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Physics 731 HOMEWORK ASSIGNMENT #3 Due: Sept. 26, 2006 (Deadline 9/28)

Read Ashcroft & Mermin (A&M), chaps. 19–20.

1. *Read but do NOT turn in this problem; solution will be supplied.* A&M 19–1 (Cf. Ibach & Lüth, 1–11 for an easier version of problem 19.) I will give a hand-waving motivation of the main result in part d. *What you learn is not worth the pain of the algebra.*
2. A&M 19–2.
3. A&M 20–1, parts a and b only.
4. A&M 20–4, parts a and b only.
5. Consider a line of 2N ions of alternating charge $\pm q$ with (in addition to the usual long-range $1/R$ Coulomb interactions) a repulsive potential energy A/R^n between nearest neighbors.

a) Show that at the equilibrium separation R_0

$$U(R_0) = -\frac{2Nq^2 \ln 2}{R_0}\left(1 - \frac{1}{n}\right)$$

b) Suppose one compresses the 1D crystal so that $R_0 \to R_0\,(1-\delta)$. Show that—to leading order—the work [per length], $U(R_0 - R_0\delta) - U(R_0)$, can be written $(1/2)C\delta^2$, where

$$C = \frac{(n-1)q^2 \ln 2}{R_0^2}$$

6. Barium oxide has the NaCl structure. Estimate the cohesive energies per molecule of the hypothetical crystals Ba^+O^- and $Ba^{++}O^{--}$ (relative to separated neutral atoms). The observed nearest-neighbor distance is R_0 = 2.76 Å; the first and second ionization potentials of Ba are 5.19 and 9.96 eV; the electron affinities (namely the energy "gain" [decrease of total energy]) for the first and second electrons added (from infinity/zero-potential) to the neutral oxygen atom are 1.5 and -9.0 eV. Which valence state (singly or doubly ionized) do you predict will occur? (Assume R_0 is the same for both forms.)

7. Estimate the Madelung constant a for a [square] checkerboard of + and - charges (2D analogue of NaCl) using the Evjen method. Specifically, find the contribution from each of the first 3 shells. (Hint: the contributions from shells 1 and 2 are 1.293 and 0.314, respectively.)

8. *Not assigned; Mathematica notebook posted on Solutions site.*

Using eqns. 9 and 10 of the Rioux article (http://www.users.csbsju.edu/%7Efrioux/h2-virial/virialh2.htm), find T(R) and V(R) for the universal binding curve rather than the Morse potential that Rioux used. In terms of the latter, the universal curve amounts to

$$E(R) = -D_e(1 + a^*)\exp(-a^*), \text{ where } a^* = (R - R_e)/\ell$$

Find ℓ in terms of the Morse potential parameters so that the curvature around the minimum of the universal curve is the same as that of the Morse curve. Redraw the figure, using the same parameters used by Rioux, using Mathematica or any other graphing program, and see if there are notable differences from Rioux's picture for the Morse potential

9. *Read but do NOT turn in the following problem; solution will be supplied. We will return to it later.*

a) A set of normalized and mutually orthogonal p-state wavefunctions for an atom can be written in the form: $p_x = x\,f(r)$; $p_y = y\,f(r)$; $p_z = z\,f(r)$.

Consider the linear combination of p wavefunctions $\psi = a_x p_x + a_y p_y + a_z p_z$. Find four sets of coefficients (a_x, a_y, a_z) that give normalized p-state wavefunctions with positive lobes pointing towards the corners of a regular tetrahedron (i.e. 4 alternating corners of a cube).

b) Consider the linear combination $\phi = bs + c\psi$, where ψ is any one of the four wavefunctions calculated above, and s is an s-state wavefunction, normalized and orthogonal to the p's. Find values of b and c which make the four resulting ϕ wavefunctions orthogonal to each other and normalized, and write out the resulting four ϕ wavefunctions (the sp^3 hybrids) in terms of $p_x + p_y + p_z$, and s. (Cf. Ibach & Lüth, 1–9.)