Computational Materials Physics

Center for Molecular Modeling

Department of Materials Science and Engineering

2nd Hohenberg-Kohn theorem

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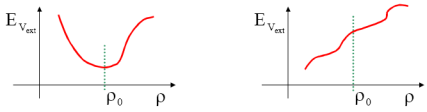
http://molmod.ugent.be
http://www.ugent.be/ea/dmse/en
my talks on Youtube: http://goo.gl/P2b1Hs

2nd Hohenberg-Kohn theorem

" The unique functional that returns the ground state total energy when applied to the ground state density, returns a higher energy for any other density. "



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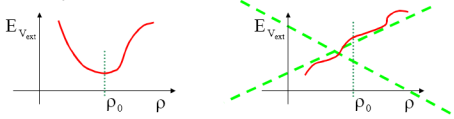

Note 1: this functional can be written as

$$E_{V_{ext}}[\rho] = F_{HK}[\rho] + \int \rho(\vec{r}) V_{ext}(\vec{r})\, d\vec{r}$$

with F_{HK} the (unknown) Hohenberg-Kohn functional that returns the kinetic and electron-electron part of the total energy.

Note 2 : this suggests a procedure to find the ground state density by minimizing the total energy functional.