UNIVERSITY OF CAMBRIDGE

Using pseudopotentials to study strongly correlated phases

Gareth Conduit
Pascal Bugnion
Richard Needs
Pablo Lopez Rios
Jonathan Lloyd-Williams
Thomas Whitehead
Lars Schonenberg

TCM Group, Department of Physics

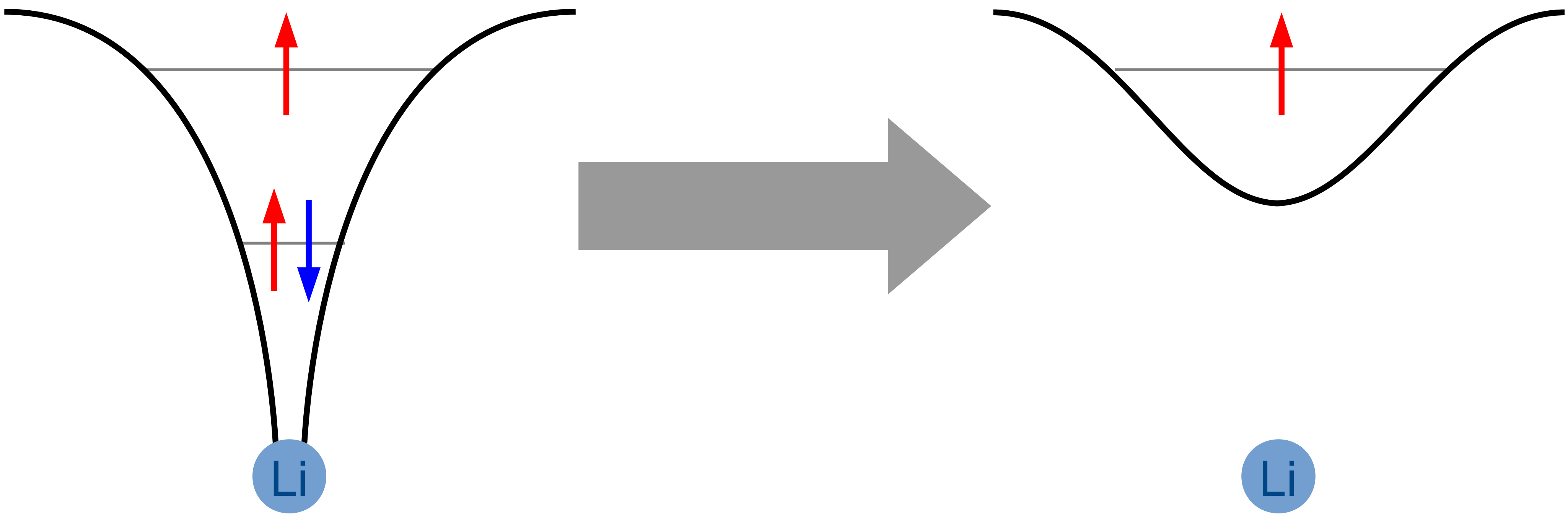
DMC study of the ground state

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

$$E = \frac{\int \bar{\psi} H \psi \, \mathrm{d}\boldsymbol{r}}{\int \bar{\psi} \psi \, \mathrm{d}\boldsymbol{r}}$$

Electron-ion pseudopotential

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

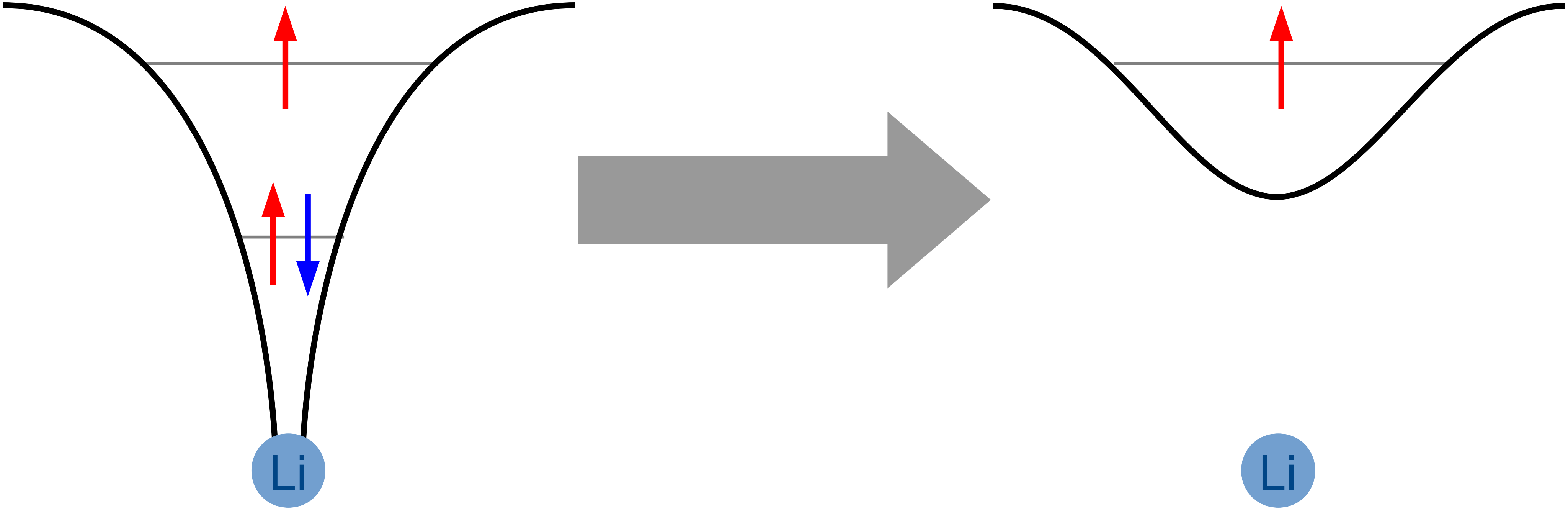


Electron-ion pseudopotential

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

Smooth background

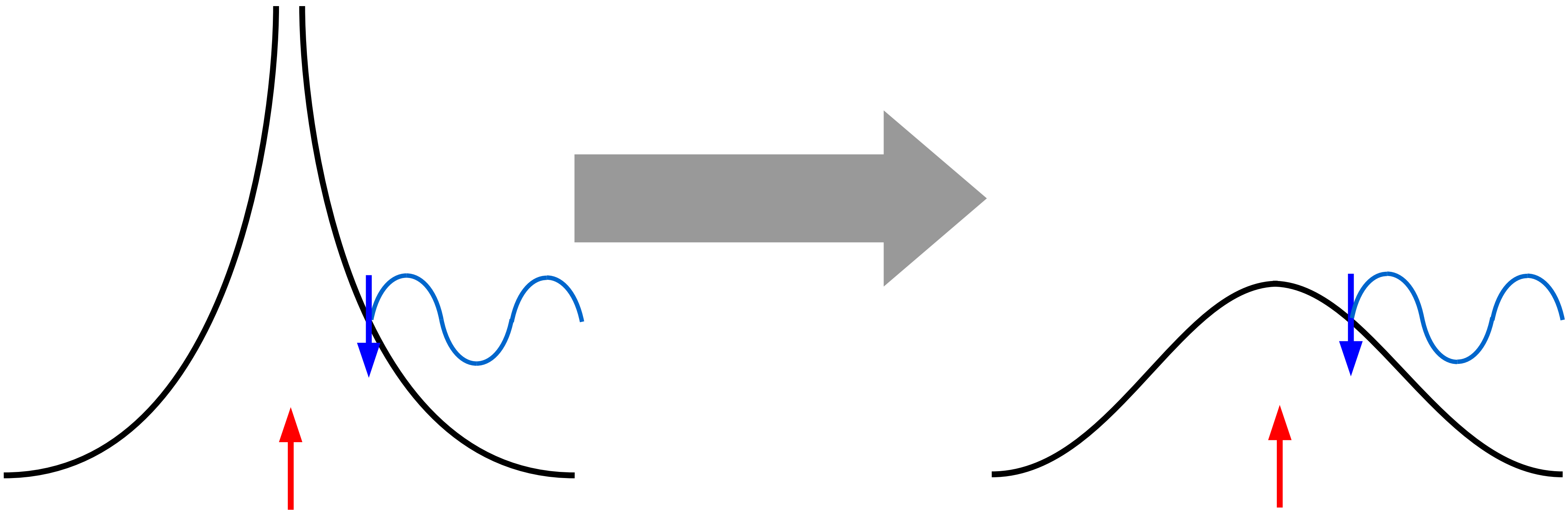
Fewer electrons



Electron-electron pseudopotential

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

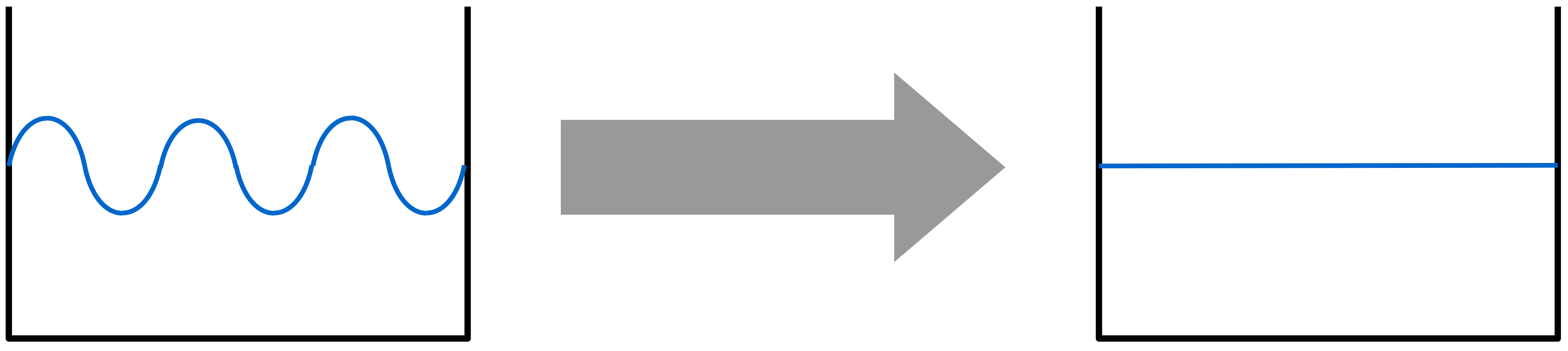
Smooth background



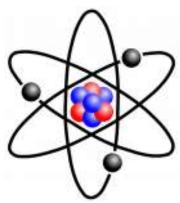
Pseudo kinetic energy

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

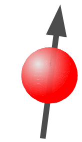
Smooth integrand

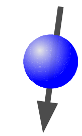


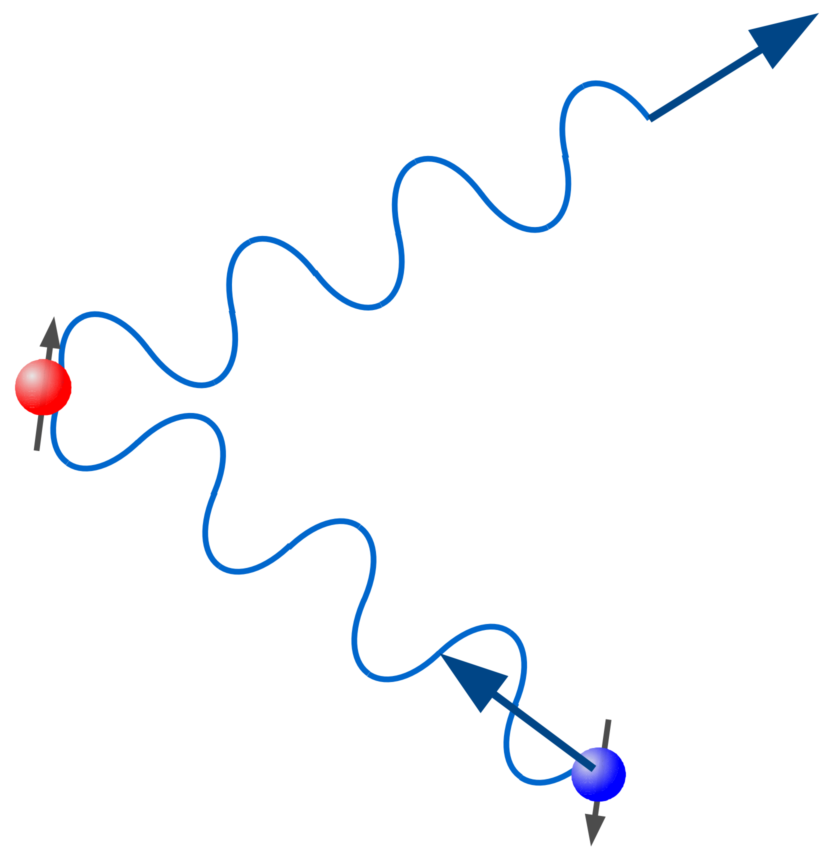
Scattering in ultracold atom gases



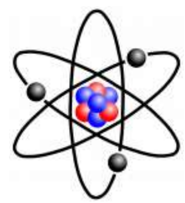
^{6}Li atom

$|F = 1/2, m_F = 1/2\rangle$ →  Up spin particle

$|F = 1/2, m_F = -1/2\rangle$ →  Down spin particle



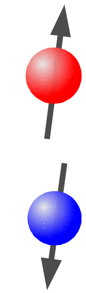
Scattering in ultracold atom gases



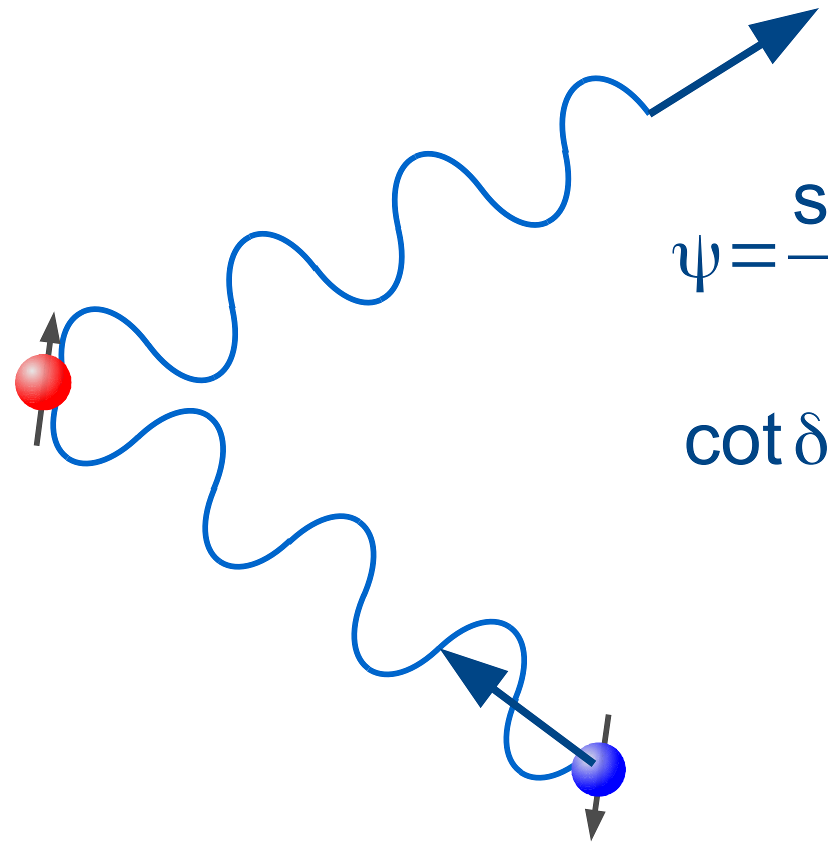
^{6}Li atom

$|F = 1/2, m_F = 1/2\rangle \rightarrow$ Up spin particle

$|F = 1/2, m_F = -1/2\rangle \rightarrow$ Down spin particle



$$V(r) = 4\pi a \delta(\boldsymbol{r}) \frac{d}{dr} r$$



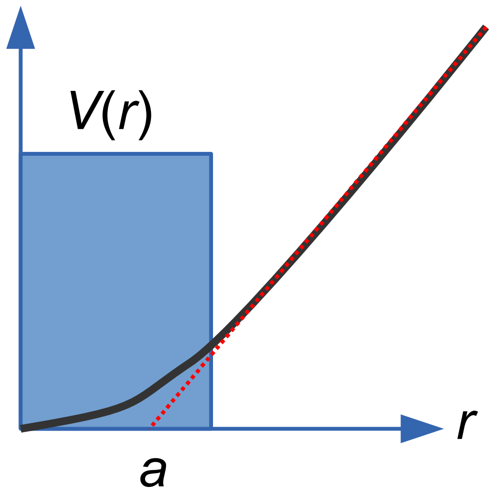
$$\psi = \frac{\sin(kr + \delta_0)}{kr}$$

$$\cot \delta_0 = -\frac{1}{ka}$$

Scattering potentials

Underlying repulsive

Effective repulsive



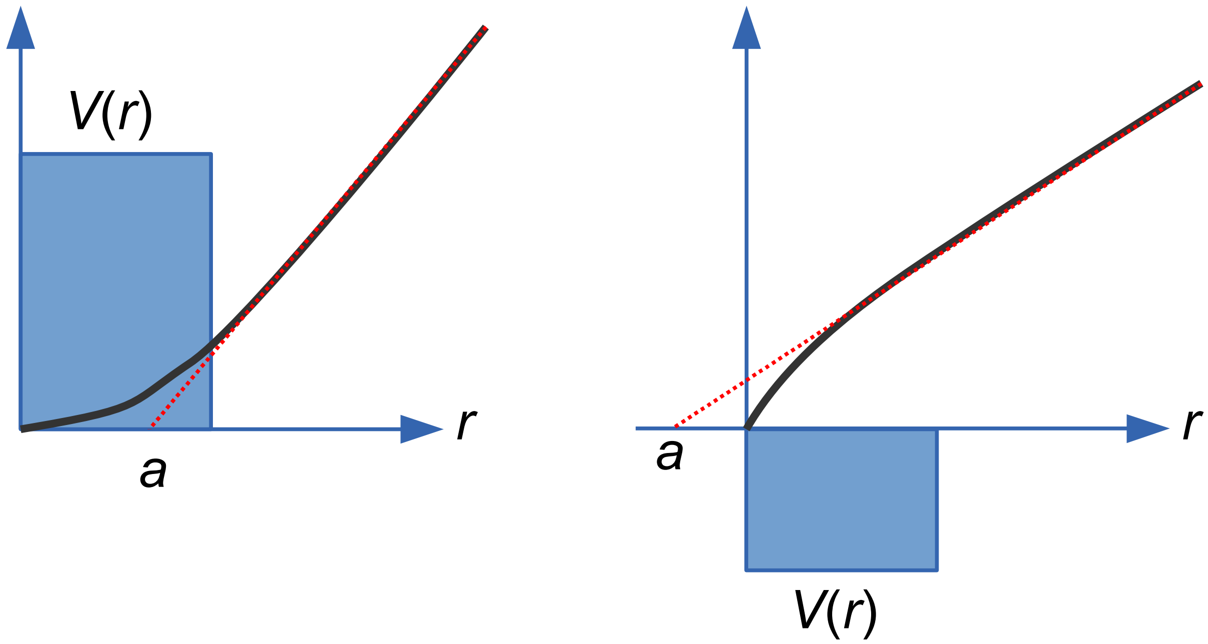
Scattering potentials

Underlying repulsive

Effective repulsive

Underlying attractive

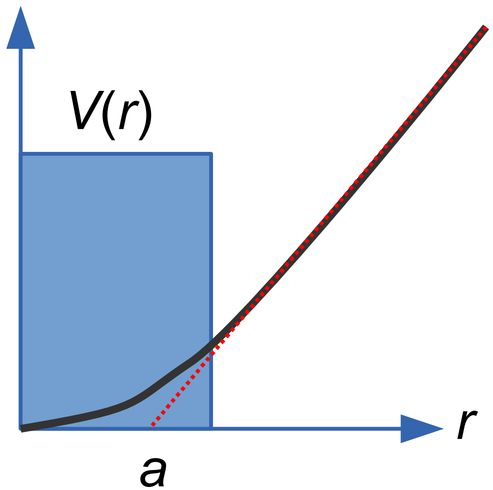
Effective attractive



Scattering potentials

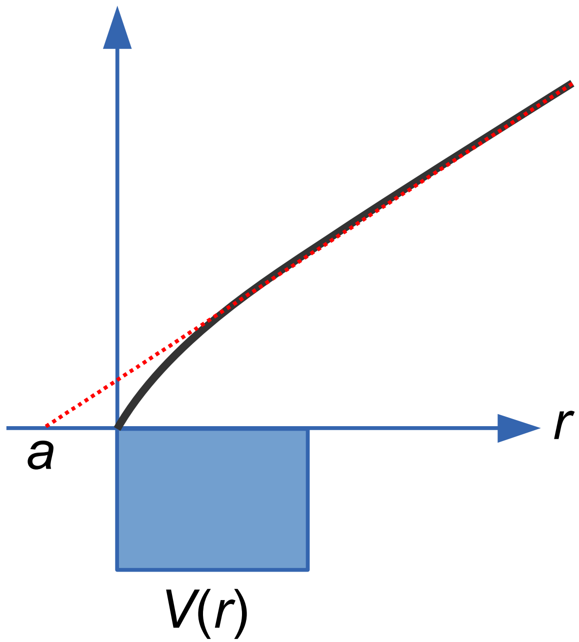
Underlying repulsive

Effective repulsive



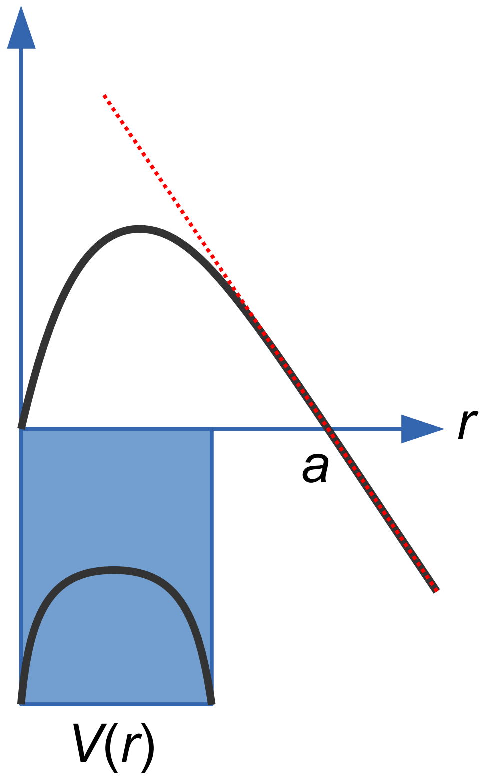
Underlying attractive

Effective attractive



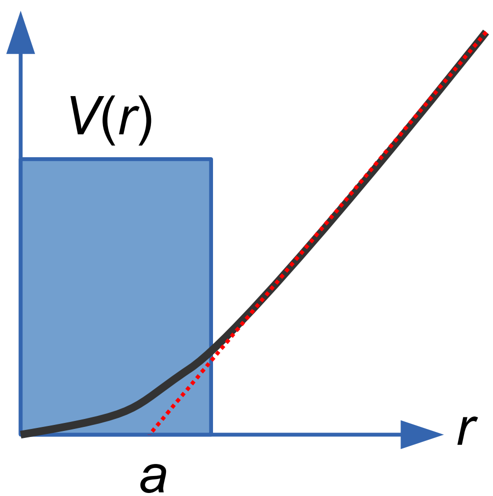
Underlying attractive

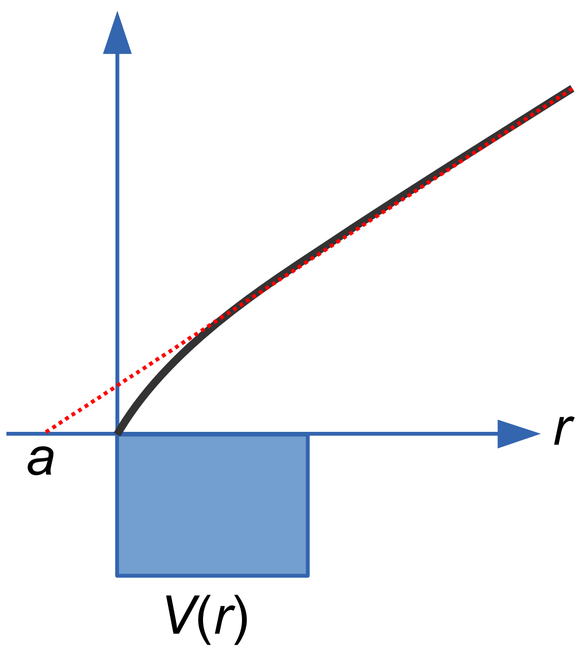
Effective repulsive

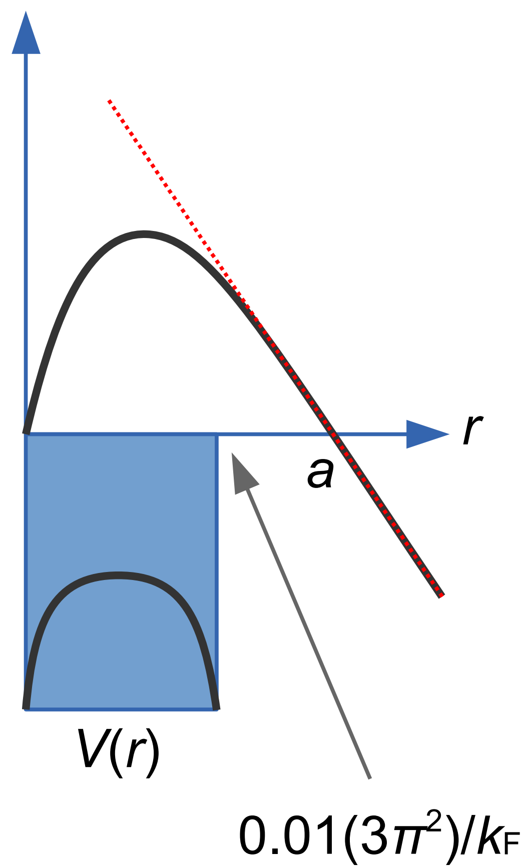


Scattering potentials

Underlying repulsive	Underlying attractive	Underlying attractive
Effective repulsive	Effective attractive	Effective repulsive

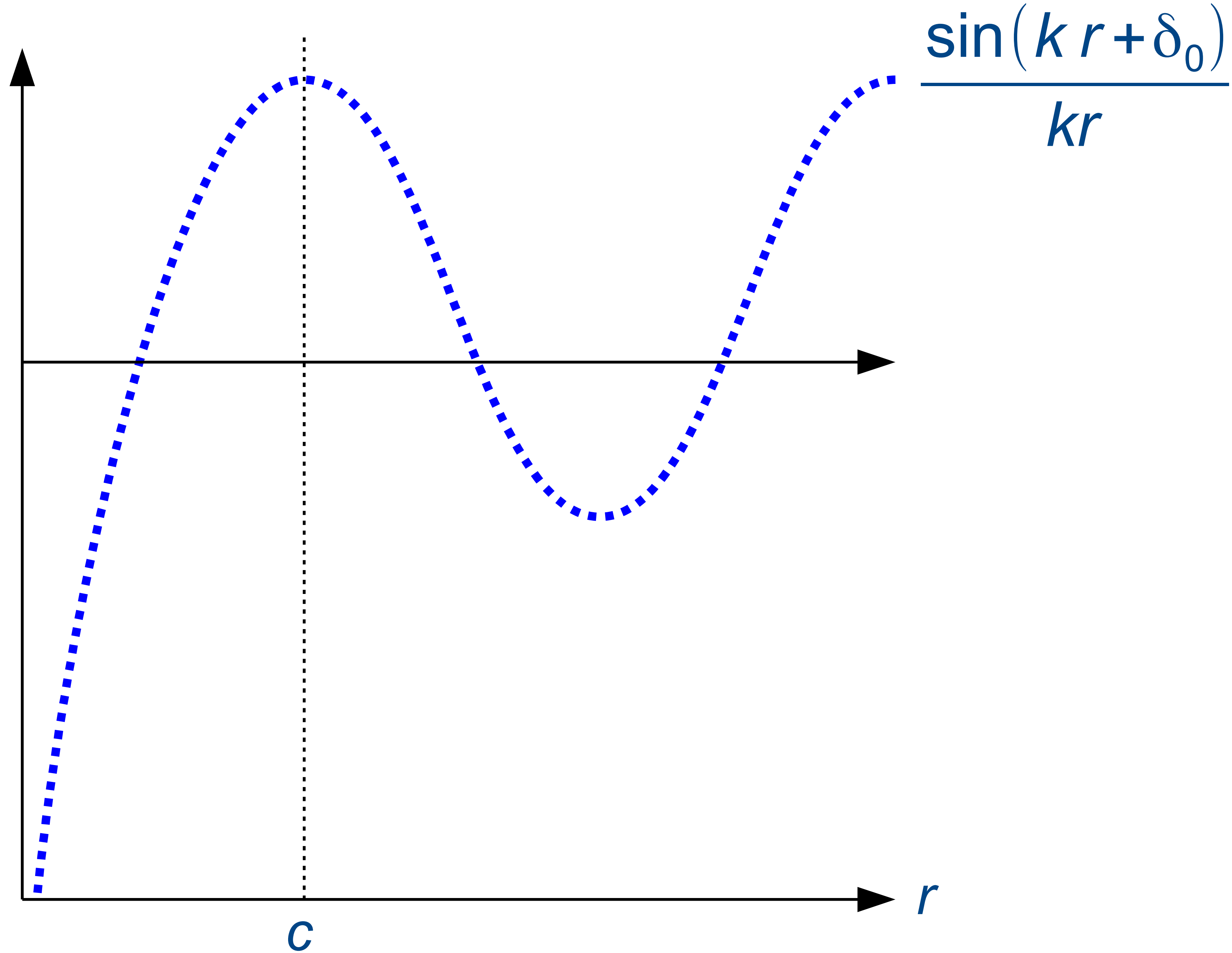




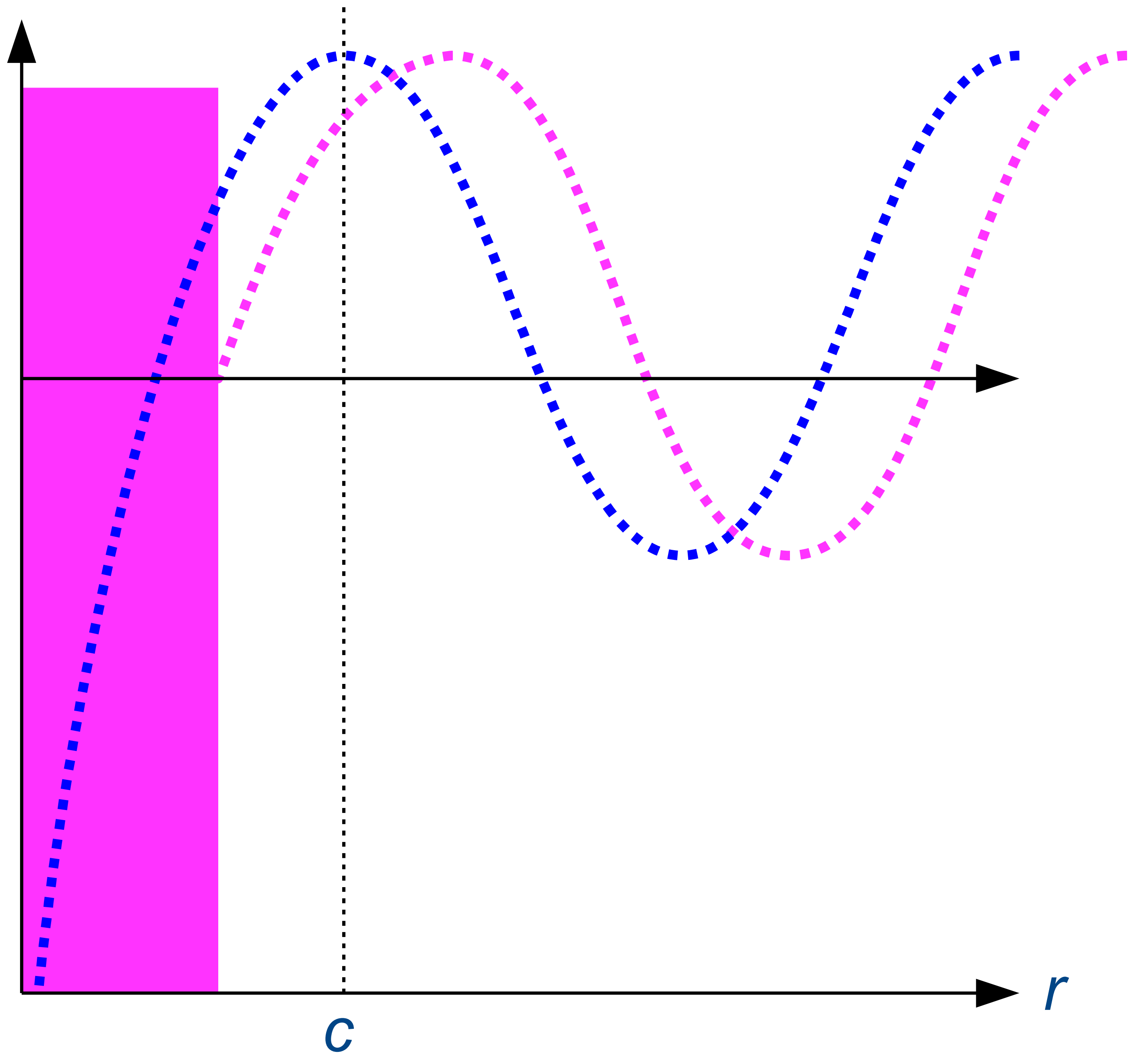


Pilati, Bertaina, Giorgini, and Troyer, PRL 105, 030405 (2010)

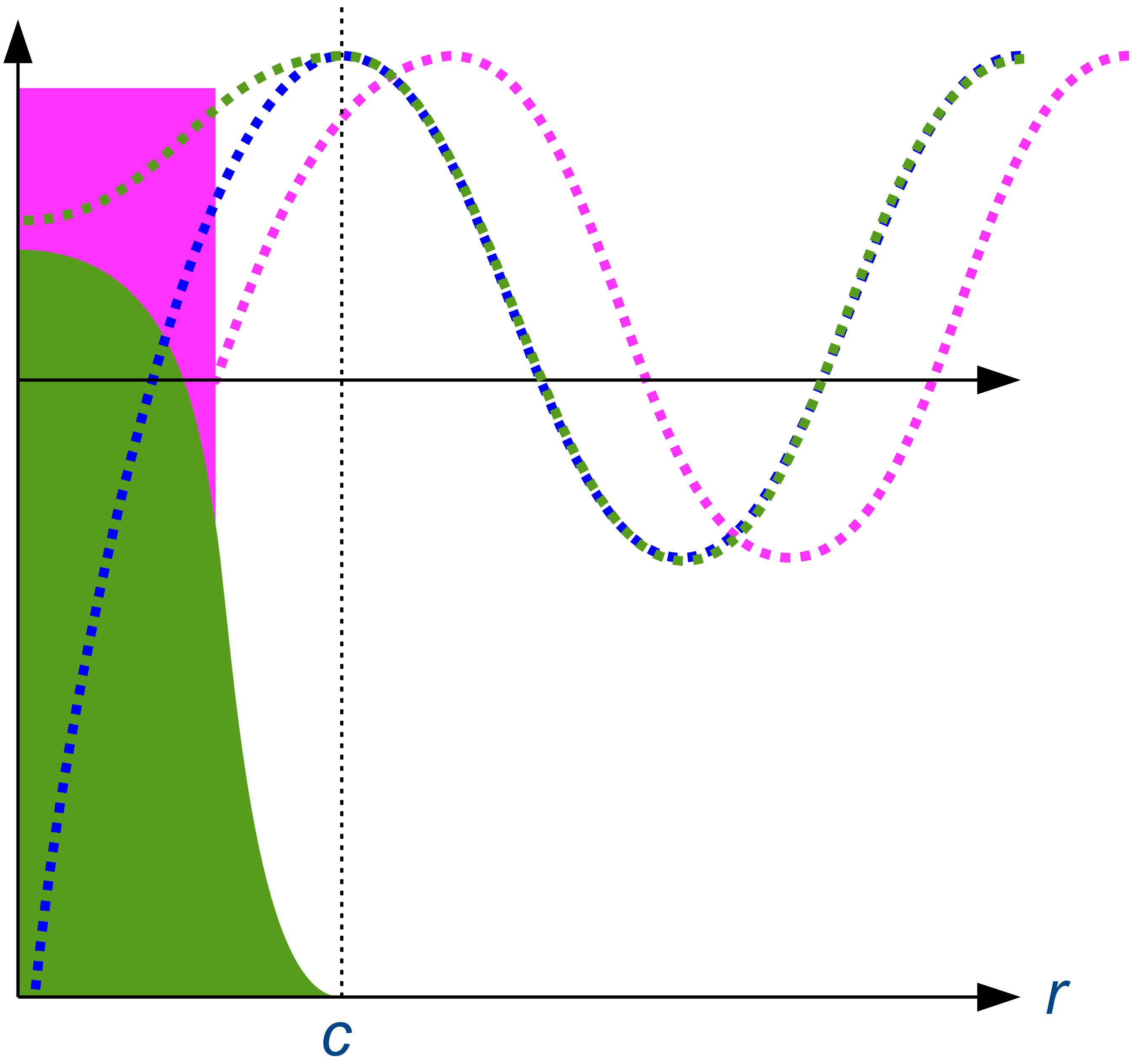
Construction of a pseudopotential



Construction of a pseudopotential



Construction of a pseudopotential

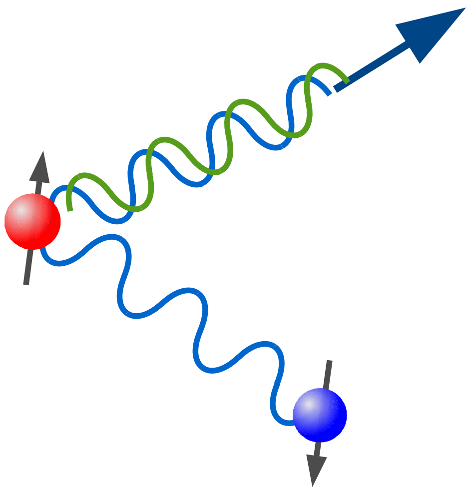


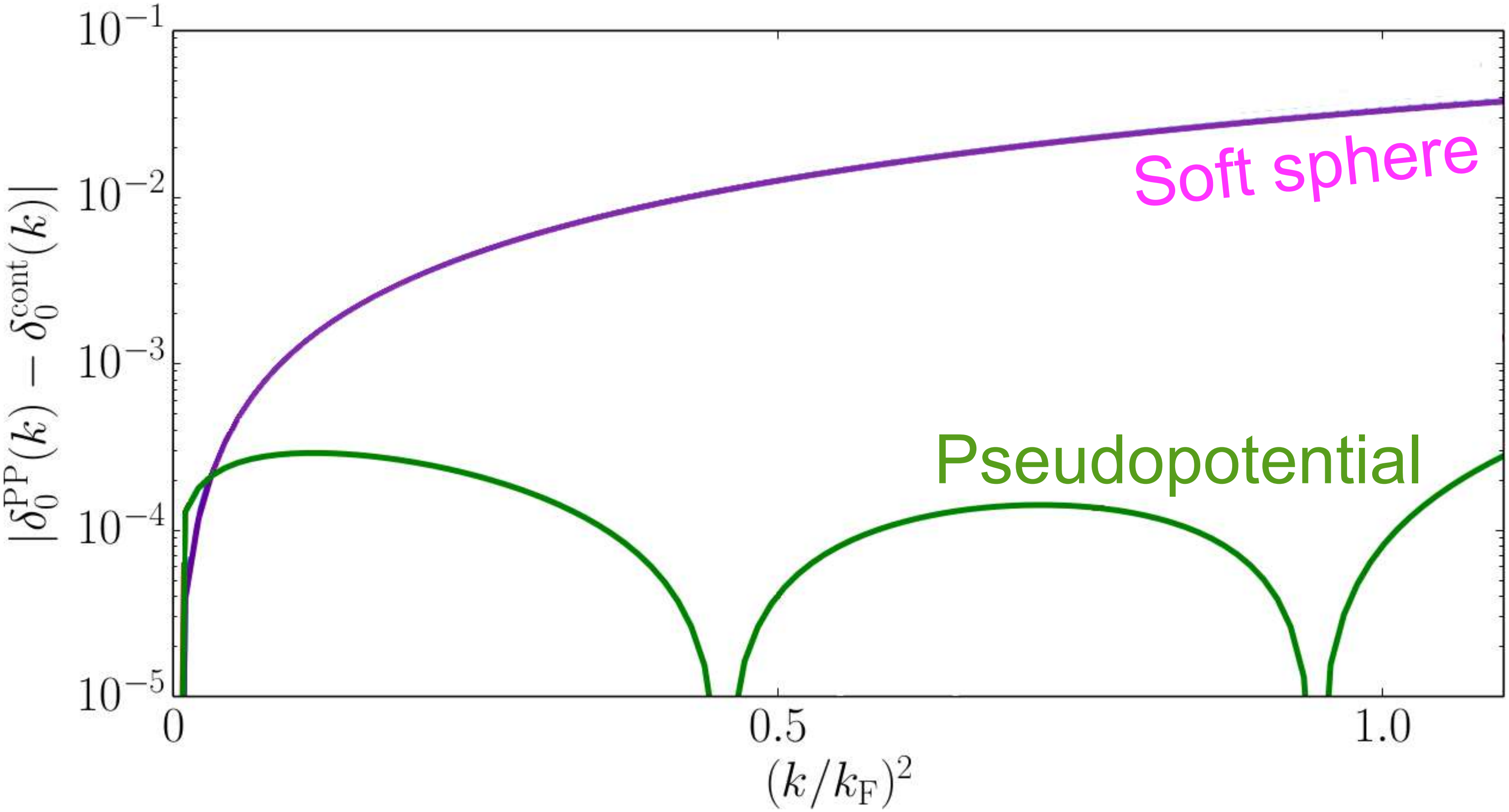
Construction of a pseudopotential

$$V_{\mathrm{PP}}(r)=\begin{cases}\left(1-\frac{r}{c}\right)^2\left[v_1\left(\frac{1}{2}+\frac{r}{c}\right)+\sum_{i=2}^{N_v} v_i\left(\frac{r}{c}\right)^i\right] & r<c\\ 0 & r>c\end{cases}$$

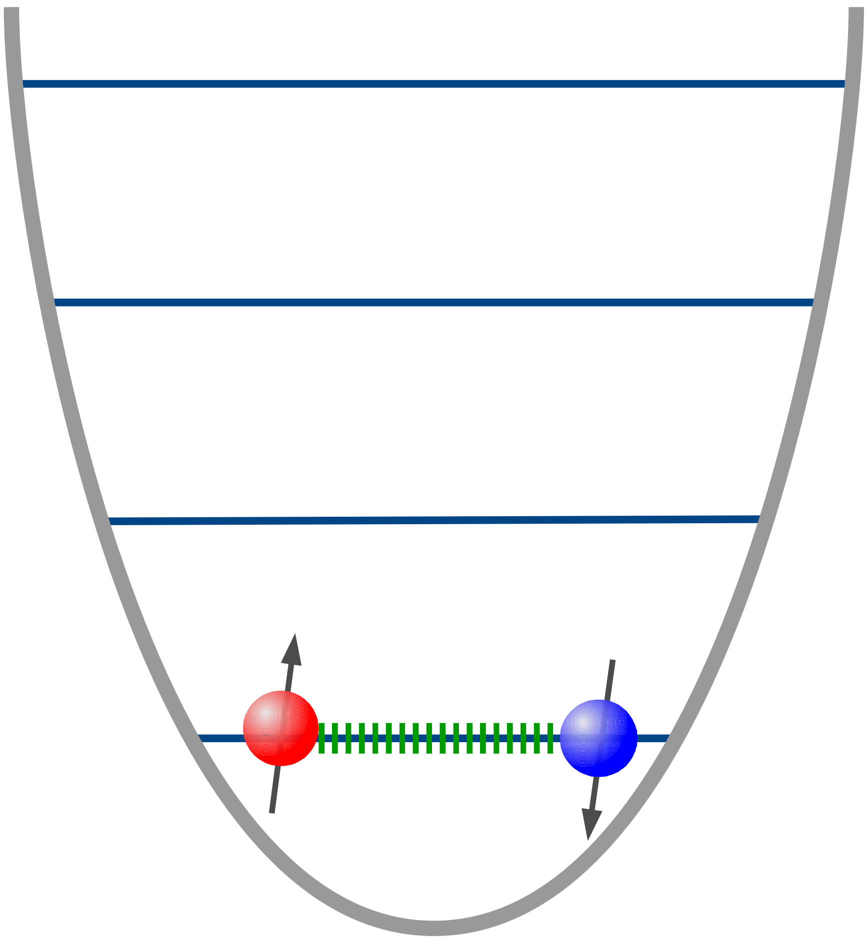
$$\sum_{l=0}^{l_{\max}}\int_0^{k_F}\left[\delta_{0,\mathrm{PP}}-\delta_{0,\mathrm{cont}}\right]^2\mathrm{d}k$$

Pseudopotential: scattering properties

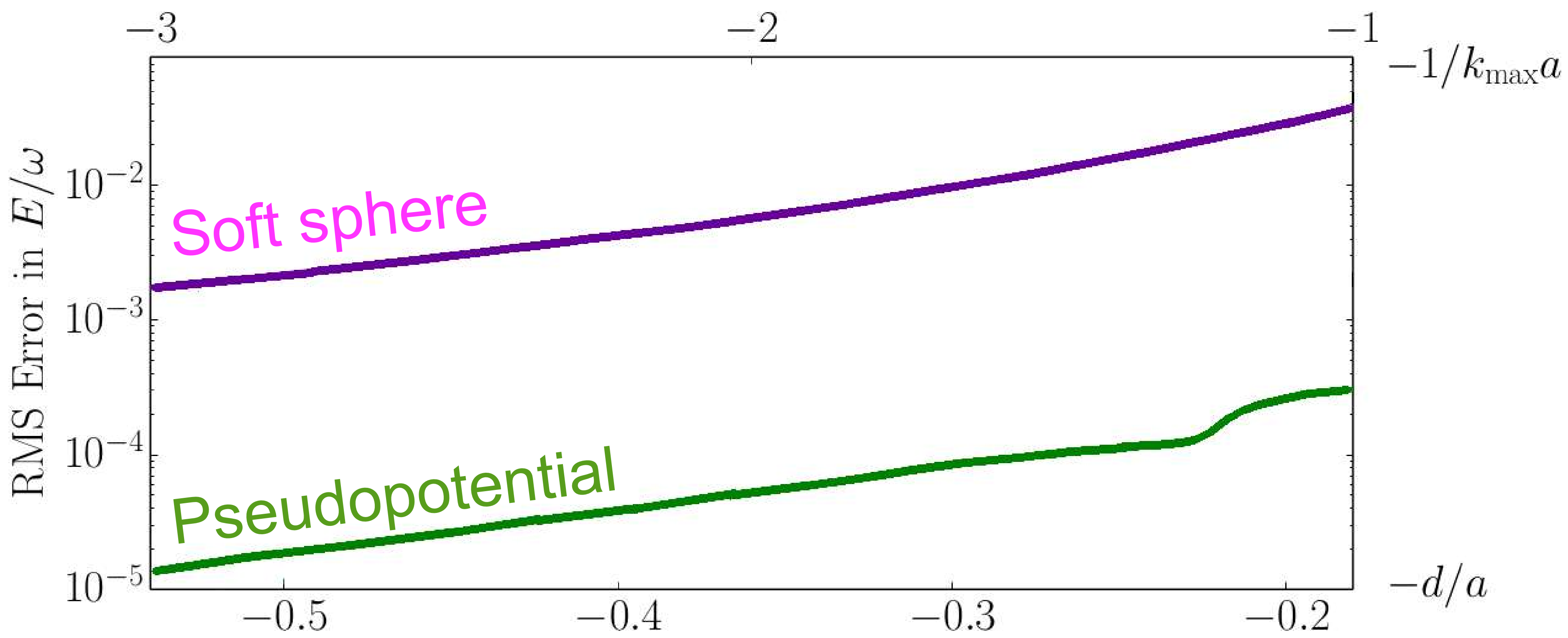




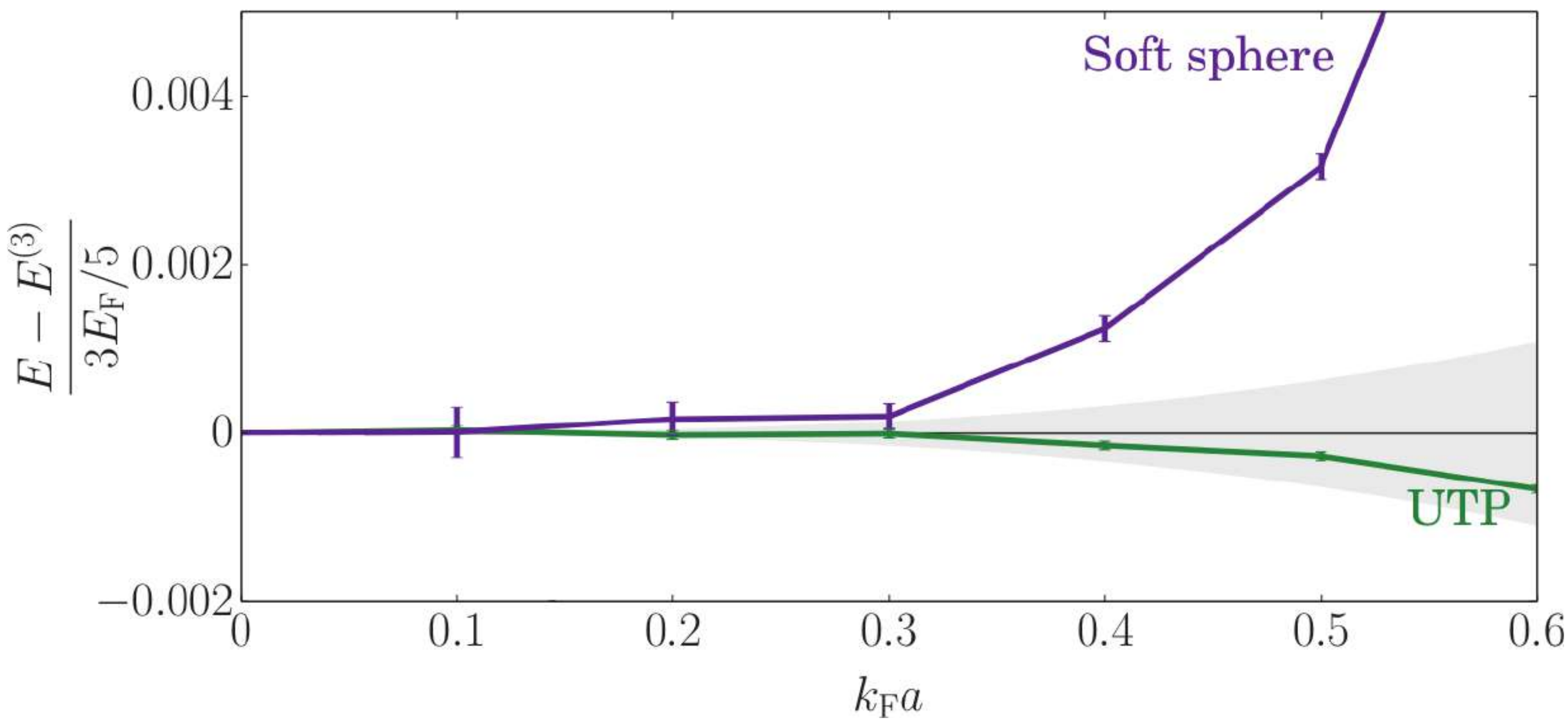
Pseudopotential: two atoms in a trap



Pseudopotential: two atoms in a trap

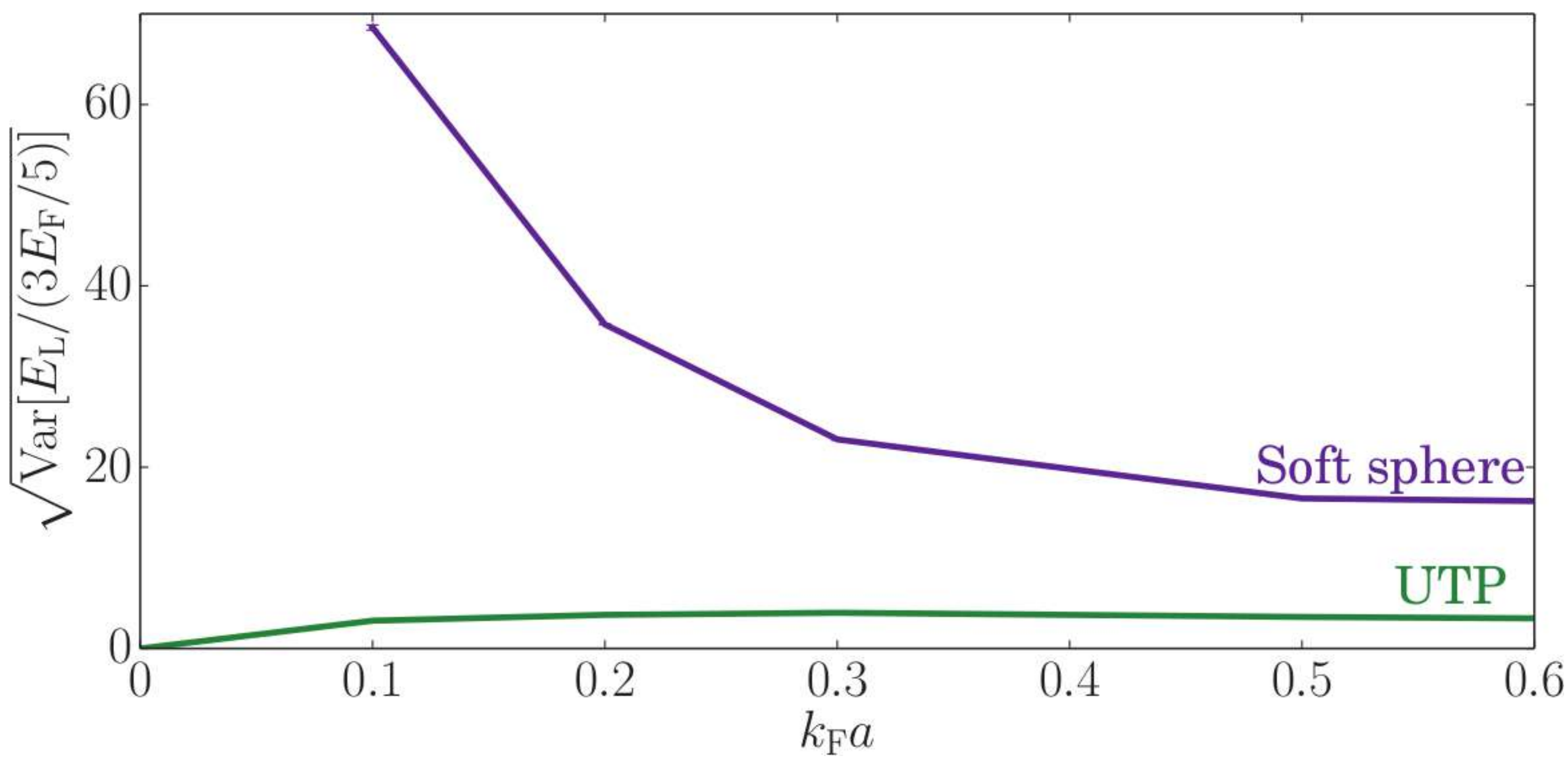


Pseudopotential: homogeneous system

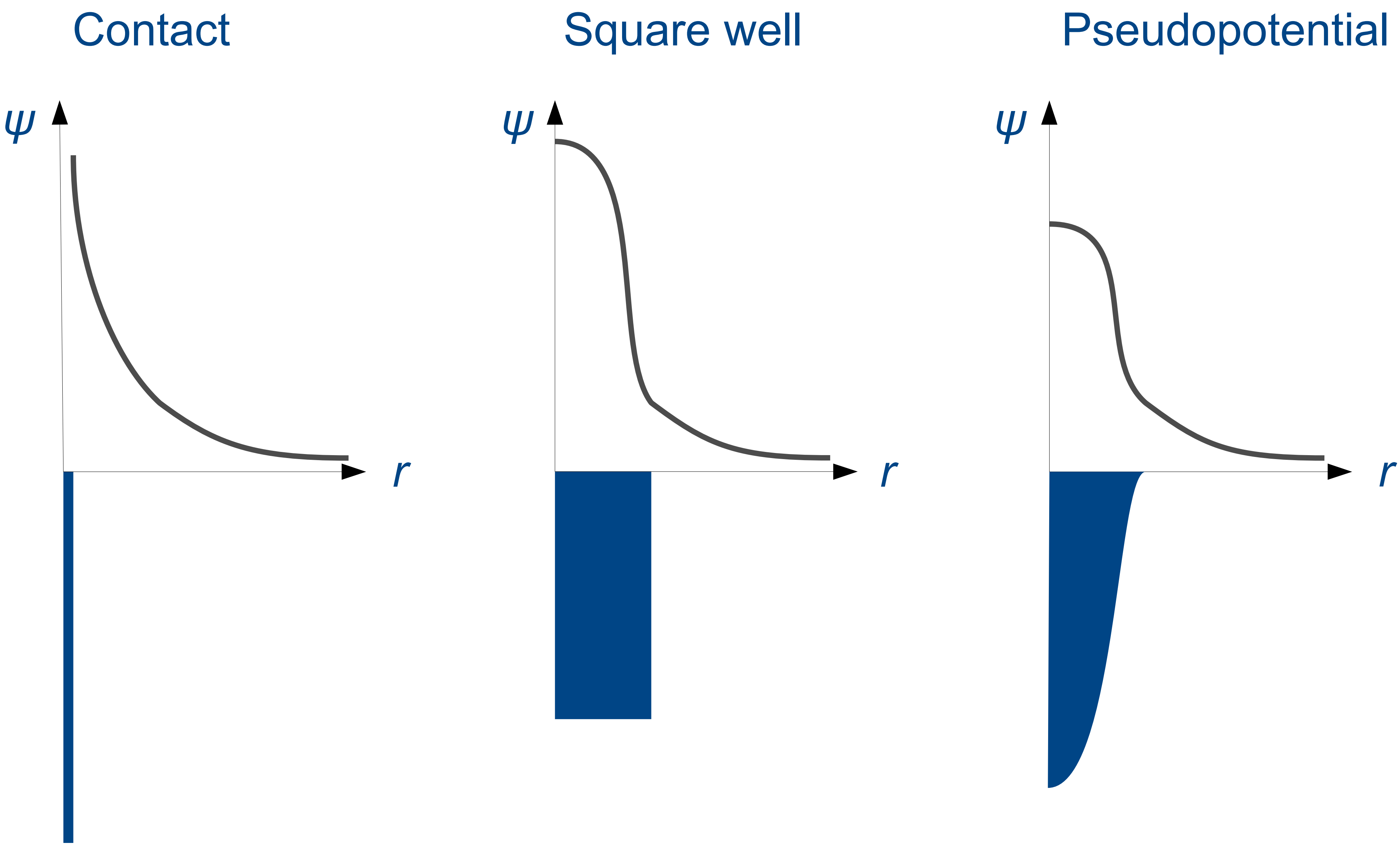


Mohling, Phys Rev 122 1043 (1961)

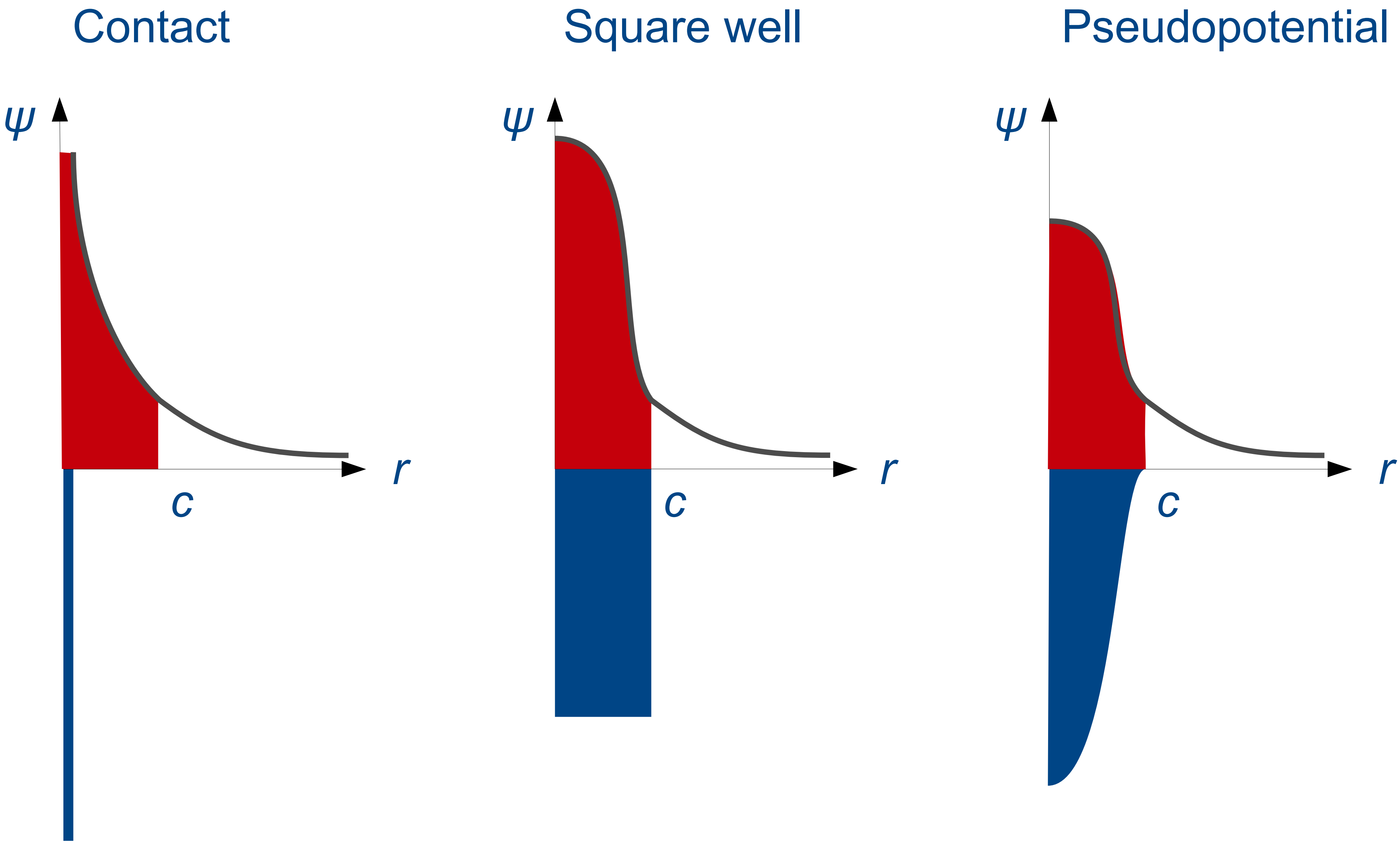
Pseudopotential: homogeneous system



Pseudopotential: bound state

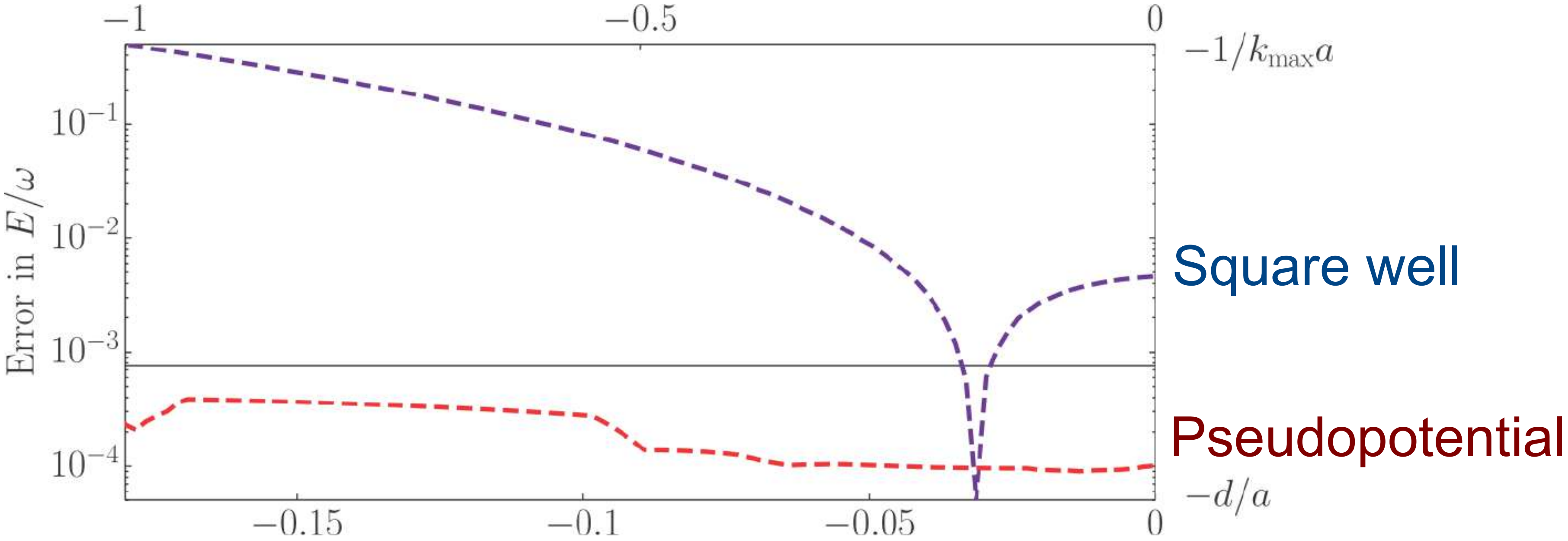


Pseudopotential: bound state



$$E = \int_0^c |\psi|^2 \, d\boldsymbol{r}$$ Troullier & Martins PRB 43 1993 (1991)

Pseudopotential: bound state



Contact interaction pseudopotential summary

Pseudopotential for repulsive, attractive, and bound state: 100 times more accurate, 1000 times faster

Formalism is systematically improvable, trading accuracy for speedup

Python tool: https://pypi.python.org/pypi/contactpp
PRA 90, 033626 (2014)

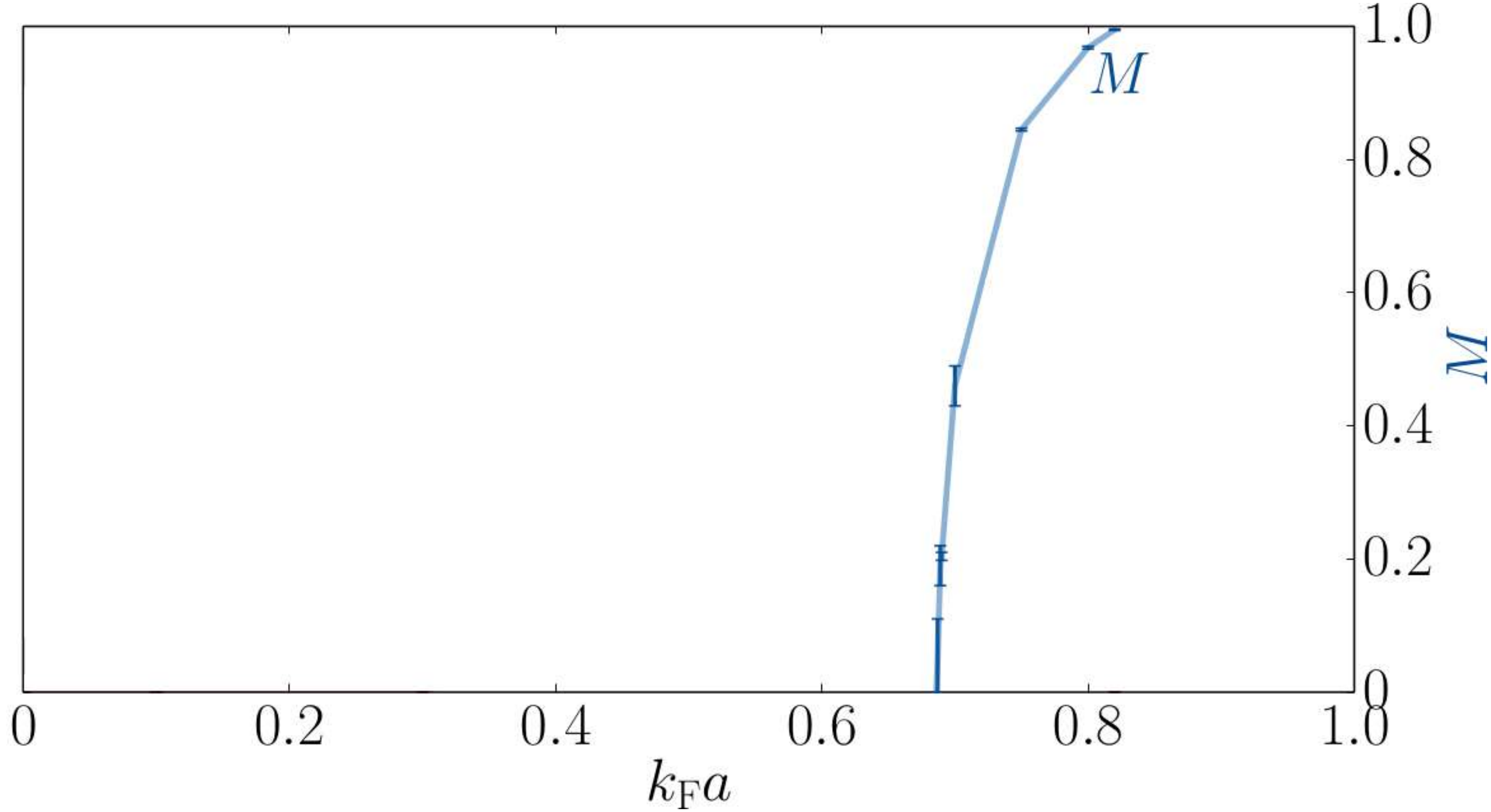
Stoner Hamiltonian

$$H = -\frac{\nabla^2}{2} + 4\pi a \delta(\boldsymbol{r}_{\uparrow} - \boldsymbol{r}_{\downarrow})$$

Theories of ferromagnetism

Stoner mean-field theory	Second order	$k_Fa=1.57$
Fluctuations beyond Hertz-Millis	First order	-
Polaron theory	First order	-
Field theory	First order	$k_Fa=1.054$
Tan relations	No magnetism	-
DMC hard sphere	First order	$k_Fa=0.81(2)$
QMC square well	First / second order	$k_Fa=0.83(2)$

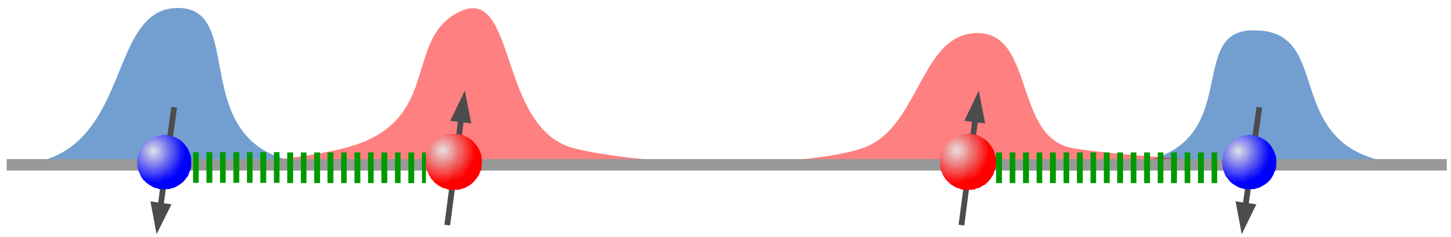
Stoner Hamiltonian



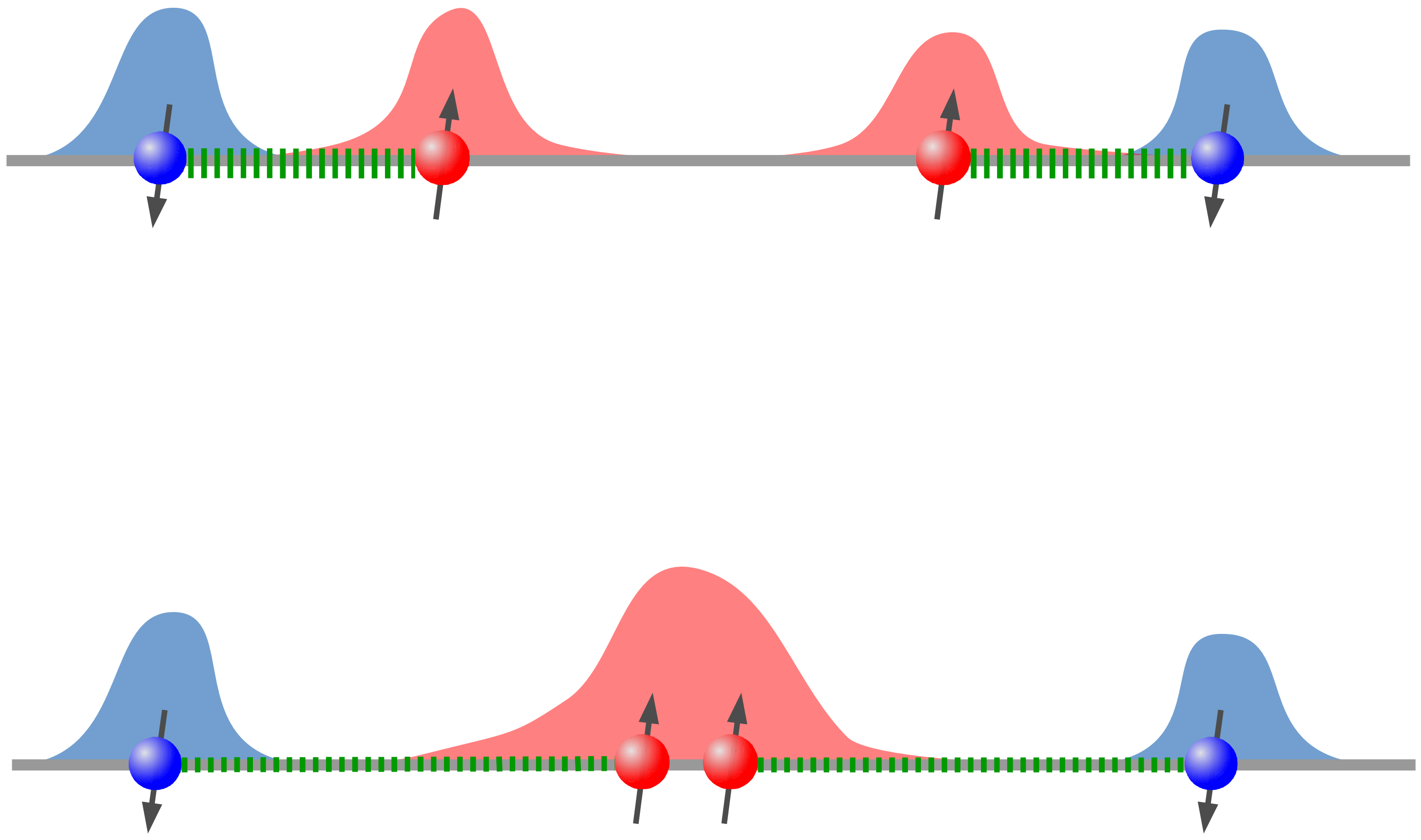
Theories of ferromagnetism

Stoner mean-field theory	Second order	$k_F a=1.57$
Fluctuations beyond Hertz-Millis	First order	-
Polaron theory	First order	-
Field theory	First order	$k_F a=1.054$
Tan relations	No magnetism	-
DMC hard sphere	First order	$k_F a=0.81(2)$
QMC square well	First / second order	$k_F a=0.83(2)$
DMC pseudopotential	Second order	$k_F a=0.683(1)$

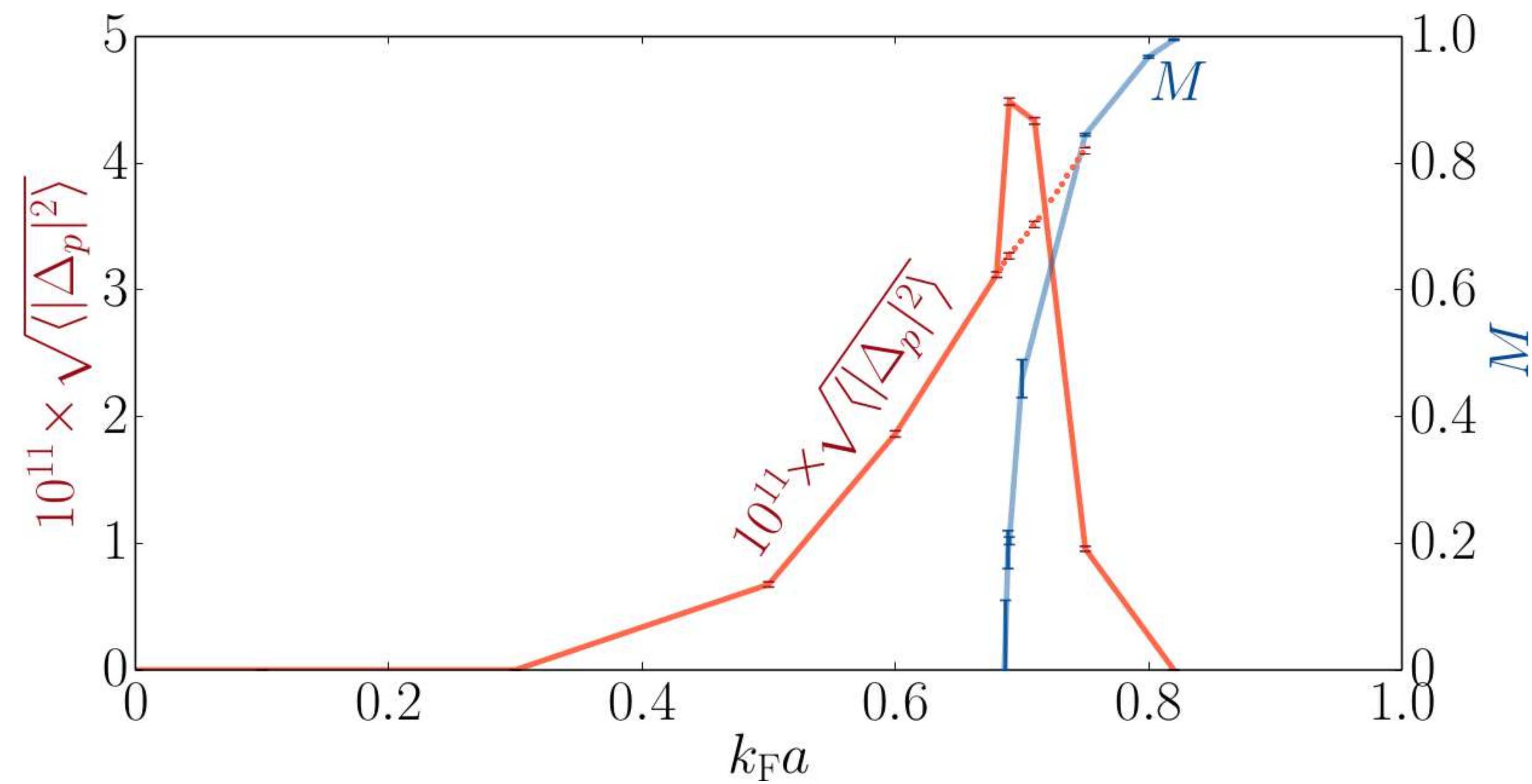
Fluctuation contributions



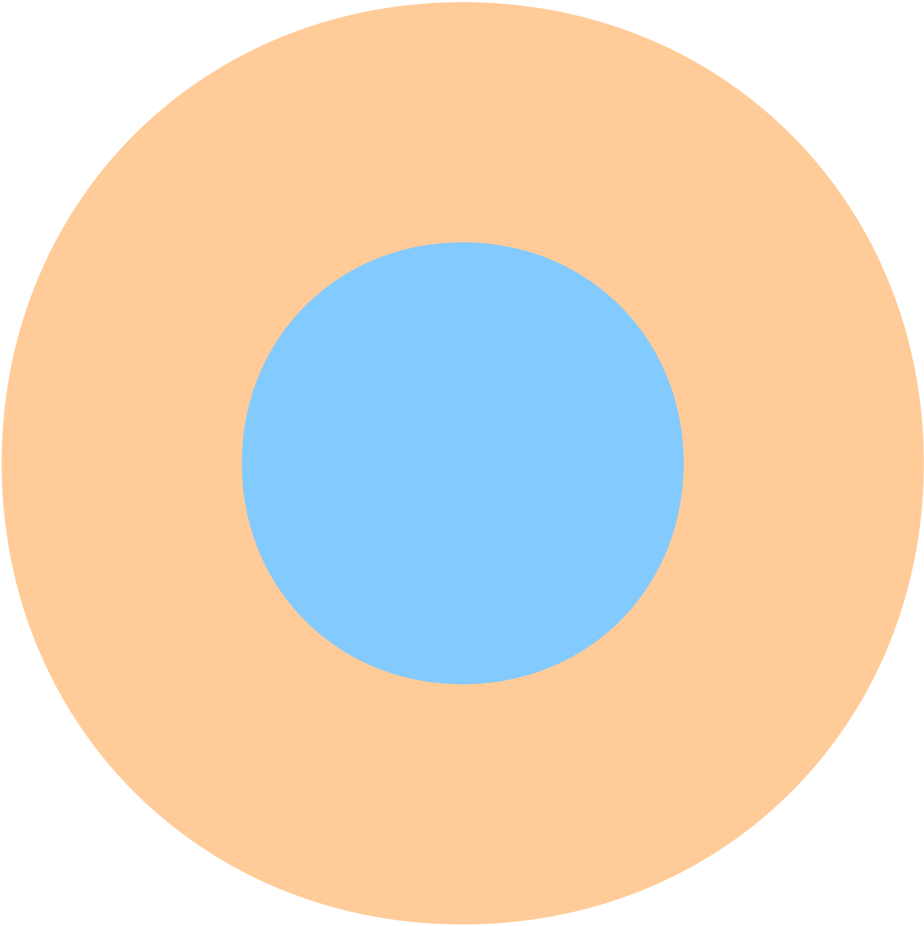
Fluctuation contributions



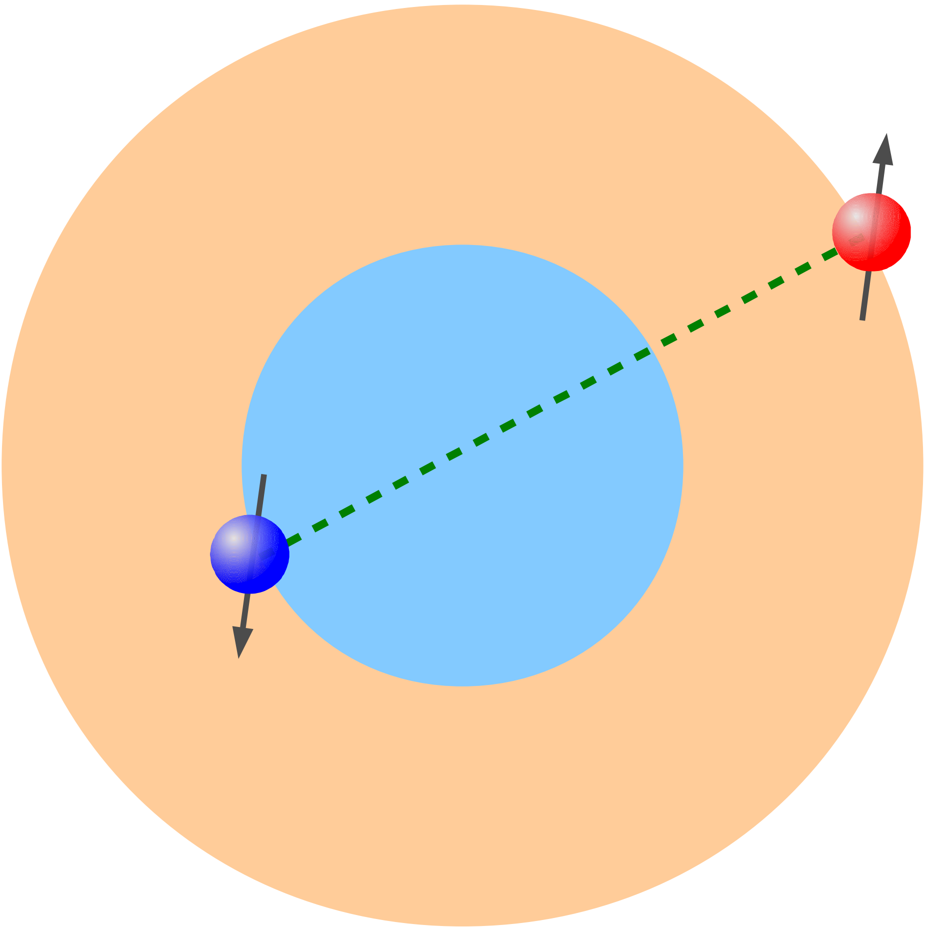
Stoner Hamiltonian



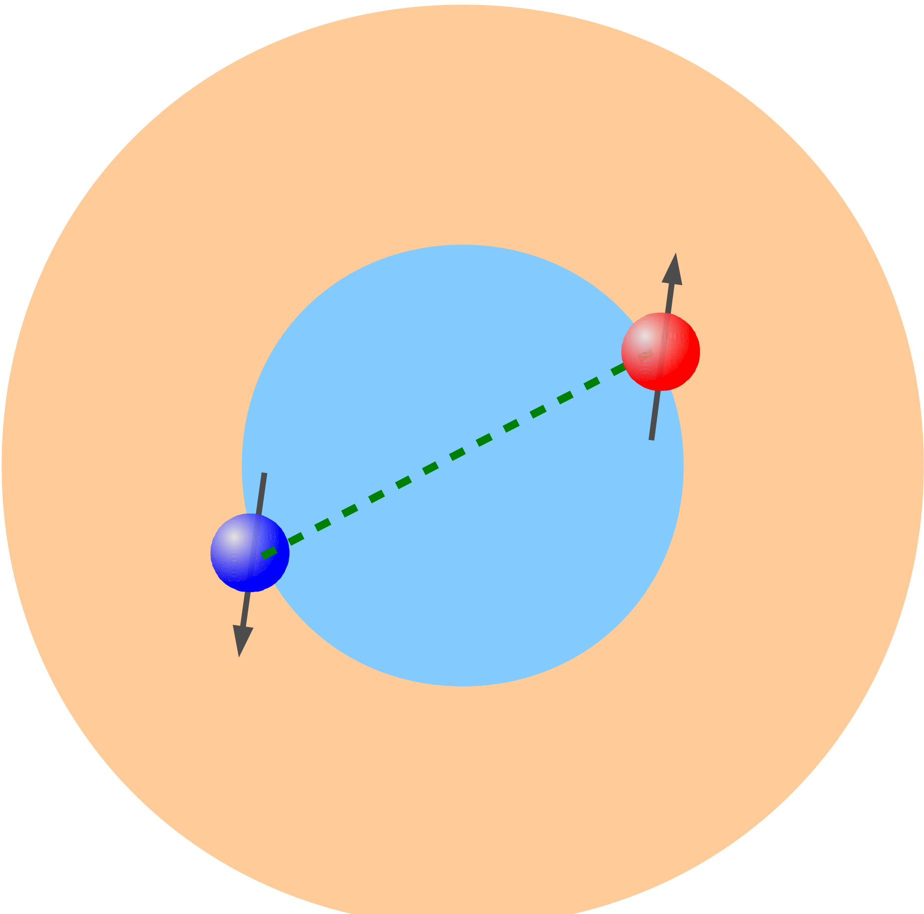
Imbalanced superfluid



FFLO superfluid



Breached superfluid

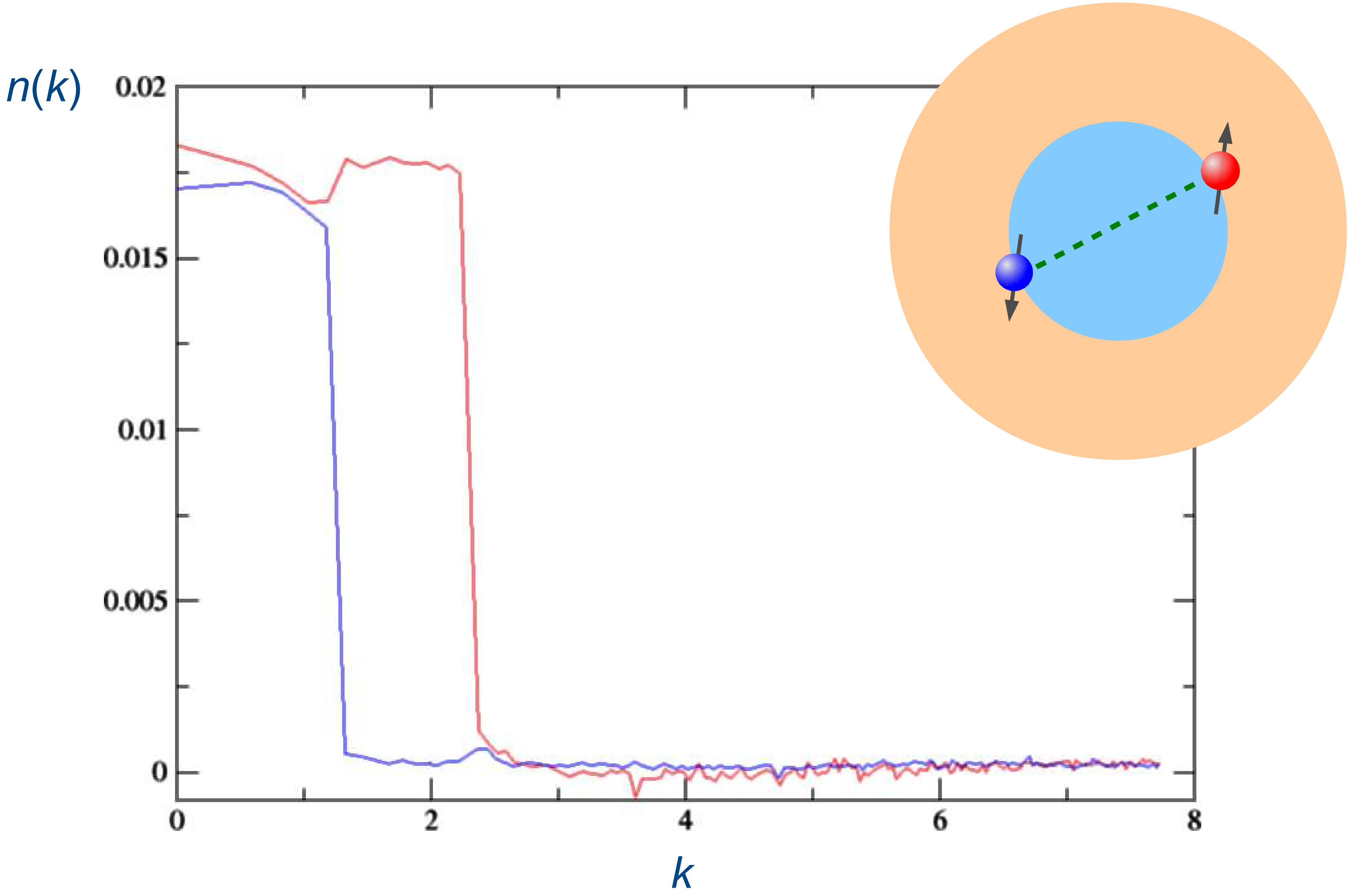


Liu & Wilczek, PRL 90, 047002 (2003)

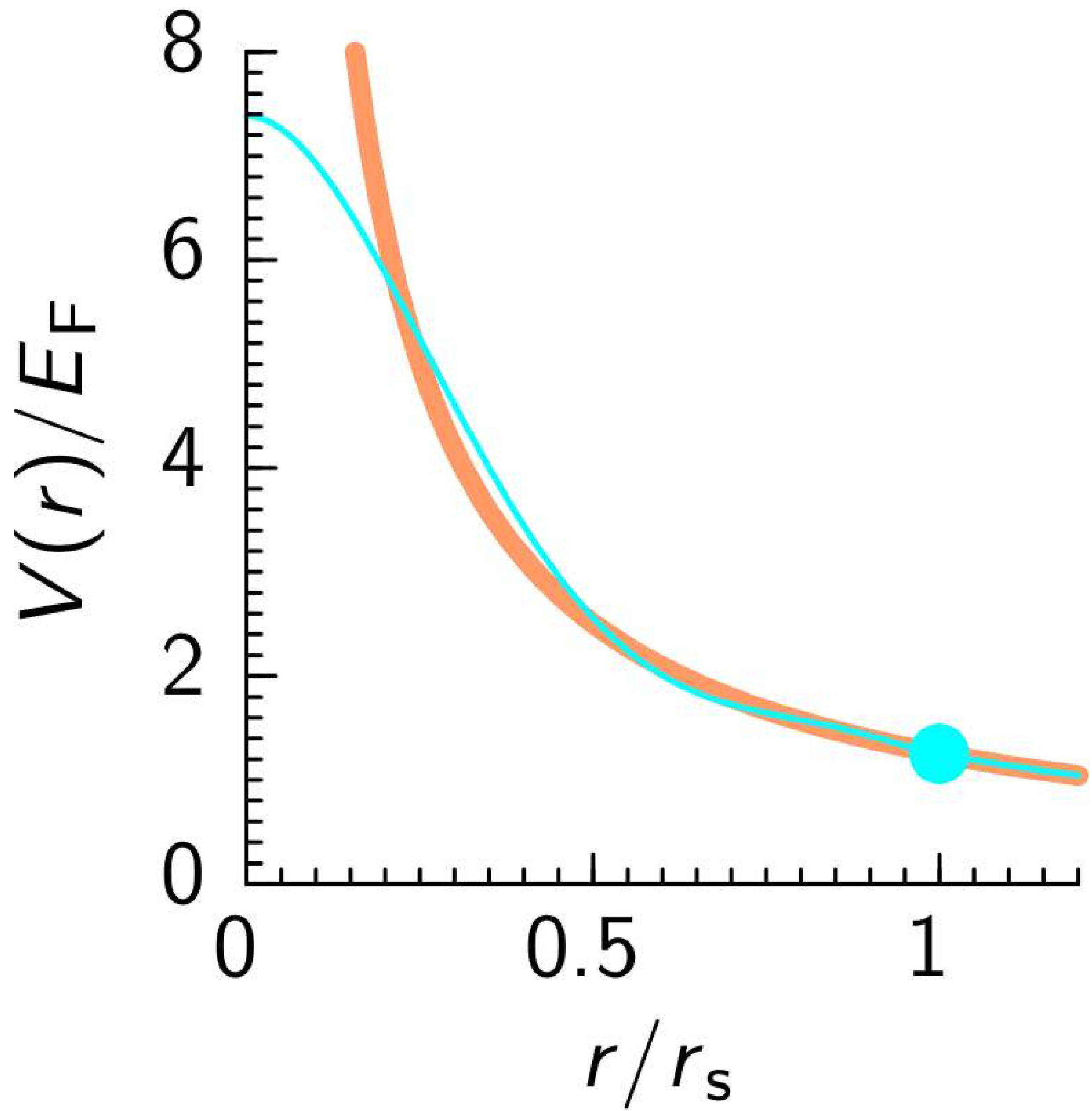
Finite ranged interactions

$$\cot \delta_0 = -\frac{1}{ka} + \frac{1}{2} k \, r_{eff}$$

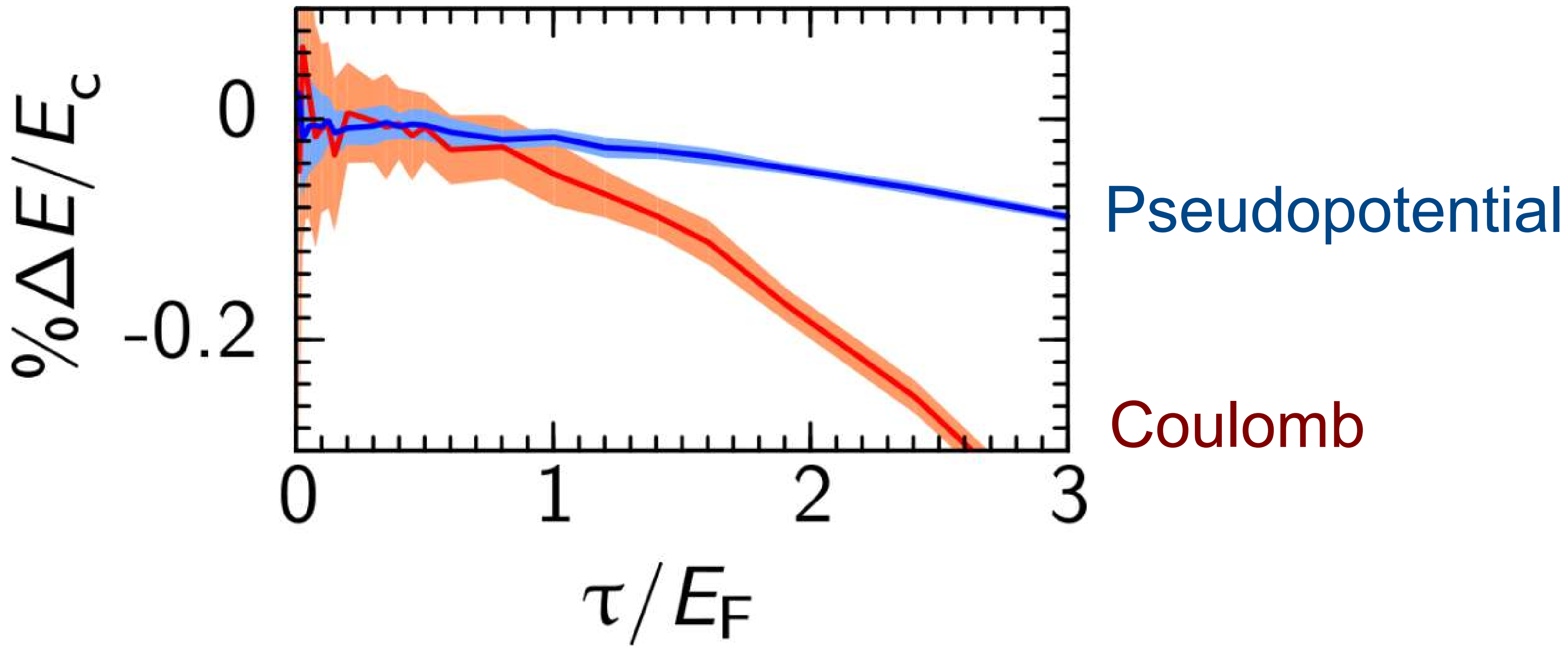
Breached superfluid



Coulomb pseudopotential

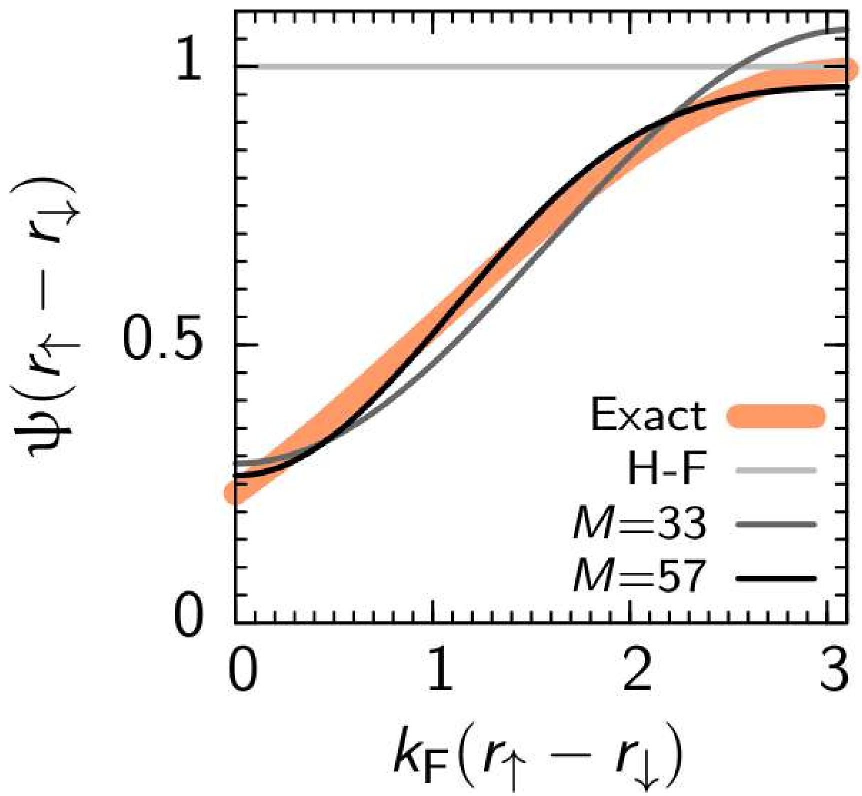


Homogeneous electron gas

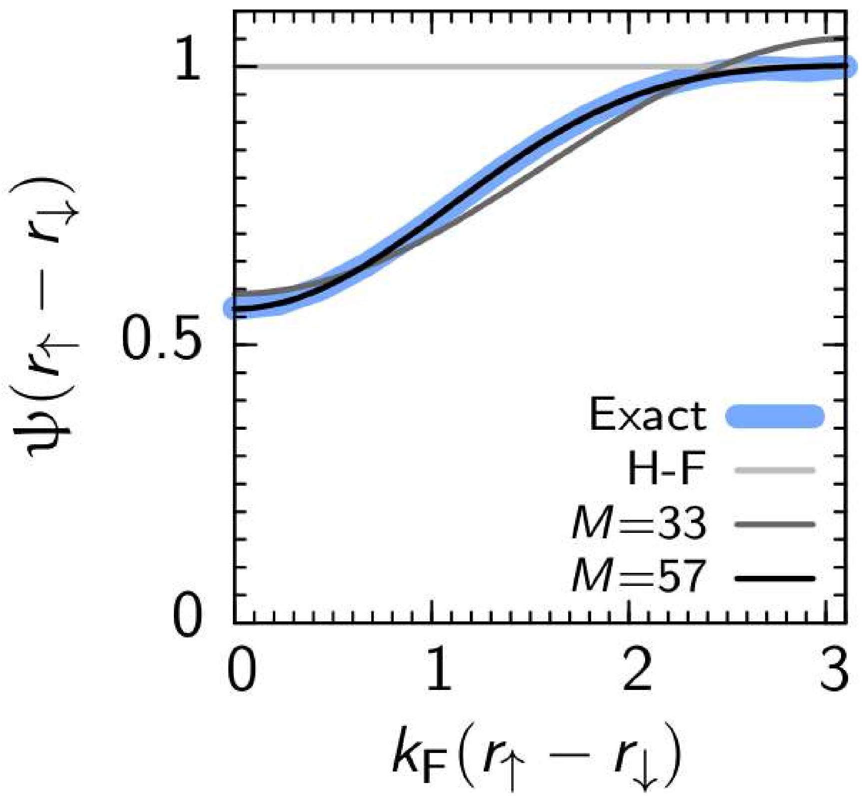


Configuration interaction

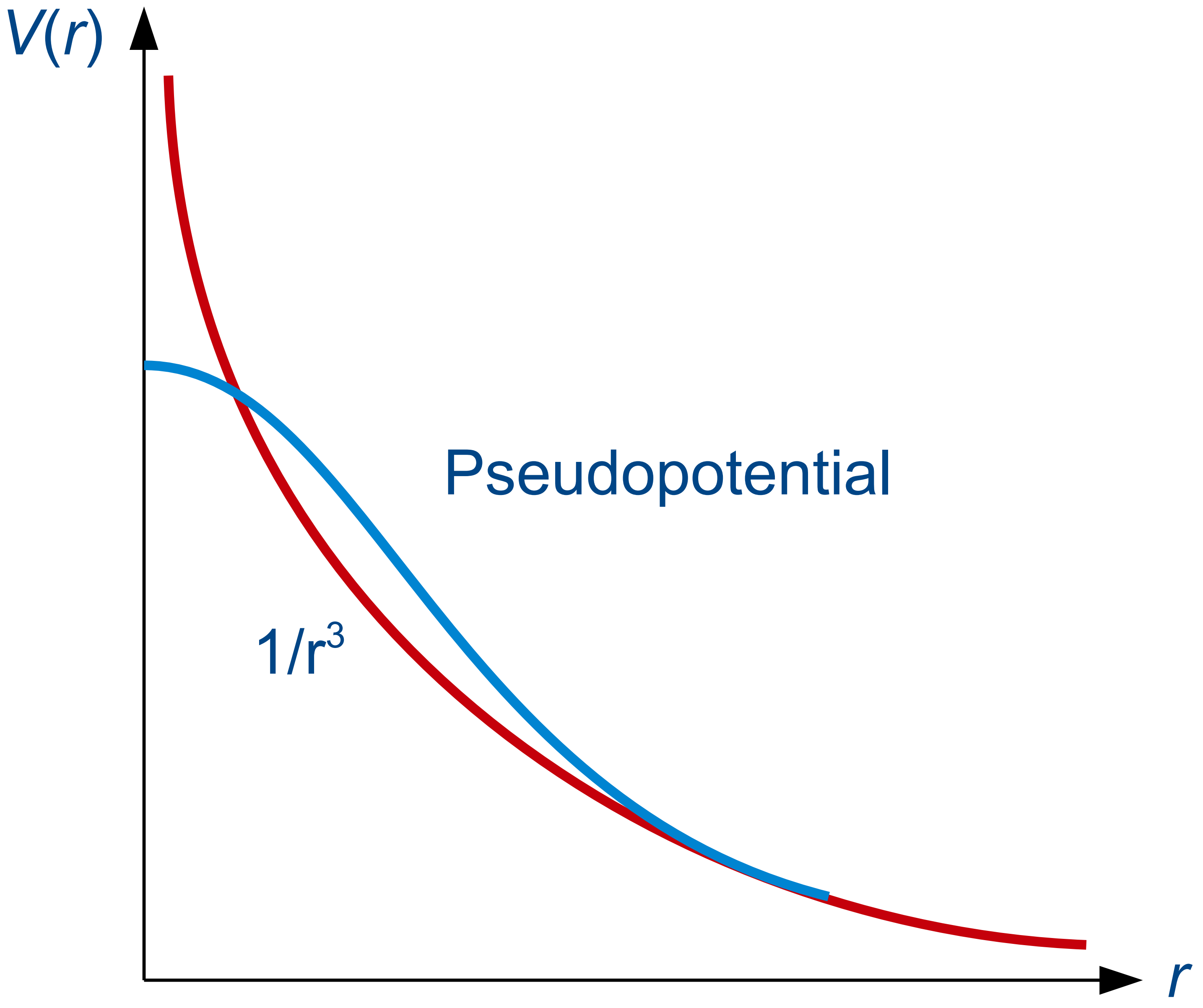
Coulomb



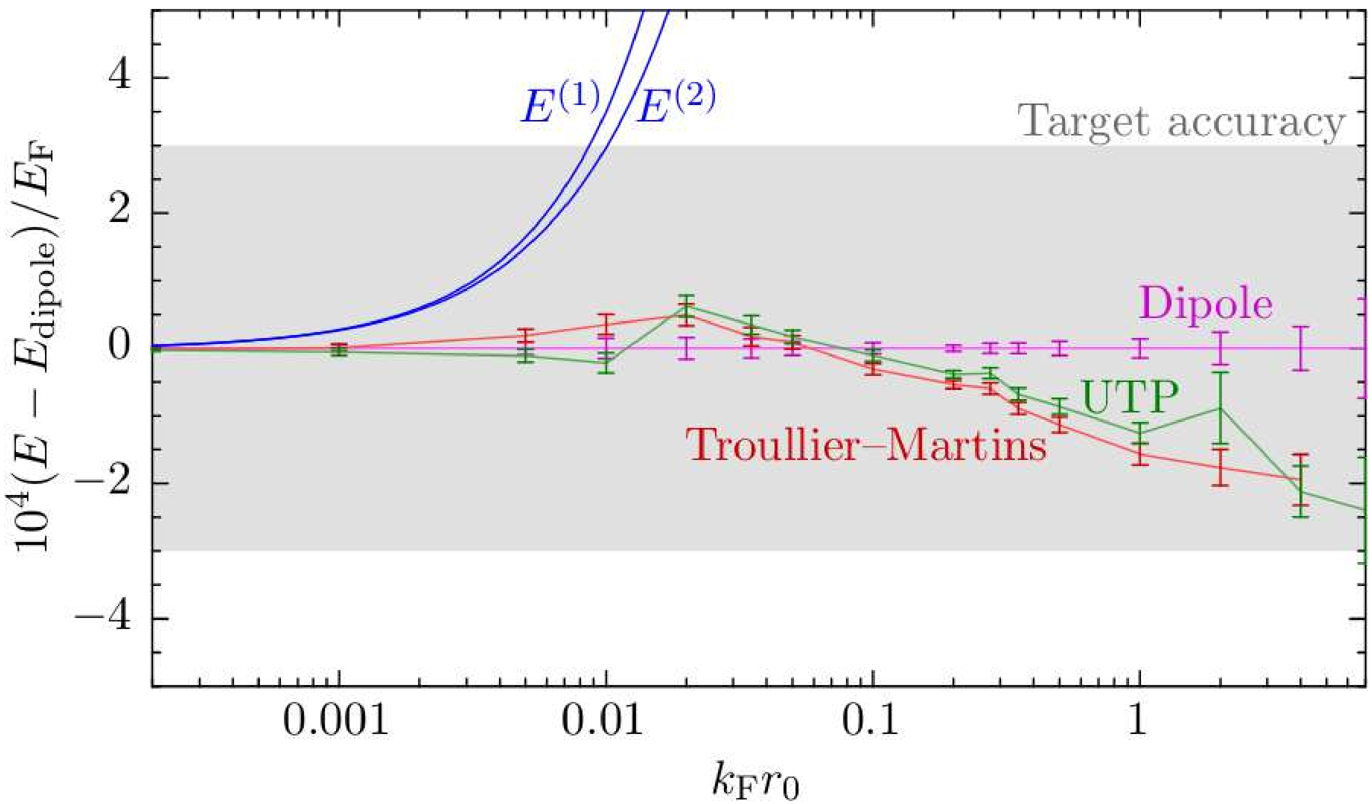
Pseudopotential



Dipolar pseudopotential

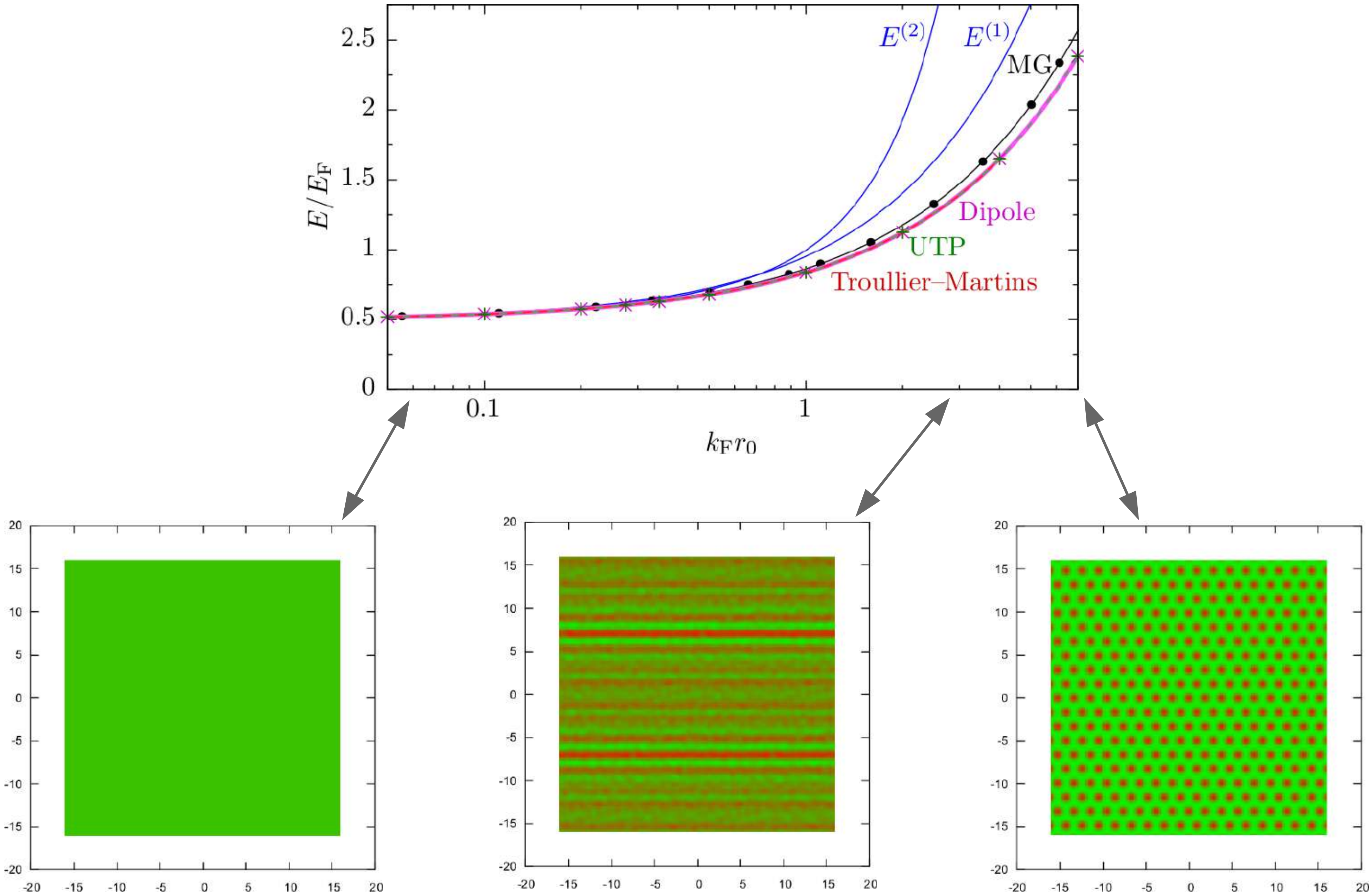


Accuracy of the ground state energy of a dipolar gas



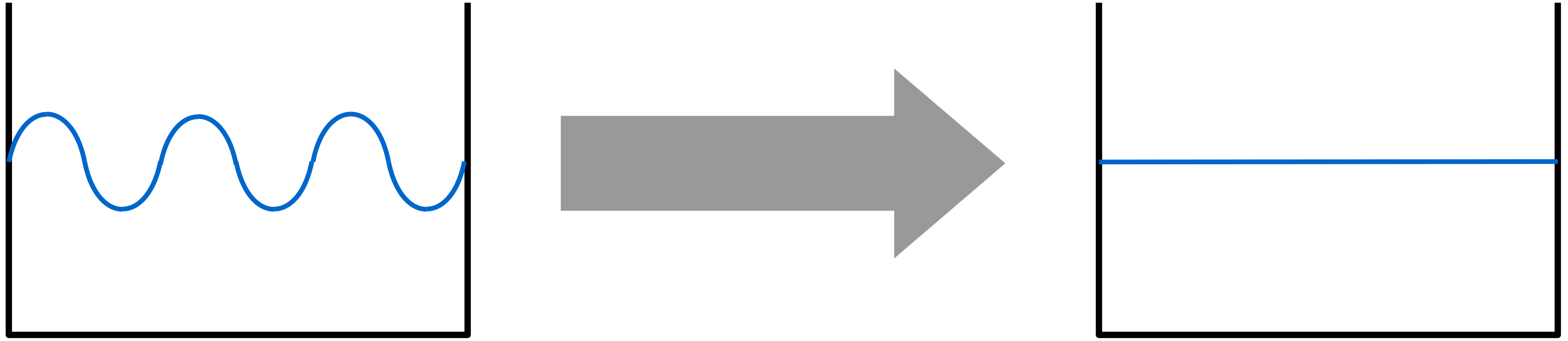
Matveeva & Giorgini, PRL 109, 200410 (2012)

Dipolar phases



Kinetic energy pseudopotential

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



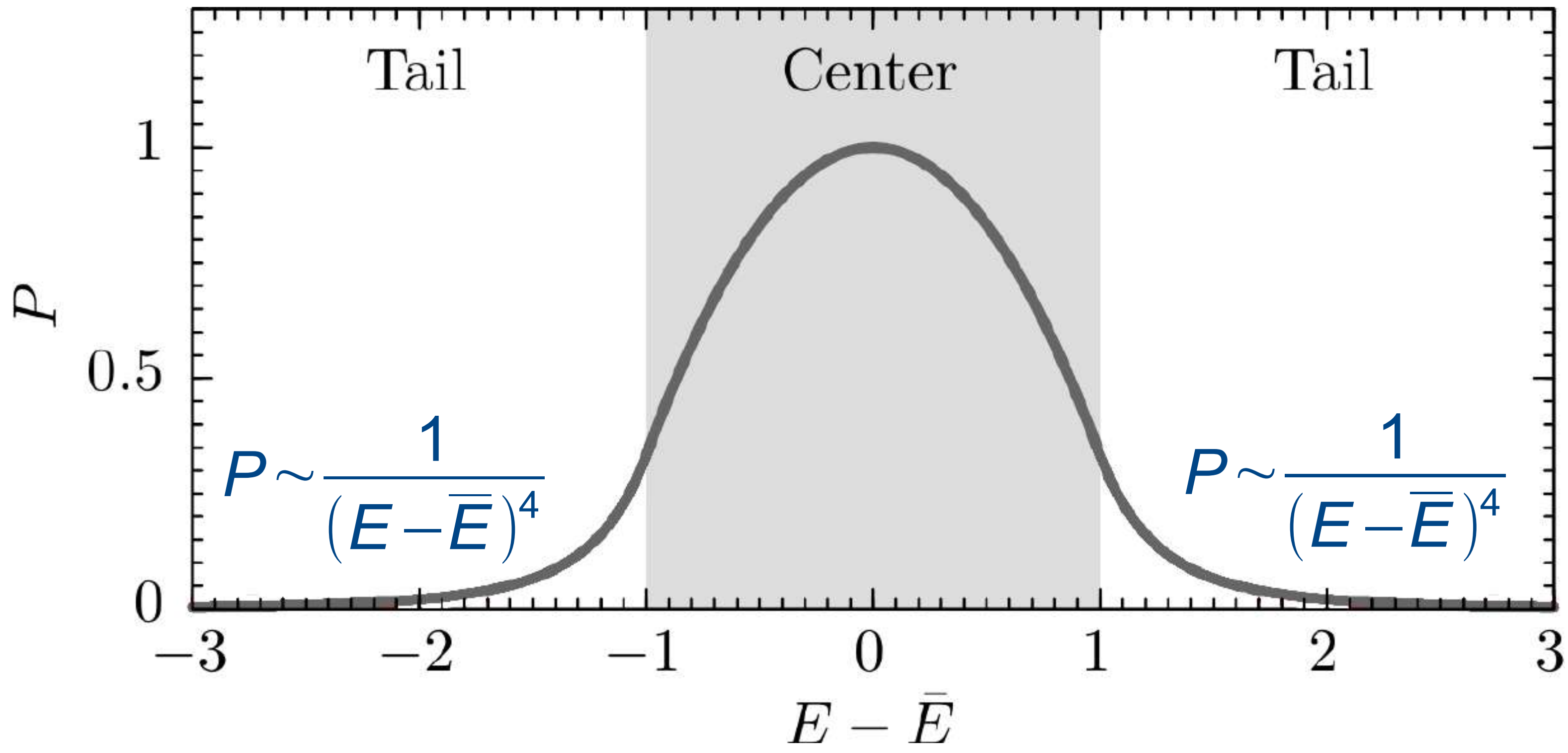
Kinetic energy pseudopotential

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

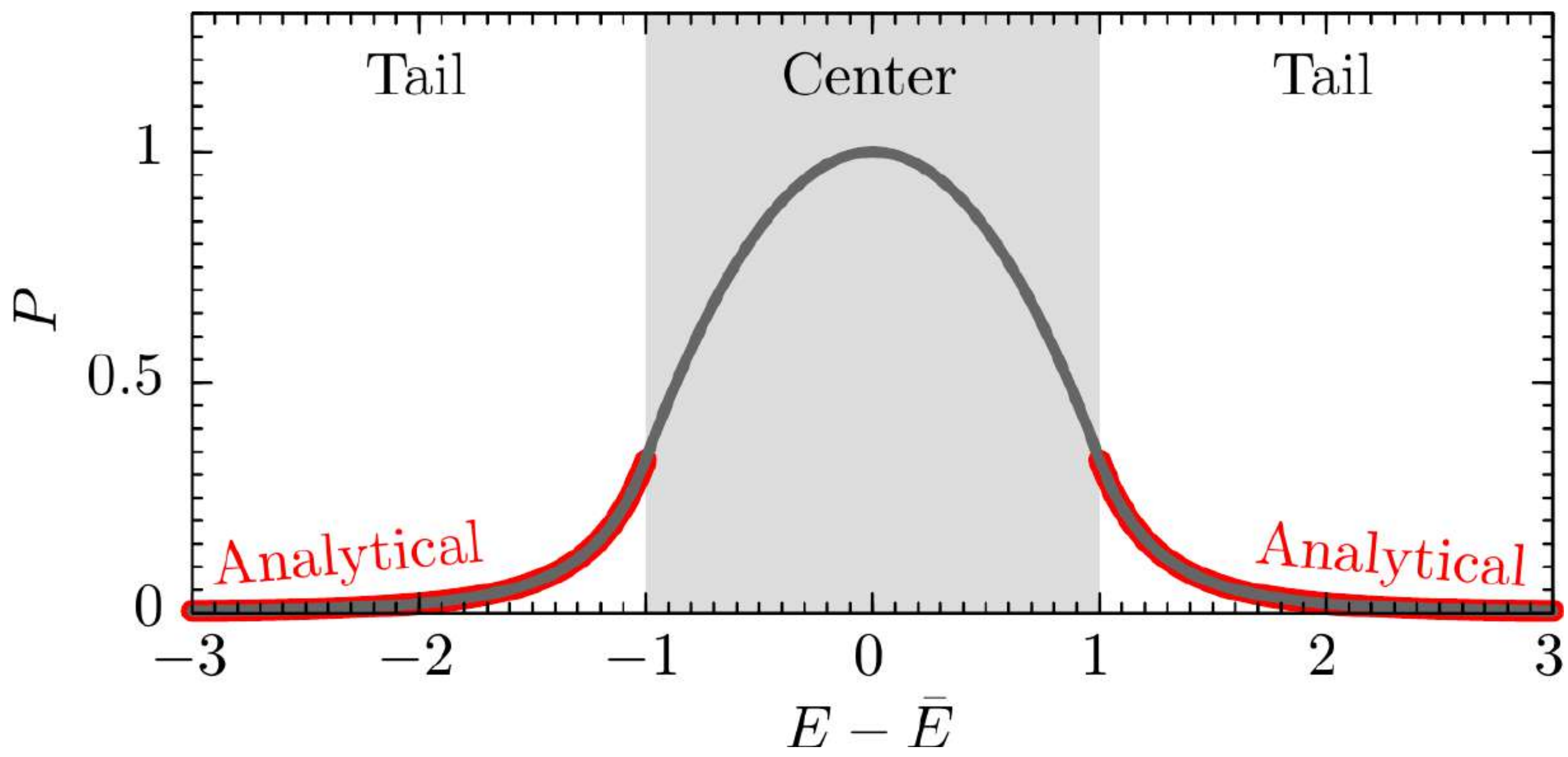
$$E = \frac{\int \bar{\psi} H \psi \, d\boldsymbol{r}}{\int \bar{\psi} \psi \, d\boldsymbol{r}} = \int_{\psi^2} \frac{H\psi}{\psi}$$

at a node $\psi \sim x$ so $E_{\text{L}} = \frac{H\psi}{\psi} \sim \frac{1}{x}$

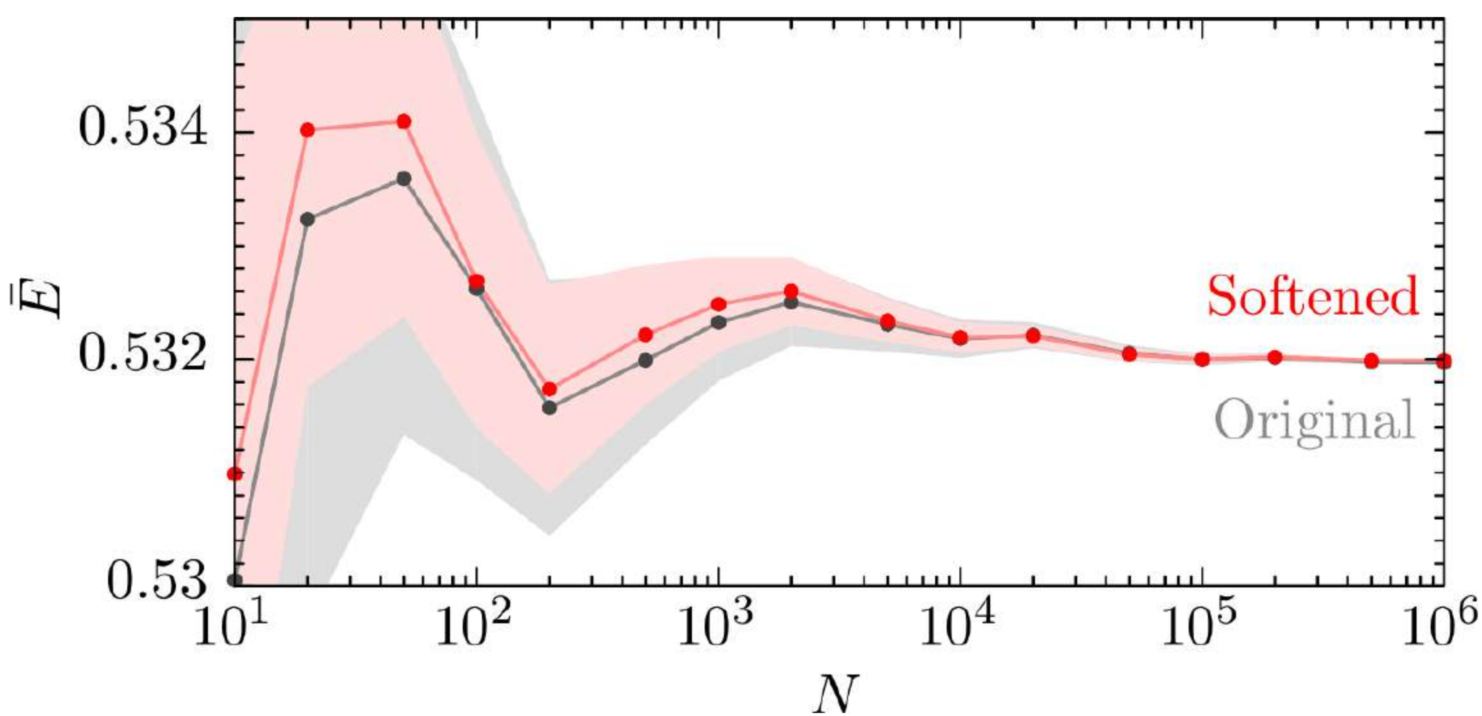
Energy distribution



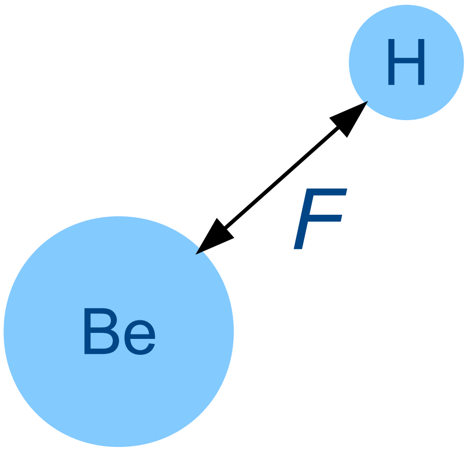
Softening the energy distribution



Accuracy of the homogeneous electron gas

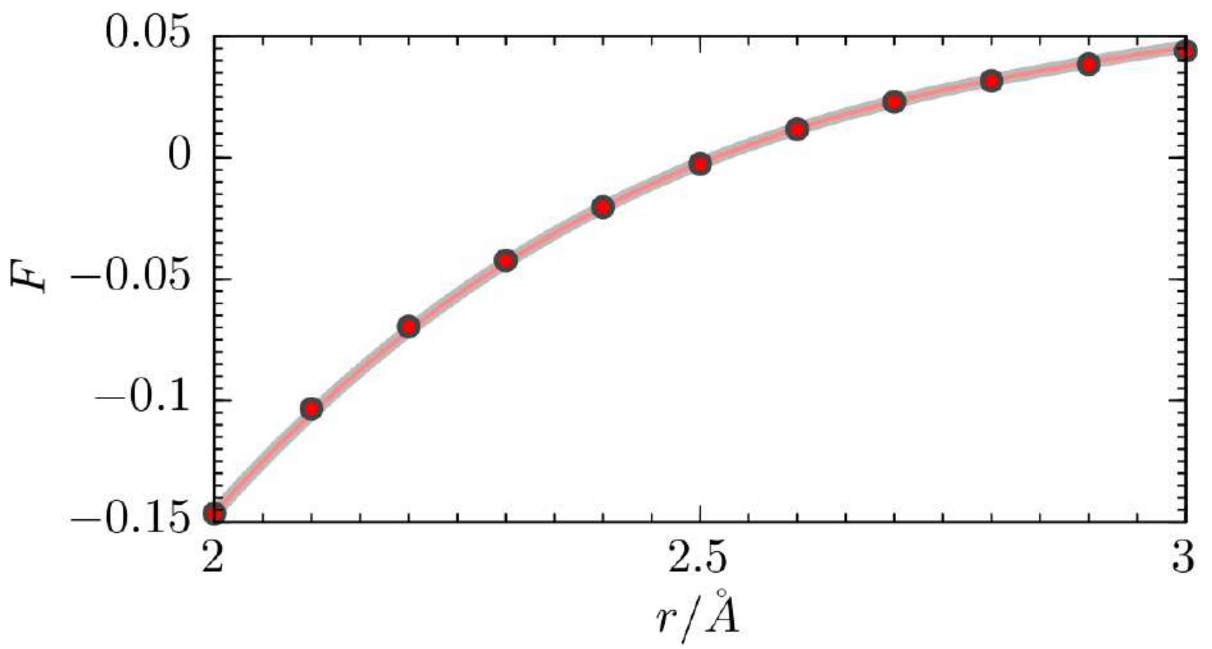


Force distribution



$$P \sim \frac{1}{F^{5/2}}$$

Force distribution



Summary

Developed a pseudopotential for the contact, Coulomb, and dipolar interactions

Studied many-body phenomena

Proposed a formalism to soften the energy and interatomic force distribution

Python tool: https://pypi.python.org/pypi/contactpp
PRA 90, 033626 (2014)