Current approach in DFT + use in real world.

Problems of DFT and in OMC.

\[
E = \frac{4}{3} \rho H^4 \\
H = \nabla^2 + V + V_{\text{ext}} + V_{\text{ion}}
\]

Derive \( H'' = H = 0 \) term.

\[
\frac{d^2E}{d\rho^2} = \left< \frac{d^2V}{d\rho^2} \right> + \frac{1}{2} \left( \frac{dV}{d\rho} \frac{d^2\rho}{d\rho^2} + \frac{d^2V}{d\rho^2} \frac{d\rho}{d\rho} \right)
\]

Results for DMC / Full 

Solving cubic quadratic nodes → phonons.

First order from

\[
V = \frac{1}{\sqrt{(x-x)^2 + (y-y)^2 + (z-z)^2}} \quad \frac{1}{\sqrt{(x+x)^2 + (y+y)^2 + (z+z)^2}}
\]

\[
+ \frac{1}{\sqrt{(x+y)^2 + (y+y)^2 + (z-z)^2}} \quad \frac{1}{\sqrt{(x+y)^2 + (y+y)^2 + (z-z)^2}}
\]

\[
+ \frac{1}{\sqrt{(x+y)^2 + (y+y)^2 + (z-z)^2}} \quad \frac{1}{\sqrt{(x+y)^2 + (y+y)^2 + (z-z)^2}}
\]

Check \( \frac{dV}{d\rho} = 0 \) by symmetry

\[
\frac{dV}{d\rho} = -\left( \frac{X-x}{(x-x)^2 + (y-y)^2 + (z-z)^2} \right)
\]

\[
\frac{d^2V}{d\rho^2} = \left( \frac{X-y}{(x-x)^2 + (y-y)^2 + (z-z)^2} \right) + \left( \frac{X-z}{(x-x)^2 + (y-y)^2 + (z-z)^2} \right)
\]

Not a surprise or \( \sigma^2 = 0 \) so by symmetry.

Holds for all max.

Holds for cubic, BCC, FCC but not HCP i.e. hex. unstable.

Holds for all cubic based structures e.g. NaCl, diamond.

What about other systems: analyze in NFE and high

limits.

N.B.
Nearly free electron limit: No change in \( \gamma \) so \( \gamma_{\text{eff}} = 0 \)

\[
V_{\text{el}} = \int \frac{\cos h x + \cos h y + \cos h z}{\sqrt{(x - x')^2 + (y - y')^2 + (z - z')^2}} \, dx \, dy \, dz
\]

\[
= -\int \frac{\frac{1}{q_x^2 + q_y^2 + q_z^2}}{2} \sum \delta(q_x - h) + \delta(q_x + h) \, dq_x \, dq_y \, dq_z
\]

\[
= -\left( \cosh X + \cosh Y + \cosh Z \right)
\]

\[
= 3. + \frac{3}{2} h^2 \left( x^2 + y^2 + z^2 \right)
\]

Electrons don't mix high density states so strictly ionic

Metals have cubic lattice (low on bond)
Tight binding:
Without electron on top of atom so no overlap.
With finite radius $R$, $\frac{\partial^2 V}{\partial R^2}$ term small due to exponentially decaying function.

Lead to next order terms $\frac{\partial^2 V}{\partial R^4}$ and $\frac{\partial^4 V}{\partial R^4}$.

Expand $\frac{\partial^2 V}{\partial R^2}$ around electron cloud, similar to $\frac{\partial^2 V}{\partial R^4}$.

Simple term $e = \pi \times \text{sign}(\nabla \cdot \mathbf{V}) = (x^2 + y^2 + z^2)(V_x, V_y, V_z)$?

Looking at more complex crystal structures.

- FCC: 1.36
- BCC: 1.83
- HCP: 1.69

What has this got to do with our stability?

Answer: How calculate energetics of these systems:

- Other ways to explain crystal stability
- „D-wave approximation
- Quasi-riegers
- $\hbar \rightarrow 0$ Issues?