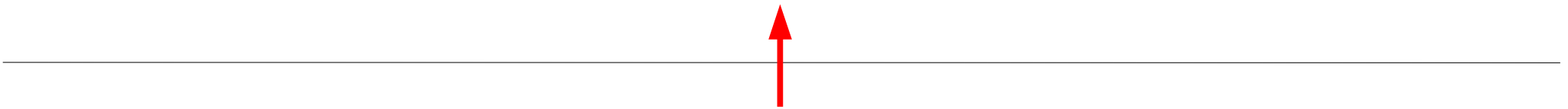
Pseudopotentials reach for the stars

Gareth Conduit

TCM Group, Department of Physics

Pseudopotential for atoms

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



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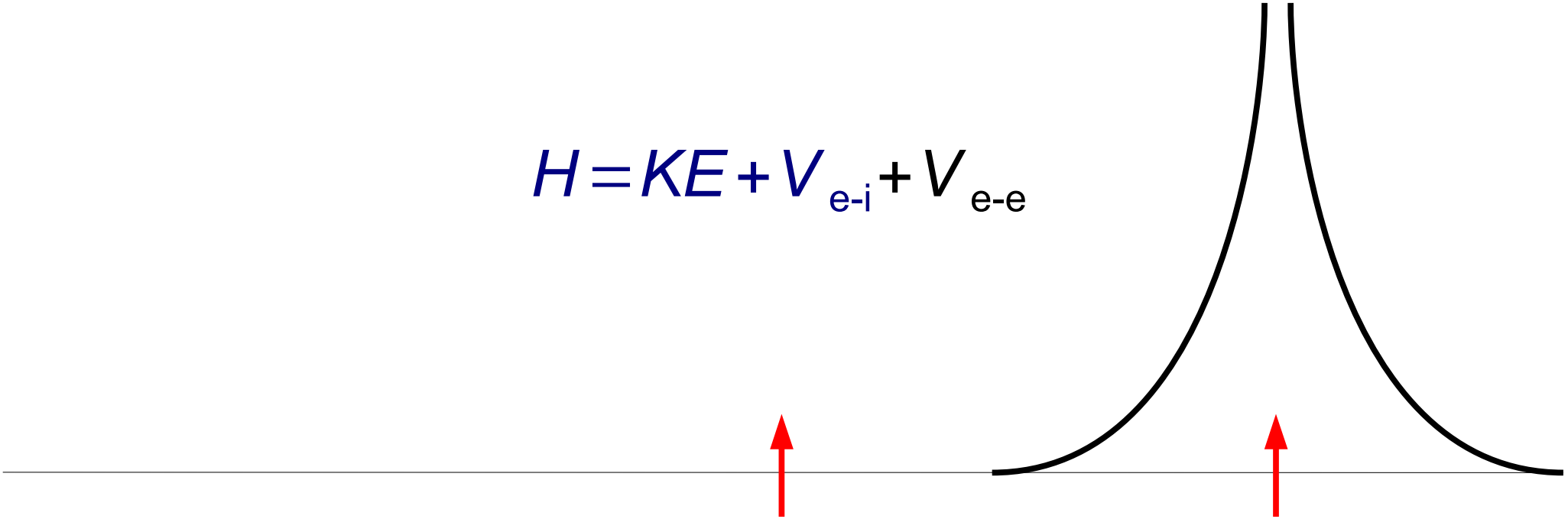

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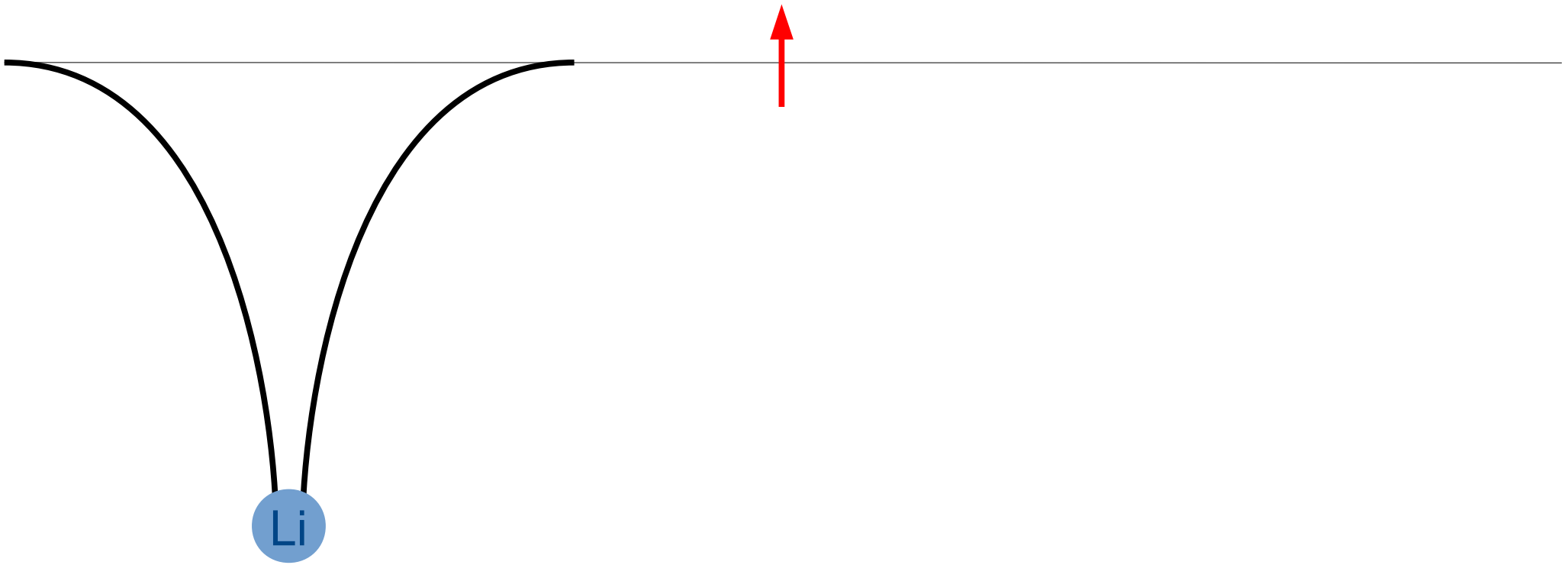
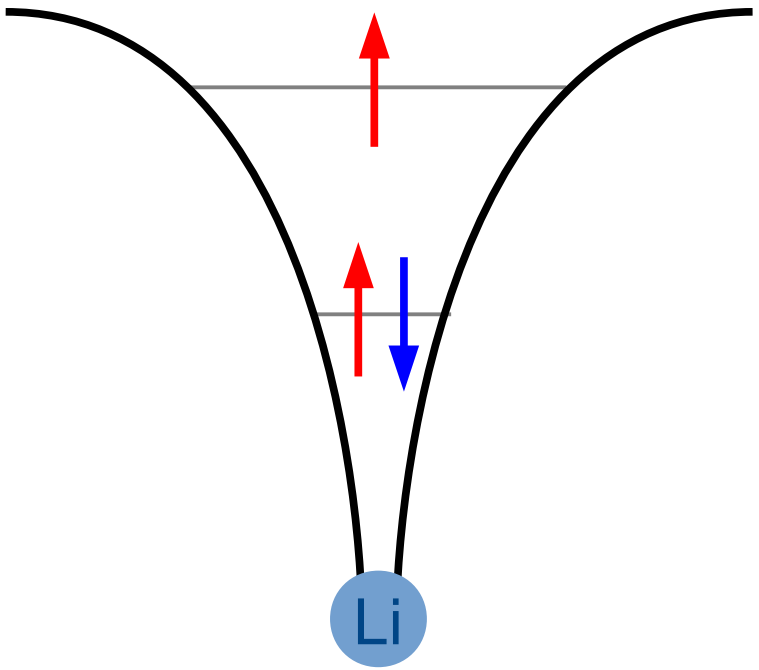
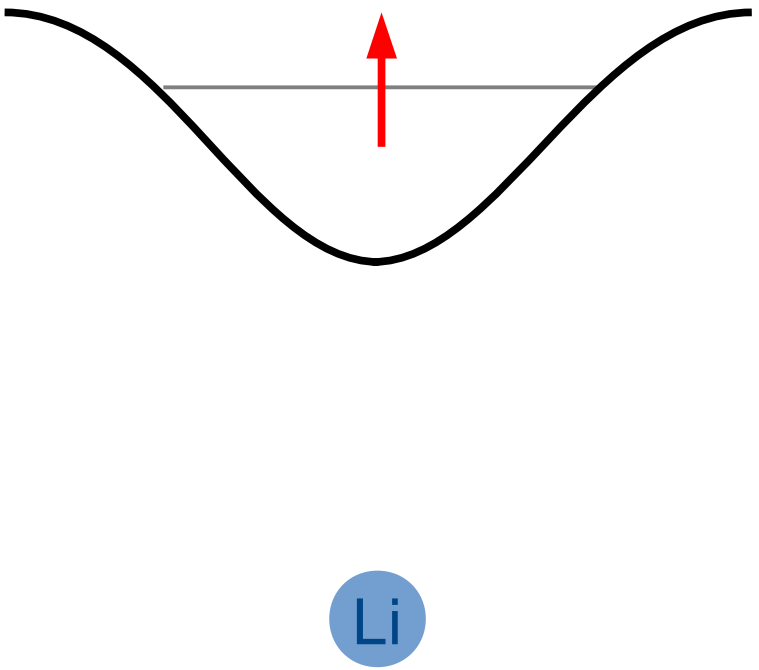


Pseudopotential for a single atom





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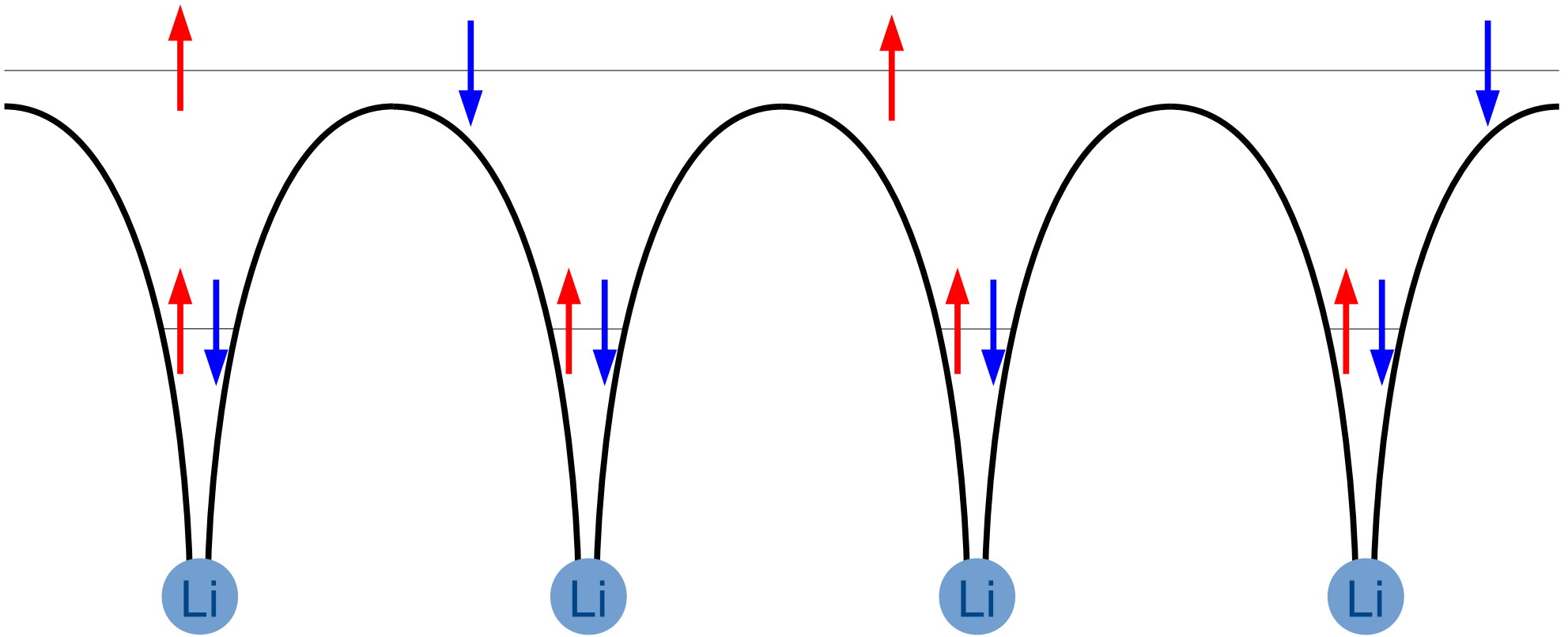

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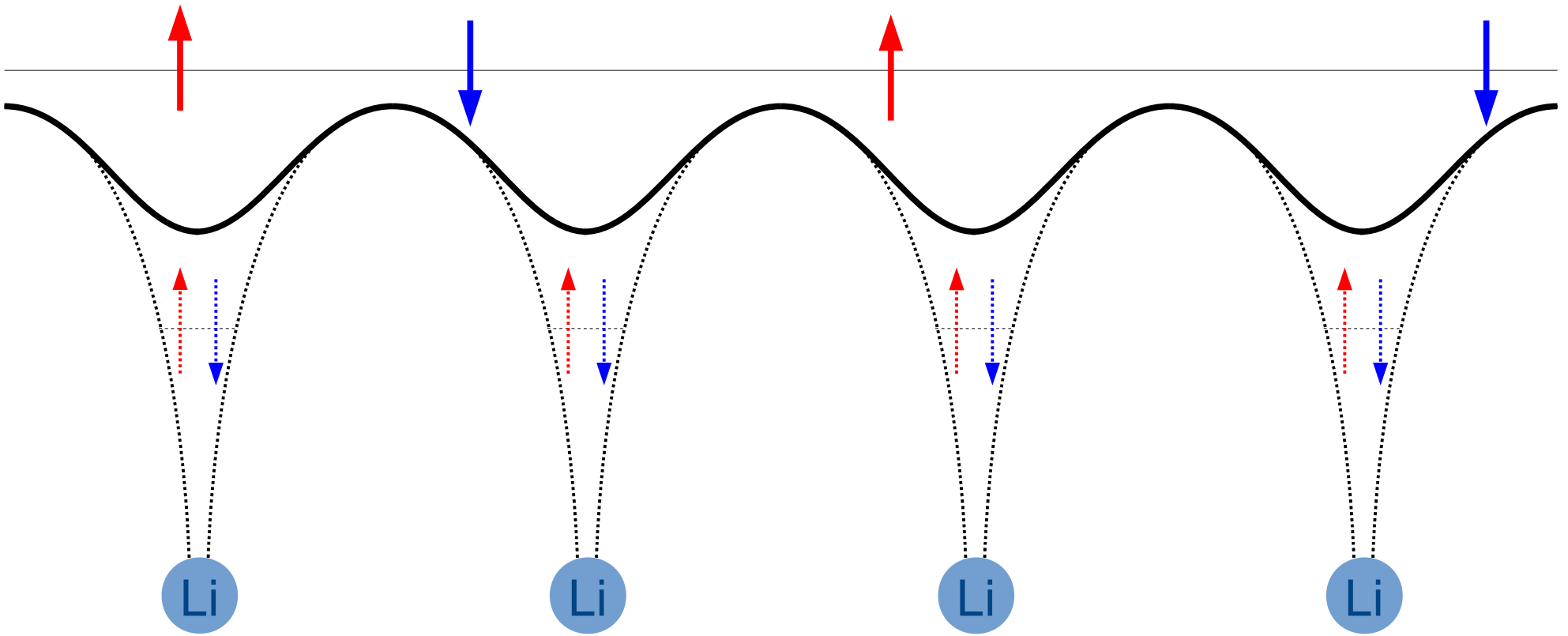

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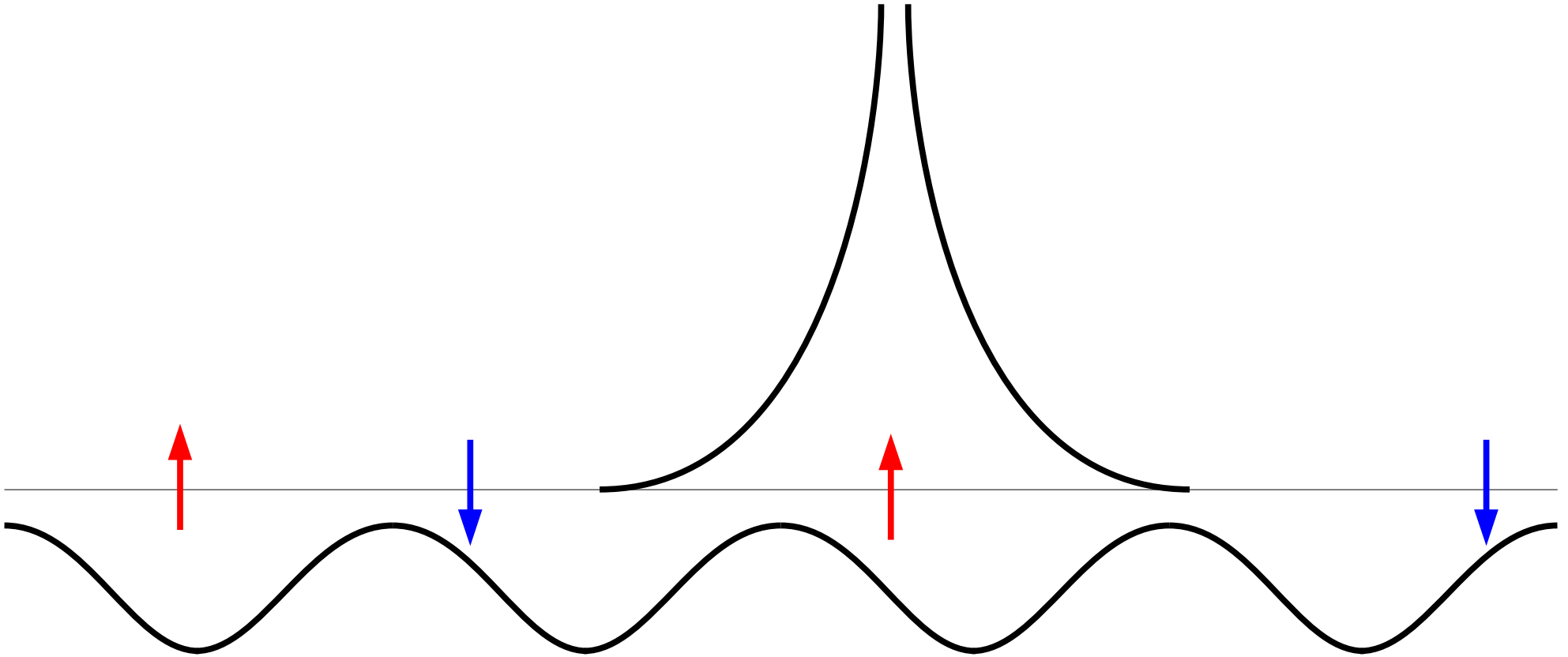
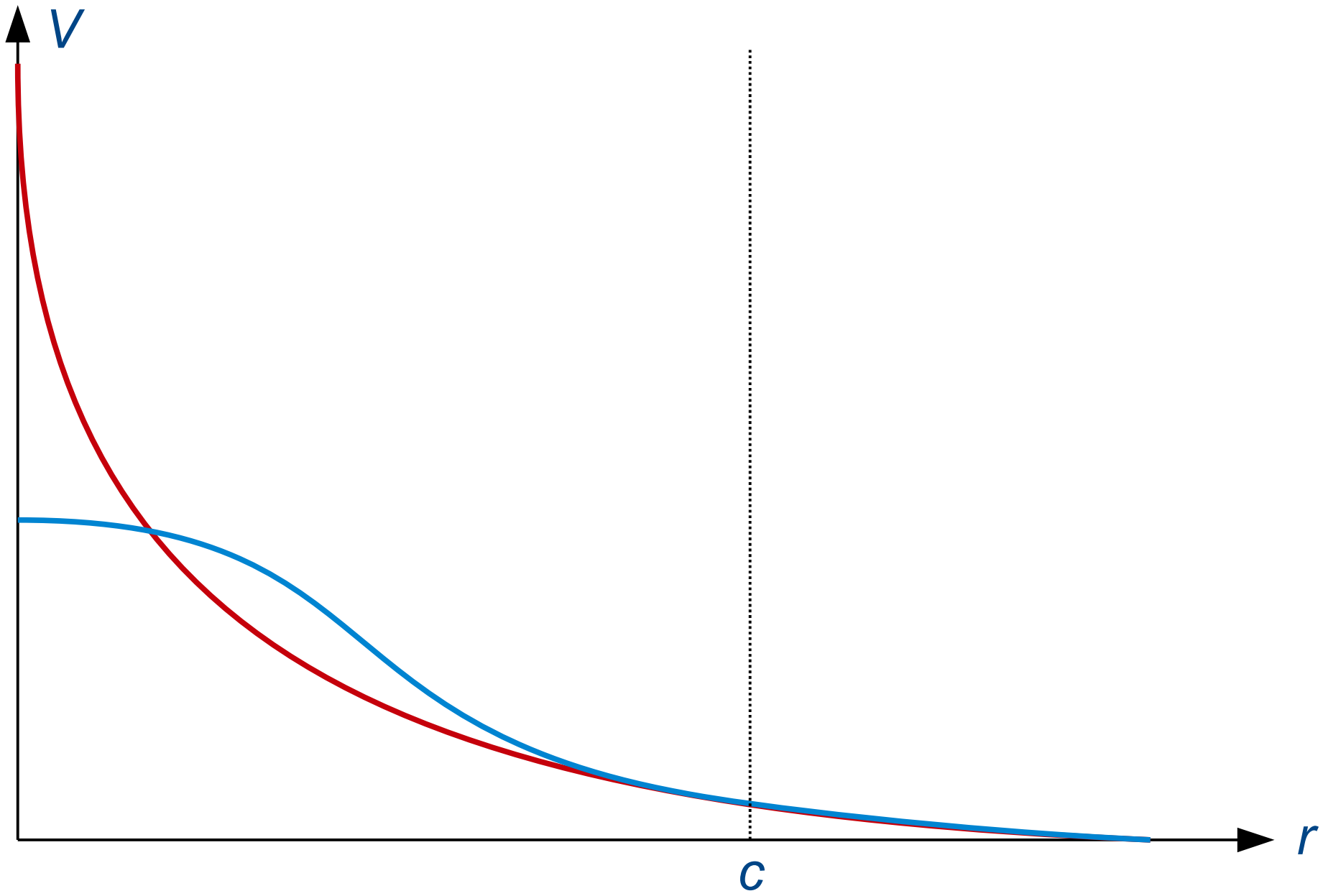


Construction of a pseudopotential



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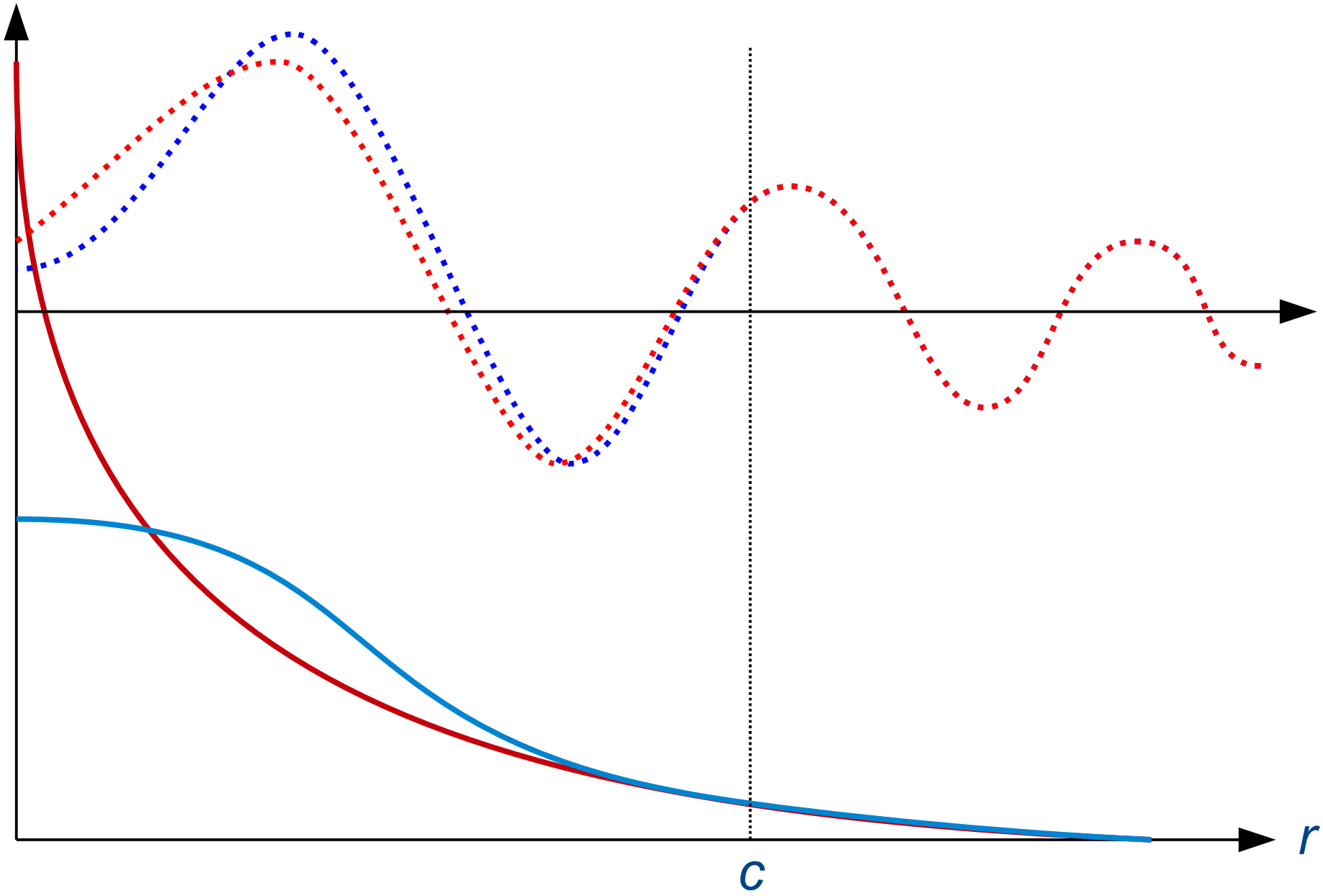

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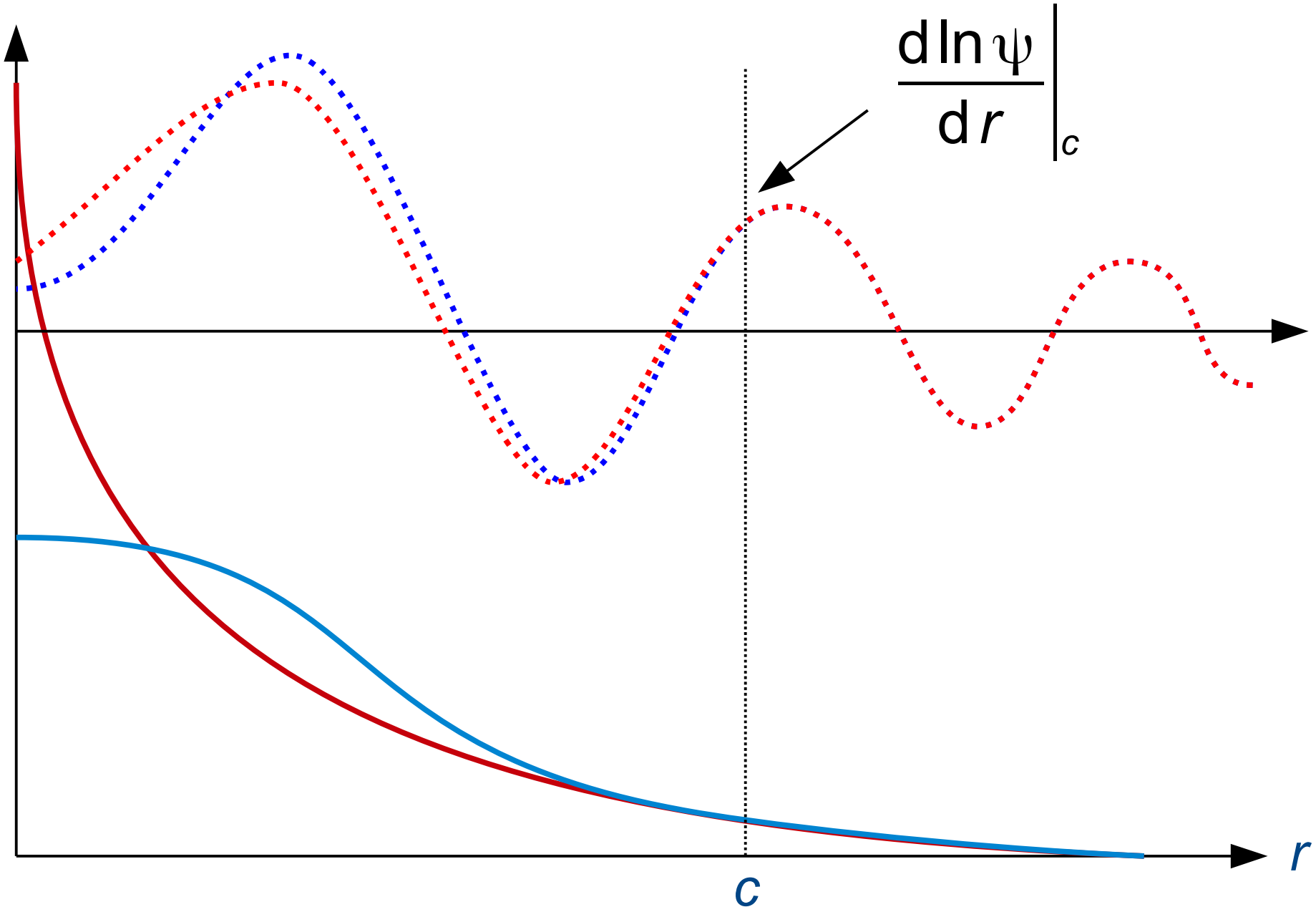
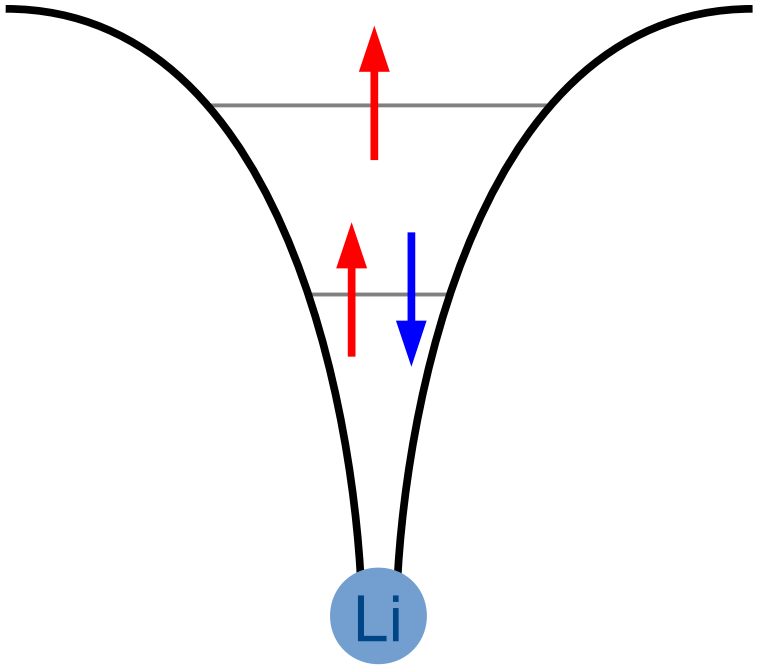


Pseudopotential atoms vs. electrons



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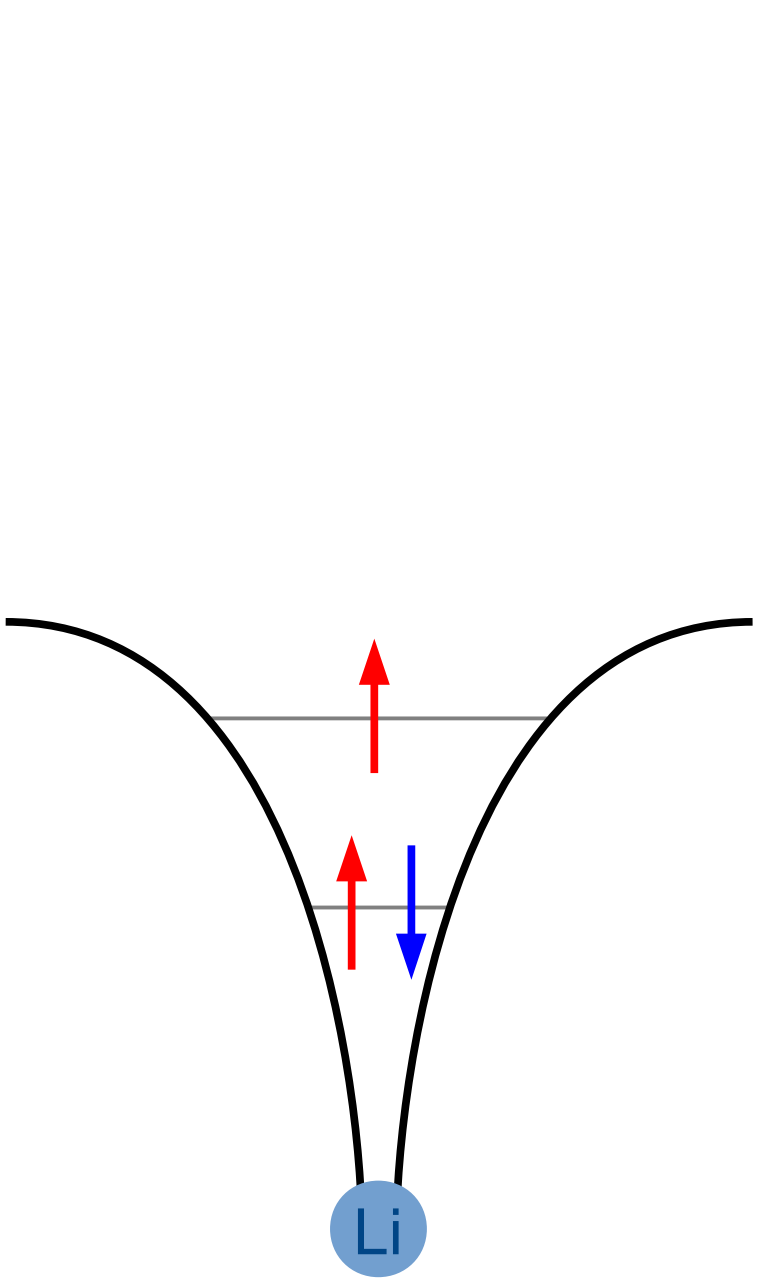

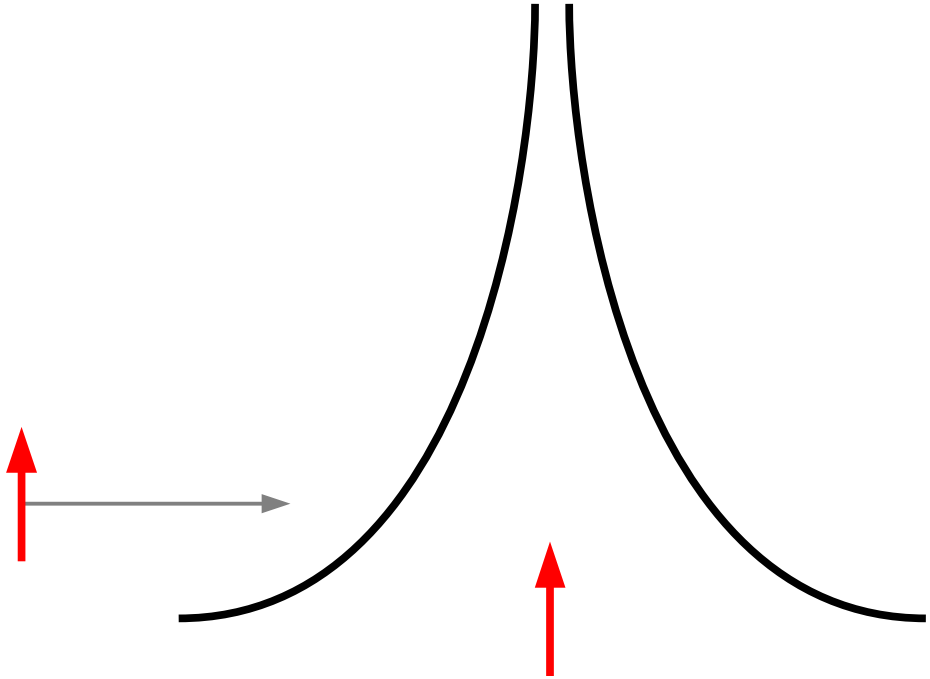

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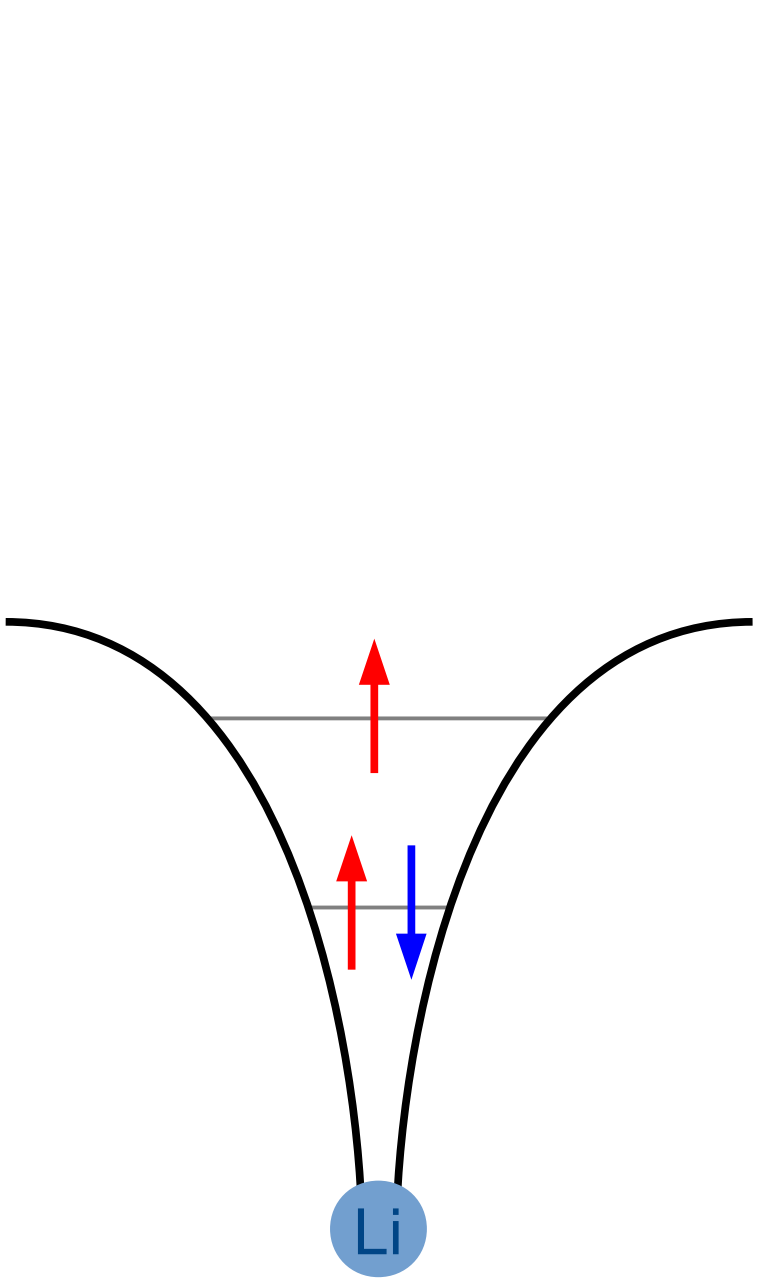

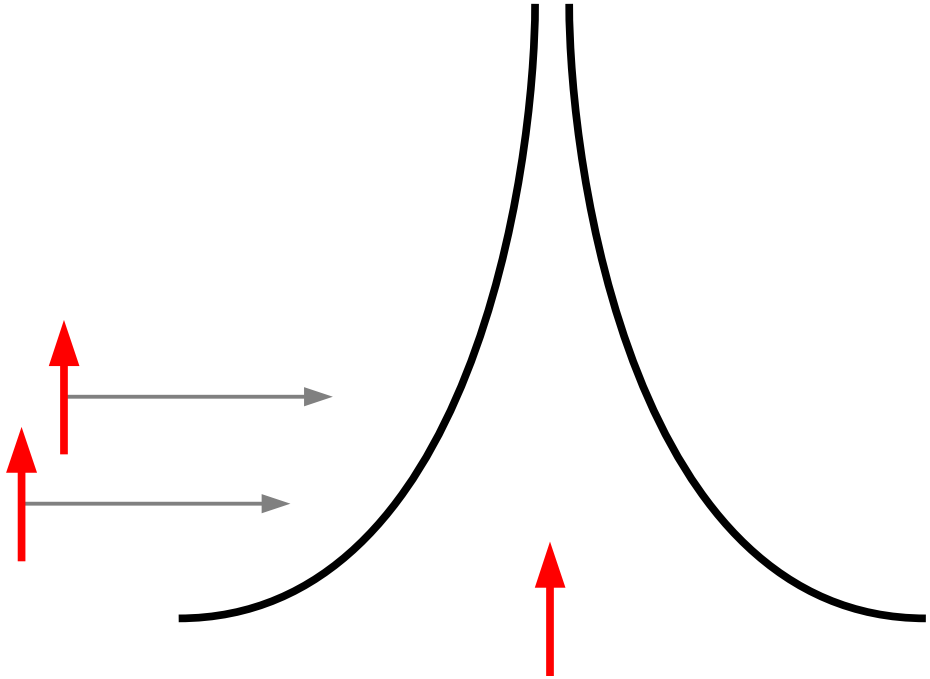

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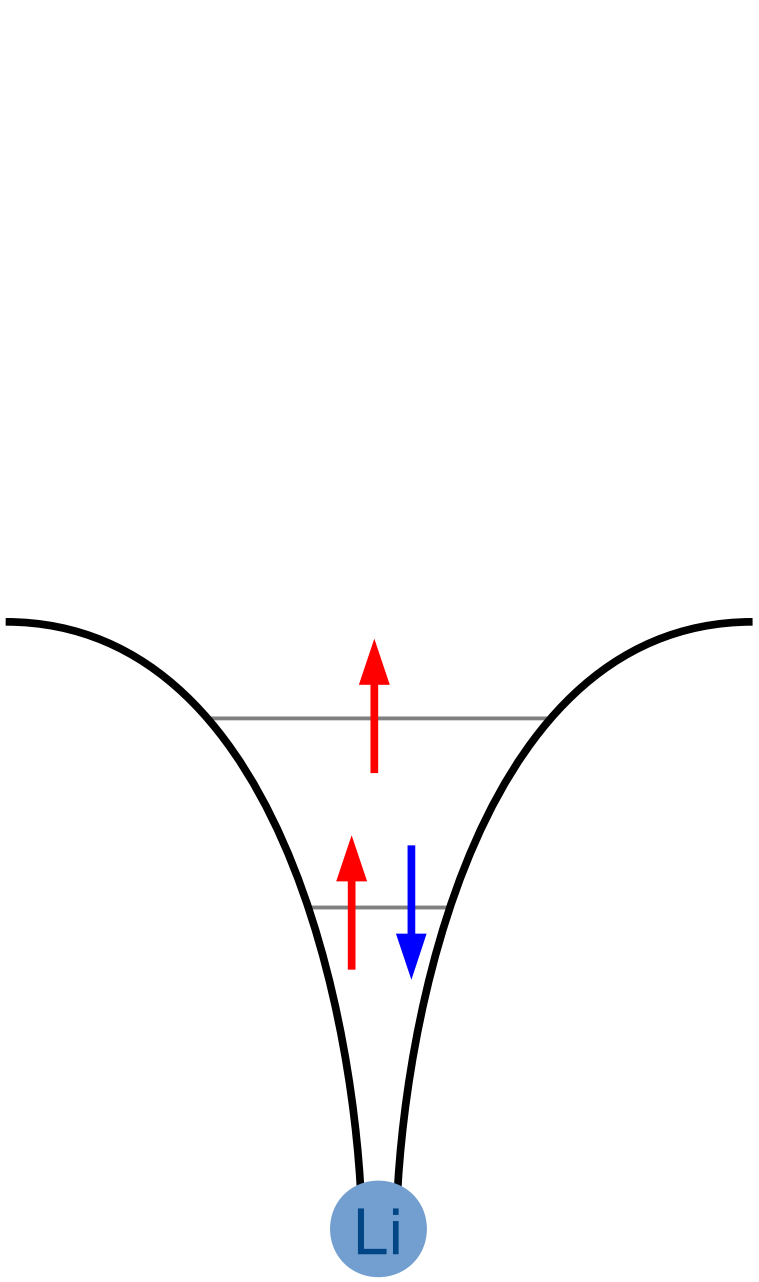
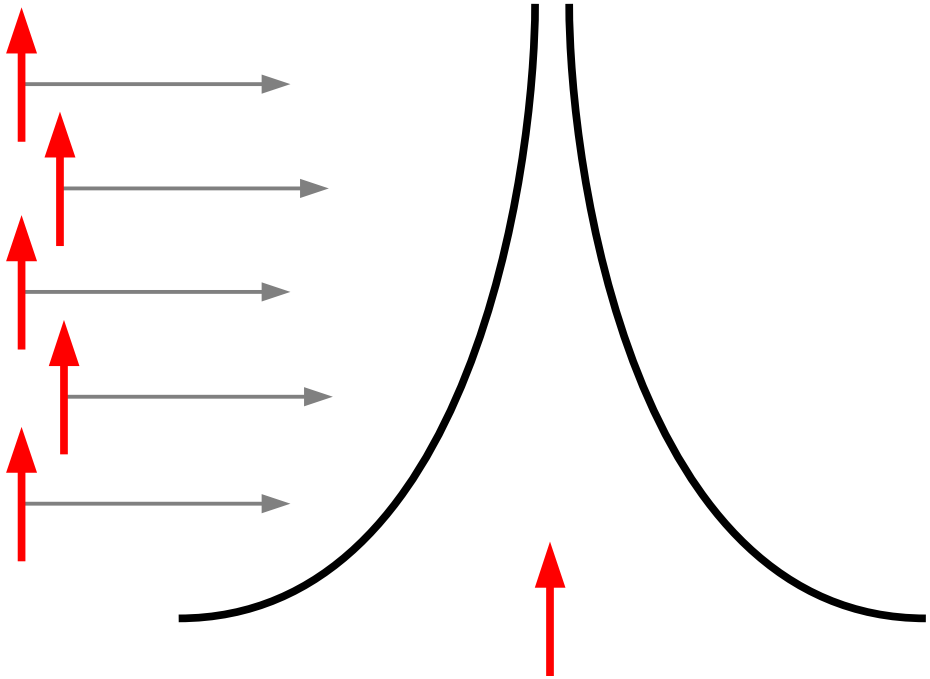
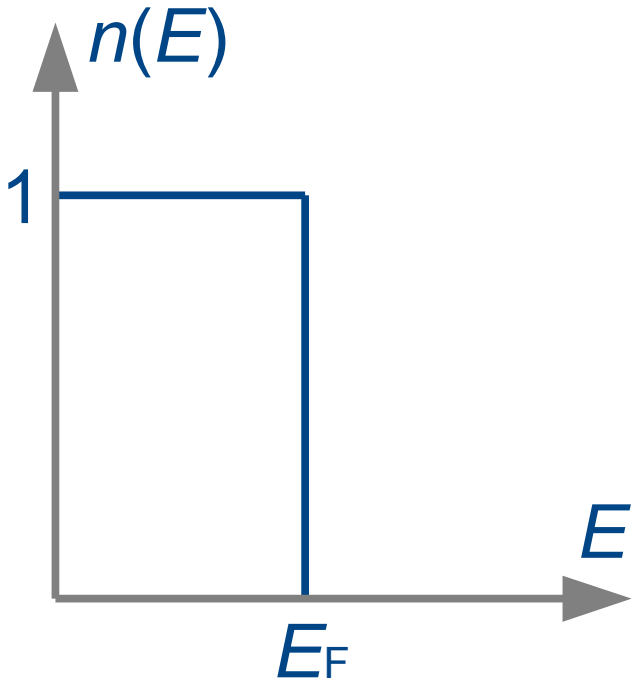


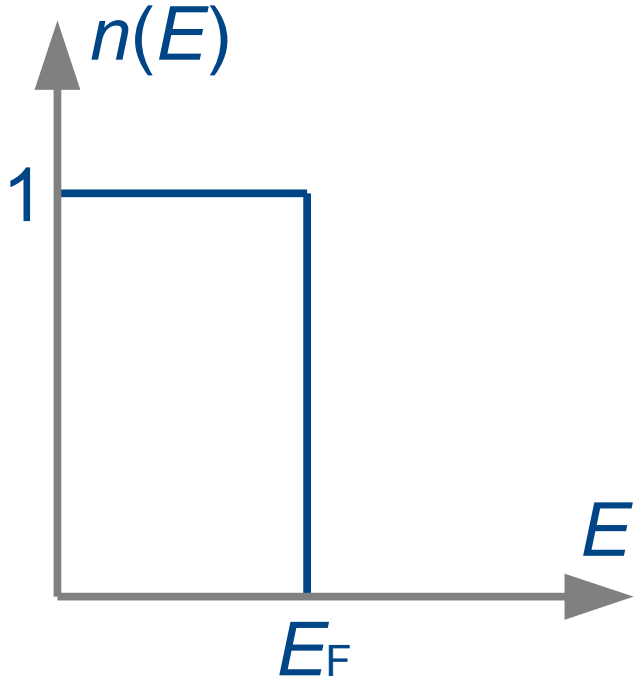


Fermi's two ideas



Fermi surface

Fermi's two ideas



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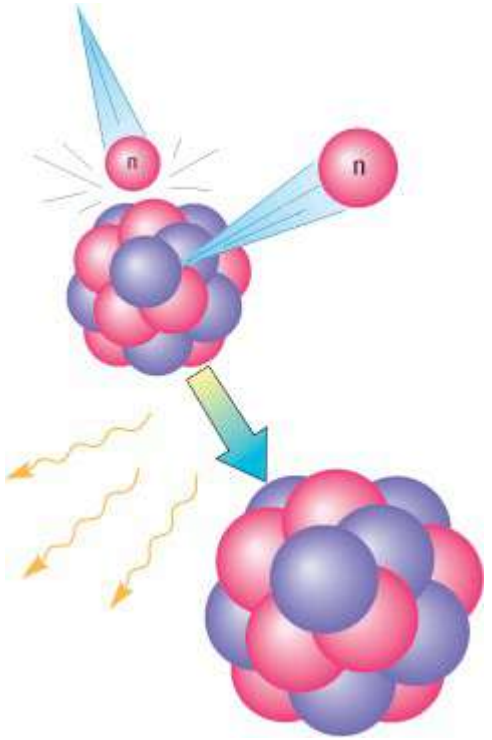


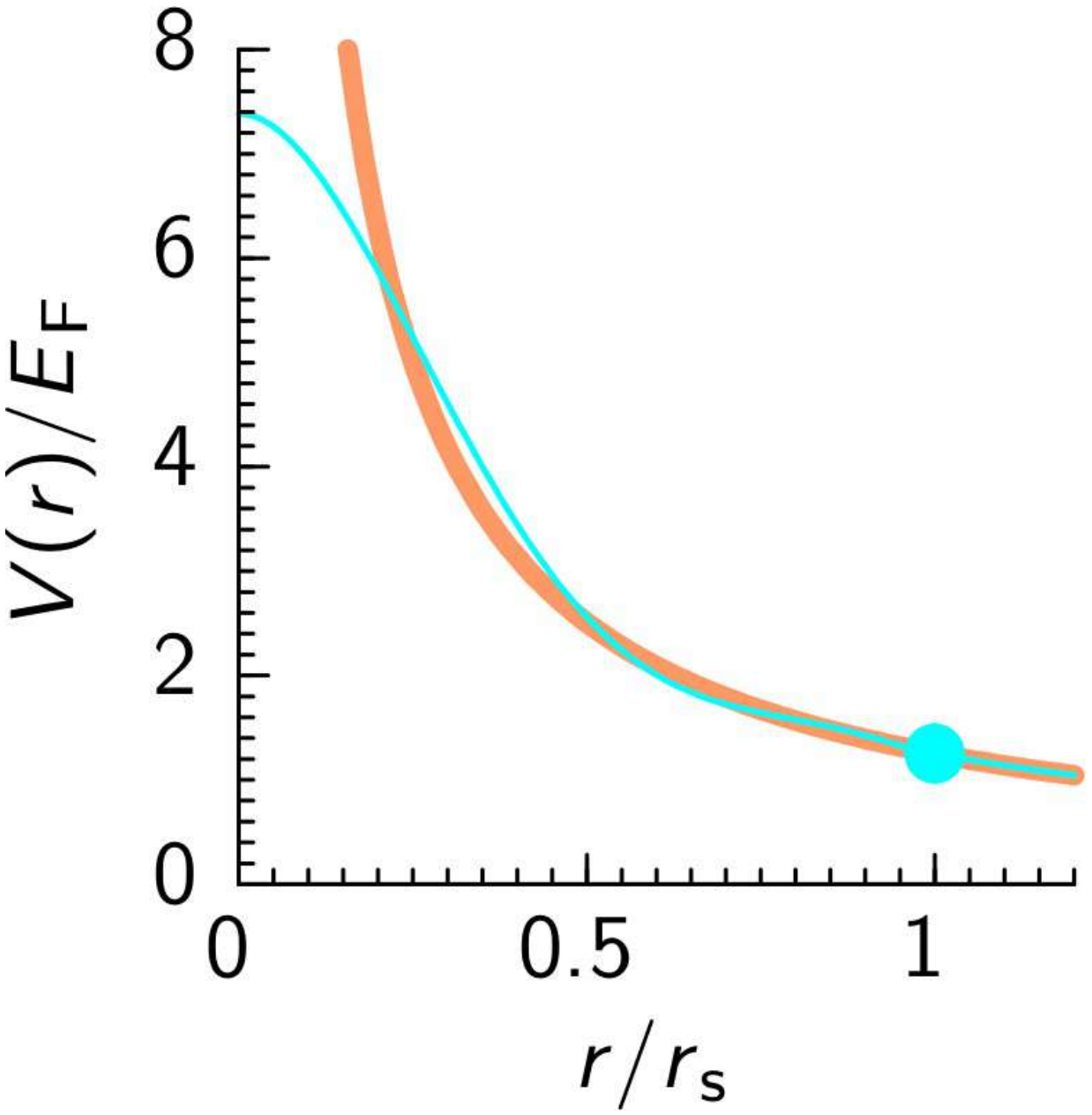
Pseudopotential for neutron scattering

Construction of a pseudopotential

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

$$\sum_{l=0}^{l_{\max}}\int_0^{2k_\mathrm{F}} \mathrm{d}k\left[\left.\frac{\mathrm{d}\ln\psi_{\mathrm{PP}}(k,l)}{\mathrm{d}r}\right|_c-\left.\frac{\mathrm{d}\ln\psi_{\mathrm{Coul}}(k,l)}{\mathrm{d}r}\right|_c\right]^2$$

Pseudopotential



Quantum Monte Carlo

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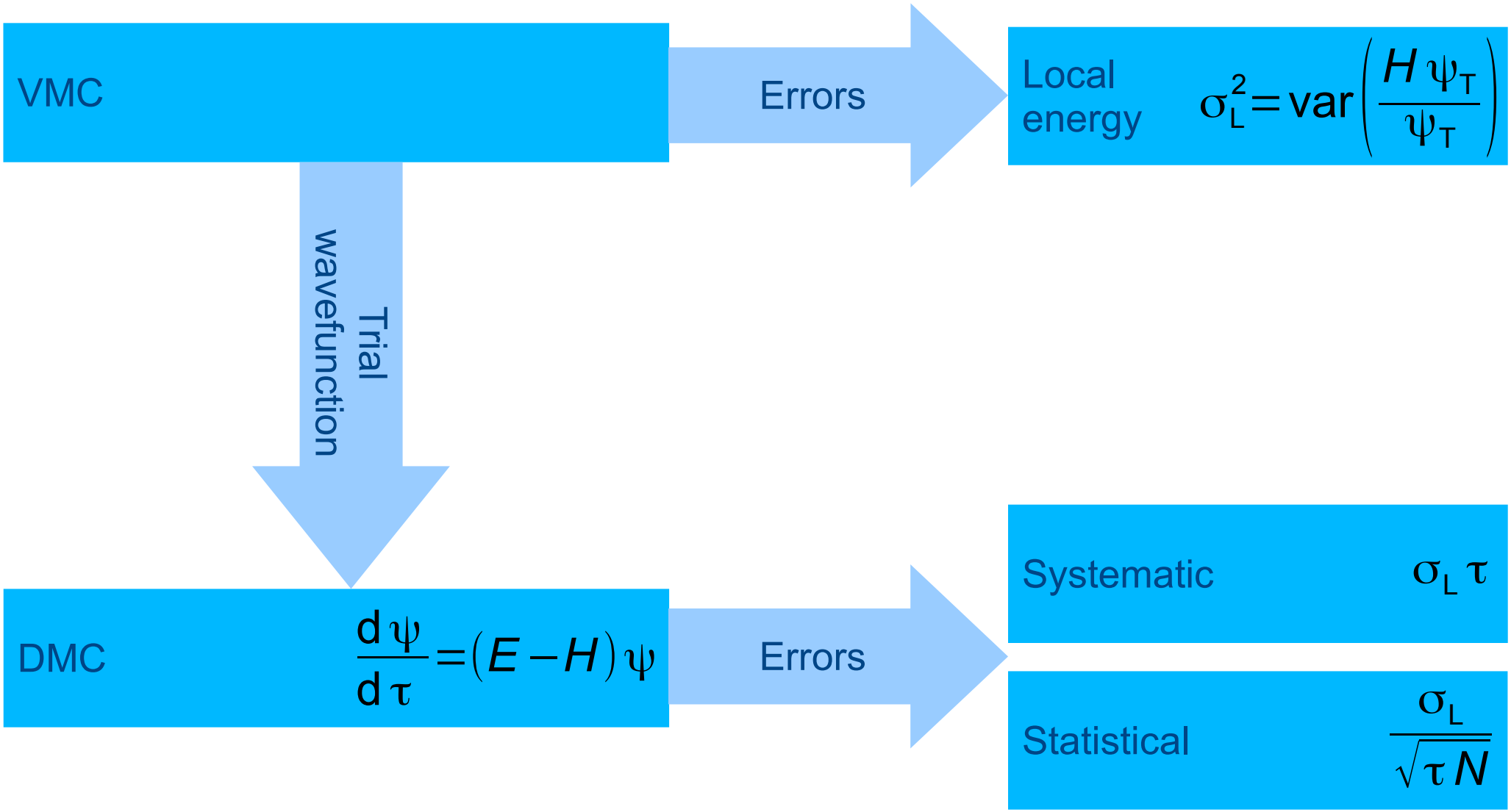
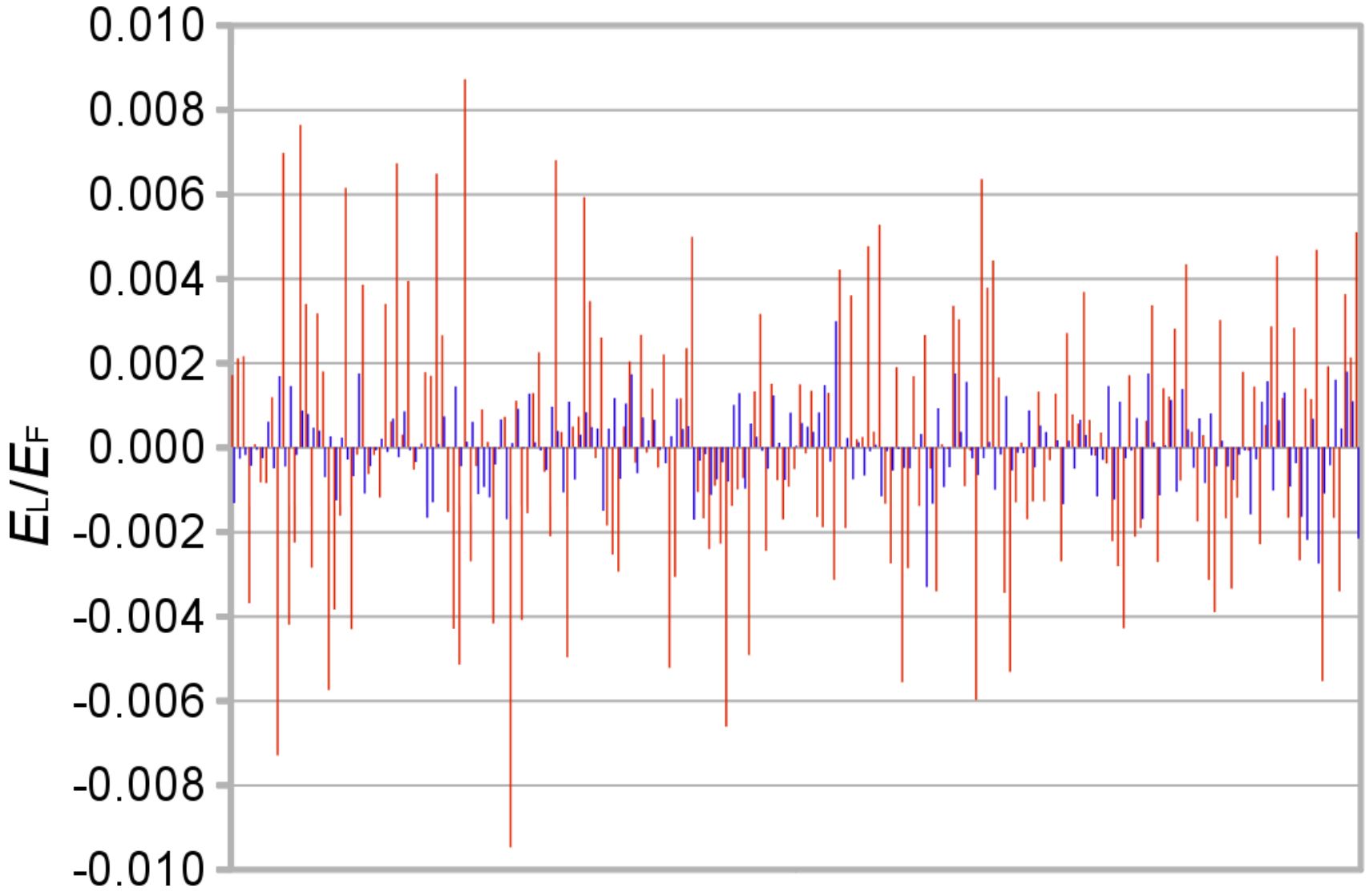
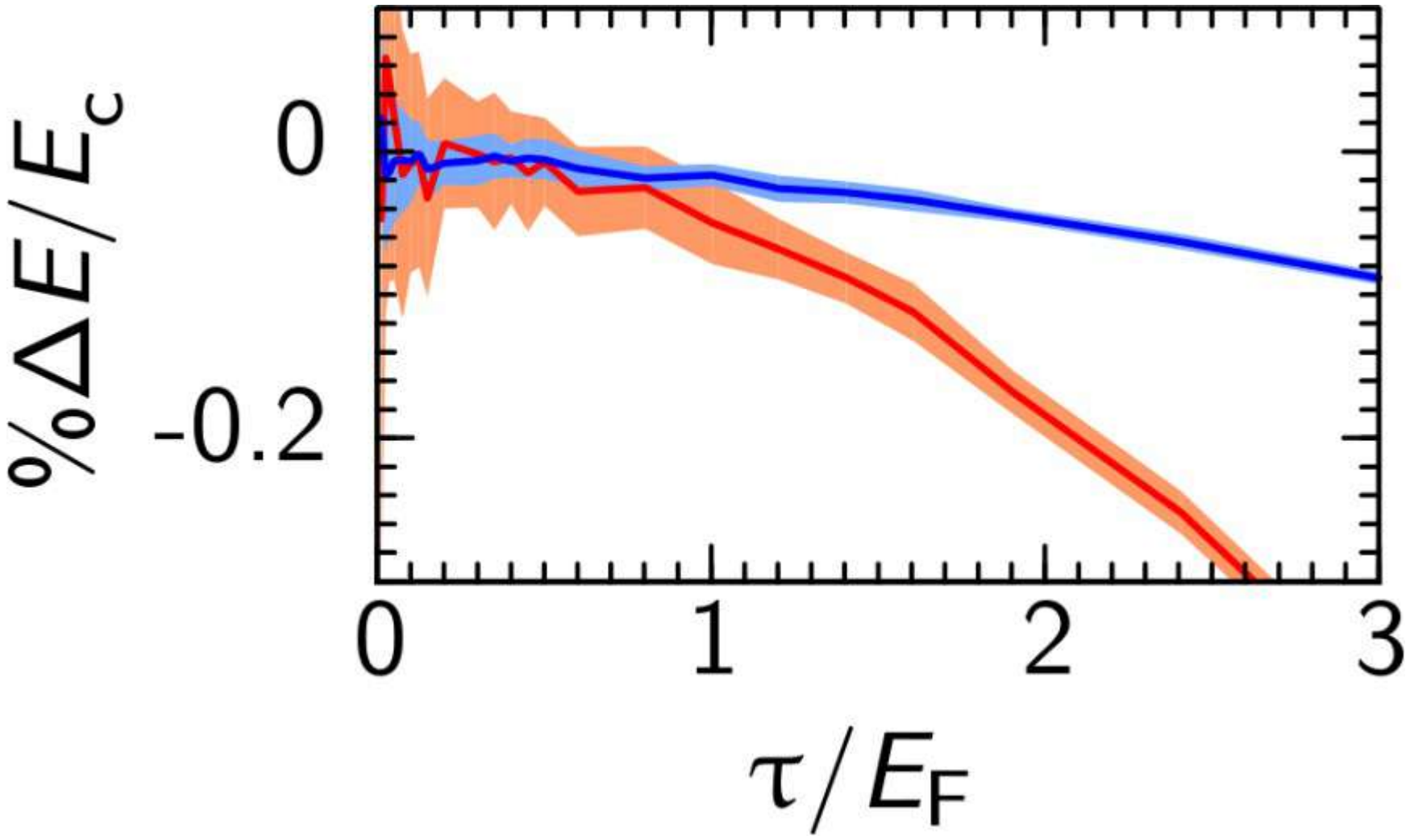


Pseudopotential: local energy



Pseudopotential: time step



Galactic dynamics

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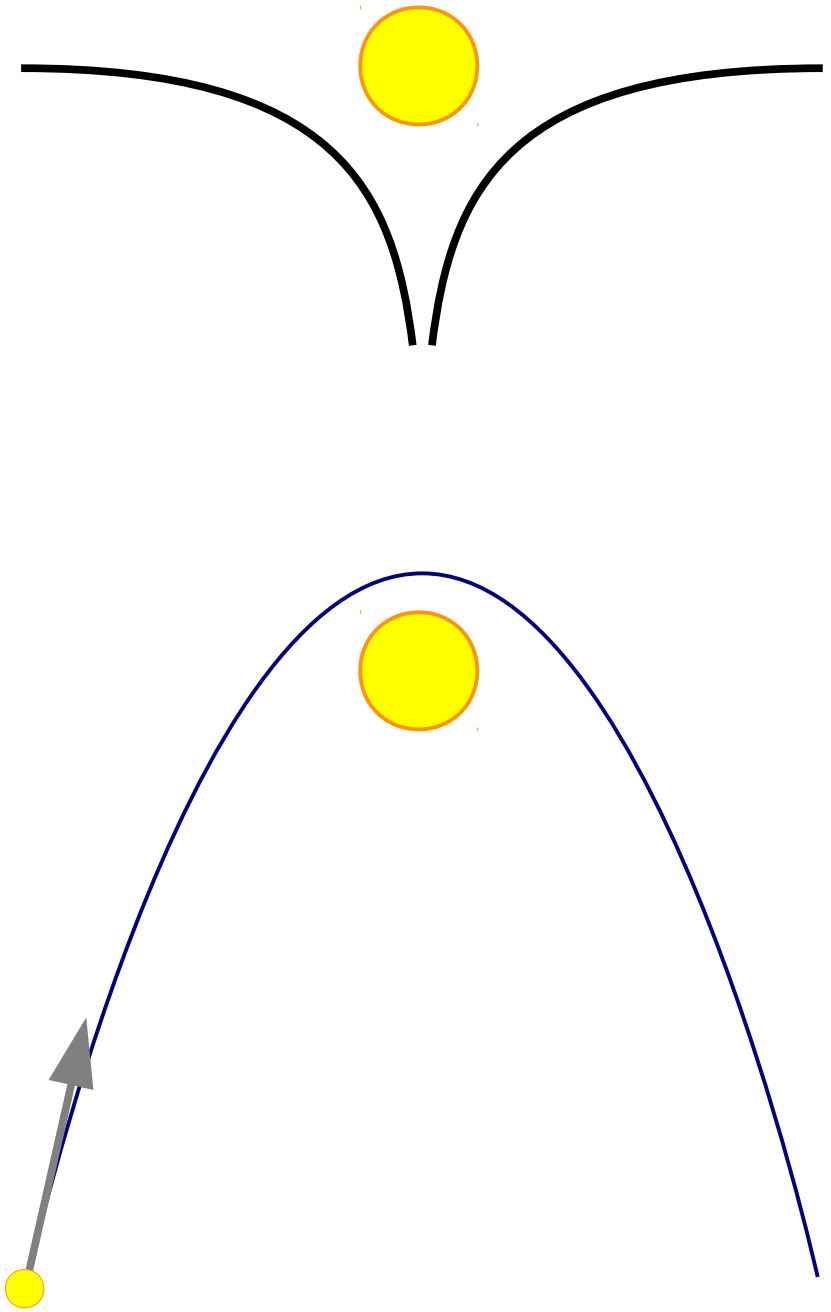

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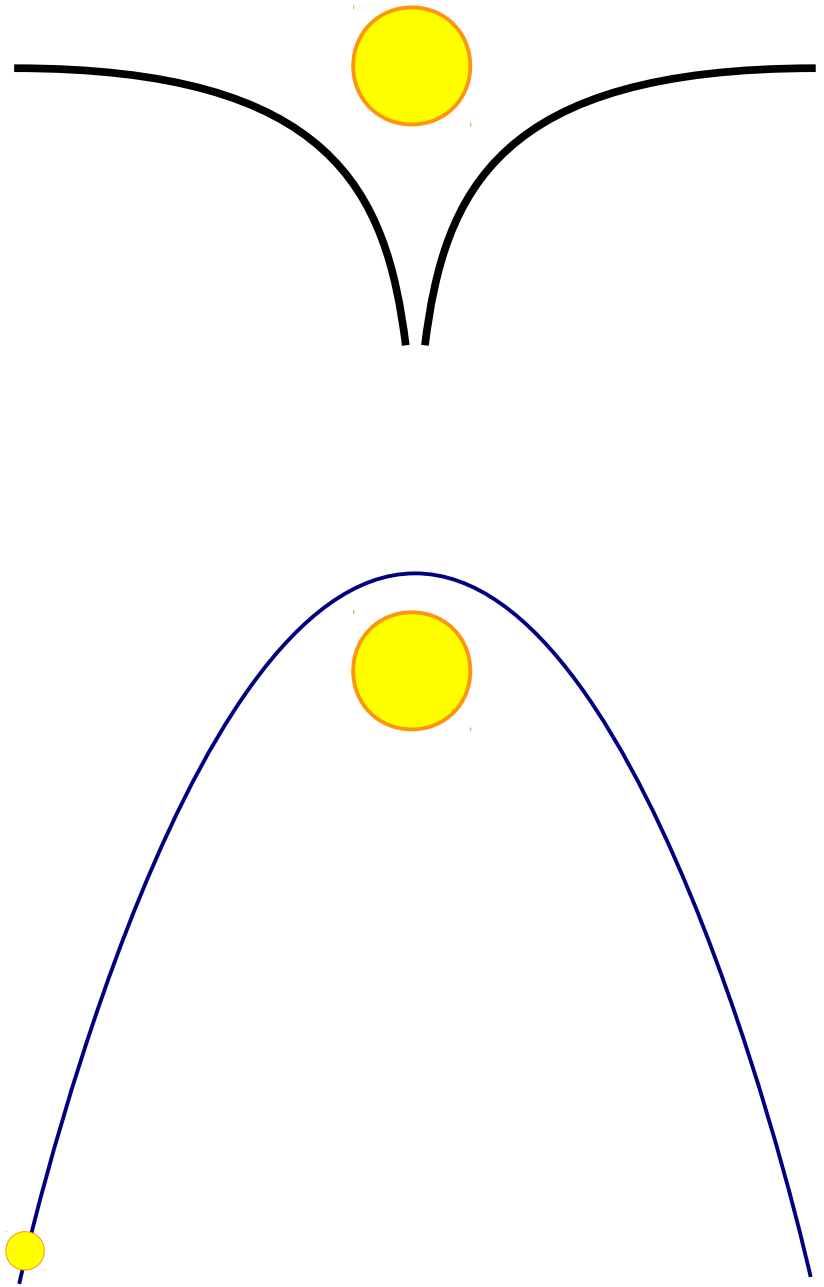

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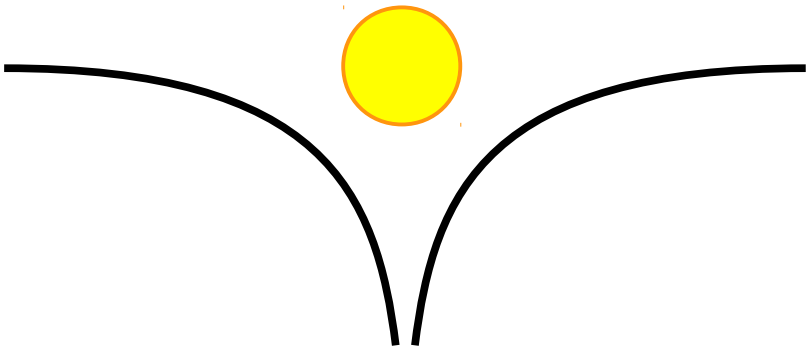

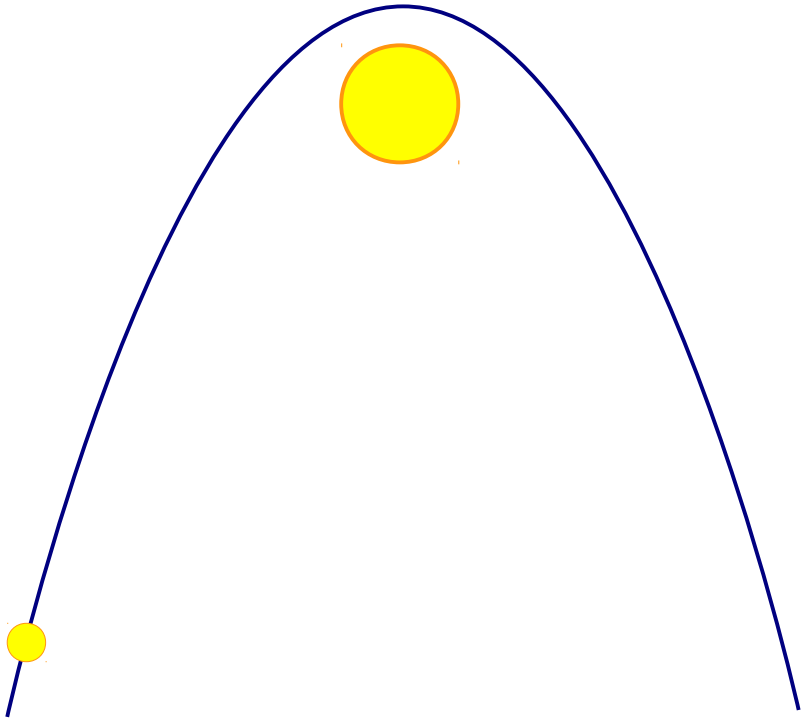

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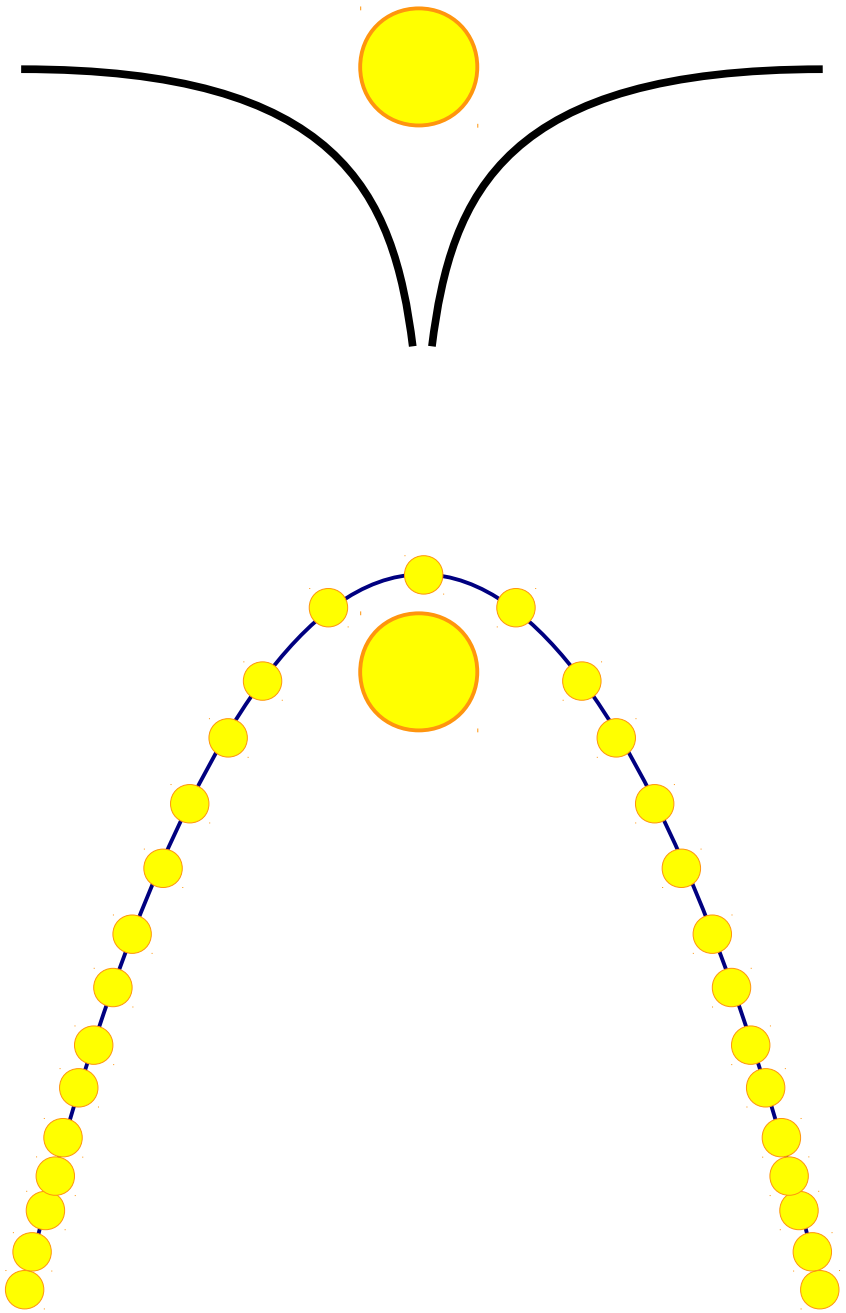

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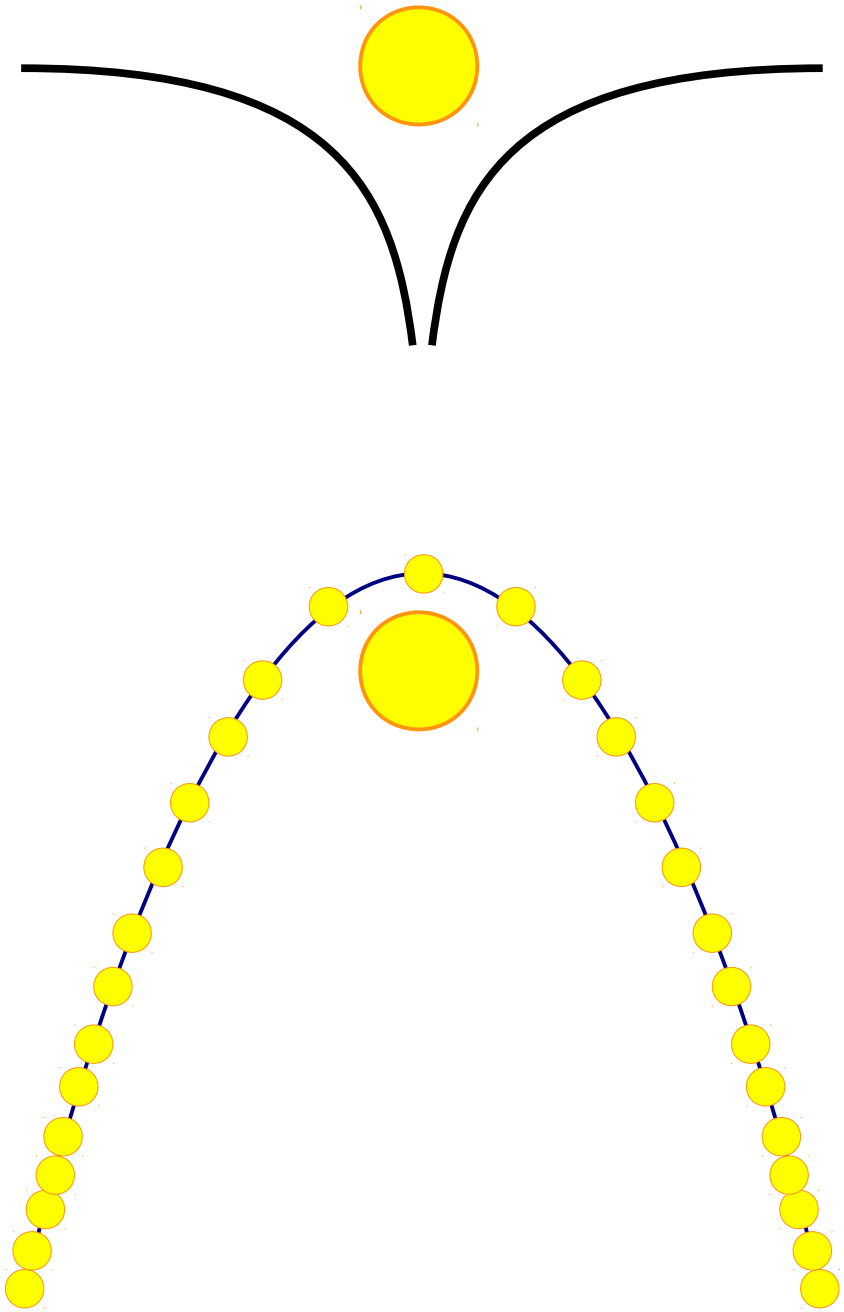

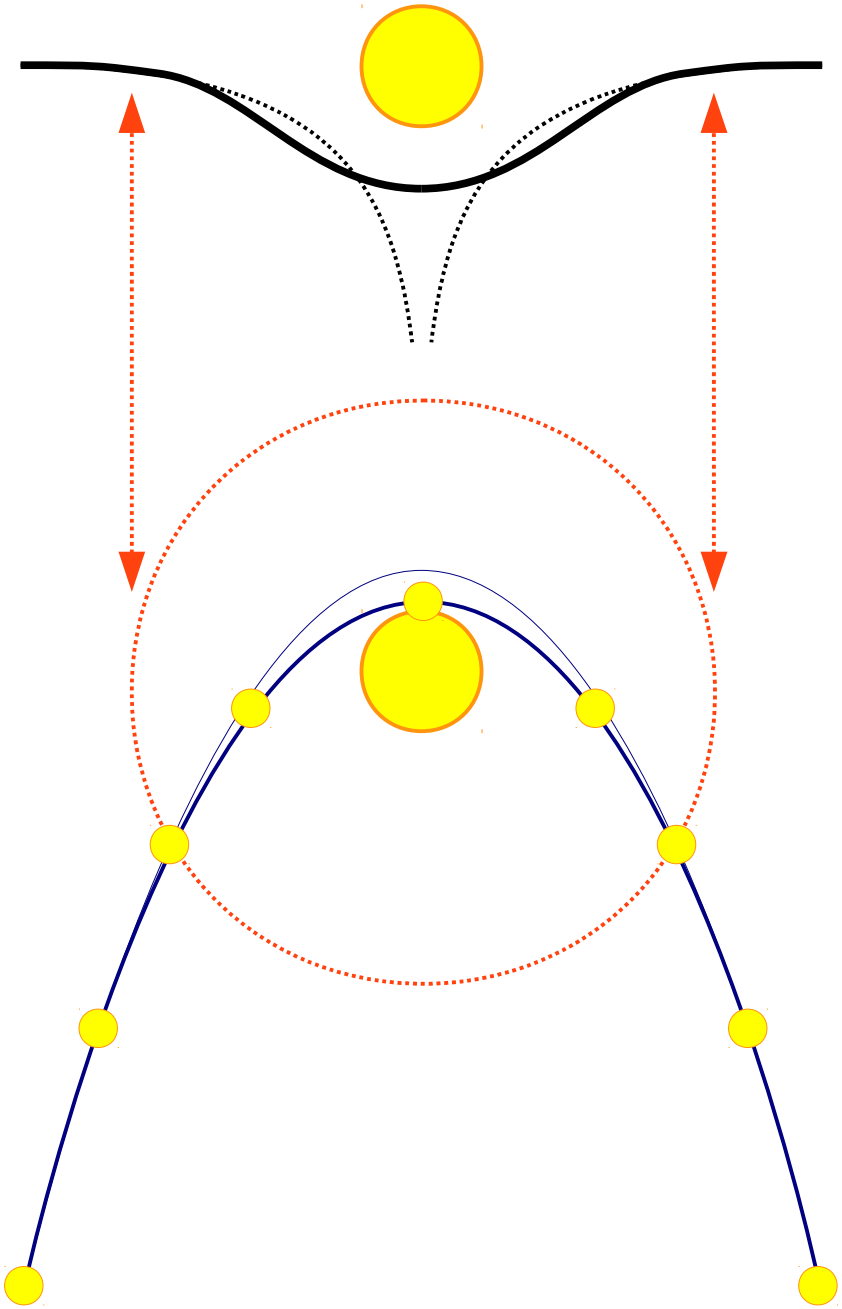

Summary

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