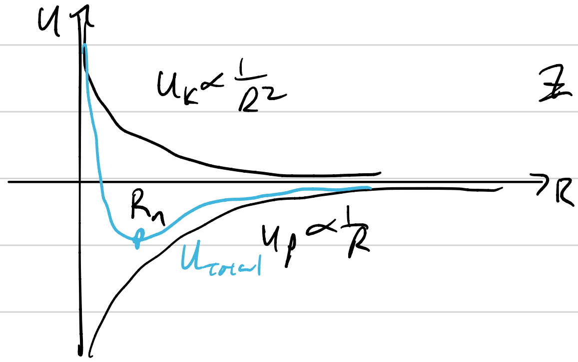
Atomic Example:

For a given n:



∃ an equilibrium point

we can take the derivative of the total energy:

$$\frac{dU}{dr} = -\frac{L^2}{mR^3} + \frac{1}{4\pi\varepsilon_0}\frac{e^2}{R^2} = 0$$

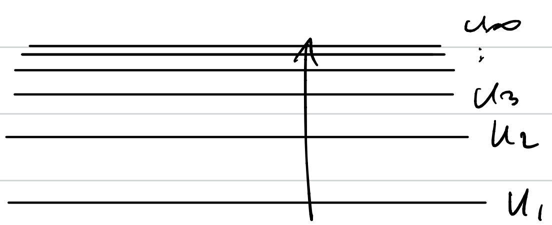
$$= -\frac{1}{R}\left(2U_K + U_p\right) = 0 \Rightarrow U_K = \frac{1}{2}U_p$$

$$R_n = \frac{4\pi\varepsilon_0}{me^2}(n\hbar)^2 \qquad U_n = -\frac{me^4}{32(\pi\varepsilon_0\hbar n)^2}$$

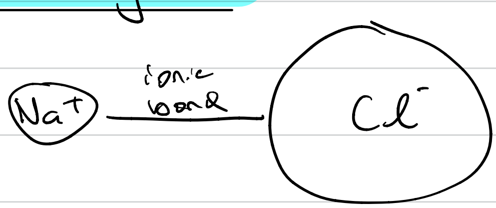
For $n=1$ ground state:

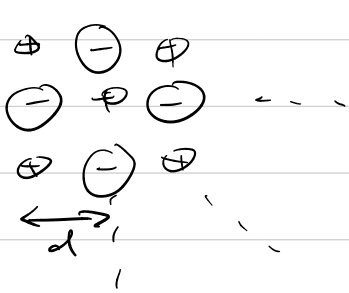
$R_1 = 5.3\times10^{-11}\,m \Rightarrow 0.53\,\text{Å} = a_0$ "Bohr's Radius"

$U_1 = -2.18\times10^{-18}\,J \Rightarrow -13.6\,eV$ (Ionization Energy)



Ionic Crystals





face-centered cubic-structure:
like the fcc 3D structure

The distance $d = 2.81\,\text{Å}$

What would be the crystal binding energy? "Energy required to separate the crystal into individual ions at infinite distance apart"

2N ions, or N molecules

$$U_{total} = \frac{1}{2}\sum_{i=1}^{2N} q_i \Phi_i = \frac{1}{8\pi\varepsilon_0}\sum_{\substack{i,j \\ i \neq j}}^{2N} \frac{q_i q_j}{|\vec{r}_i - \vec{r}_j|}$$

Average Energy per Molecule

$$\frac{U_{tot}}{N} \sim \frac{-e^2}{4\pi\varepsilon_0}\sum_{j=2}^{2N} \frac{\pm 1}{|\vec{r}_i - \vec{r}_j|}$$

$$= -\frac{e^2}{4\pi\varepsilon_0 R}\underbrace{\sum_{j=2}^{2N} \frac{\pm 1}{|\vec{r}_i - \vec{r}_j|/R}}$$

"Madelung Constant" determined by the crystal structure.

For the crystal to be stable: $M > 0$

NaCl $M = 1.748$

$$\frac{U_{tot}}{N} \simeq -1.43 \times 10^{-18}\ \text{J/molecule} = -8.95\ \text{eV/molecule}$$

Experimentally $\Rightarrow -8\ \text{eV/molecule}$

Chapter 3: Laplace's Equation

- Motivation

$$\rho \leftrightarrow \phi \ : \ \phi(\vec{r}) = \frac{1}{4\pi\varepsilon_0}\int \frac{\rho(\vec{r}')}{|\vec{r} - \vec{r}'|}\, dV'$$

$$\nabla^2 \phi = -\frac{\rho}{\varepsilon_0} \quad \text{(poisson equation)}$$

+ boundary condition ϕ ⟶ then we can easily solve for the potential

$\left(\phi, \frac{\partial \phi}{\partial n} \text{ at boundary}\right)$ ($\hookrightarrow \hat{n} \perp d\ell$)

If we have no free charges $\Rightarrow$ Poisson Eq. → Laplace's Eq.

where the solutions are harmonic functions

$$\boxed{\nabla^2 \phi = 0}$$

Laplace in 1-D

x: $\frac{d^2\phi}{dx^2} = 0$