a) The effective nuclear charge experienced by a given electron shows the shielding effects of the other electrons present. If r goes to zero, the potential has the form ~-Z/r , if r goes to infinity, the potential has the form ~ -1/r. In those two cases, the effective potential function (2) does not work well.

c) To calculate the ionization potential of He and Li, using the Slater's rules.

$$For\ He\ Ip = E(He^+) - E(He)$$

$$E(He^+) = \varepsilon_{1s}$$

$$\varepsilon_{1s} = -\frac{1}{2}\left(\frac{Z - \sigma_{1s}}{n_{effective,1s}}\right)^2, \ n_{effective,1s} = 1$$

$$\sigma_{1s} = \sum_{j \le 1s} (q_j - \delta_{j1s})\Delta\sigma_j = (q_{1s} - 1)\Delta\sigma_{1s} = 0$$

$$\therefore\ E(He^+) = \varepsilon_{1s} = -\frac{1}{2} \times 4 = -2\ Hartree$$

$$E(He) = 2 \times \varepsilon_{1s}$$

$$\varepsilon_{1s} = -\frac{1}{2}\left(\frac{Z - \sigma_{1s}}{n_{effective,1s}}\right)^2, \ n_{effective,1s} = 1$$

$$\sigma_{1s} = (2 - 1)\Delta\sigma_{1s} \quad \Delta\sigma_{1s} = 0.30$$

$$E(He) = 2 \times \left(-\frac{1}{2} \times 1.7^2\right) = -2.89\ Hartree$$

$$IP = -2 + 2.89 = 0.89\ Hartree \approx 24.22\ eV$$

For lithium, calculated IP is about 5.75 eV

d) Using Koopmans-Theory, for He IP is about 39.32 eV and for Li IP is about 5.75 eV. Koopmans-Theory works well only for the atoms which have the similar valence electron configuration with lithium.

e) Calculated ionization potentials for Na, K ,Rb are 7.32 eV, 4.8 eV, 4.12 eV respectively, using Koopmans-Theory.

f) The smaller its radius, the bigger the effective nuclear charge felt by a valence electron. So the ionization energy increase when we go through the row (Li-Ne) of the periodic table.