$ $\hbar = h/2\pi$ $= 1.05 \times 10^{-34} \text{ J} \cdot \text{s}$ $= 6.58 \times 10^{-16} \text{ eV} \cdot \text{s}$
Rydberg constant:	$R = m_e k^2 e^4 / (4\pi\hbar^3)$ $= 1.10 \times 10^{-2} \text{ nm}^{-1}$
Rydberg energy:	$E_R = \hbar c R = m_e k^2 e^4 / (2\hbar^2)$ $= 13.6 \text{ eV}$
Speed of light:	$c = 3.00 \times 10^8 \text{ m/s}$

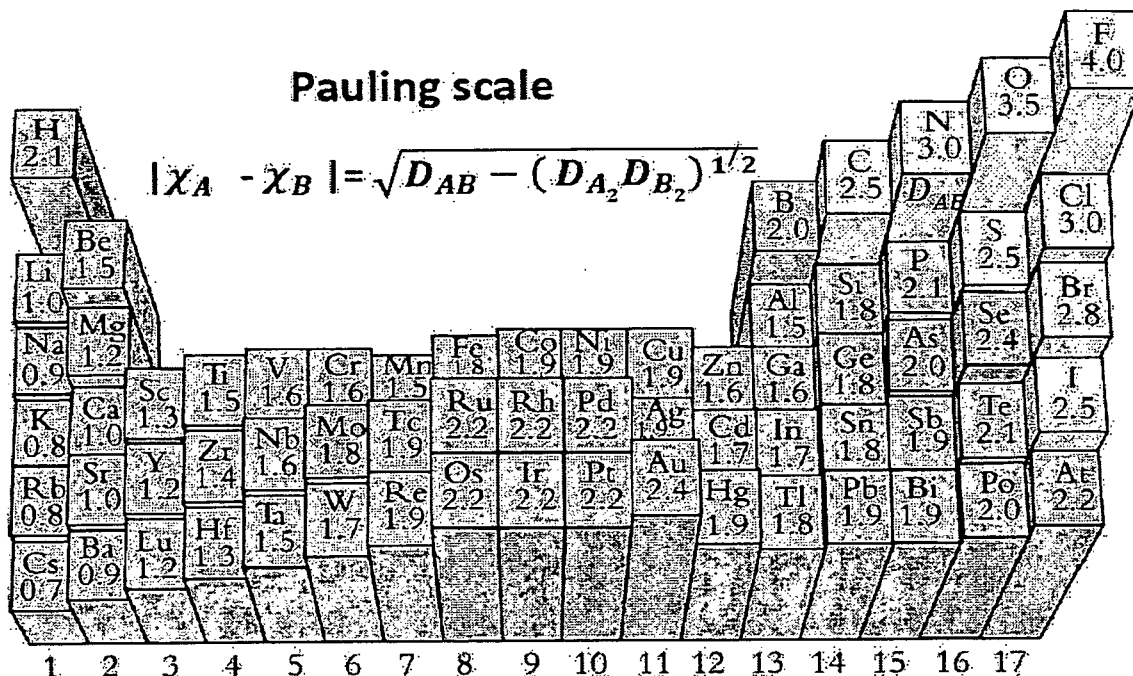
Useful Combinations

$\hbar c = 1240 \text{ eV} \cdot \text{nm} = 1240 \text{ MeV} \cdot \text{fm}$
$\hbar c = 197 \text{ eV} \cdot \text{nm} = 197 \text{ MeV} \cdot \text{fm}$
$k e^2 = 1.44 \text{ eV} \cdot \text{nm} = 1.44 \text{ MeV} \cdot \text{fm}$
$N_A \times (1 u) = 1 \text{ gram}$
$k_B T = 0.0252 \text{ eV}$ at room temperature (293-K)

Conversion Factors

Area:	$1 \text{ barn} = 10^{-28} \text{ m}^2$
Energy:	$1 \text{ cal} = 4.184 \text{ J}$ $1 \text{ eV} = 1.60 \times 10^{-19} \text{ J}$
Length:	$1 \text{ Å} = 1 \text{ angstrom}$ $= 10^{-10} \text{ m}$ $1 \text{ ft} = 30.48 \text{ cm}$ $1 \text{ in} = 2.54 \text{ cm}$ $1 \text{ mi} = 1609 \text{ m}$
Mass:	$1 \text{ lb (mass)} = 0.454 \text{ kg}$ $1 \text{ MeV}/c^2 = 1.074 \times 10^{-3} u$ $= 1.783 \times 10^{-30} \text{ kg}$ $1 u = \frac{1}{12} m(^{12}\text{C atom})$ $= 931.5 \text{ MeV}/c^2$ $= 1.66 \times 10^{-27} \text{ kg}$
Momentum:	$1 \text{ MeV}/c = 5.34 \times 10^{-22} \text{ kg} \cdot \text{m/s}$

Periodic Table: Electronegativities



Periodic table of the elements

period	group																		18
	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17		
1	<div><div></div><div>H</div></div>																	2	
2	<div><div></div><div>Li</div></div>	<div><div></div><div>Be</div></div>											<div><div></div><div>B</div></div>	<div><div></div><div>C</div></div>	<div><div></div><div>N</div></div>	<div><div></div><div>O</div></div>	<div><div></div><div>F</div></div>	10	
3	<div><div></div><div>Na</div></div>	<div><div></div><div>Mg</div></div>											<div><div></div><div>Al</div></div>	<div><div></div><div>Si</div></div>	<div><div></div><div>P</div></div>	<div><div></div><div>S</div></div>	<div><div></div><div>Cl</div></div>	18	
4	<div><div></div><div>K</div></div>	<div><div></div><div>Ca</div></div>	<div><div></div><div>Sc</div></div>	<div><div></div><div>Ti</div></div>	<div><div></div><div>V</div></div>	<div><div></div><div>Cr</div></div>	<div><div></div><div>Mn</div></div>	<div><div></div><div>Fe</div></div>	<div><div></div><div>Co</div></div>	<div><div></div><div>Ni</div></div>	<div><div></div><div>Cu</div></div>	<div><div></div><div>Zn</div></div>	<div><div></div><div>Ga</div></div>	<div><div></div><div>Ge</div></div>	<div><div></div><div>As</div></div>	<div><div></div><div>Se</div></div>	<div><div></div><div>Br</div></div>	36	
5	<div><div></div><div>Rb</div></div>	<div><div></div><div>Sr</div></div>	<div><div></div><div>Y</div></div>	<div><div></div><div>Zr</div></div>	<div><div></div><div>Nb</div></div>	<div><div></div><div>Mo</div></div>	<div><div></div><div>Tc</div></div>	<div><div></div><div>Ru</div></div>	<div><div></div><div>Rh</div></div>	<div><div></div><div>Pd</div></div>	<div><div></div><div>Ag</div></div>	<div><div></div><div>Cd</div></div>	<div><div></div><div>In</div></div>	<div><div></div><div>Sn</div></div>	<div><div></div><div>Sb</div></div>	<div><div></div><div>Te</div></div>	<div><div></div><div>I</div></div>	54	
6	<div><div></div><div>Cs</div></div>	<div><div></div><div>Ba</div></div>	<div><div></div><div>La</div></div>	<div><div></div><div>Hf</div></div>	<div><div></div><div>Ta</div></div>	<div><div></div><div>W</div></div>	<div><div></div><div>Re</div></div>	<div><div></div><div>Os</div></div>	<div><div></div><div>Ir</div></div>	<div><div></div><div>Pt</div></div>	<div><div></div><div>Au</div></div>	<div><div></div><div>Hg</div></div>	<div><div></div><div>Tl</div></div>	<div><div></div><div>Pb</div></div>	<div><div></div><div>Bi</div></div>	<div><div></div><div>Po</div></div>	<div><div></div><div>At</div></div>	86	
7	<div><div></div><div>Fr</div></div>	<div><div></div><div>Ra</div></div>	<div><div></div><div>Ac</div></div>	<div><div></div><div>Rf</div></div>	<div><div></div><div>Db</div></div>	<div><div></div><div>Sg</div></div>	<div><div></div><div>Bh</div></div>	<div><div></div><div>Hs</div></div>	<div><div></div><div>Mt</div></div>	<div><div></div><div>Ds</div></div>	<div><div></div><div>Rg</div></div>	<div><div></div><div>Cn</div></div>	<div><div></div><div>Nh</div></div>	<div><div></div><div>Fl</div></div>	<div><div></div><div>Mc</div></div>	<div><div></div><div>Lv</div></div>	<div><div></div><div>Ts</div></div>	118	
<div> <div>lanthanoid series 6</div> <div>actinoid series 7</div> </div>																			<div> <div>58</div><div>Ce</div> <div>59</div><div>Pr</div> <div>60</div><div>Nd</div> <div>61</div><div>Pm</div> <div>62</div><div>Sm</div> <div>63</div><div>Eu</div> <div>64</div><div>Gd</div> <div>65</div><div>Tb</div> <div>66</div><div>Dy</div> <div>67</div><div>Ho</div> <div>68</div><div>Er</div> <div>69</div><div>Tm</div> <div>70</div><div>Yb</div> <div>71</div><div>Lu</div> </div> <div> <div>90</div><div>Th</div> <div>91</div><div>Pa</div> <div>92</div><div>U</div> <div>93</div><div>Np</div> <div>94</div><div>Pu</div> <div>95</div><div>Am</div> <div>96</div><div>Cm</div> <div>97</div><div>Bk</div> <div>98</div><div>Cf</div> <div>99</div><div>Es</div> <div>100</div><div>Fm</div> <div>101</div><div>Md</div> <div>102</div><div>No</div> <div>103</div><div>Lr</div> </div>

Alkali metals

Alkaline-earth metals

Transition metals

Other metals

Other nonmetals

Halogens

Noble gases

Rare-earth elements (21, 39, 57-71) and lanthanoid elements (57-71) only

Actinoid elements

*Numbering system adopted by the International Union of Pure and Applied Chemistry (IUPAC).

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The ideal gas law is $pV = NkT$. The energy of a single-atomic classical ideal gas of N atoms is $U = \frac{3}{2}NkT$. The work done by the gas in a quasistatic process along some curve $p(V)$ in the $p - V$ plane is $W = \int_{V_1}^{V_2} p(V)dV$. The thermal de Broglie wavelength of a particle of mass m at temperature T is $\lambda_{th} \sim \frac{h}{\sqrt{mkT}}$. The ratio between the thermal de Broglie wavelength and the typical distance between particles in the gas (as determined by the number density of the gas) determines, roughly, under what conditions a gas can be considered classical and obeying the ideal gas law. The energy levels of an oscillator, ignoring the zero-point energy, are $\hbar\omega n$, where $n \geq 0$ is the (integer) number of quanta. The first law of TD expresses energy conservation: the energy of a system of fixed number of particles can change because of the heat transfer and work performed.

The microcanonical distribution (for an (E, V, N) -system) states that all accessible microstates are equally likely. The TD potential is the entropy, $S = k \ln \Omega(E, V, N)$, where Ω is the multiplicity function. The TD identity $dS = \frac{1}{T}dE + \frac{p}{T}dV - \frac{\mu}{N}dN$ can be used to determine the temperature, pressure and chemical potential as partial derivatives of S .

The canonical distribution (for a (T, V, N) system), upon denoting $\beta = \frac{1}{kT}$, is: $P(\text{microstate}) = Z^{-1}e^{-\beta E_{\text{microstate}}}$, where Z is the Boltzmann partition function $Z = \sum_{\text{microstates}} e^{-\beta E_{\text{microstate}}}$. The TD potential is the free energy $F = E - TS$. The partition function determines F : $F = -\frac{1}{\beta} \log Z(T, V, N)$. The average energy of a system is $E = -\frac{\partial}{\partial \beta} \ln Z$. The TD identity is $dF = -SdT - pdV + \mu dN$.

Nuclear energy excitations are measured in eV and are typically of order GeV , or $10^9 eV$, where $1eV \sim 10^{-19} J$. The “fundamental string” (of the putative “theory of everything”) presumably has a characteristic scale of excitations $10^{19} GeV$. The Boltzmann constant is $k \sim 10^{-23} J/K$.

Some useful mathematical expressions are:

$\frac{d \ln x}{dx} = \frac{1}{x}$, $\ln x^a = a \ln x$, $\ln e = 1$, $e^{\ln x} = x$, $\frac{d e^{a(x)}}{dx} = e^{a(x)} \frac{da(x)}{dx}$, $\frac{dx^k}{dx} = kx^{k-1}$. The function $e^{-\frac{1}{x}} \rightarrow 0$ as $x \rightarrow 0$ and is positive for $x > 0$ (also $\frac{d^n e^{-\frac{1}{x}}}{dx^n} \big|_{x \rightarrow 0} = 0$, for all $n > 0$). As $x \rightarrow 0$, $e^{-x} \simeq 1 - x + \frac{x^2}{2}$.

Various Gaussian integrals are as follows:

$$\int_0^\infty dx e^{-ax^2} = \frac{\sqrt{\pi}}{2a^{\frac{1}{2}}}, \quad \int_0^\infty dx x e^{-ax^2} = \frac{1}{2a}, \quad \int_0^\infty dx x^2 e^{-ax^2} = \frac{\sqrt{\pi}}{4a^{\frac{3}{2}}}, \quad \int_0^\infty dx x^3 e^{-ax^2} = \frac{1}{2a^2}$$