Computational Materials Physics

Center for Molecular Modeling

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correlation

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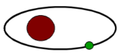
http://molmod.ugent.be
http://www.ugent.be/ea/dmse/en
my talks on Youtube: http://goo.gl/P2b1Hs

correlation in classical mechanics

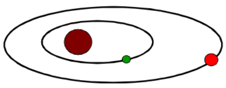
two-body problem: Sun-Earth



analytical solution

Energy:
- kinetic (translational)
- kinetic (rotational)
- potential

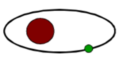
three-body problem: Sun-Earth-Jupiter

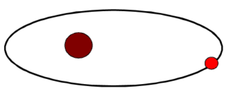


only numerical solutions possible

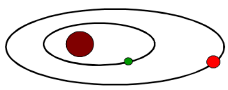
correlation in classical mechanics

total energy of Sun-Earth + total energy of Sun-Jupiter





difference = (classical) correlation energy



total energy of Sun-Earth-Jupiter

correlation in quantum mechanics

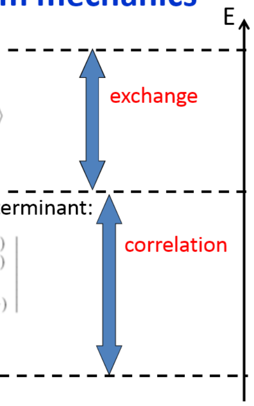
Independent electron solution,
many-body wave function is product:

$$\left|\Psi_0^H(\vec{\alpha}_1,\ldots,\vec{\alpha}_N)\right\rangle = |\Psi_1(\vec{\alpha}_1)\Psi_2(\vec{\alpha}_2)\ldots\Psi_N(\vec{\alpha}_N)\rangle$$

Independent electron solution,
many-body wave function is Slater determinant:

$$\left|\Psi_0^{HF}\right\rangle = \frac{1}{\sqrt{N!}}\begin{vmatrix} \Psi_1(\vec{\alpha}_1) & \Psi_1(\vec{\alpha}_2) & \ldots & \Psi_1(\vec{\alpha}_N) \\ \Psi_2(\vec{\alpha}_1) & \Psi_2(\vec{\alpha}_2) & \ldots & \Psi_2(\vec{\alpha}_N) \\ \vdots & \vdots & \ddots & \vdots \\ \Psi_N(\vec{\alpha}_1) & \Psi_N(\vec{\alpha}_2) & \ldots & \Psi_N(\vec{\alpha}_N) \end{vmatrix}$$

Exact solution (unknown)



correlation (summary)

Correlation in classical physics =
energy difference between independent particle solution and exact solution

Correlation in quantum physics =
energy difference between Hartree-Fock solution and exact solution