

<p>(b) Shells are filled in the order</p> $1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d \dots$ <p>with s,p,d shells containing 2,6,10 electrons respectively.</p> <p>(i) ^{16}S: $[\text{Ne}]3s^23p^4$ (ii) ^{23}V: $[\text{Ar}]4s^23d^3$ (iii) ^{40}Zr: $[\text{Kr}]5s^24d^2$ (iv) ^{54}Xe: $[\text{Xe}]$ (All filled shells) (v) ^{66}Dy: $[\text{Xe}]6s^24f^{10}$</p> <p>Where filled shell configurations $[\text{Ne}]$ contains 10 electrons, $[\text{Ar}]$ contains 18, $[\text{Kr}]$ contains 36 and $[\text{Xe}]$ contains 54.</p> <p>Thus</p> <p>(i) Sulfur has 4 electrons in a p-shell, these fill $l_z = -1, 0, 1$ with spin up and $l_z = 1$ with spin down. Thus $L = 1$ and $S = 1$, and since the shell is more than half full $J = L + S = 2$.</p> <p>(ii) Vanadium has 3 electrons in a d-shell, these fill $l_z = 2, 1, 0$ with spin up giving $L = 3$ and $S = 3/2$. Since the shell is less than half filled $J = L - S = 3/2$.</p> <p>(iii) Zirconium has 2 electrons in a d-shell, these fill $l_z = 2, 1$ with spin up giving $L = 3$ and $S = 1$. Since the shell is less than half filled $J = L - S = 2$.</p> <p>(iv) Xenon is a noble gas, meaning all shells are filled, so $J = L = S = 0$.</p> <p>(v) Dysprosium has 10 electrons in an f-shell, these fill all the spin up state (7 of them) and $l_z = 3, 2, 1$ for spin down giving $L = 6$ and $S = 2$. Since the shell is more than half filled $J = L + S = 8$.</p> <p>Note that none of these atoms violate the Madelung rule which dictates the filling order or violates Hund's rules when the atoms are isolated. (Violations do sometimes occur but these atoms work as they are supposed to).</p> <p>Er typically is in a +3 state. 2 of those are from the core s-orbitals. 1 is from the f orbital.</p> <p>(a) For 11 electrons in an f-shell, using Hund's first rule we obtain $S = 3/2$ and Hund's second rule we have $L = 6$. Since the shell is more than half filled, J is given by the sum $J = 6 + 3/2 = 15/2$. Using the formula for the Lande g factor (with $g = 2$) we have</p> $\tilde{g} = \frac{1}{2}(g + 1) + \frac{1}{2}(g - 1) \left[\frac{S(S + 1) - L(L + 1)}{J(J + 1)} \right] = 6/5$ <p>(b) The counting here is messed up. There are 7 electrons before losing one. For 7 electrons in an f-shell, $L = 0$ and $S = 7/2$ and $J = S$. is purely spin, so $\tilde{g} = g = 2$ (it also comes out of the above formula as well). In fact, we should have 6 electrons when one is lost, and we get $L = 3 = S$ and $J = 0$. However, This is a van-vleck ion, so in fact the result is not what is predicted here.</p> <p>The shell has $2l + 1$ orbital states and 2 spin states per orbital. Hund's first rule tells us that</p> $S(n, l) = \begin{cases} \frac{n}{2} & 0 \leq n \leq 2l + 1 \\ \frac{4l + 2 - n}{2} & 2l + 1 \leq n \leq 4l + 2 \end{cases}$ <p>The second rule tells us that for $n \leq 2l + 1$ we have</p> $L(n, l) = \sum_{x=l-n+1}^{x=l} x$ <p>We can do this sum to obtain</p> $L(n, l) = \frac{1}{2}n(2l + 1 - n)$ <p>For $2l + 1 \leq n \leq 4l + 2$ we can consider only the electrons in addition to the $L = 0$ half-filled shell, so $L(n, l) = L(n - (2l + 1), l)$ So we have in all,</p> $L(n, l) = \begin{cases} \frac{1}{2}n(2l + 1 - n) & 0 \leq n \leq 2l + 1 \\ \frac{1}{2}(n - 2l - 1)(4l + 2 - n) & 2l + 1 \leq n \leq 4l + 2 \end{cases}$ <p>And thus we have (using Hund's third rule) $J = L - S$ for less than half filled and $J = L + S$ for more than half filled so</p> $J(n, l) = \begin{cases} \frac{1}{2}n(2l - n) & 0 \leq n < 2l + 1 \\ \frac{1}{2}(n - 2l)(4l + 2 - n) & 2l + 1 \leq n \leq 4l + 2 \end{cases}$ <p>It is useful here to recall that</p> $\mathbf{S}_i \cdot \mathbf{S}_j = \frac{1}{2}(\mathbf{S}_i^+ \mathbf{S}_j^- + \mathbf{S}_i^- \mathbf{S}_j^+) + S_i^z S_j^z$ <p>Indeed, students often need to be reminded of this! Maybe it is worth giving this as a hint!</p> <p>(a) If each spin is aligned in the \hat{z} direction (it has $S_z = 1$), then the energy is $-g\mu_B B$ per spin and for each bond we have energy $-J\mathbf{S}_i \cdot \mathbf{S}_j = JS_i^z S_j^z = -JS^2$ since S^+ on the spins all give zero. The system is in an energy eigenstate with energy</p> $E = -Ng\mu_B B - NzJS^2/2$ <p>with z the number of neighbors of each site (=6 for a cubic lattice).</p> <p>(a) Let $\cos \theta = z$. The function $E(z)$ is an upside-down parabola with maximum at $z = -B/(2\kappa M) < 0$. If this parameter is $z > -1$ then there are two minima, one at $\theta = 0$ and the other at $\theta = \pi$. The absolute minimum is always at $\theta = 0$.</p>	<p>Probably here I should have stated explicitly that all three spins have the same \mathbf{S} (might be interesting to consider a case where they don't all have the same spin!).</p> <p>(a) The Hamiltonian is</p> $\mathcal{H} = J(\mathbf{S}_1 \cdot \mathbf{S}_2 + \mathbf{S}_1 \cdot \mathbf{S}_3 + \mathbf{S}_2 \cdot \mathbf{S}_3)$ <p>Since $\mathbf{S}_1 \cdot \mathbf{S}_1 = S^2$ is a constant we can write</p> $\mathcal{H} = (J/2)(\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3)^2 + \text{constant}$ <p>To minimize the energy, we must have</p> $\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 = 0$ <p>which implies that the spins are at 120 degree angles from each other – but can lie in any plane.</p> <p>(b) For a triangular lattice, each triangle must have three spins each at 120 degree angles from its neighbors. So choose three directions all at 120 degree angles from each other in any given plane. Call these three directions A, B, C. Now we must assign each site on the triangular lattice one of the three values A, B, or C in such a way that all triangles contain one site of type A, one of type B, and one of type C. One can think of this as being now a crystal whose unit cell has three times the area of the original unit cell, and now contains one spin of each type A, B, C.</p> <p>Note the obvious typo, it should read $2\mathbf{S}_1 \cdot \mathbf{S}_2 = (\mathbf{S}_1 + \mathbf{S}_2)^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2$.</p> <p>(a)</p> $\mathcal{H} = -(J/2)[(\mathbf{S}_1 + \mathbf{S}_2)^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2]$ <p>Since $(\mathbf{S})^2 = S(S + 1)$ for spin-1/2 we have $(\mathbf{S})^2 = 3/4$. Further, when two spin 1/2's are added they can form either a spin-0 singlet or a spin-1 triplet (three S_z states). So $(\mathbf{S}_1 + \mathbf{S}_2)^2$ takes the values 0 for the singlet or $S(S + 1) = 2$ for the $S = 1$ triplet. Thus the Hamiltonian has eigenstates $3J/4$ for the singlet (one eigenstate) and $-J/4$ for the triplet (three eigenstates).</p> <p>(b) Similarly</p> $\mathcal{H} = -(J/2)[(\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3)^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2 - \mathbf{S}_3^2]$ <p>Here, again for spin 1/2 we have $(\mathbf{S})^2 = 3/4$. When adding three spin-1/2s, we can obtain spin-1/2 in two ways and spin-3/2 in one way. (To see this, think about adding the first two spin-1/2 to get spin-0 or spin-1. Now adding a spin-1/2 the spin-0 gives spin-1/2 and adding spin-1/2 to the spin-1 gives either spin-1/2 or spin-3/2. Note that counting the total number of eigenstates we should get 8 since each spin-1/2 has two possible S_z states. Each of the two possible spin-1/2's can take two possible S_z states and the spin-3/2 can take 4 possible S_z states, which gives a total of 8 possible S_z states.</p> <p>In the case that the three spins add to spin-1/2, we obtain energy $3J/4$ (four eigenstates) whereas if the three spins add to spin-3/2, $\mathbf{S}^2 = S(S + 1) = 15/4$, so the energy is $-3J/4$ (four eigenstates).</p> <p>(c) Same story</p> $\mathcal{H} = -(J/2)[(\mathbf{S}_1 + \mathbf{S}_2 + \mathbf{S}_3 + \mathbf{S}_4)^2 - \mathbf{S}_1^2 - \mathbf{S}_2^2 - \mathbf{S}_3^2 - \mathbf{S}_4^2]$ <p>The sum of the four spins can give spin 0 in two ways, spin 1 in 3 ways, and spin 2 in one way. Again we should add up the total number of eigenstates to check that it is $2^4 = 16$. We have 2 spin 0's + 3 states for spin 1 in 3 ways + 5 states in spin 2. So we have $2 + 9 + 5 = 16$. The spin-0 singlets (two eigenstates) have energy $(-J/2)[0 - 4(3/4)] = 3J/2$. The three spin-1 triplets (9 eigenstates) have energy $(-J/2)[2 - 4(3/4)] = J/2$ and the spin-2 fiveplets (5 eigenstates) have energy $(-J/2)[2 \times 3 - 4(3/4)] = -3J/2$</p> <p>(a) The first spin can be either in the spin-up or spin down state, so we leave σ_1 as a variable to be summed over. The remaining spins are defined by R_i for $i = 1, \dots, N - 1$ where each R_i can take the values ± 1. The Hamiltonian in terms of the R variables is</p> $\mathcal{H} = -J \sum_{i=1}^{N-1} R_i$ <p>So the partition function is</p> $Z = 2(e^{-\beta J} + e^{\beta J})^{N-1} = 2(2 \cosh(\beta J))^{N-1}$ <p>with the factor of 2 out front being the sum over the first spin. The free energy is thus</p> $F = -k_B T \log Z = -k_B T N \log 2 - k_B T N \log \cosh(\beta J)$ <p>which is a completely continuous function with no cusps or discontinuities at finite β.</p> <p>(a) Following the hint, the magnetic energy between two monopoles of charge q_m and q'_m separated by distance r is given by</p> $E = \frac{\mu_0 q_m q'_m}{4\pi r}$ <p>Here we have charge of magnitude $q_m = \mu_B A \rho$ where $A = \pi r^2$ is the area of the end. Check that this has the right dimensions, recall that a dipole is a charge times a length, so q_m correctly has dimension of a charge.</p> <p>Thus the energy is</p> $\frac{\mu_0 (\mu_B \rho (\pi r^2))^2}{4\pi L}$ <p>(b) This problem, on the other hand is analogous to the energy of a capacitor. The energy stored in a capacitor is $q^2/(2C)$ where electrically the capacitance is $\epsilon_0 A/d$ with A the area and d the spacing. The analogy here is thus $A/(d\mu_0)$. Thus the total energy stored is</p> $E = q_m^2 \mu_0 d / (2A) = \frac{\mu_0 (\mu_B \rho (\pi r^2))^2 L}{2}$
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