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Physics 731 HOMEWORK ASSIGNMENT #3 Due: Sept. 20/25, 2001?

No class on Tues., Sept. 18; make-up class, rm. 1304 Wednesday, Sept. 19, 7:15-8:30p.m.

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

1. A&M 19–1 b, c, d (cf. Ibach & Lüth, 1–11 for an easier version of this problem).
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 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 $R_0 \rightarrow R_0\,(1-\delta)$. 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 of the first and second electrons added 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. *Read but do NOT turn in this problem; solution will be supplied*

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 <u>normalized</u> 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.)

8. 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 4 shells.