Computational Materials Physics

Center for Molecular Modeling

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classical forces

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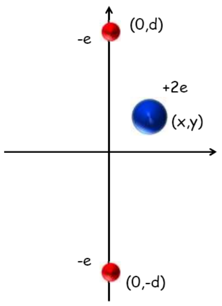
http://molmod.ugent.be
http://www.ugent.be/ea/dmse/en
my talks on Youtube: http://goo.gl/P2b1Hs

Classical forces



Total electrostatic energy as a function of the position of the 'nucleus' :

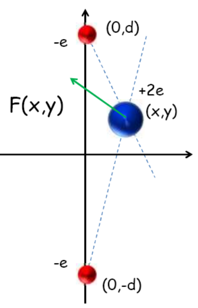
$$\underbrace{E(x,y)}_{\text{position of the nucleus}} = \underbrace{\frac{-2C}{\sqrt{x^2+(d-y)^2}} + \frac{-2C}{\sqrt{x^2+(d+y)^2}}}_{\text{electron-nucleus}} + \underbrace{\frac{C}{2d}}_{\text{electron-electron}}$$

For dynamic problems, kinetic energy terms of 'electrons' and 'nuclei' will appear as well.

$$C = \frac{e^2}{4\pi\epsilon_0}$$

(Instructive: plot a 3D graph of E(x,y))

Classical forces



Use Coulomb's law to get the components of the force on the 'nucleus' :

$$F_x(x,y) = \frac{-2xC}{\left(x^2+(d-y)^2\right)^{3/2}} + \frac{-2xC}{\left(x^2+(d+y)^2\right)^{3/2}}$$

$$F_y(x,y) = \frac{2C(d-y)}{\left(x^2+(d-y)^2\right)^{3/2}} + \frac{-2C(d+y)}{\left(x^2+(d+y)^2\right)^{3/2}}$$

You can verify that:

$$F_x = \frac{\partial E}{\partial x}$$

$$F_y = \frac{\partial E}{\partial y}$$

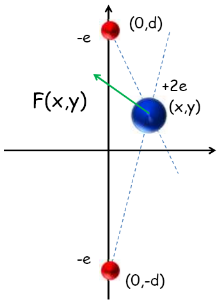
Or more generally:

$$\vec{F} = -\nabla_{\vec{r}} E$$

Force associated with moving the nucleus

Position of the nucleus

Classical forces



These are specific examples of the Hamilton formulation of classical mechanics :

$$\mathcal{H}\,(p,\,q,\,t) = T + V$$

Hamilton equations:

$$\dot{p} = -\frac{\partial \mathcal{H}}{\partial q}$$

$$\dot{q} = \frac{\partial \mathcal{H}}{\partial p}$$

Classical forces

One of the H-equations leads to a force associated to a generalized coordinate.

$$F_q = \dot{p} = -\frac{\partial \mathcal{H}}{\partial q}$$

This is a general expression !

- Applicable to static as well as dynamic problems
- Applicable to any generalized coordinate
- Applicable to classical and quantum problems