Condensed Matter Theory (MP473) — Assignment 1

Please hand in your solutions no later than Tuesday, February 18. If you have questions about this assignment, please ask your lecturer,

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Ex. 1.1: Aufbau & Hund: magnetism of atoms

Periodic Table of the Elements

1 IA	2 IIA	3 IIIB	4 IVB	5 VB	6 VIB	7 VIIB	8 VIII	9 VIII	10 VIII	11 IB	12 IIB	13 IIIA	14 IVA	15 VA	16 VIA	17 VIIA	18 VIIIA
1 **H** Hydrogen 1.00794																	2 **He** Helium 4.002602
3 **Li** Lithium 6.941	4 **Be** Beryllium 9.012182											5 **B** Boron 10.811	6 **C** Carbon 12.0107	7 **N** Nitrogen 14.00674	8 **O** Oxygen 15.9994	9 **F** Fluorine 18.9984032	10 **Ne** Neon 20.1797
11 **Na** Sodium 22.989770	12 **Mg** Magnesium 24.3050											13 **Al** Aluminum 26.981538	14 **Si** Silicon 28.0855	15 **P** Phosph. 30.973761	16 **S** Sulfur 32.066	17 **Cl** Chlorine 35.4527	18 **Ar** Argon 39.948
19 **K** Potassium 39.0983	20 **Ca** Calcium 40.078	21 **Sc** Scandium 44.955910	22 **Ti** Titanium 47.867	23 **V** Vanadium 50.9415	24 **Cr** Chromium 51.9961	25 **Mn** Manganese 54.938049	26 **Fe** Iron 55.845	27 **Co** Cobalt 58.933200	28 **Ni** Nickel 58.6934	29 **Cu** Copper 63.546	30 **Zn** Zinc 65.39	31 **Ga** Gallium 69.723	32 **Ge** German. 72.61	33 **As** Arsenic 74.92160	34 **Se** Selenium 78.96	35 **Br** Bromine 79.904	36 **Kr** Krypton 83.80
37 **Rb** Rubidium 85.4678	38 **Sr** Strontium 87.62	39 **Y** Yttrium 88.90585	40 **Zr** Zirconium 91.224	41 **Nb** Niobium 92.90638	42 **Mo** Molybd. 95.94	43 **Tc** Technet. (97.907215)	44 **Ru** Ruthen. 101.07	45 **Rh** Rhodium 102.90550	46 **Pd** Palladium 106.42	47 **Ag** Silver 107.8682	48 **Cd** Cadmium 112.411	49 **In** Indium 114.818	50 **Sn** Tin 118.710	51 **Sb** Antimony 121.760	52 **Te** Tellurium 127.60	53 **I** Iodine 126.90447	54 **Xe** Xenon 131.29
55 **Cs** Cesium 132.90545	56 **Ba** Barium 137.327	57–71 Lantha-nides	72 **Hf** Hafnium 178.49	73 **Ta** Tantalum 180.9479	74 **W** Tungsten 183.84	75 **Re** Rhenium 186.207	76 **Os** Osmium 190.23	77 **Ir** Iridium 192.217	78 **Pt** Platinum 195.078	79 **Au** Gold 196.96655	80 **Hg** Mercury 200.59	81 **Tl** Thallium 204.3833	82 **Pb** Lead 207.2	83 **Bi** Bismuth 208.98038	84 **Po** Polonium (208.982415)	85 **At** Astatine (209.987131)	86 **Rn** Radon (222.017570)
87 **Fr** Francium (223.019731)	88 **Ra** Radium (226.025402)	89–103 Actinides	104 **Rf** Rutherford. (261.1089)	105 **Db** Dubnium (262.1144)	106 **Sg** Seaborg. (263.1186)	107 **Bh** Bohrium (262.1231)	108 **Hs** Hassium (265.1306)	109 **Mt** Meitner. (266.1378)	110 (269, 273)	111 (272)	112 (277)						

Lanthanide series	57 **La** Lanthanum 138.9055	58 **Ce** Cerium 140.116	59 **Pr** Praseodym. 140.90765	60 **Nd** Neodym. 144.24	61 **Pm** Prometh. (144.912745)	62 **Sm** Samarium 150.36	63 **Eu** Europium 151.964	64 **Gd** Gadolin. 157.25	65 **Tb** Terbium 158.92534	66 **Dy** Dyspros. 162.50	67 **Ho** Holmium 164.93032	68 **Er** Erbium 167.26	69 **Tm** Thulium 168.93421	70 **Yb** Ytterbium 173.04	71 **Lu** Lutetium 174.967
Actinide series	89 **Ac** Actinium (227.027747)	90 **Th** Thorium 232.0381	91 **Pa** Protactin. 231.03588	92 **U** Uranium 238.0289	93 **Np** Neptunium (237.048166)	94 **Pu** Plutonium (244.064197)	95 **Am** Americium (243.061372)	96 **Cm** Curium (247.070346)	97 **Bk** Berkelium (247.070298)	98 **Cf** Californ. (251.079579)	99 **Es** Einstein. (252.08297)	100 **Fm** Fermium (257.095096)	101 **Md** Mendelev. (258.098427)	102 **No** Nobelium (259.1011)	103 **Lr** Lawrenc. (262.1098)

Figure 1: Periodic Table of the Elements (from *Schroeder*).

a. Find the electron configurations and term symbols for the ground states of the following atoms and ions. Use the aufbau principle and Hund's rules and explain what you are doing.

Atom/Ion	Ne	K	Si	Ti	Co	Cl^-	Fe^{2+}	Fe^{2+}	Nd	Pt
Atomic number	10	19	14	22	27	17	26	26	60	78

Note: Pt is actually an example of an atom that is not described correctly by the Aufbau principle. Its observed electron configuration ends with $5d^9 6s^1$. Challenge: See if you can find the correct term symbol from that configuration.

b. Discuss briefly why there are no Neon magnets, while some of the strongest permanent magnets are Neodymium compounds.

Ex. 1.2: Particles in a 3D harmonic oscillator potential

a. Describe the ground state of a system of N non-interacting bosons in terms of the occupation numbers of single particle states.
   Do the same for a system of N non-interacting fermions. For fermions, give an argument that, at $T = 0$, we must have $\mu = \epsilon_F$, where ϵ_F is the energy of the highest occupied state.

Consider N identical fermions of spin $\frac{1}{2}$ and mass m subject to a potential $V(\vec{r}) = \frac{1}{2}m\omega^2(x^2 + y^2 + z^2)$. The single particles energy levels in the presence of this potential are $E_{\vec{n}} = \hbar\omega(n_x + n_y + n_z + \frac{3}{2})$. Here n_x, n_y and n_z are nonnegative integers.

b. Calculate the density of states $g(E)$ for this system.

c. Calculate the Fermi energy ϵ_F

d. Express the average energy per particle in the ground state in terms of ϵ_F.

Ex. 1.3: Spinless fermions in a 1D harmonic oscillator potential

Recall that the one-dimensional harmonic oscillator with angular frequency ω has energy levels $E_n = \hbar\omega(n + \frac{1}{2})$ and corresponding eigenstates $|n\rangle$ whose wavefunctions are

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)$$

where H_n are the Hermite polynomials, given by

$$H_n(z) = (-1)^n e^{z^2} \frac{d^n}{dz^n}\left(e^{-z^2}\right)$$

a. Calculate the first three Hermite polynomials (give them in polynomial form).

b. Find the ground state of a system of two spinless (or spin polarized) fermions in a 1D harmonic osccilator potential
   Do the same for three spinless fermions.

c. Argue that the ground state of a system of N spinless fermions in this potential is, up to a normalization constant, given by

$$\Psi(x_1, ..., x_N) \sim \prod_{i<j}^{N}(x_i - x_j)e^{-\frac{m\omega\sum_i x_i^2}{2\hbar}}$$