Coupling Molecular Dynamics and Quantum Mechanics

A (hopefully) lightweight introduction to a not so lightweight topic.

Jørgen Høgberget

Outline

Recap of Molecular Dynamics

- Why do we need quantum mechanics?

Introducing Quantum Mechanics

- Difference from Statistical Mechanics
- Benefits and Problems

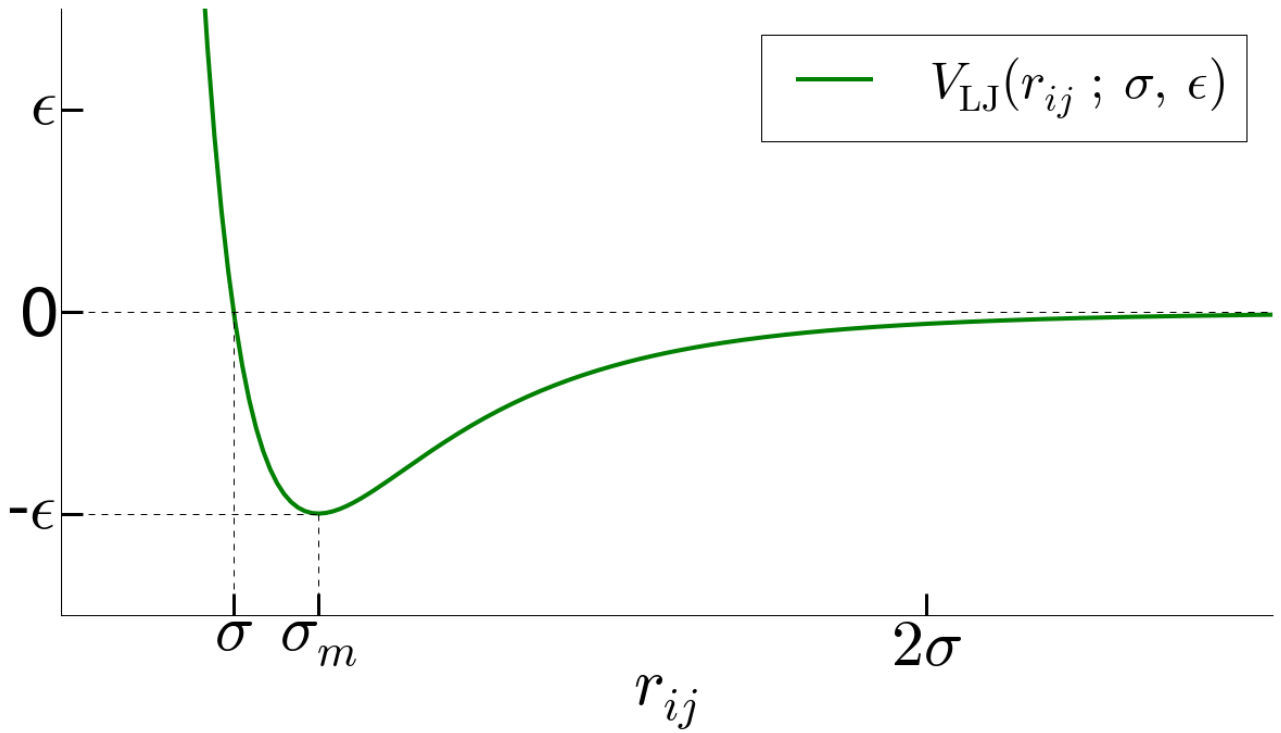
Parameterizing Potentials using Quantum Mechanics

- Connecting the scales
- Practical calculations
- Examples
- State of the art

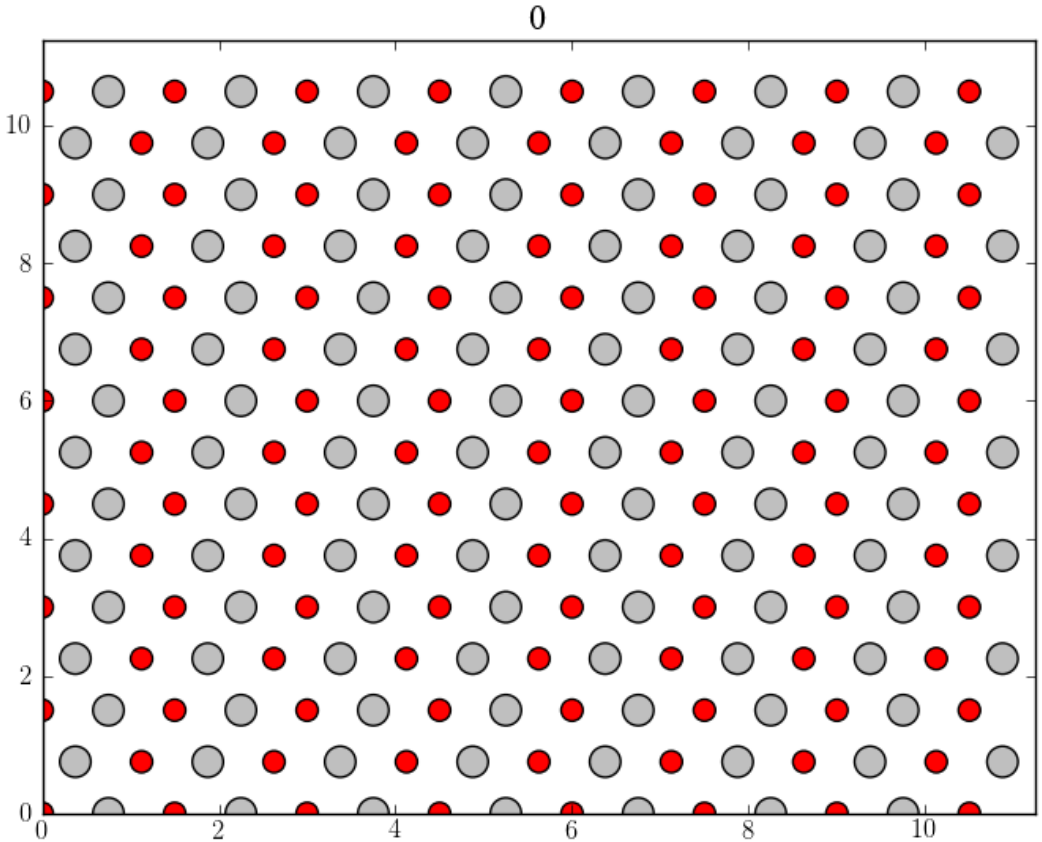
Recap of Molecular Dynamics

Coupling Molecular Dynamics and Quantum Mechanics

- Integrate Newton's equations for a dynamic ensemble of point particles.
- Molecular interactions are described by potentials.



Coupling Molecular Dynamics and Quantum Mechanics



The force is expressed as the gradient of the potential

Why do we need quantum mechanics?

Introducing Quantum Mechanics

Difference from Statistical Mechanics

Benefits and Problems

[1]

Parameterizing Potentials using Quantum Mechanics

Connecting the scales

Practical calculations

Examples

State of the art

References

[1] Moskowitz Kalos. A new Look at Correlations in Atomic and Molecular Systems. Application of Fermion Monte Carlo Variational Method. *Int. J. Quant. Chem.*, **XX**:1107, 1981.

Questions?

$$V_{\mathrm{LJ}}(r_{ij}\,;\,\sigma,\,\epsilon) = 4\epsilon\left(\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right)$$