

Pseudopotentials reach for the stars

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TCM Group, Department of Physics

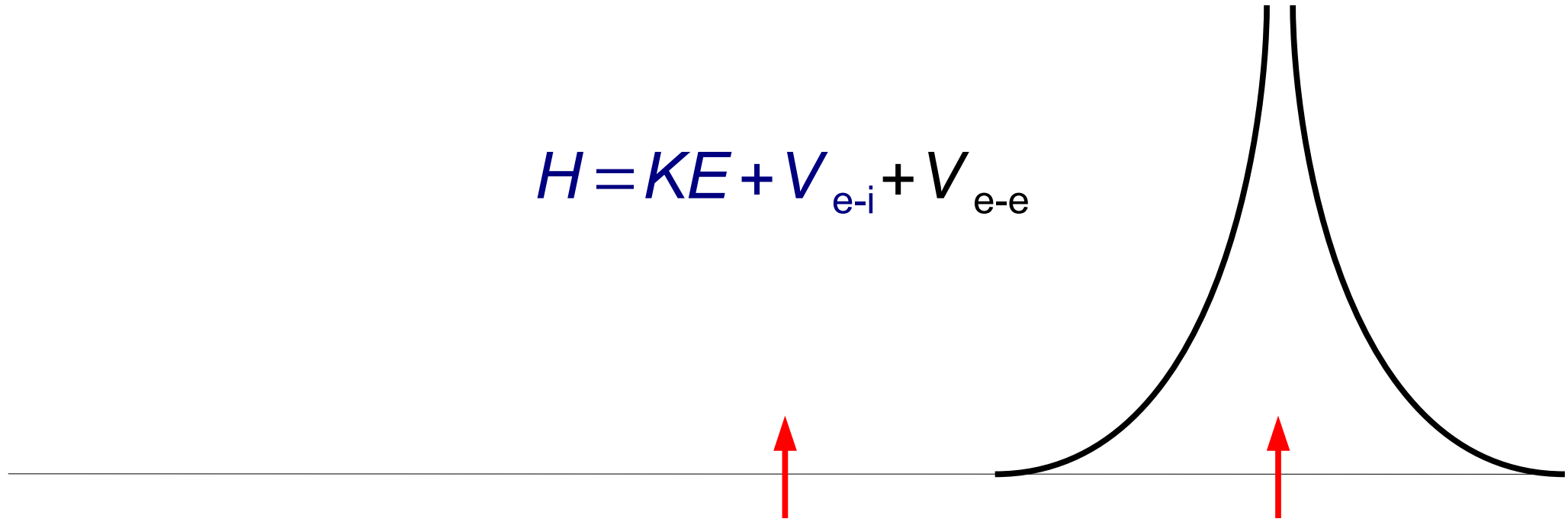
Pseudopotential for atoms

$$H = KE + V_{e-i} + V_{e-e}$$



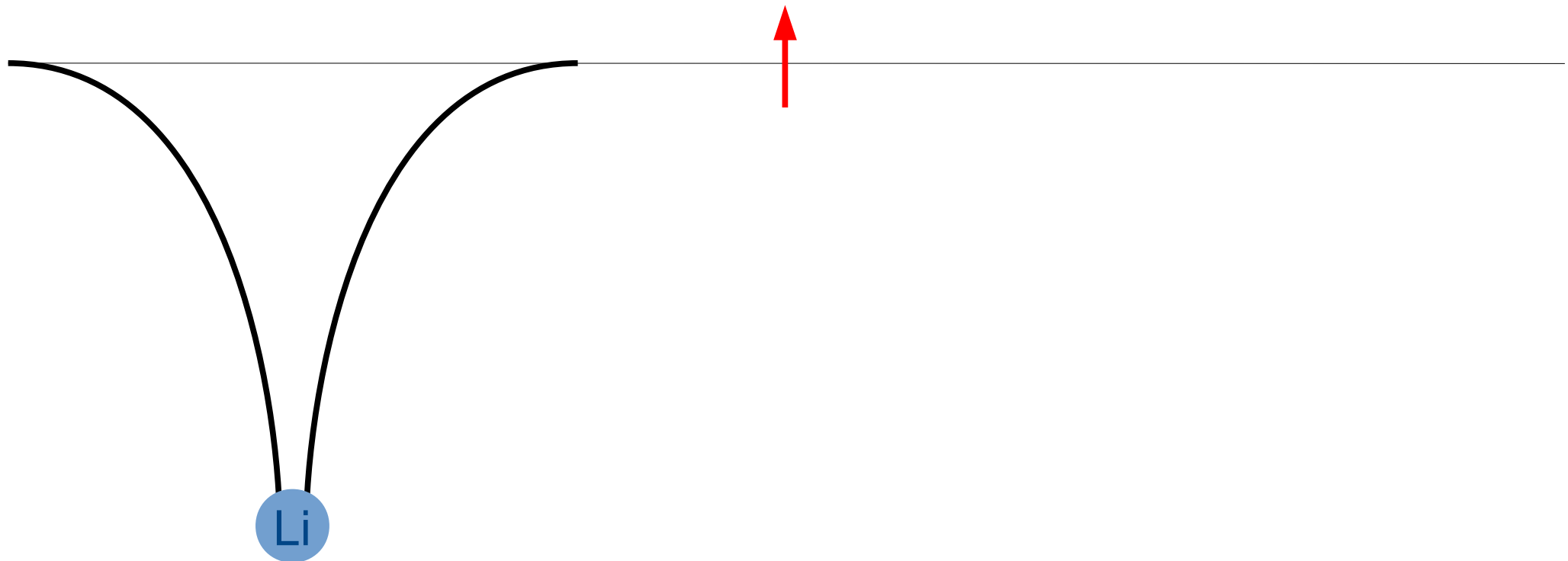
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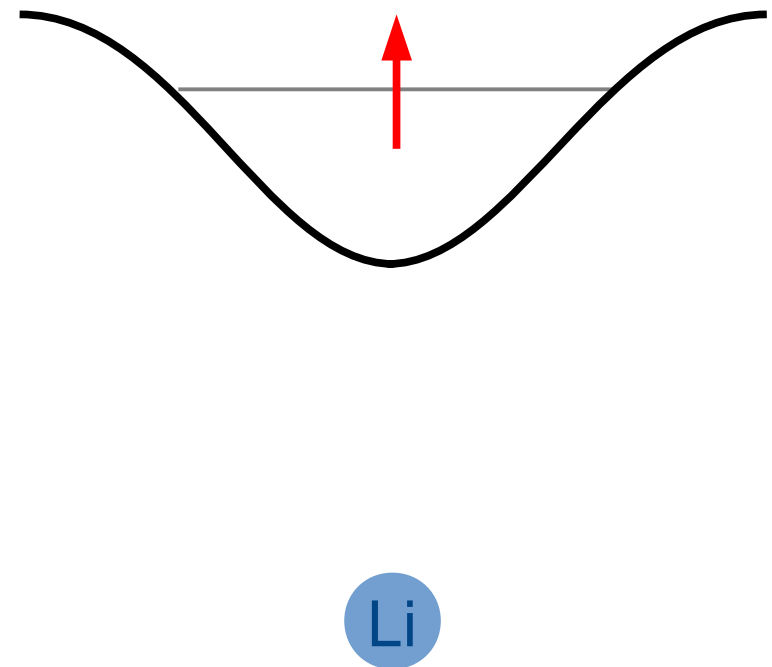
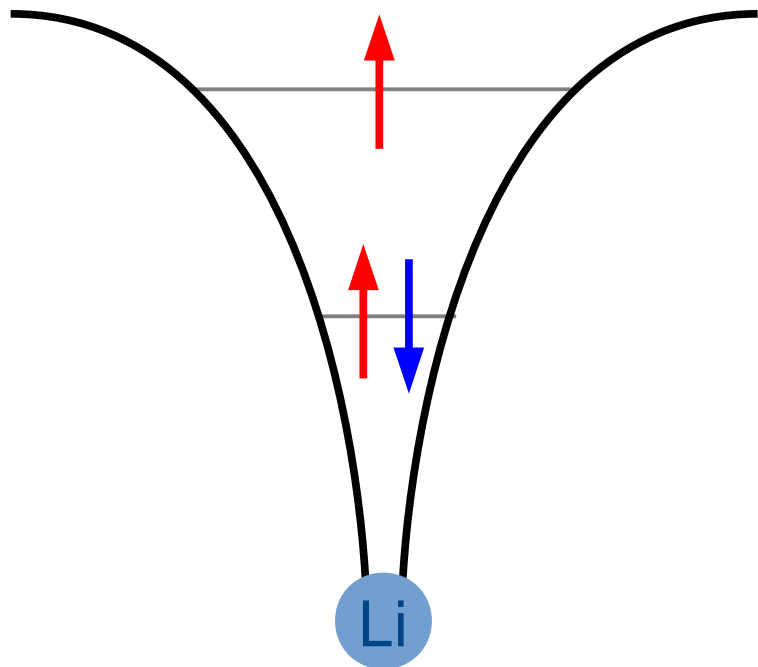


Pseudopotential for atoms

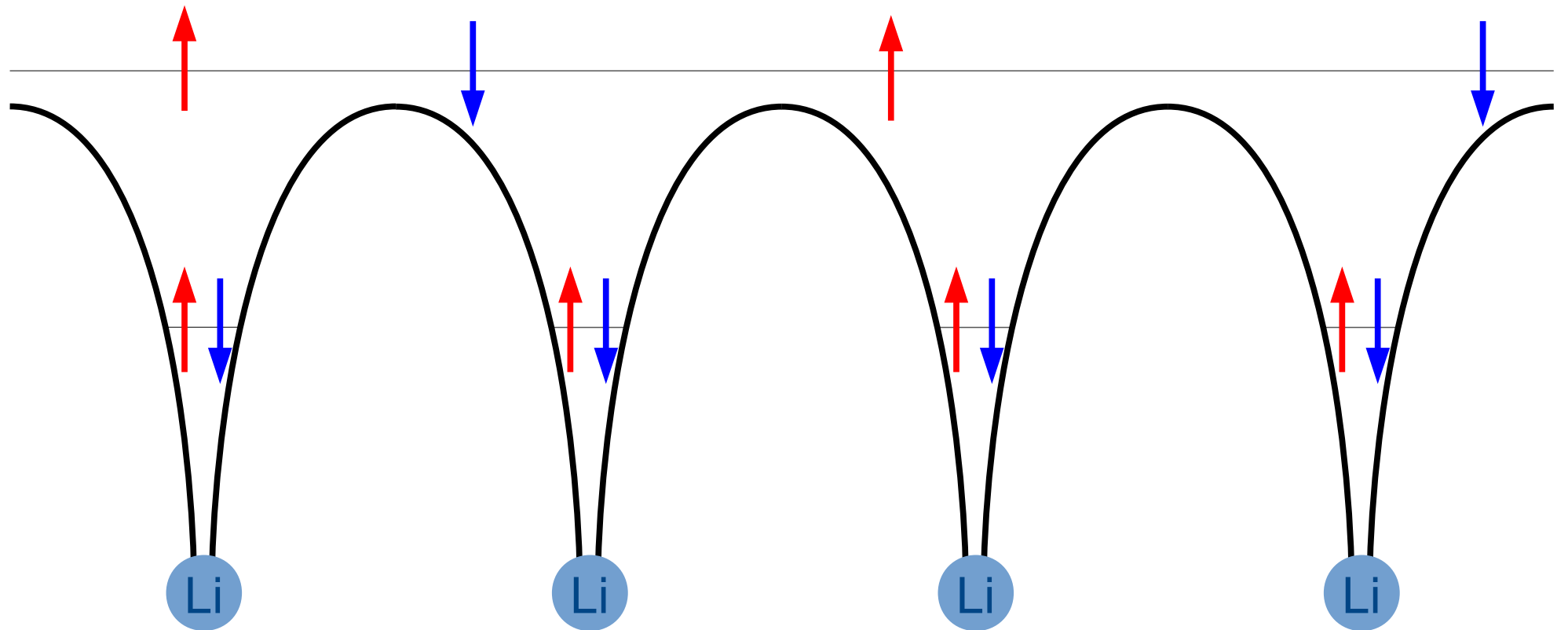
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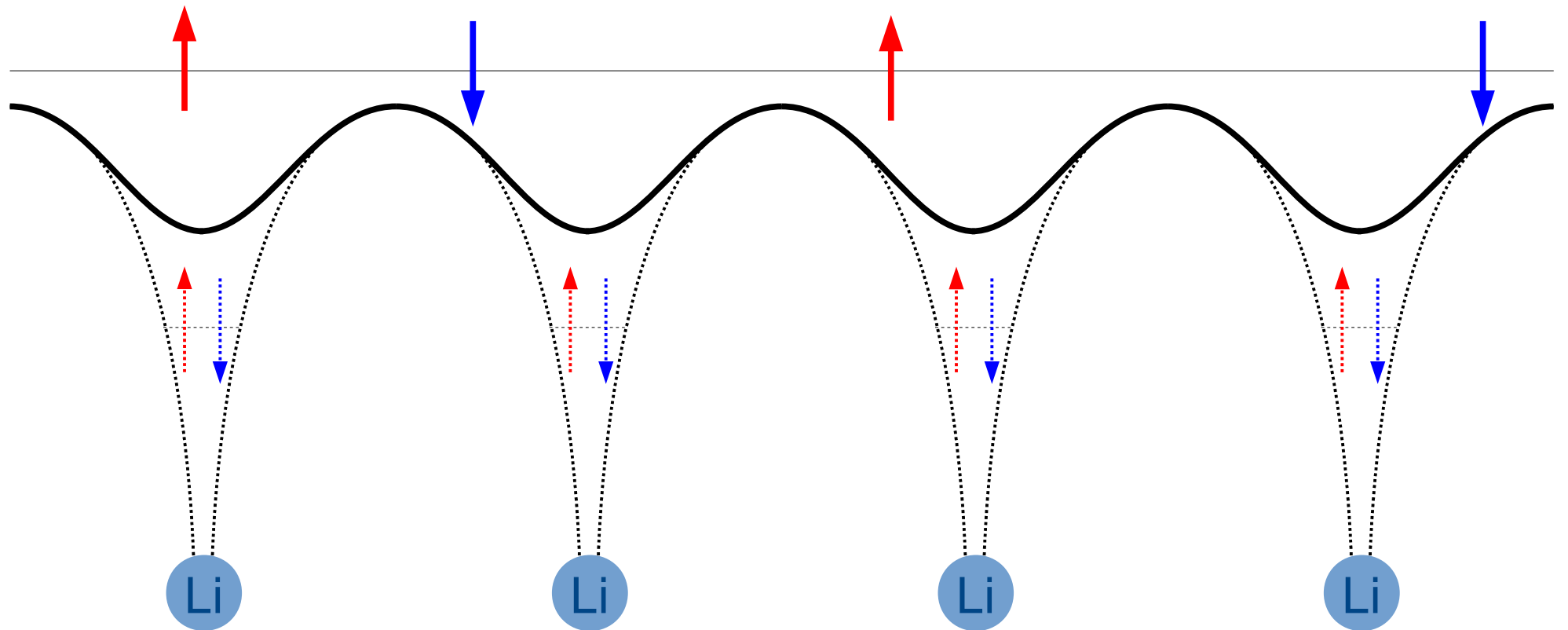
Pseudopotential for a single atom



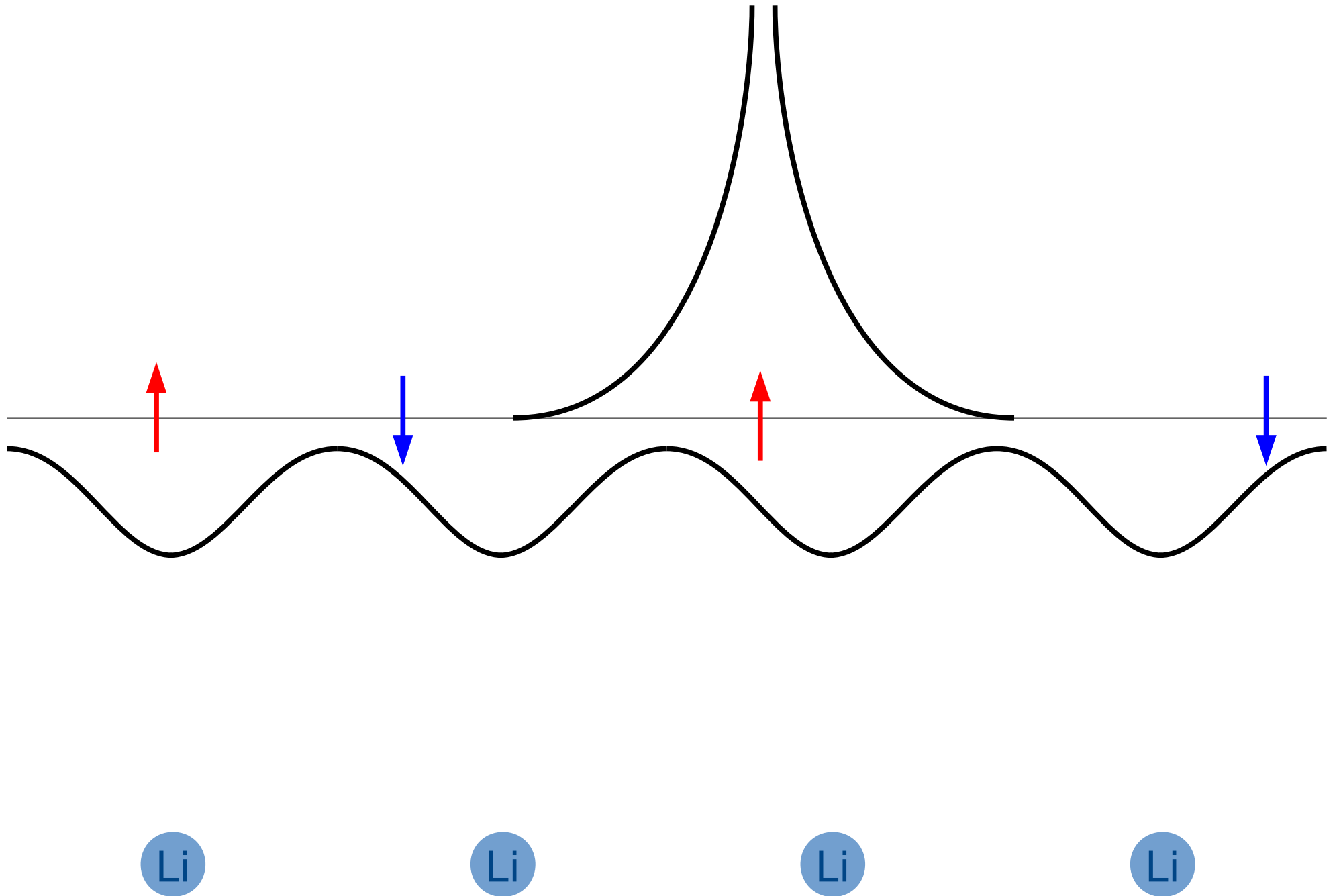
Pseudopotential for atoms



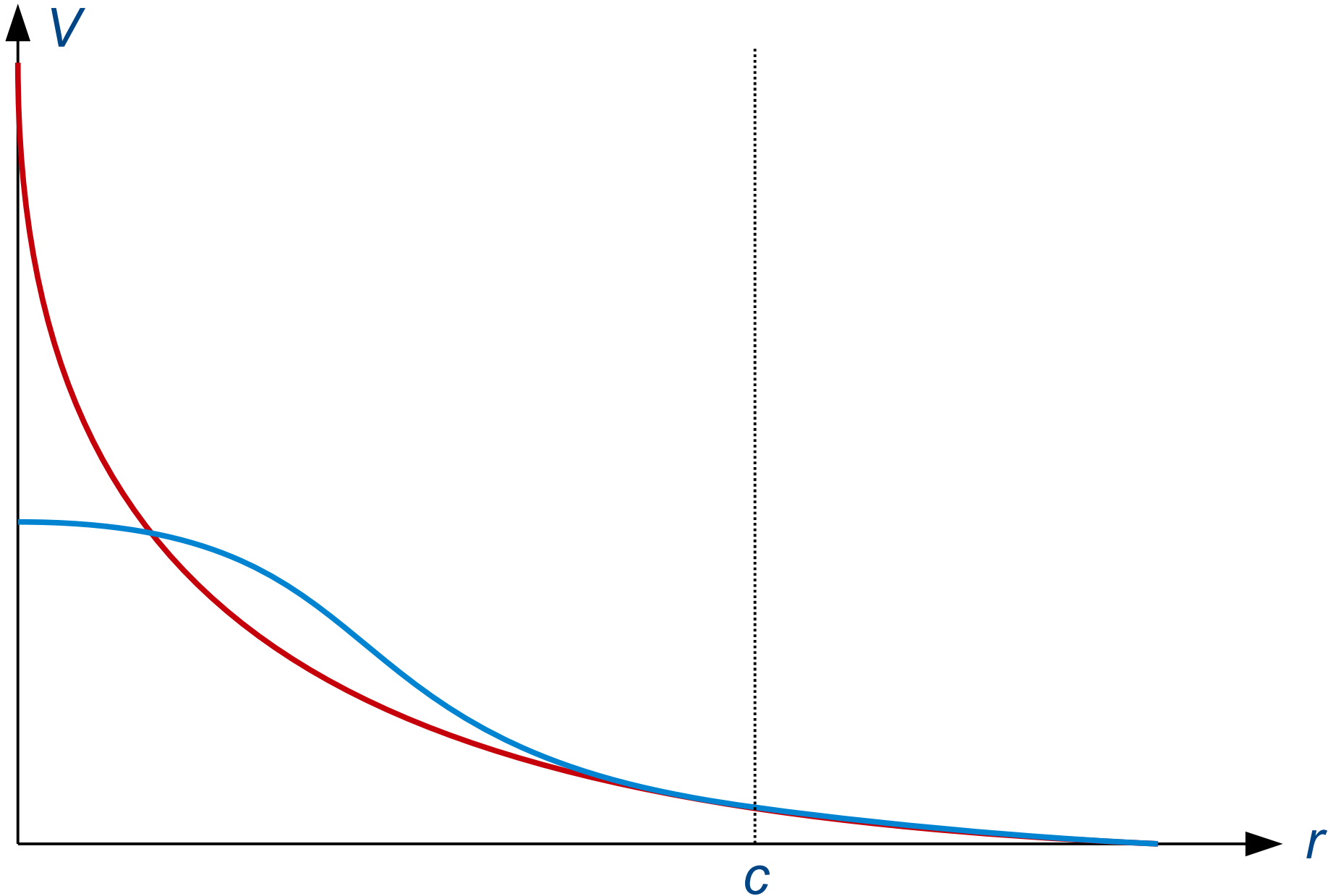
Pseudopotential for atoms



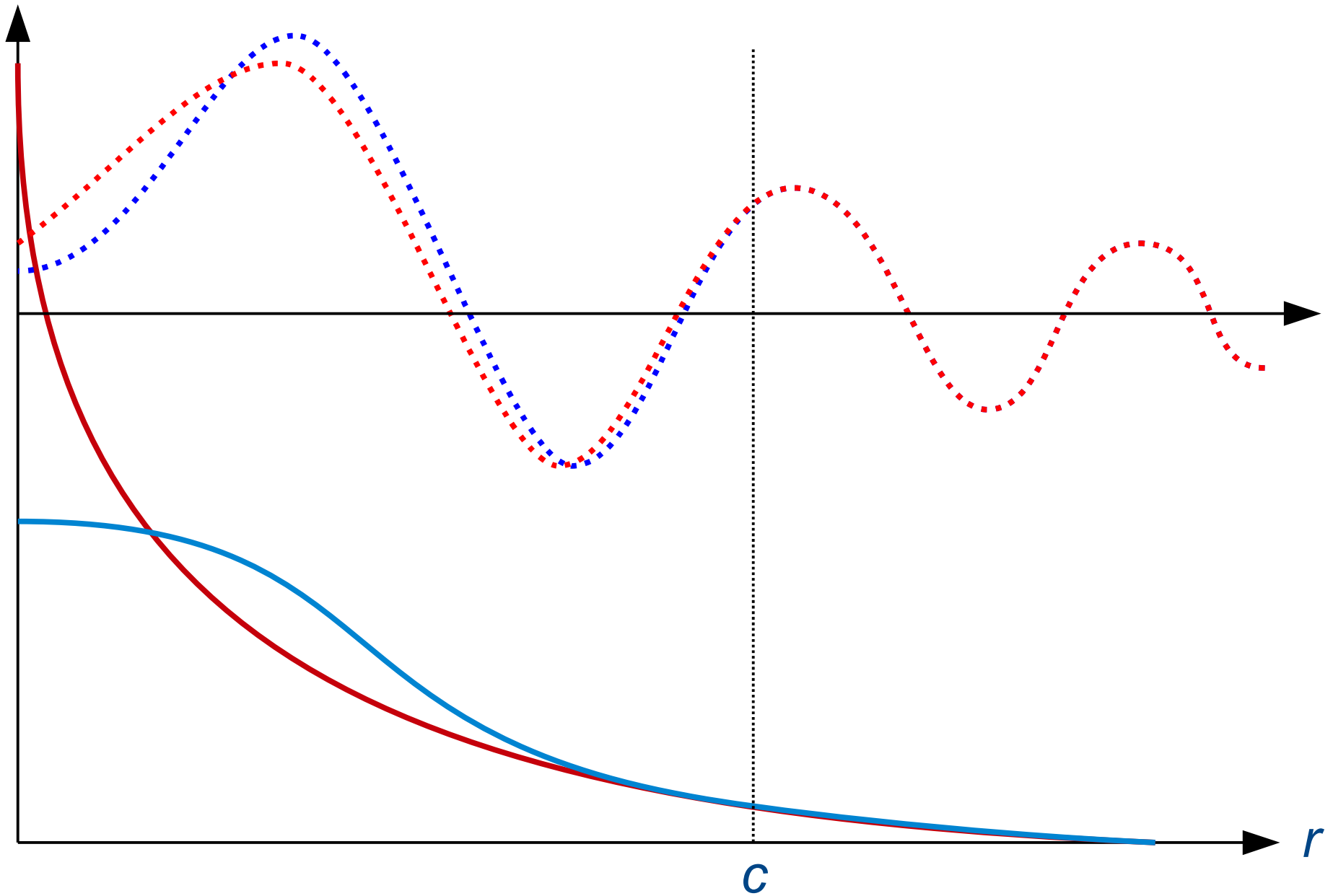
Pseudopotential for atoms



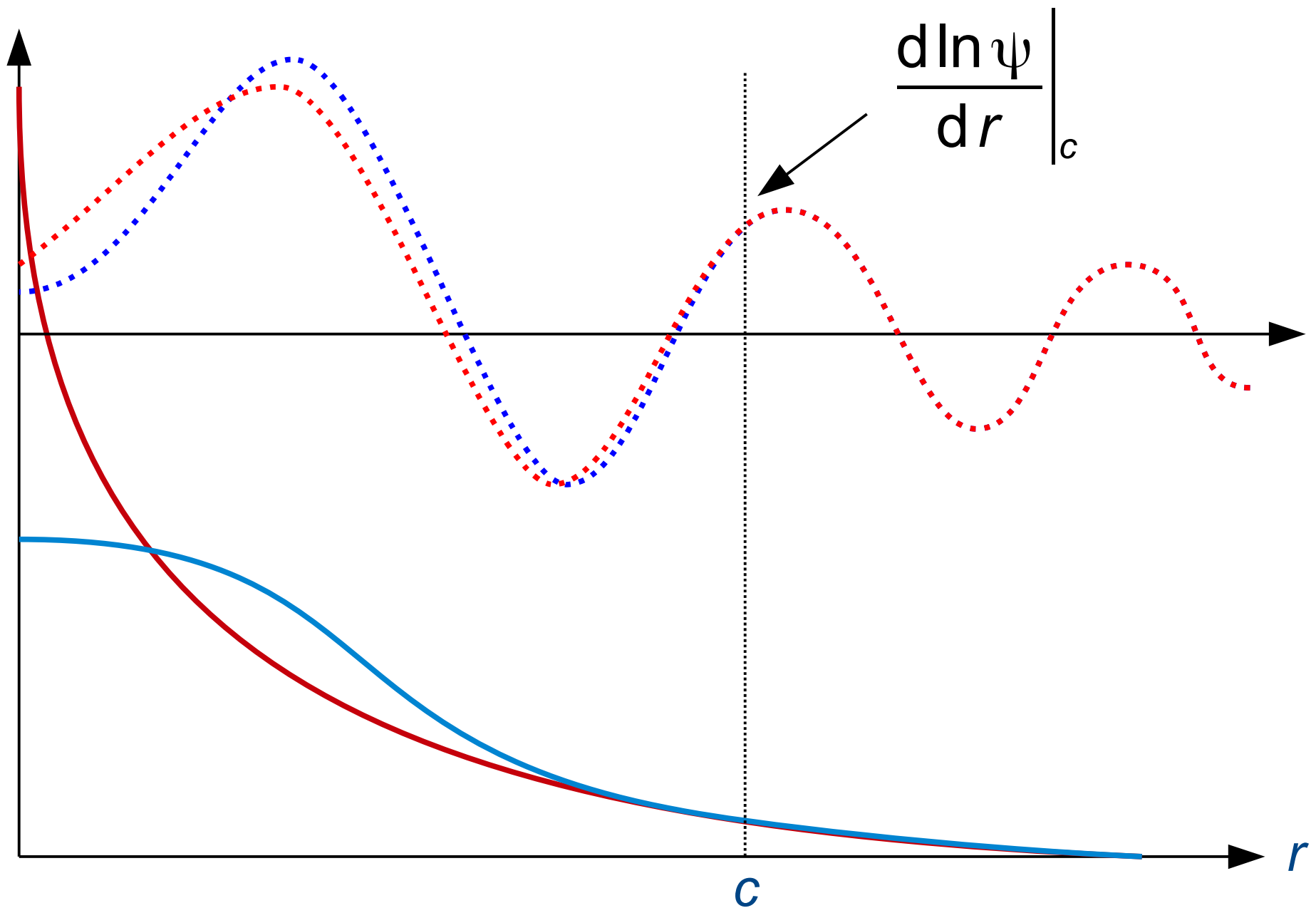
Construction of a pseudopotential



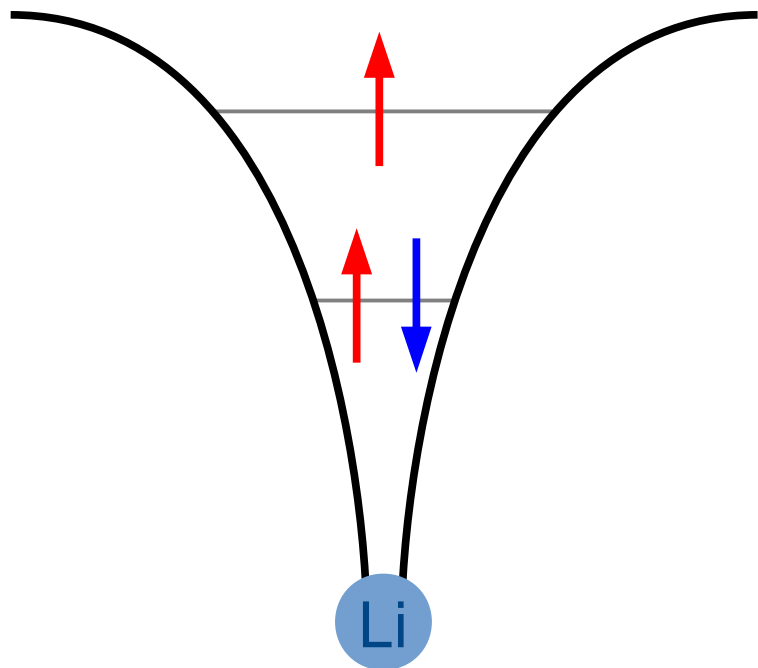
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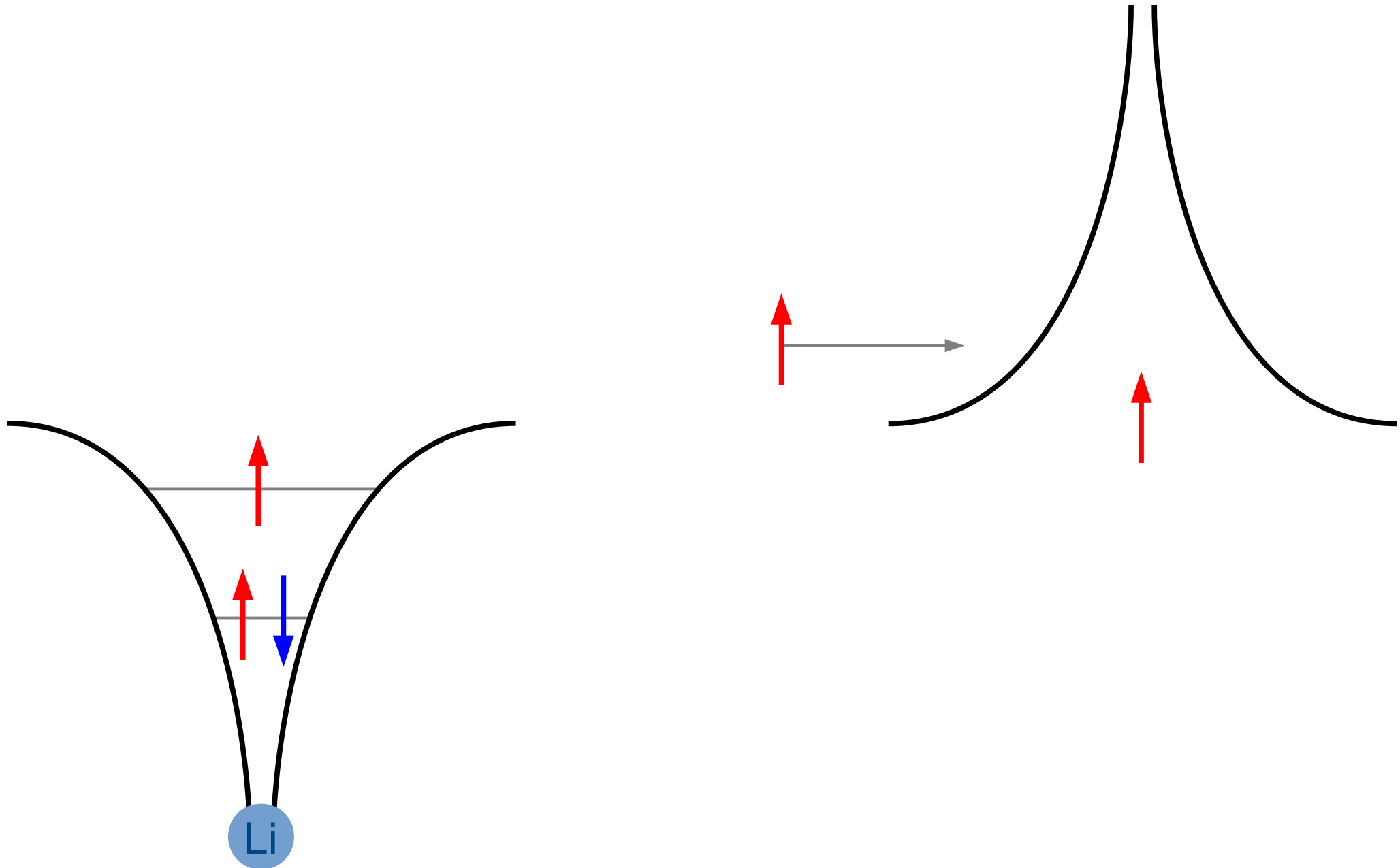
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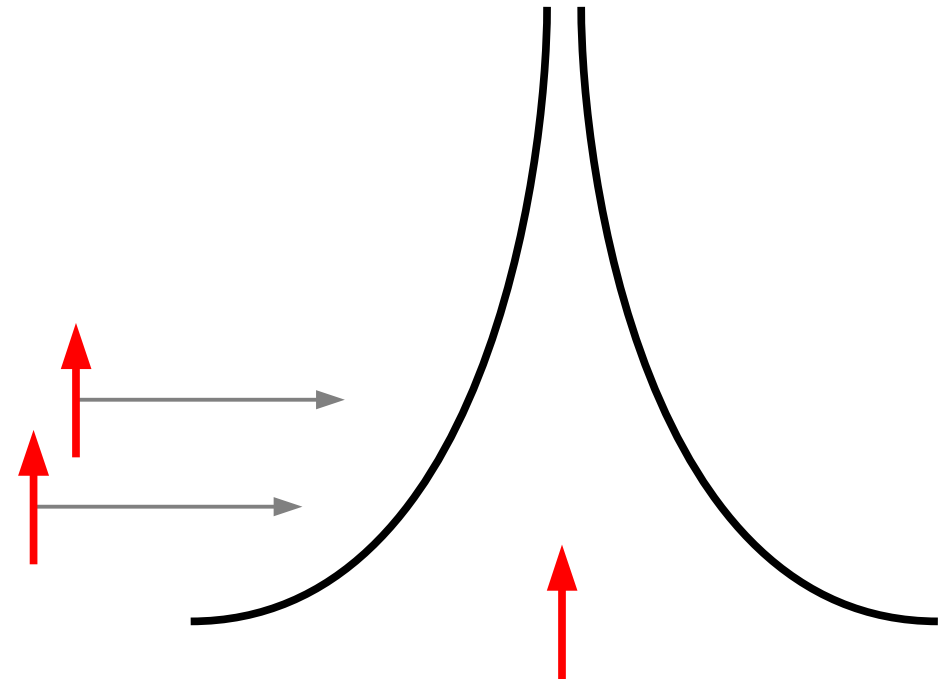
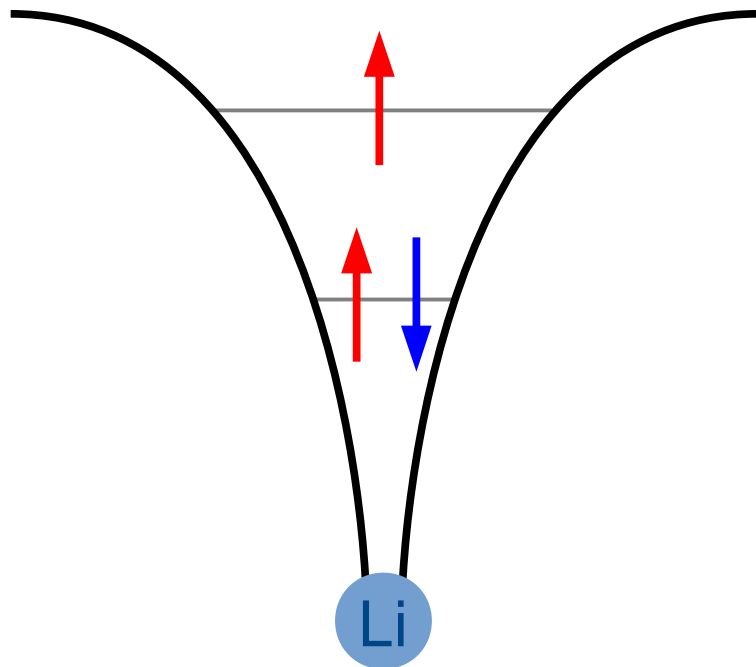
Pseudopotential atoms vs. electrons



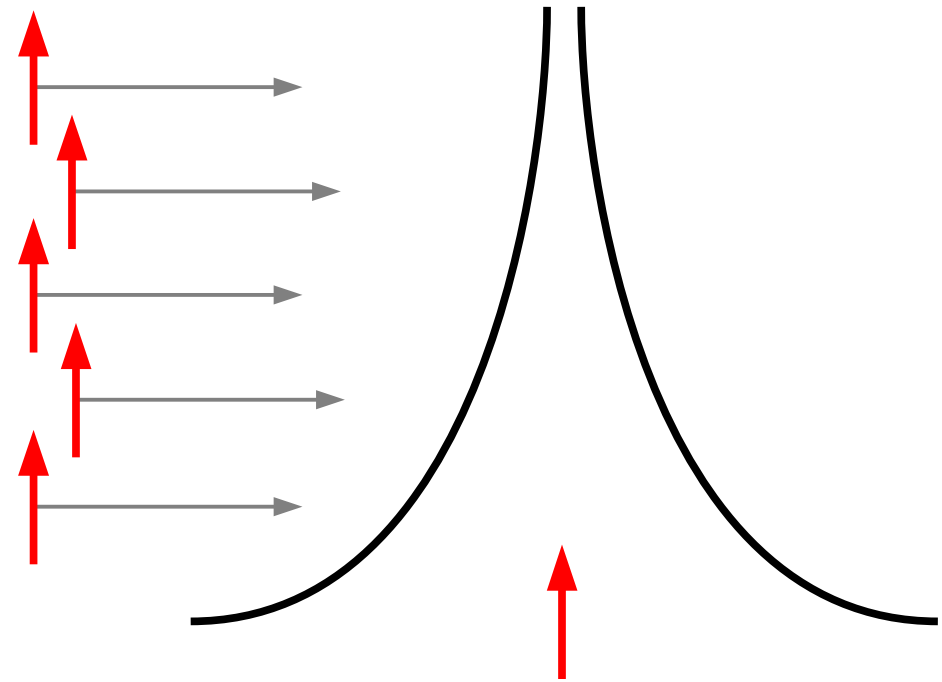
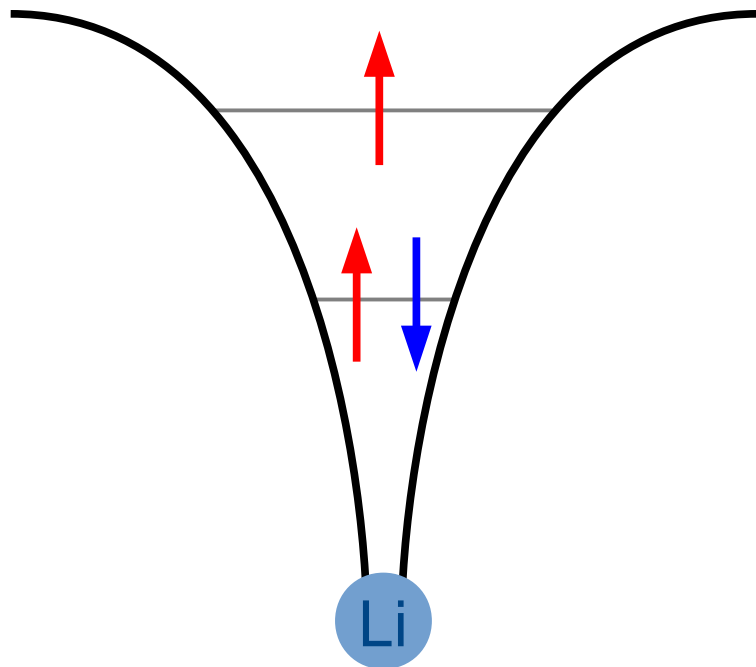
Pseudopotential atoms vs. electrons



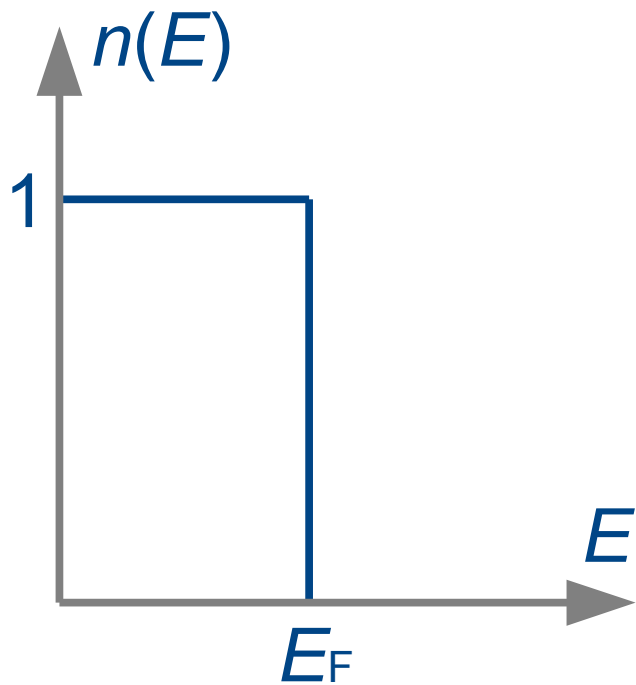
Pseudopotential atoms vs. electrons



Pseudopotential atoms vs. electrons

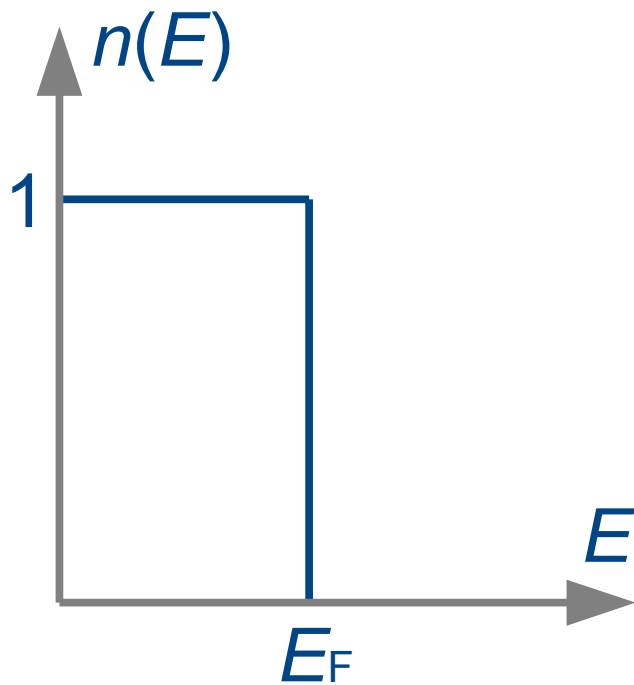


Fermi's two ideas

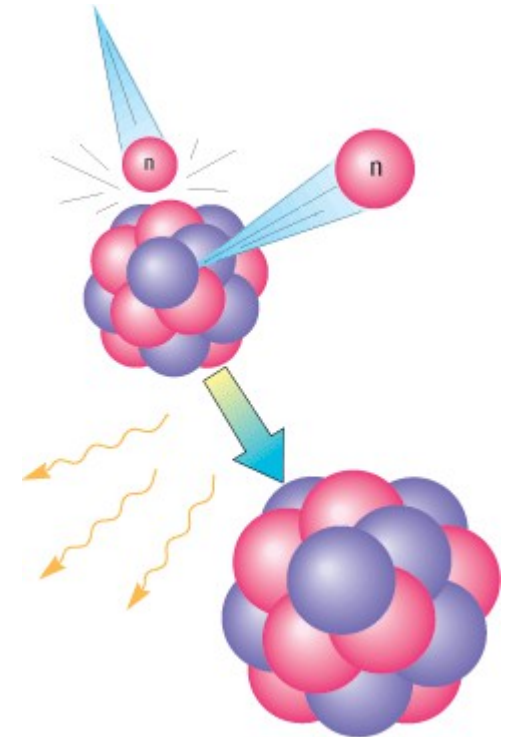


Fermi
surface

Fermi's two ideas



Fermi
surface



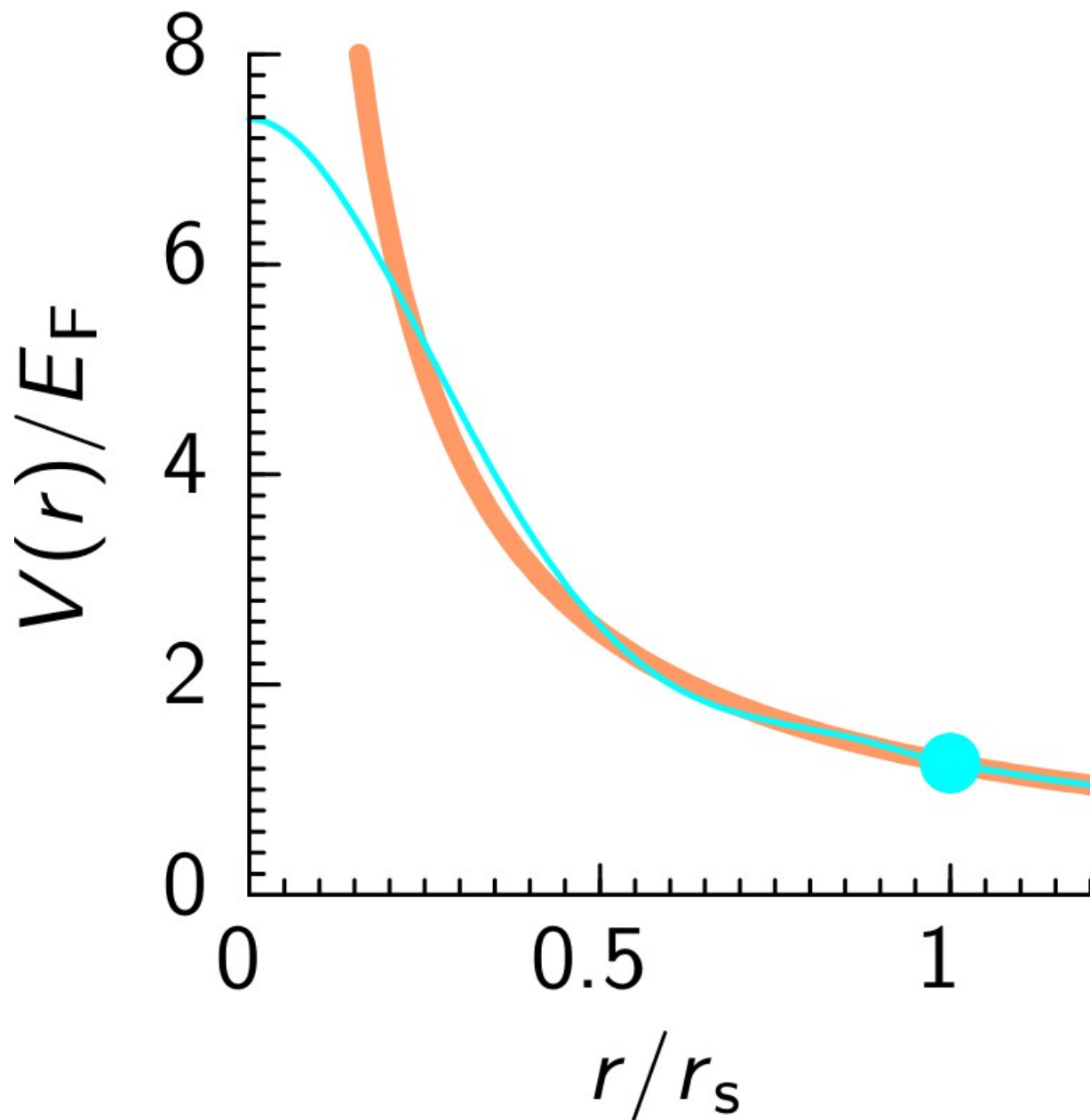
Pseudopotential for
neutron scattering

Construction of a pseudopotential

$$V_{\text{PP}}(r) = \begin{cases} \frac{1}{c} + \left(1 - \frac{r}{c}\right)^2 \left[v_1 \left(\frac{1}{2} + \frac{r}{c}\right) + \sum_{i=2}^{N_v} v_i \left(\frac{r}{c}\right)^i \right] & r < c \\ \frac{1}{r} & r > c \end{cases}$$

$$\sum_{l=0}^{l_{\max}} \int_0^{2k_F} dk \left[\left. \frac{d \ln \psi_{\text{PP}}(k, l)}{dr} \right|_c - \left. \frac{d \ln \psi_{\text{Coul}}(k, l)}{dr} \right|_c \right]^2$$

Pseudopotential



Quantum Monte Carlo

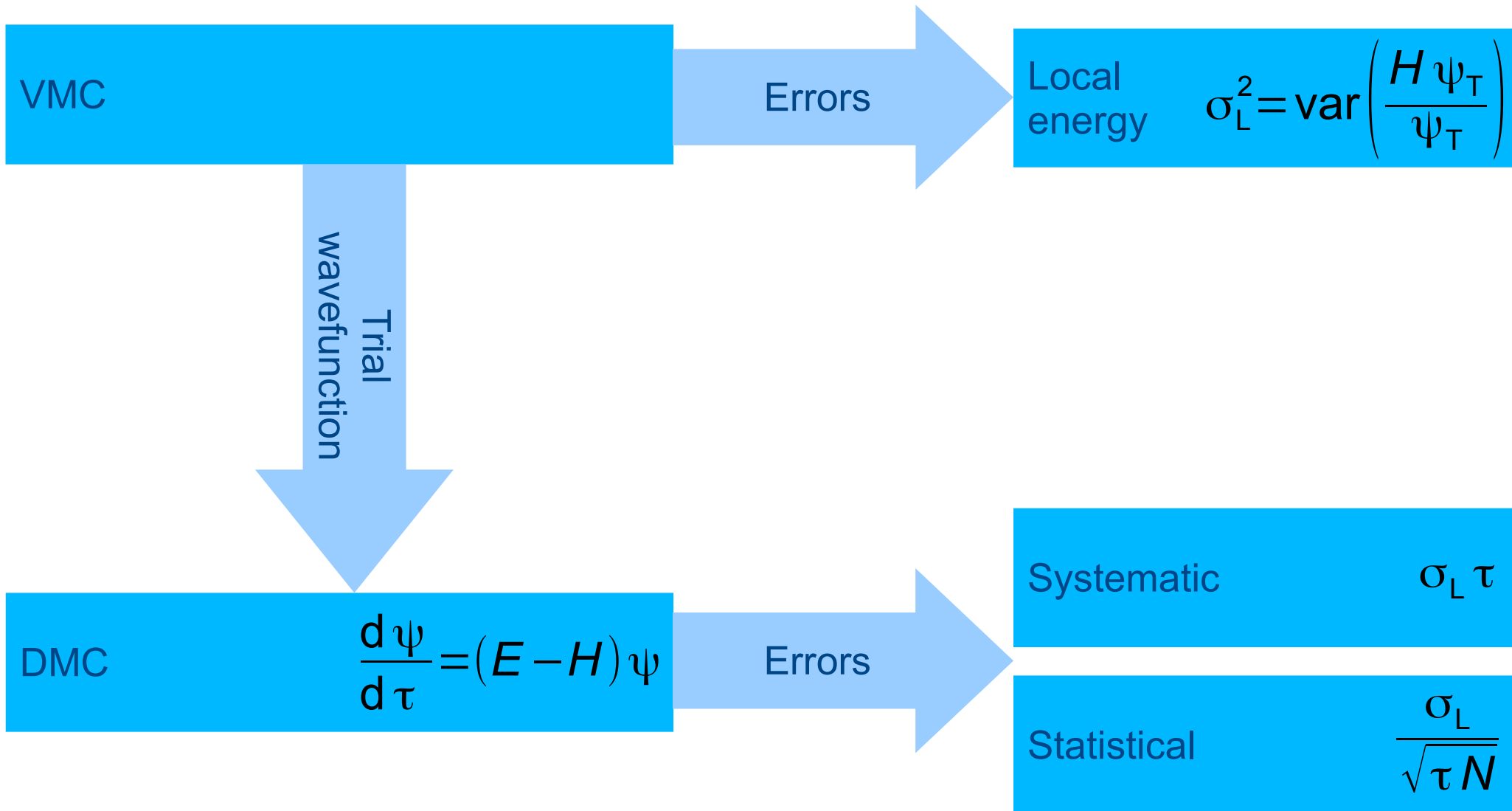
VMC

Errors

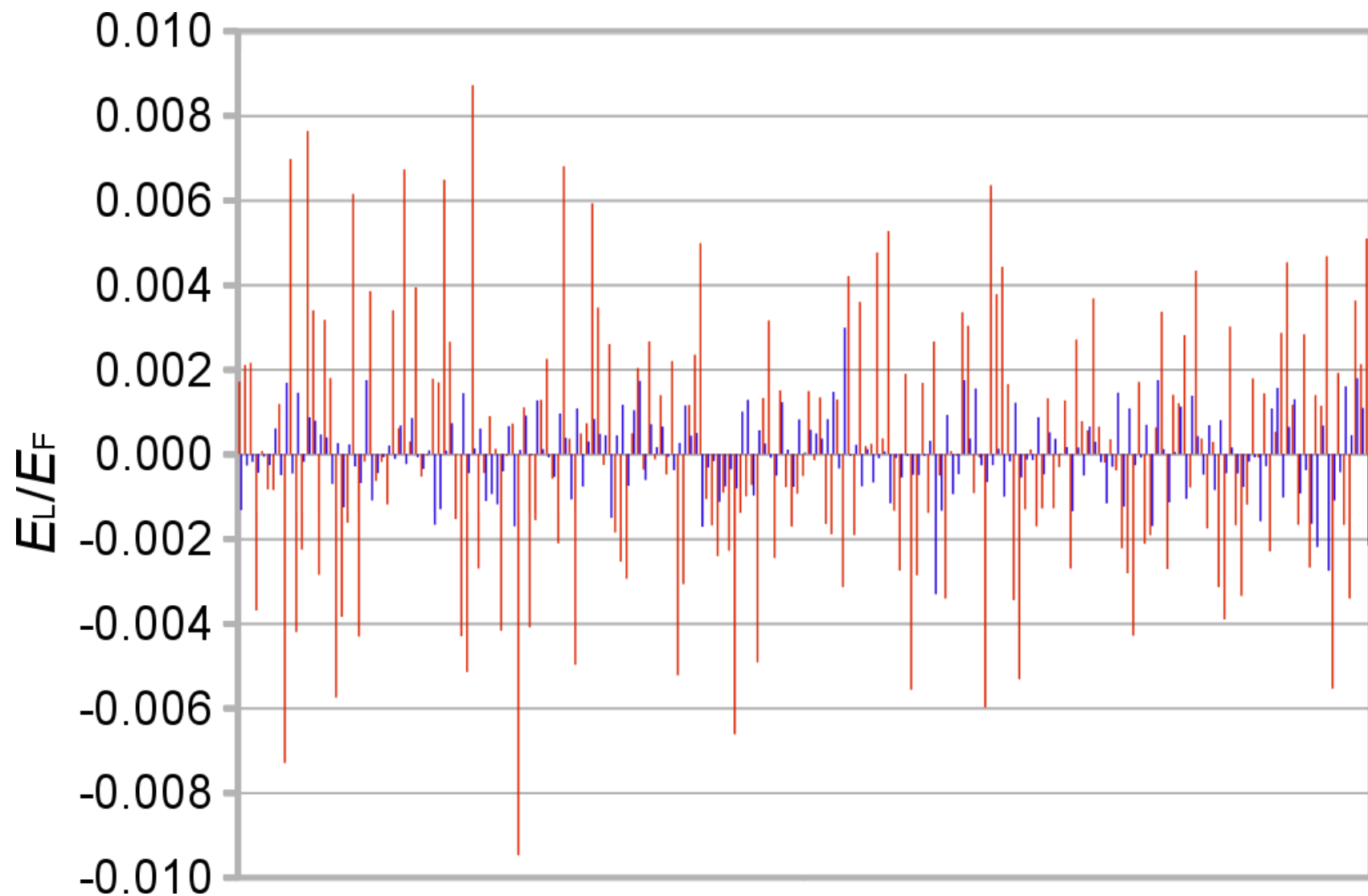
Local
energy

$$\sigma_L^2 = \text{var} \left(\frac{H \psi_T}{\psi_T} \right)$$

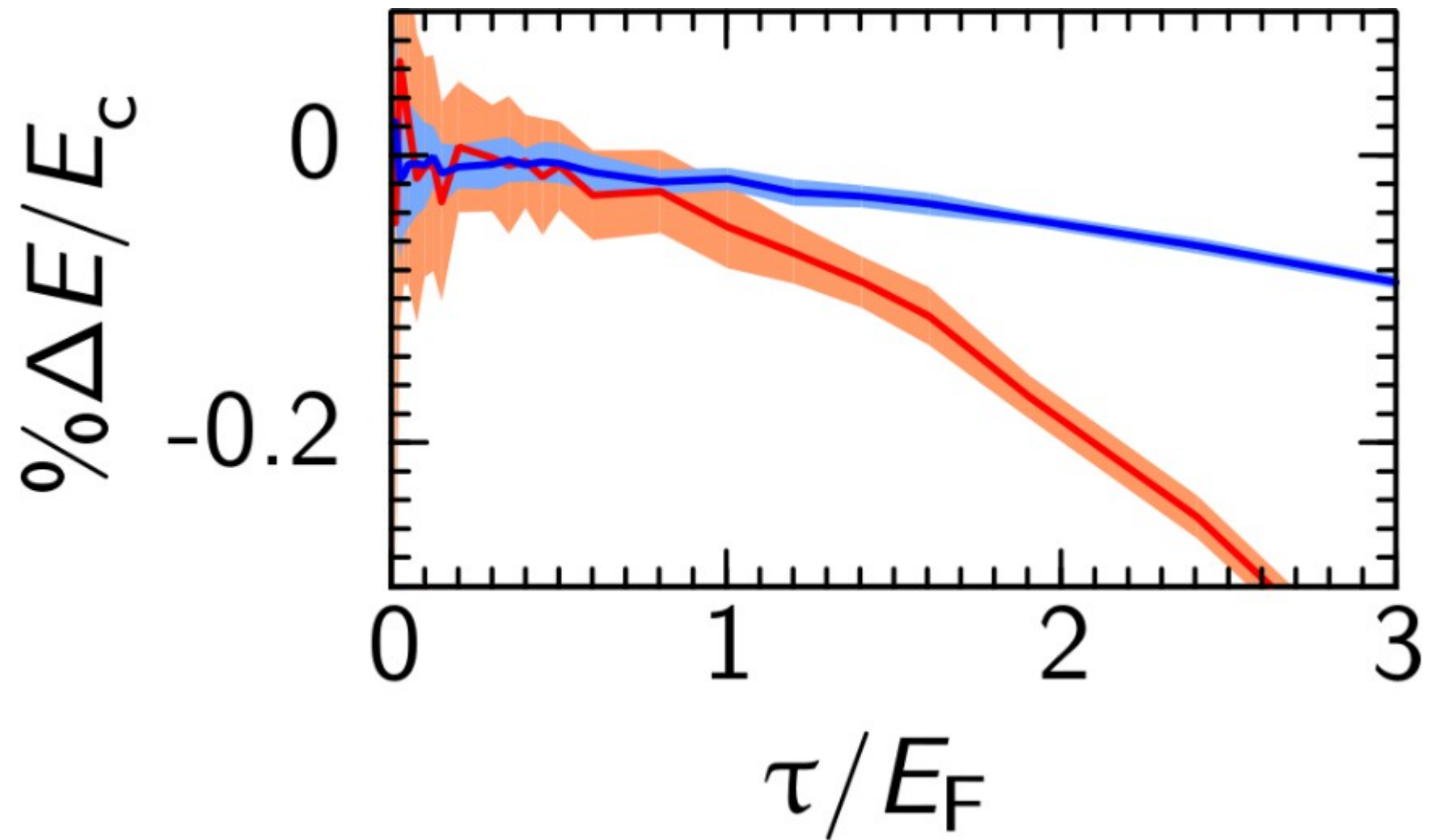
Quantum Monte Carlo



Pseudopotential: local energy



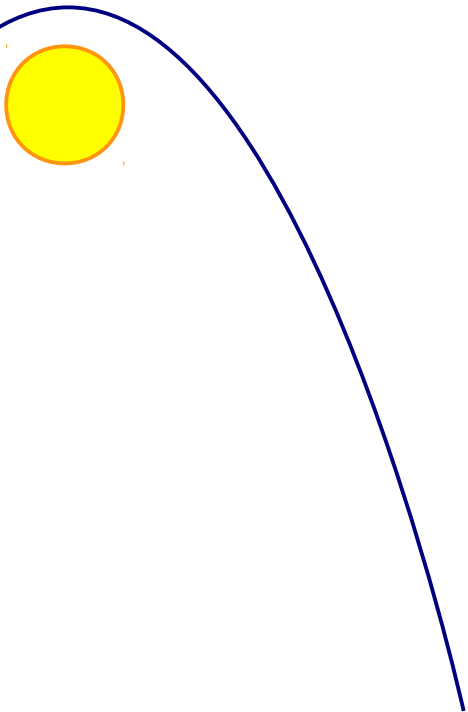
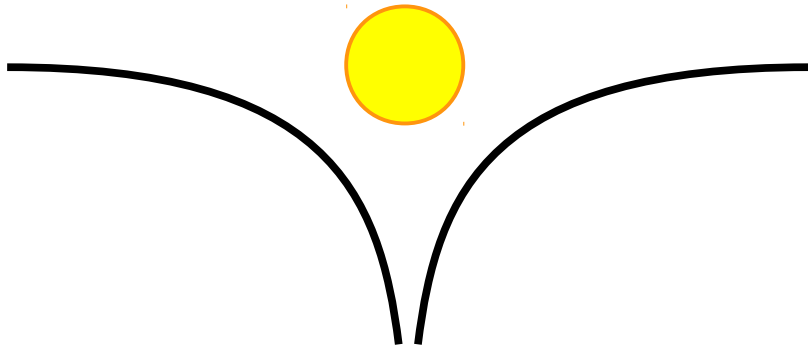
Pseudopotential: time step



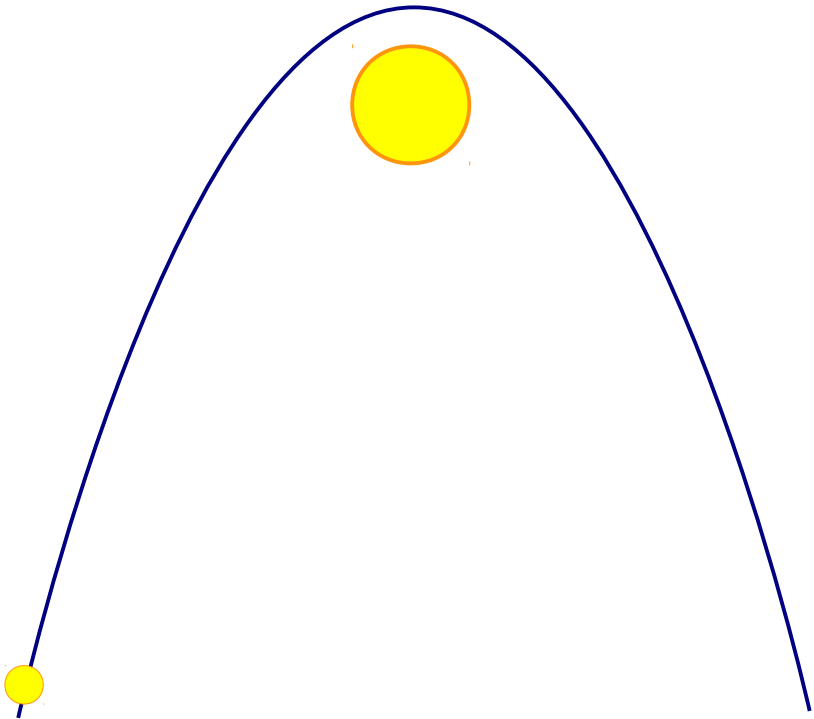
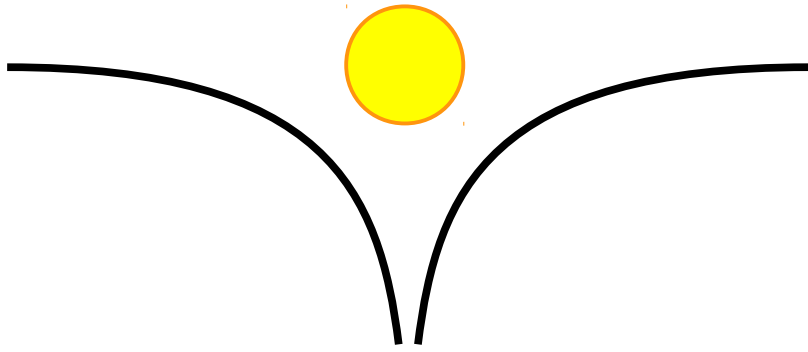
Galactic dynamics



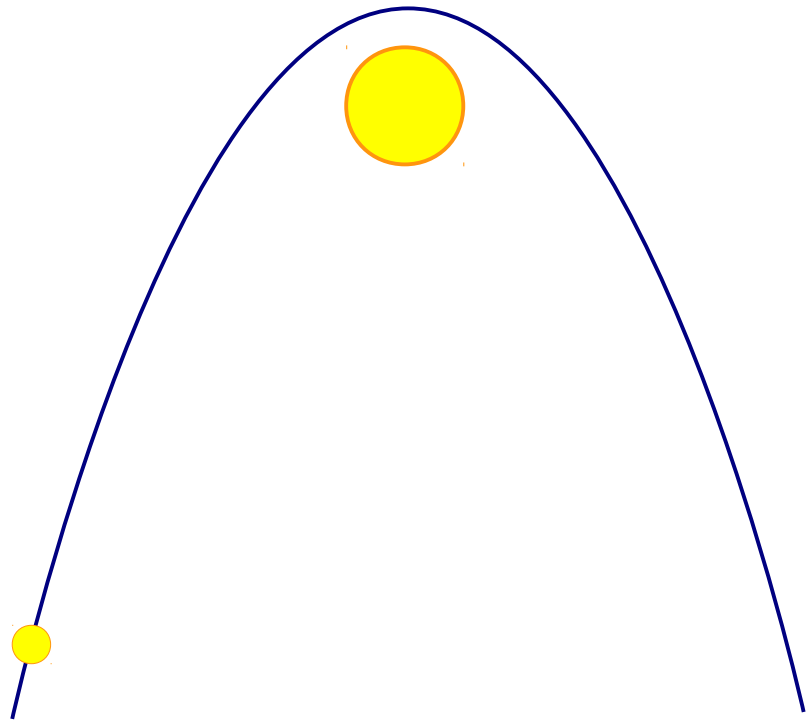
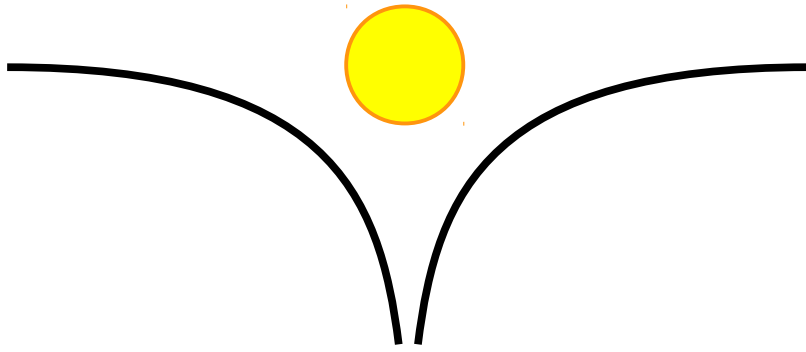
Galactic dynamics



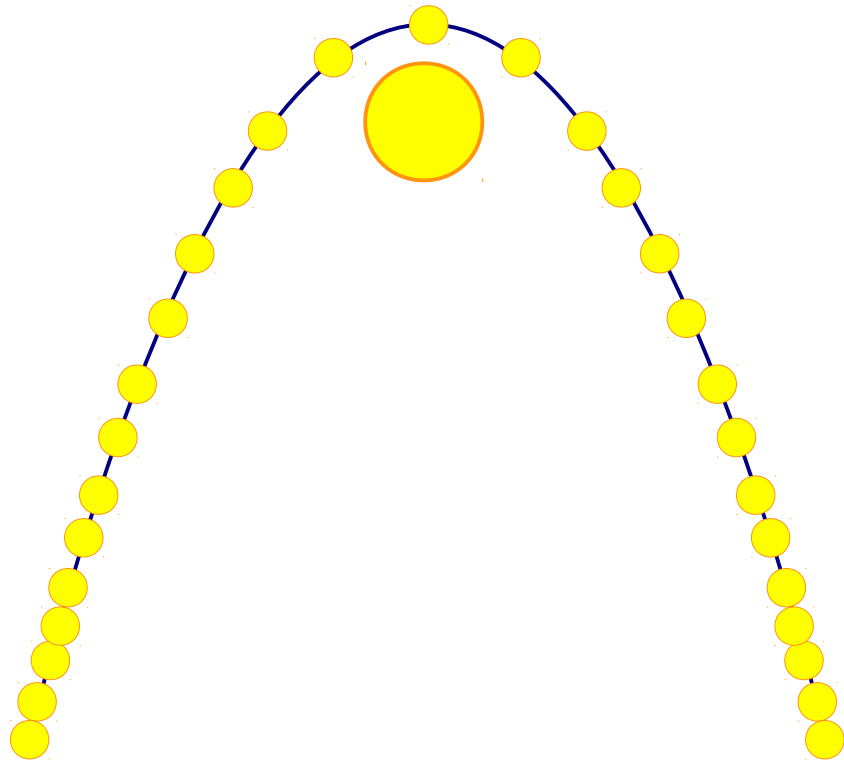
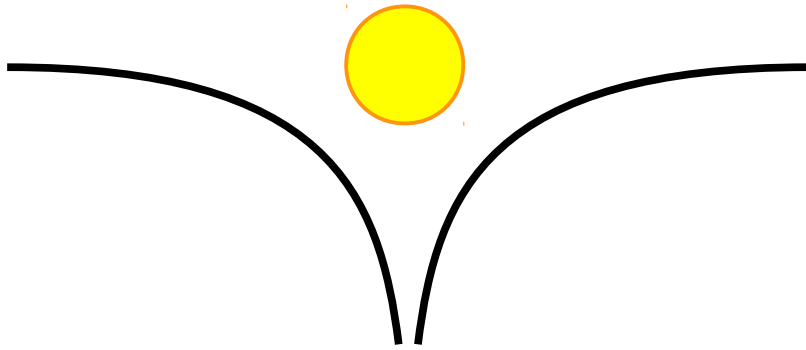
Galactic dynamics



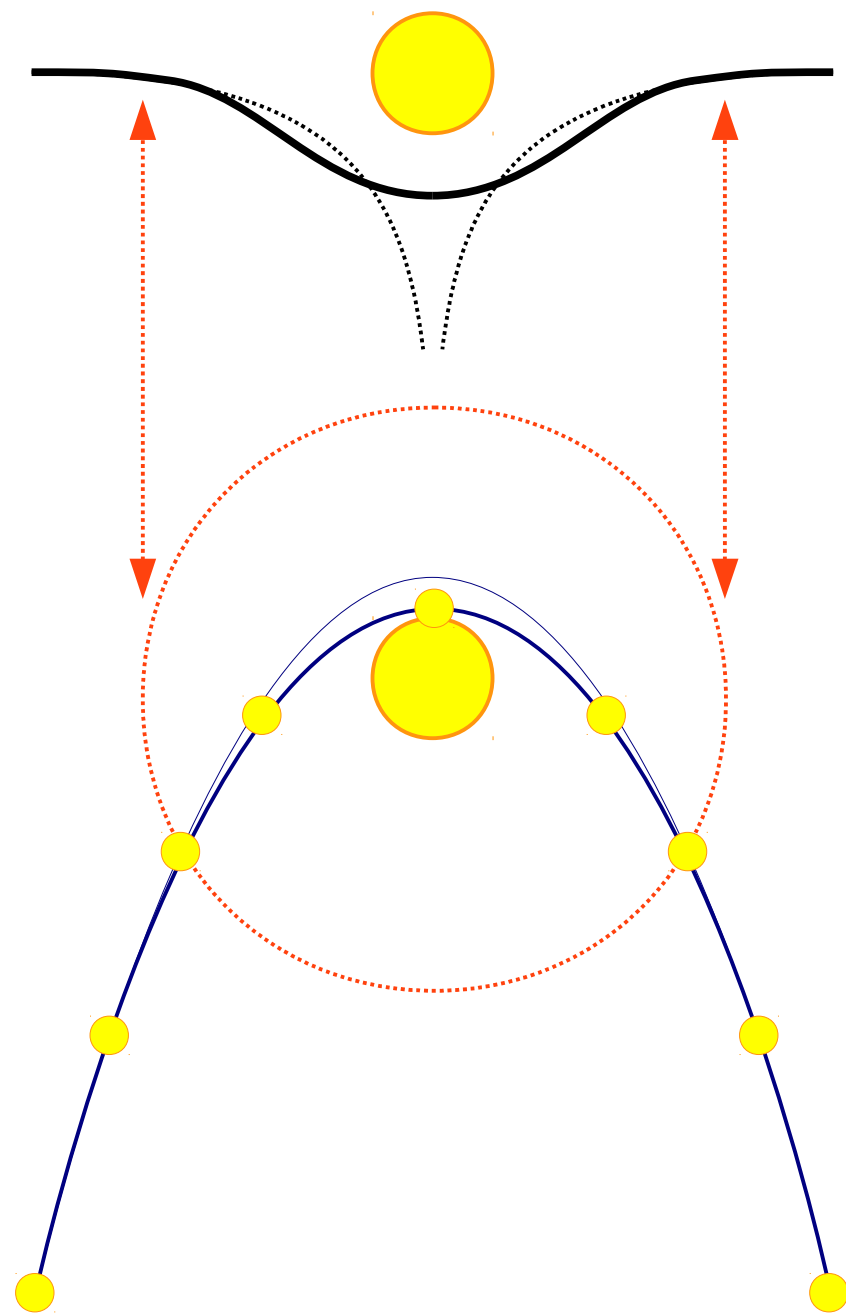
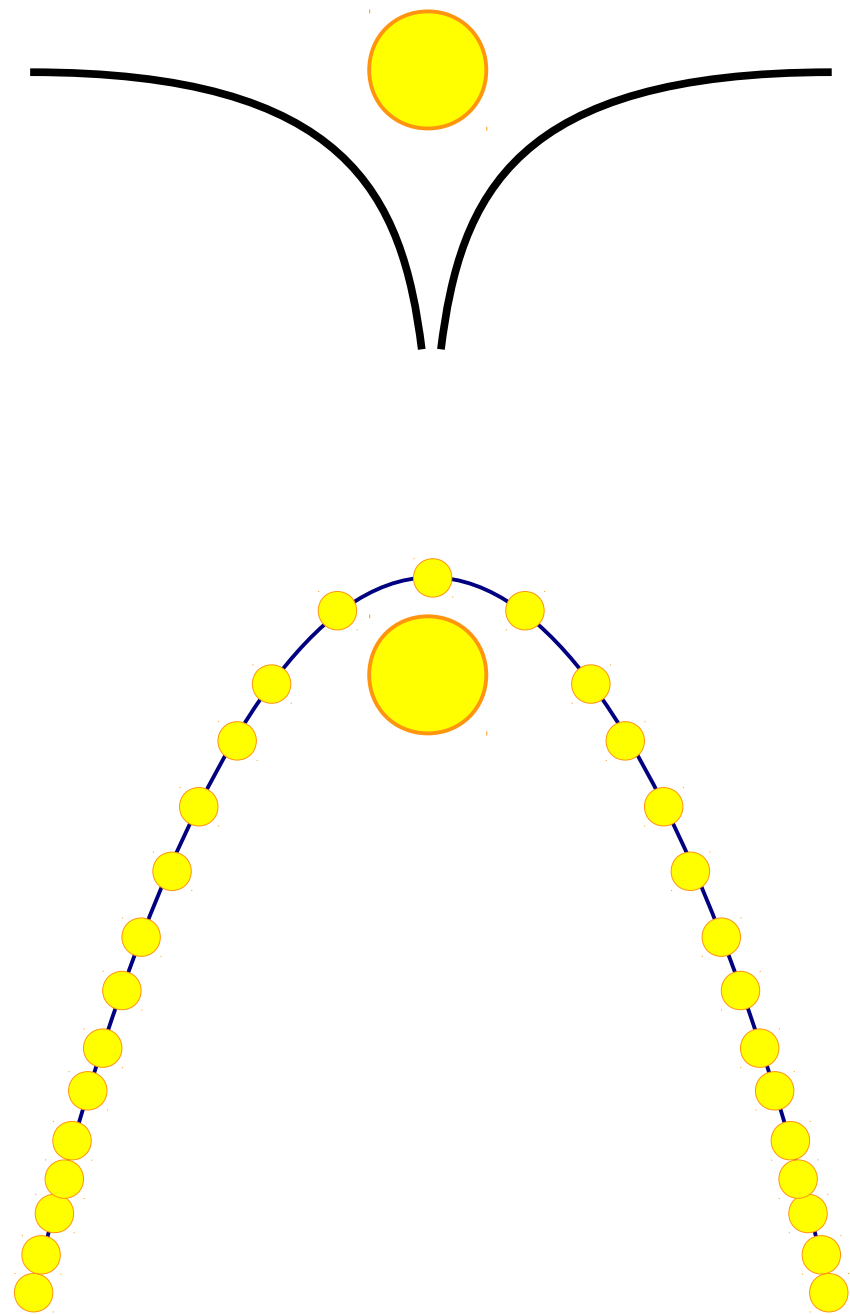
Galactic dynamics



Galactic dynamics



Galactic dynamics



Summary

Developed a pseudopotential for the repulsive Coulomb interaction

Accelerates numerical calculations by a factor of 30

Pseudopotentials could be applied to cold atoms contact interaction and galactic dynamics