equilibrium lattice constant, a_o, [20]. (The difference between the V total energy at its minimum and the spin-polarized Xα energy of the ^4F multiplet of the $3d^3 4s^2$ configuration of the isolated V atom [which corresponds to the experimental ground state of the atom] is −0.45 Ry/atom. Thus, this figure and the equilibrium cohesive energy calculated with reference to the $3d^4\ 4s^1$ configuration bracket the experimental value of the cohesive energy.) The Xα approximation thus predicts for V, as for Cs, a cohesive energy, compressibility [3], and lattice constant in good agreement with experiment.

The kink in the cohesive energy curve, near the transition point ($a \approx 7$ a.u.), is indicative of the possibility of a phase transition in which a discontinuous volume change is associated with the onset of magnetic polarization. Unfortunately, detailed examination of this transition will probably require more detailed knowledge of the cohesive energy as a function of lattice constant near the transition point than is reported here.

The densities of states are illustrated in Fig. 6 for two non-magnetic lattice constants, to show the increasing density of states at the Fermi energy which eventually leads to the stability of the magnetic state as the lattice constant is further increased. Fig. 7 shows the spin-polarized densities of states for the majority (α) and minority (β) spins, for magnetic V at a lattice constant of 8.5 a.u., well beyond the transition point. Note that the Fermi energy has passed through a minimum in the majority-spin (α) density of states in order to make the transition from the non-magnetic to the magnetized state. This may be associated with the phase transition mentioned above in which a discontinuous change in lattice constant may occur

at the onset of magnetic behavior. It is precisely in this region of the transition that the minimum in the majority-spin density of states must pass through the Fermi energy.