UNIVERSITY OF CAMBRIDGE

Pseudizing the Hamiltonian

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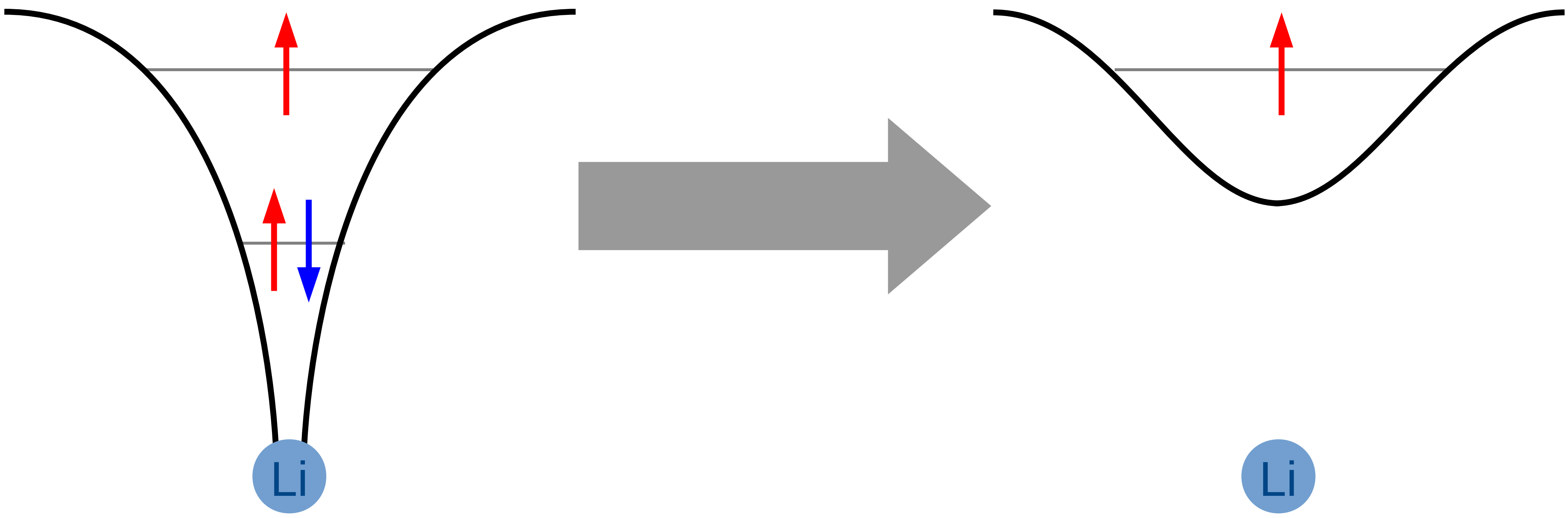
Pseudopotentials

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

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

Pseudopotentials

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

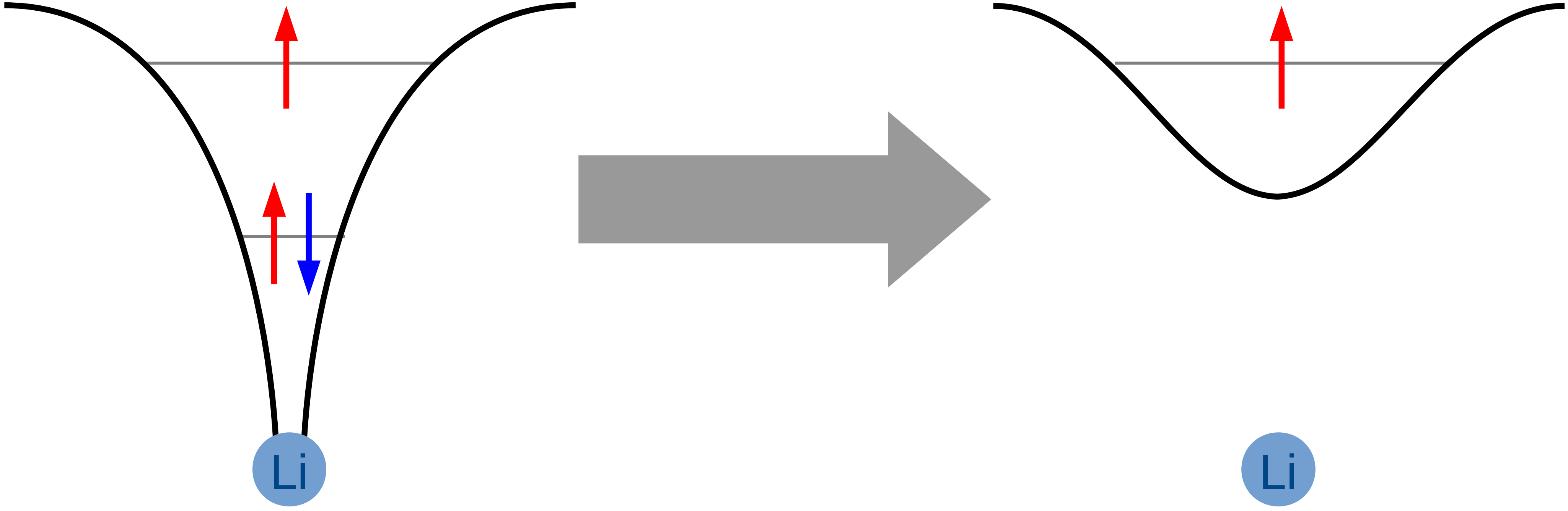


Pseudopotentials

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

Smooth background

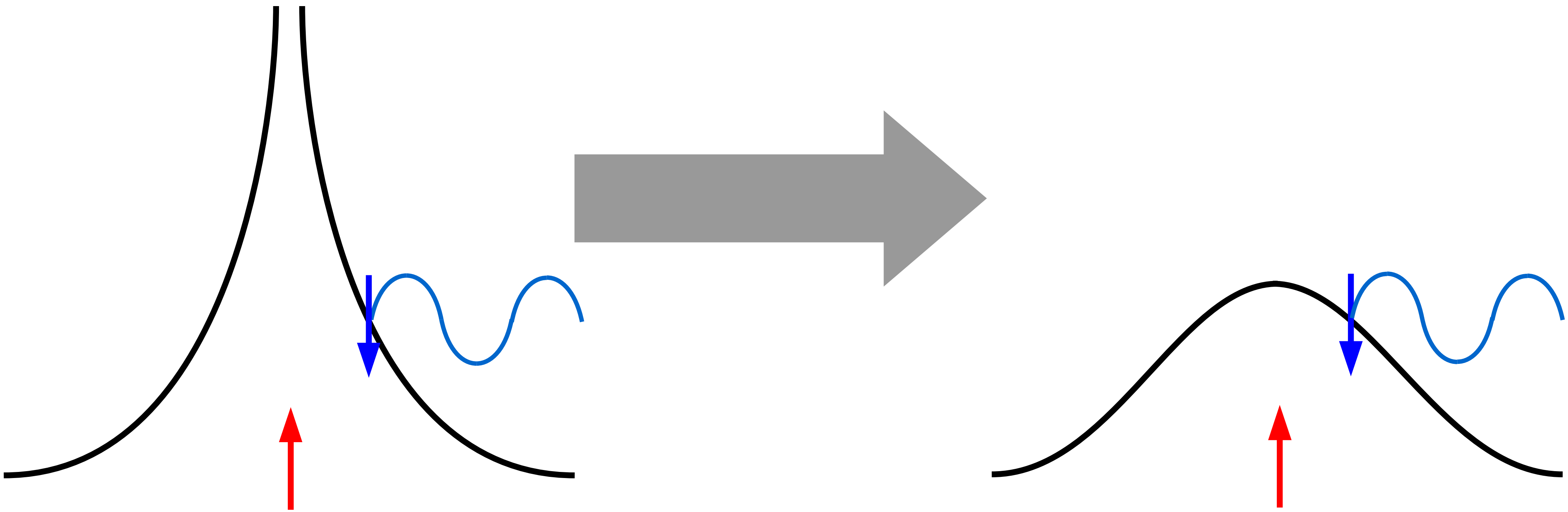
Fewer electrons



Pseudopotentials

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

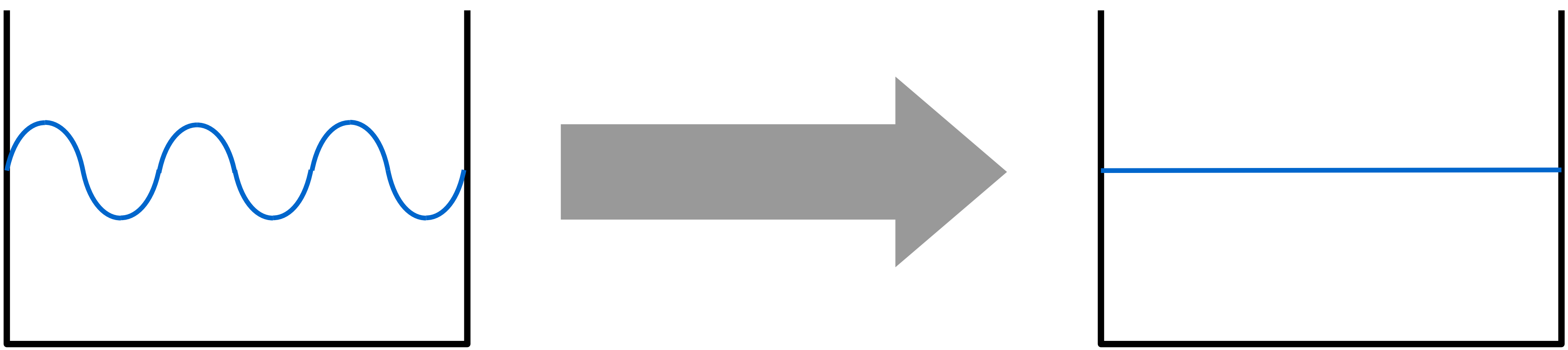
Smooth background



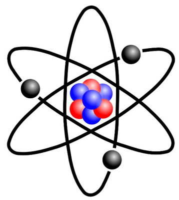
Pseudopotentials

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

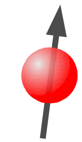
Smooth integrand

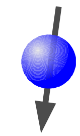


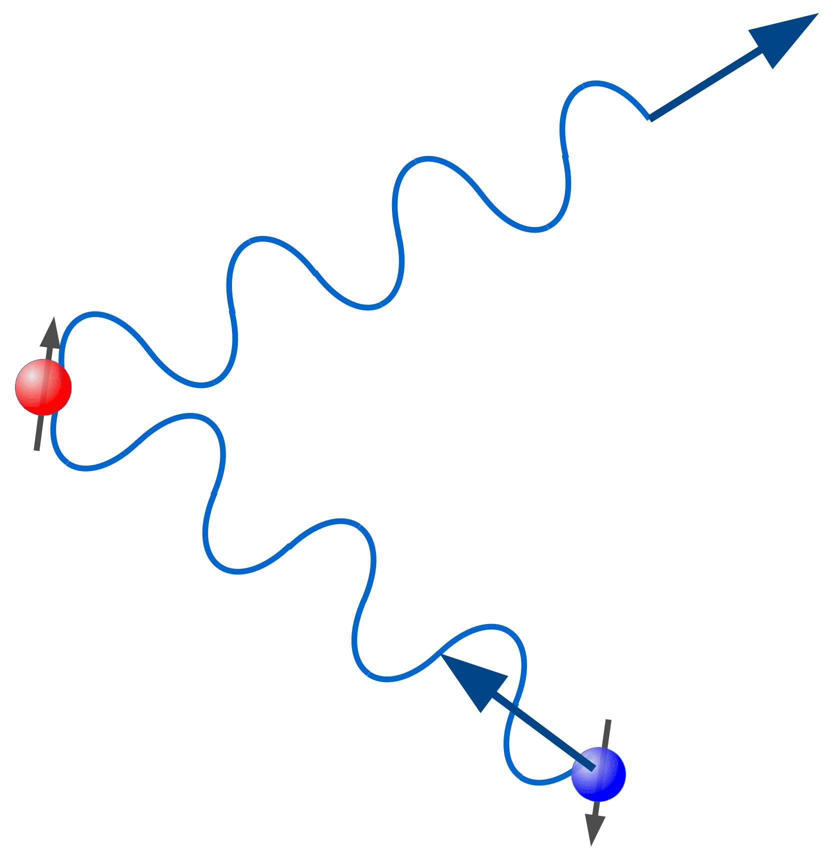
Scattering in ultracold atom gases



^{6}Li atom

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

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



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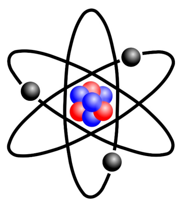

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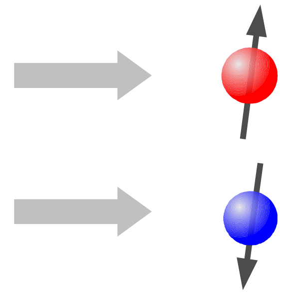
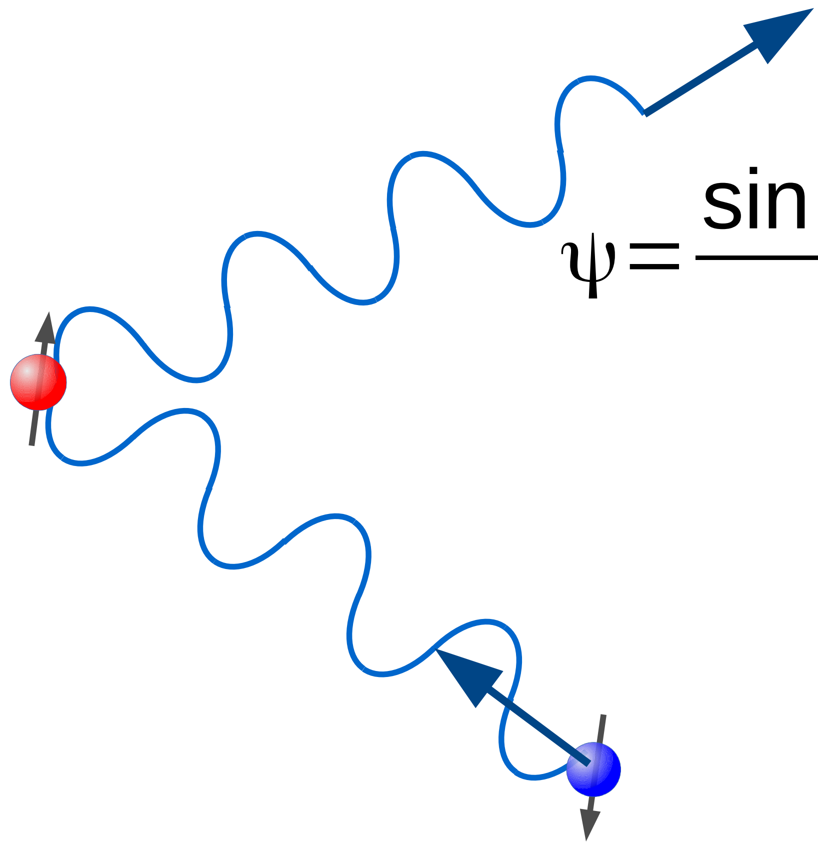


Up spin electron

Down spin electron

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

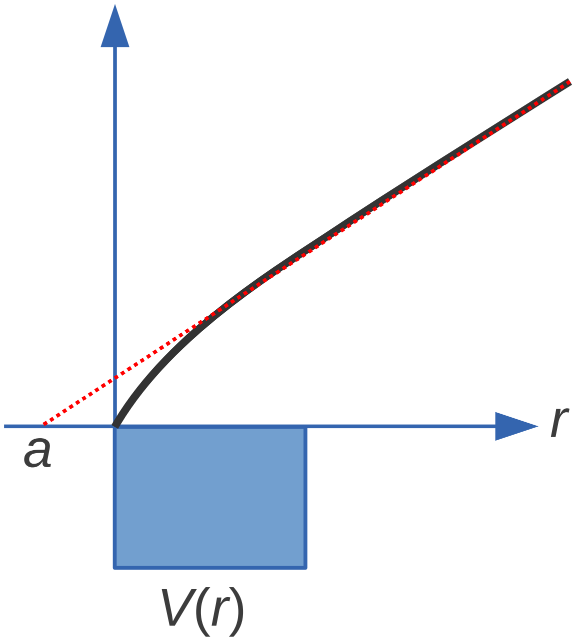
$$V(r) = \frac{a}{2r^2}\delta(r)$$



Scattering potentials

Underlying attractive

Effective attractive



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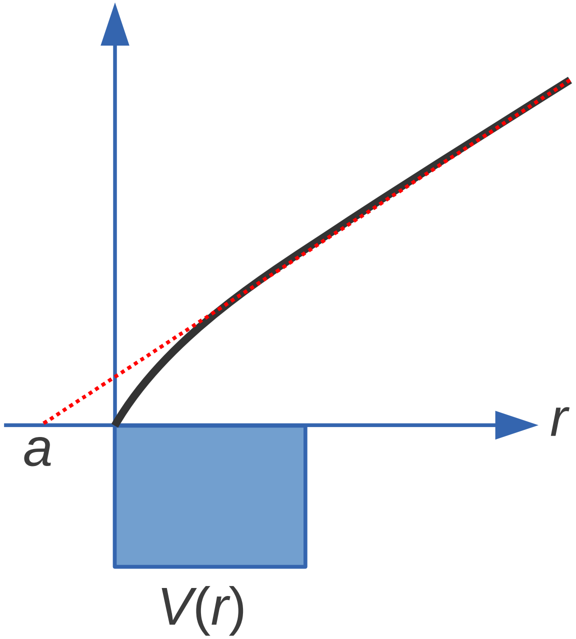
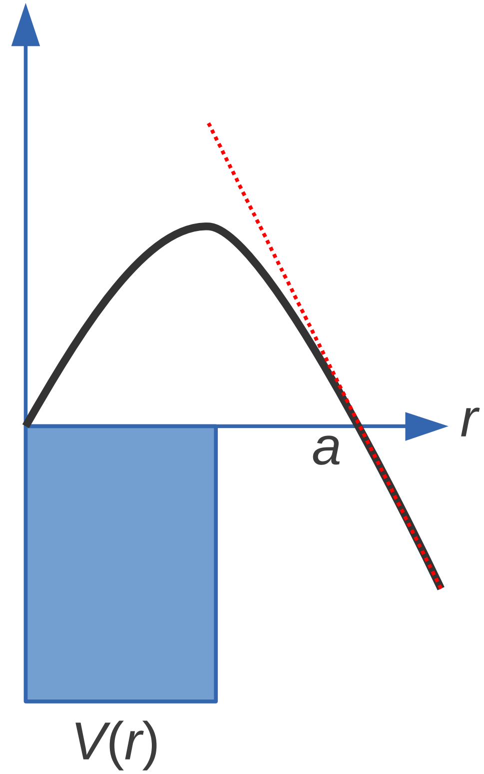


Underlying attractive

Effective repulsive



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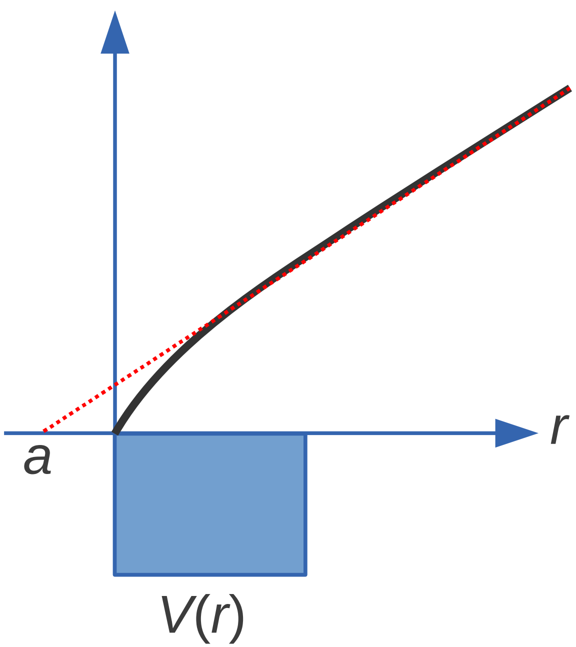

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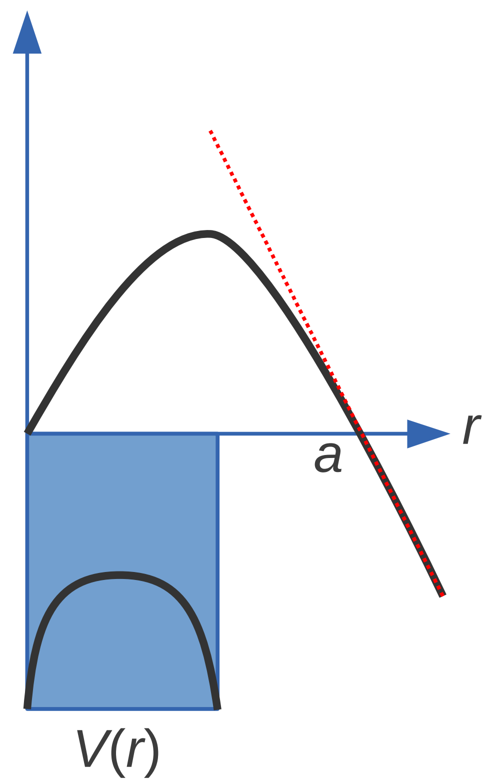

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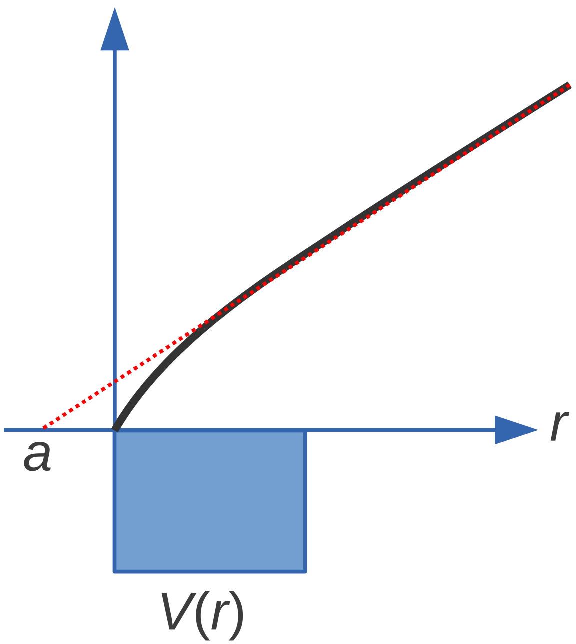

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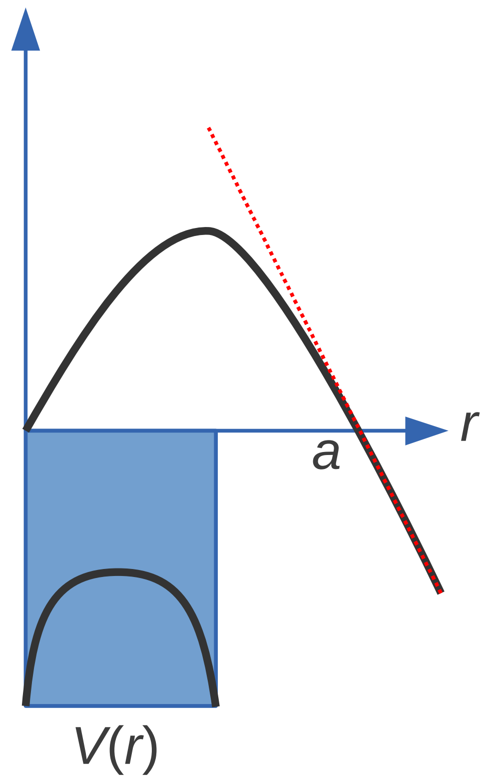
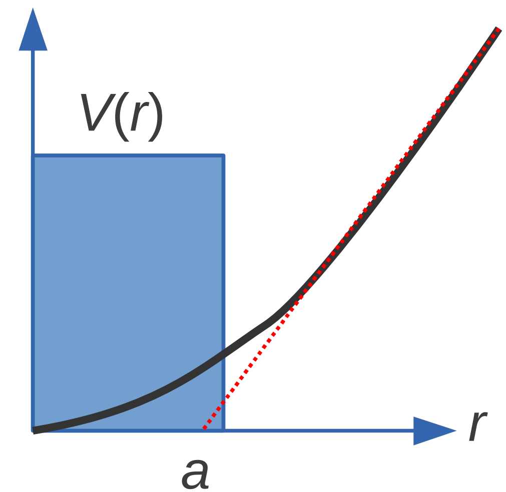
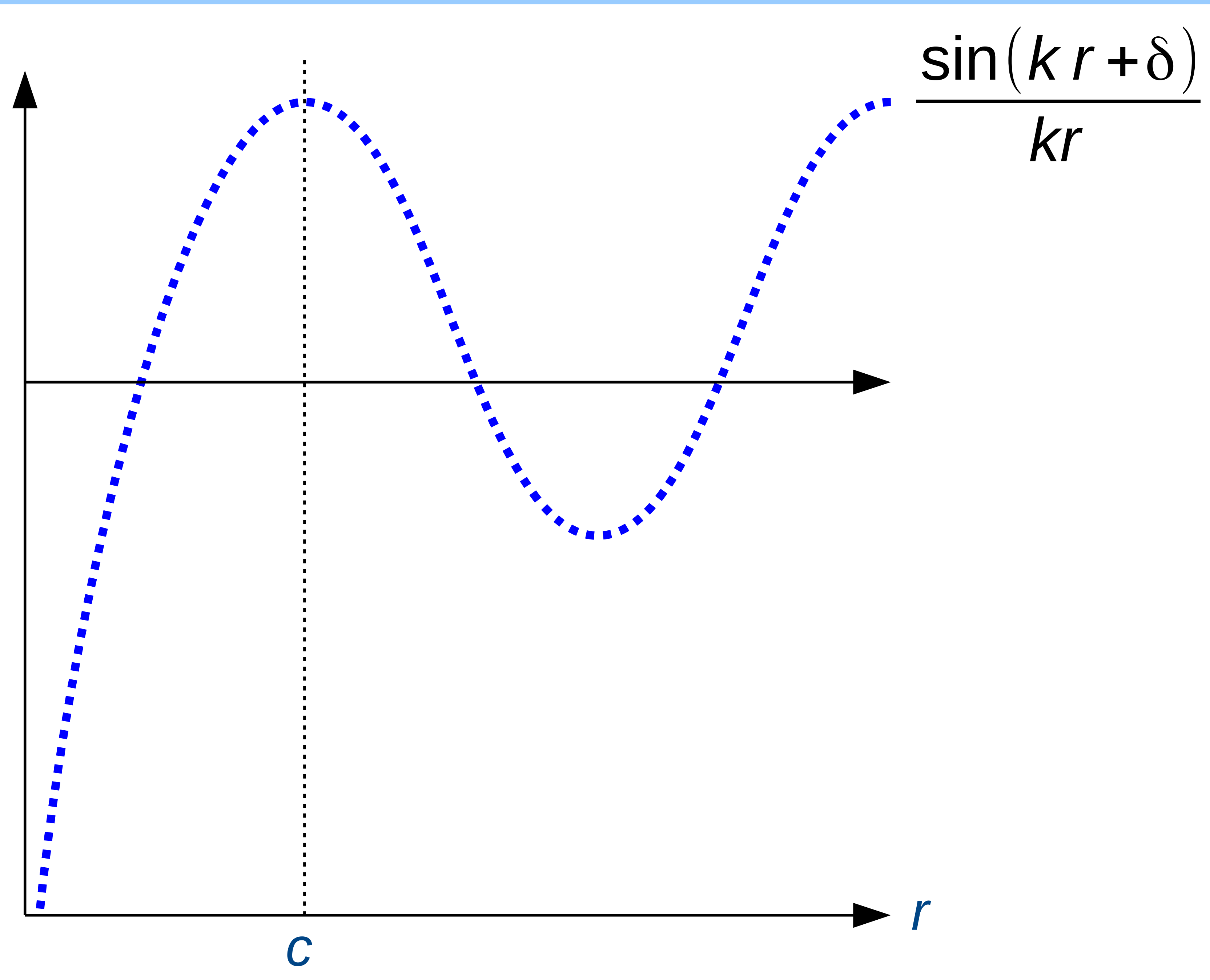


Underlying repulsive

Effective repulsive



Construction of a pseudopotential



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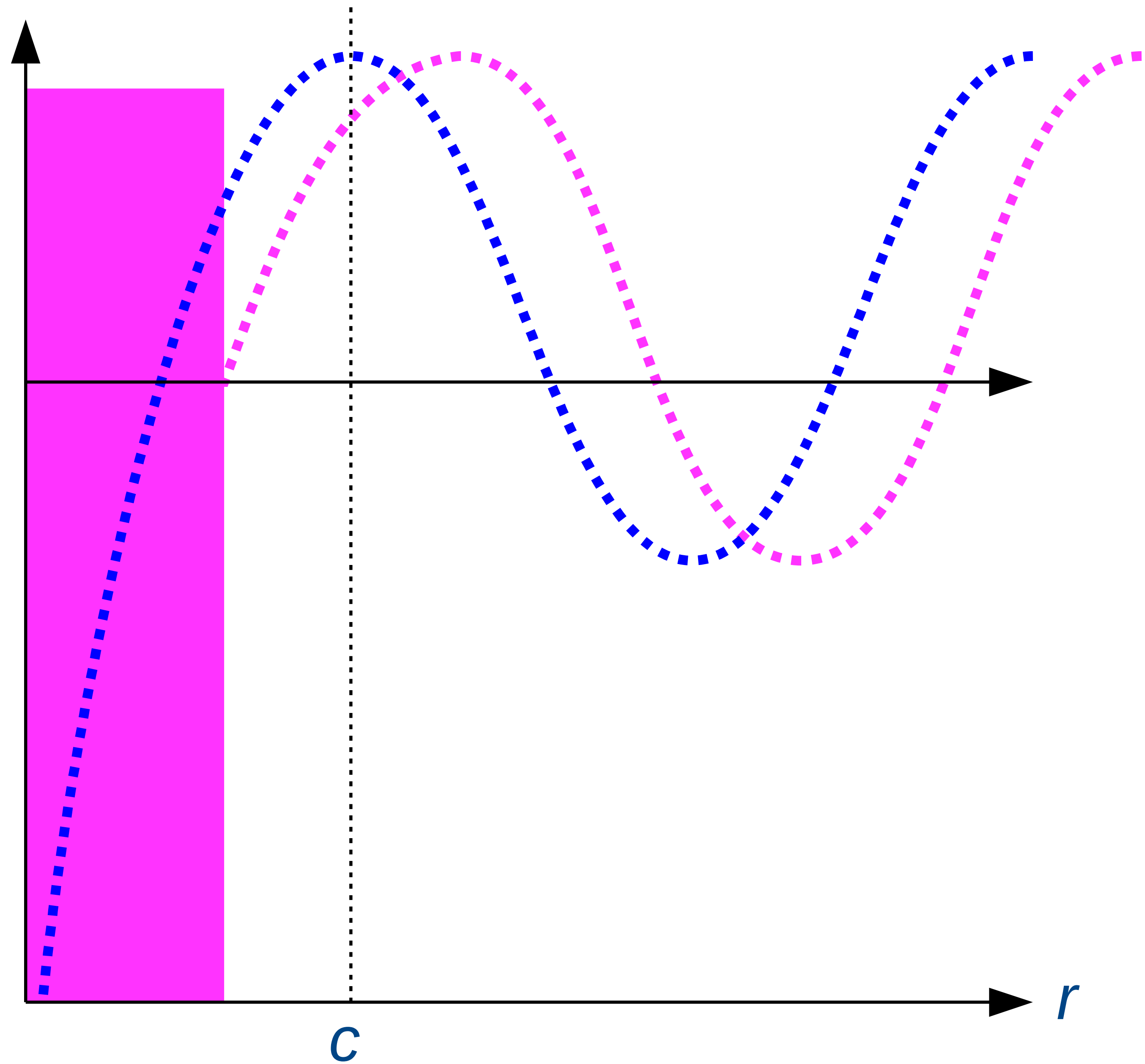

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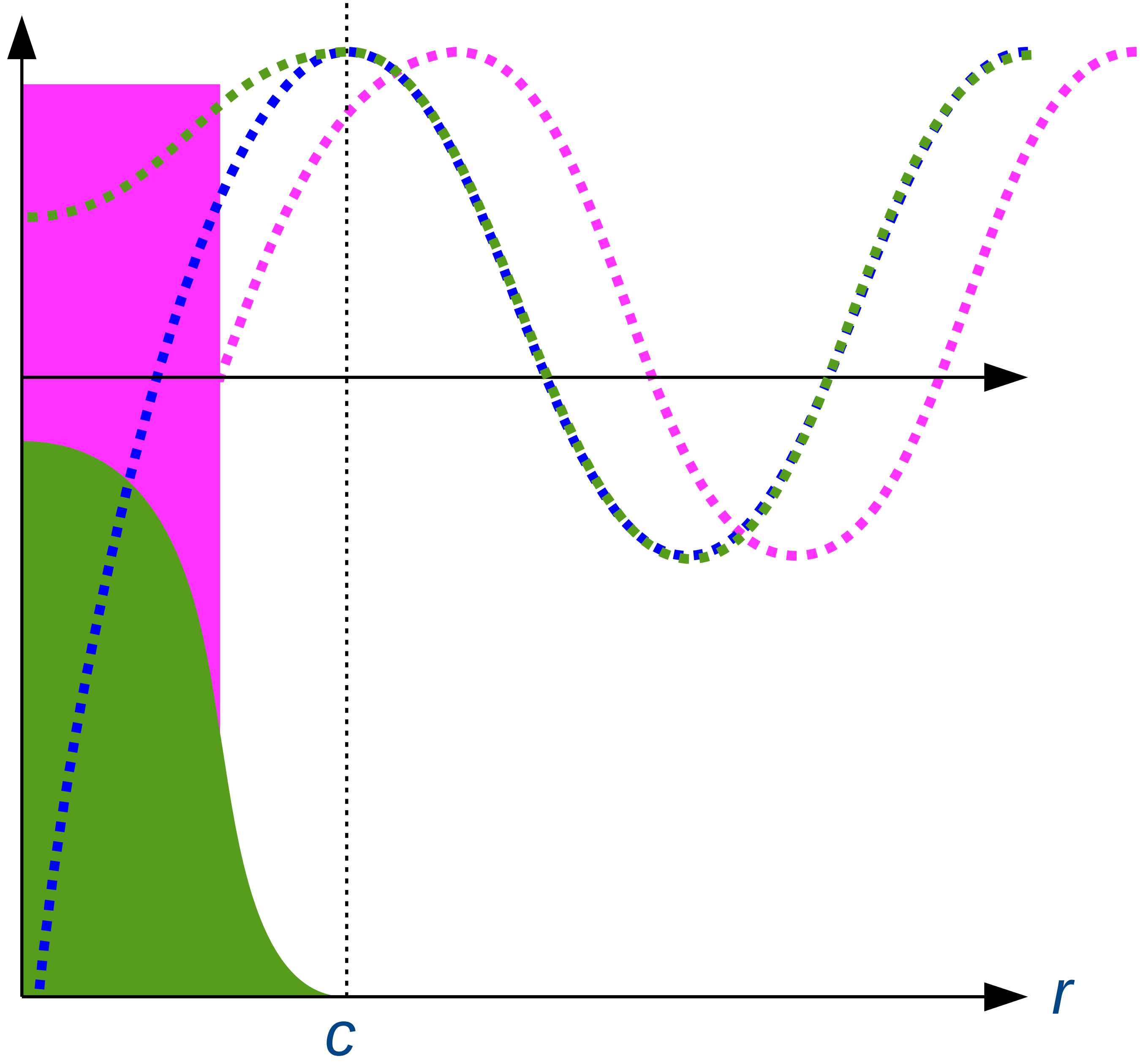
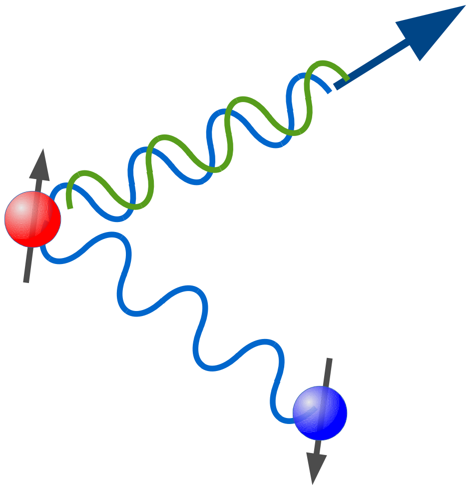


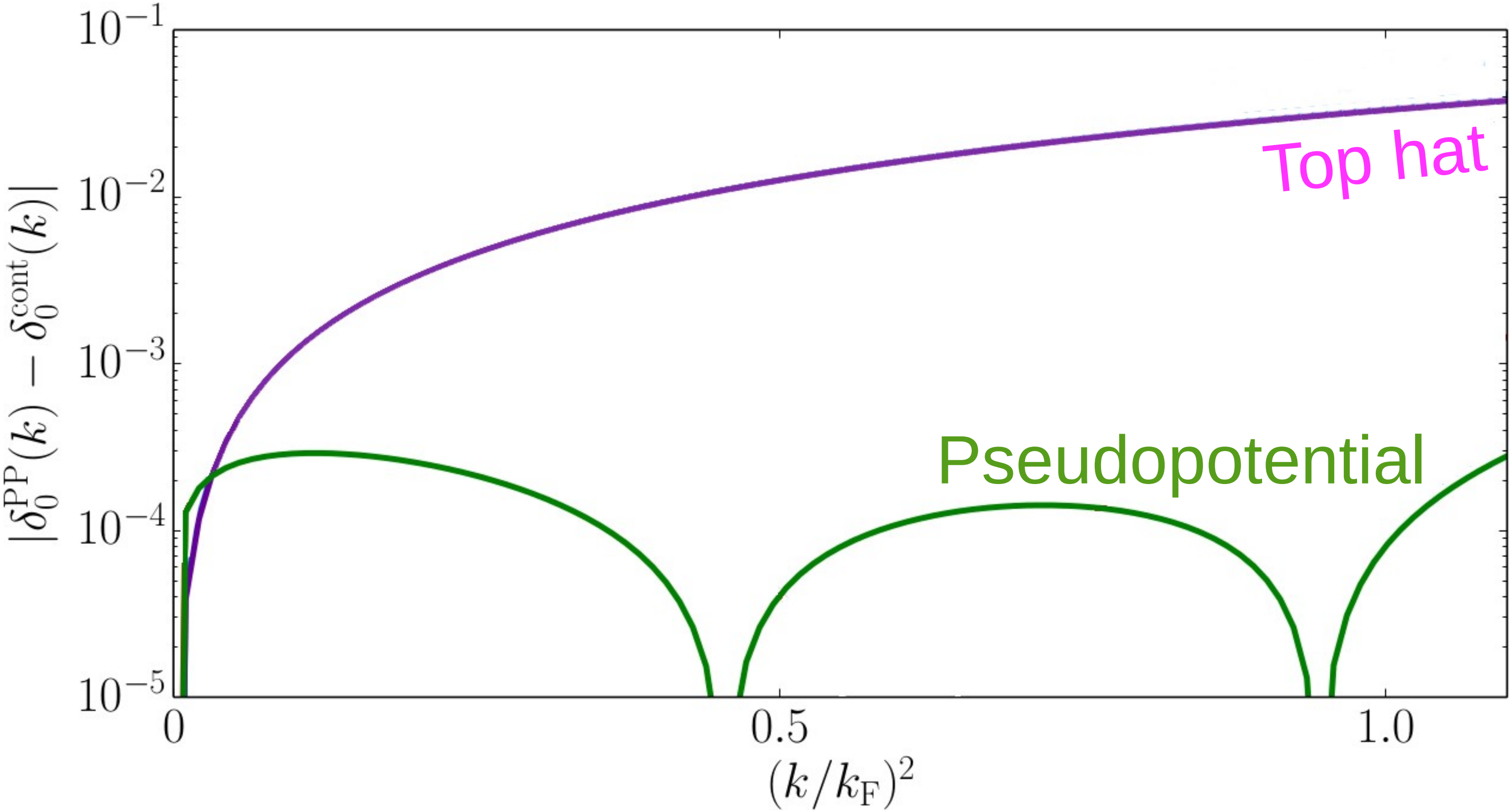
Construction of a pseudopotential

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

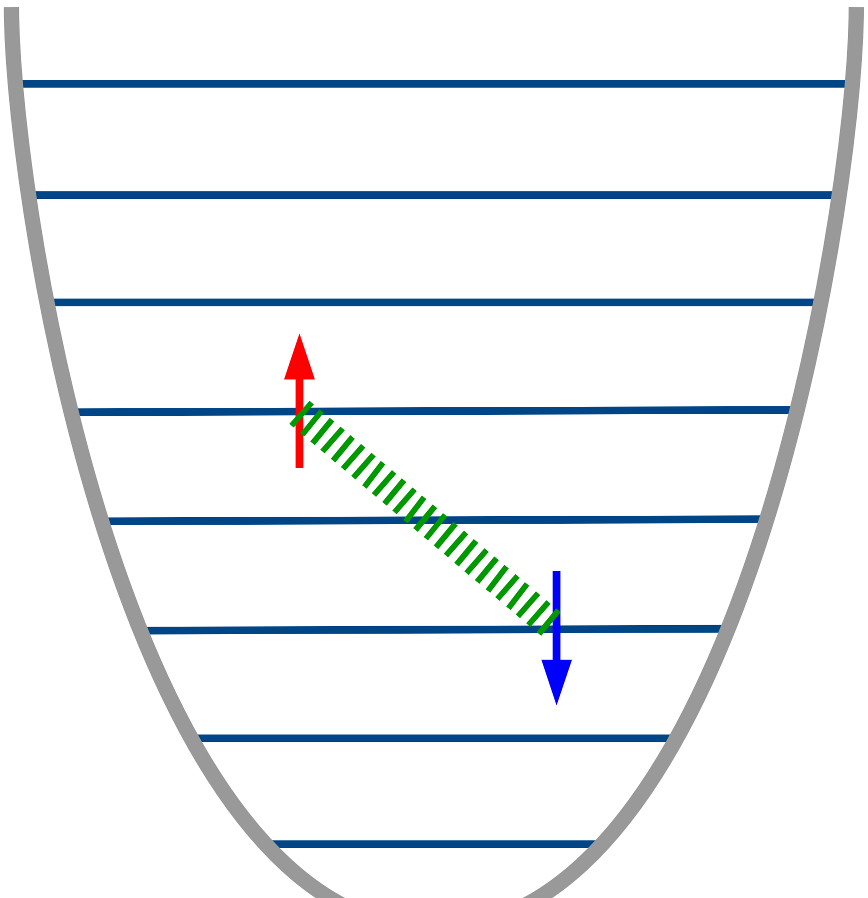
$$\sum_{l=0}^{l_{\max}}\int_{0}^{k_{\mathrm{F}}}\left[\left.\frac{\mathrm{d}\ln\psi_{\mathrm{PP}}(k,l)}{\mathrm{d}r}\right|_{c}-\frac{\mathrm{d}\ln\psi_{\mathrm{cont}}(k,l)}{\mathrm{d}r}\Big|_{c}\right]^{2}\mathrm{d}k$$

Pseudopotential: scattering properties





Pseudopotential: two atoms in a trap



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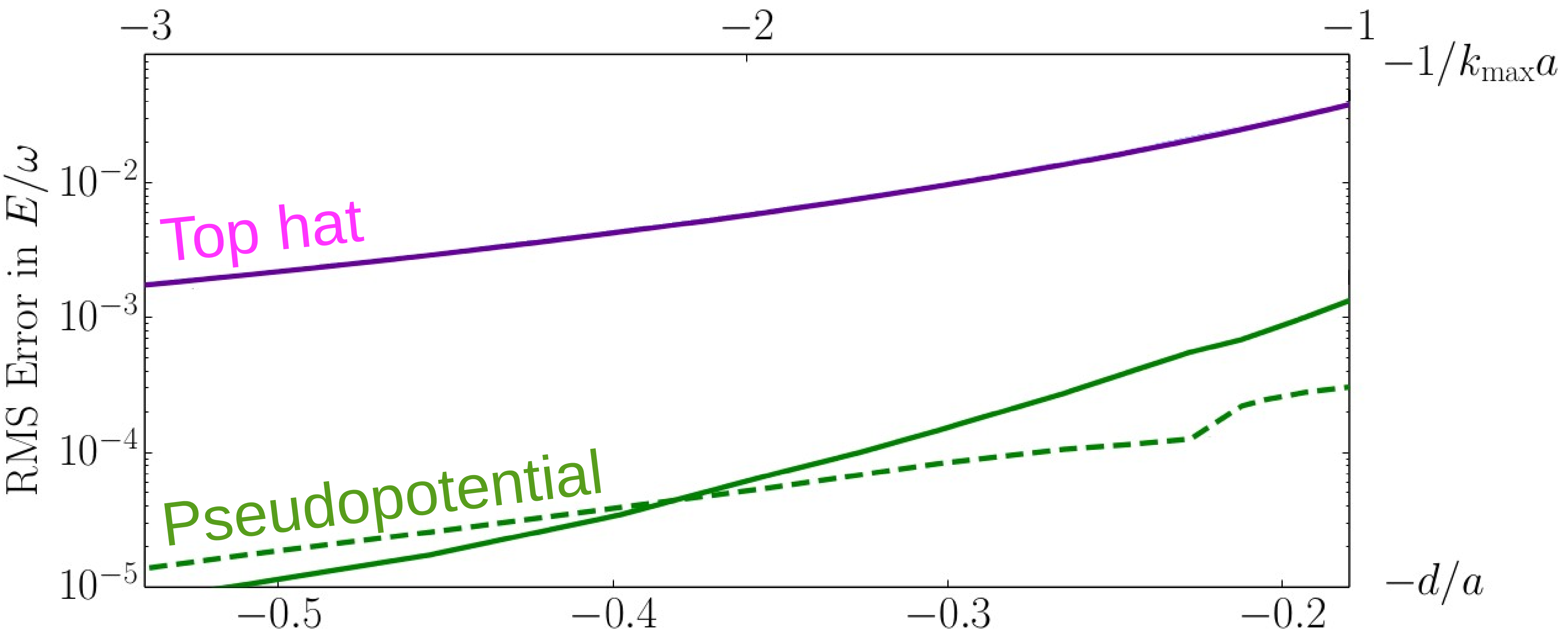


Pseudopotentials summary

Repulsive & attractive state: 100 times more accurate, 1000 times faster

Bound state: 1000 times more accurate, 1000 times faster

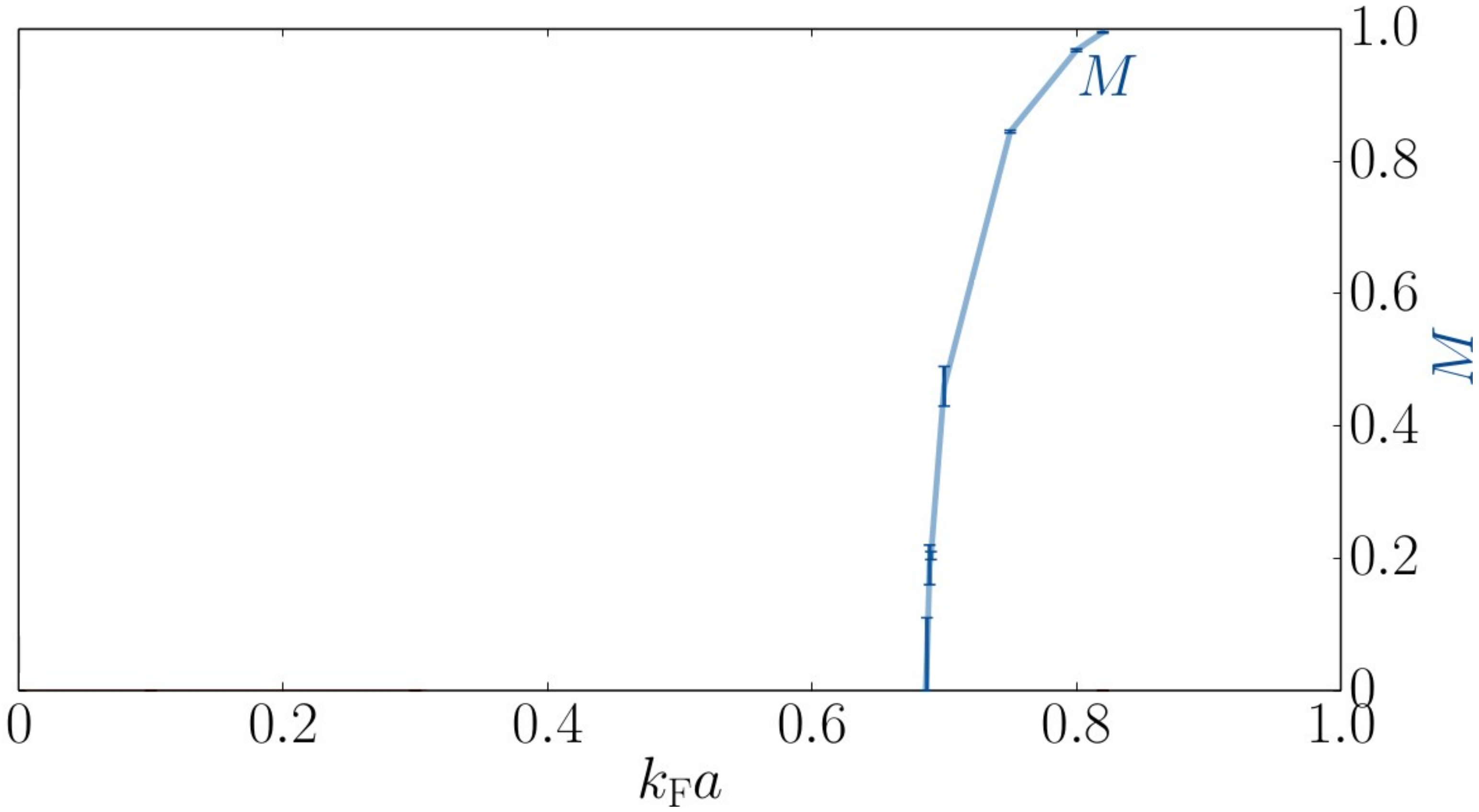
Stoner Hamiltonian

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

Theories of ferromagnetism

Stoner mean-field theory	Second order	$k_F a=1.57$
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	$k_F a=0.81(2)$
Hartree Fock MC	First / second order	$k_F a=0.83(2)$

Stoner Hamiltonian



Theories of ferromagnetism

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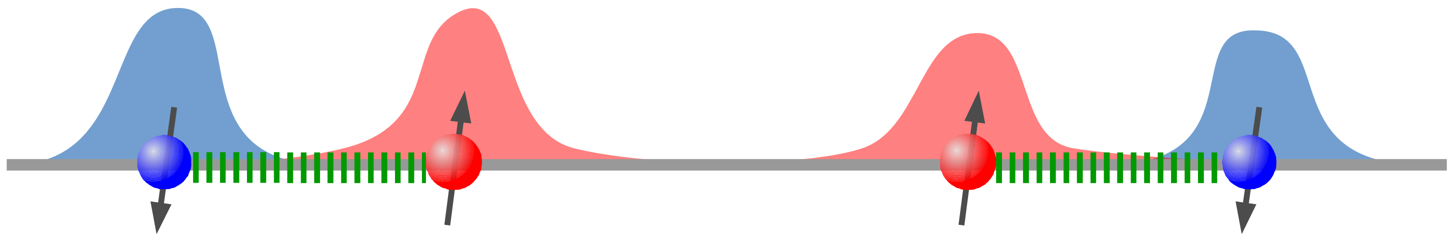
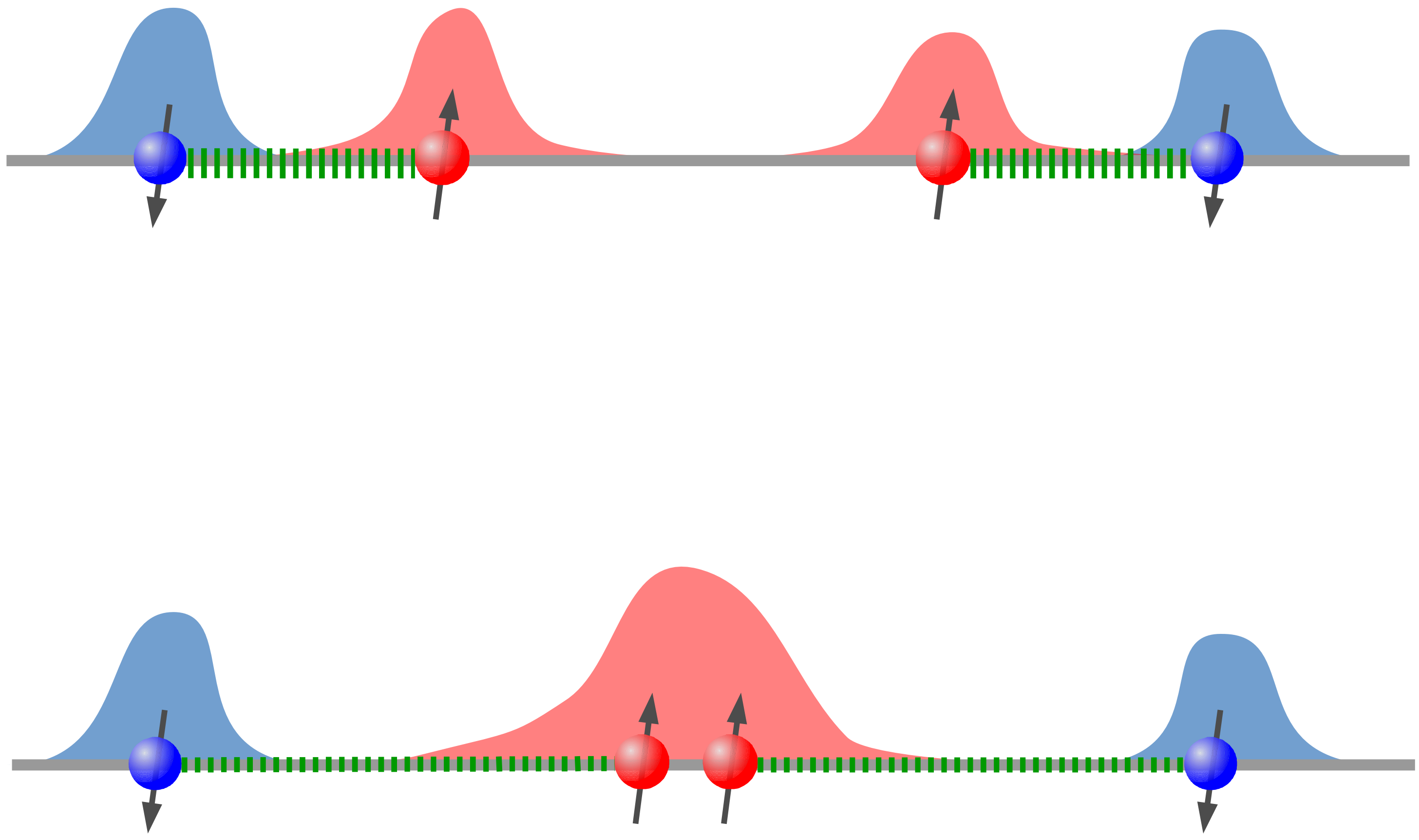
Tan relations	No magnetism	-
DMC hard sphere	First order	$k_F a=0.81(2)$
Hartree Fock MC	First / second order	$k_F a=0.83(2)$
DMC pseudopotential	Second order	$k_F a=0.683(1)$

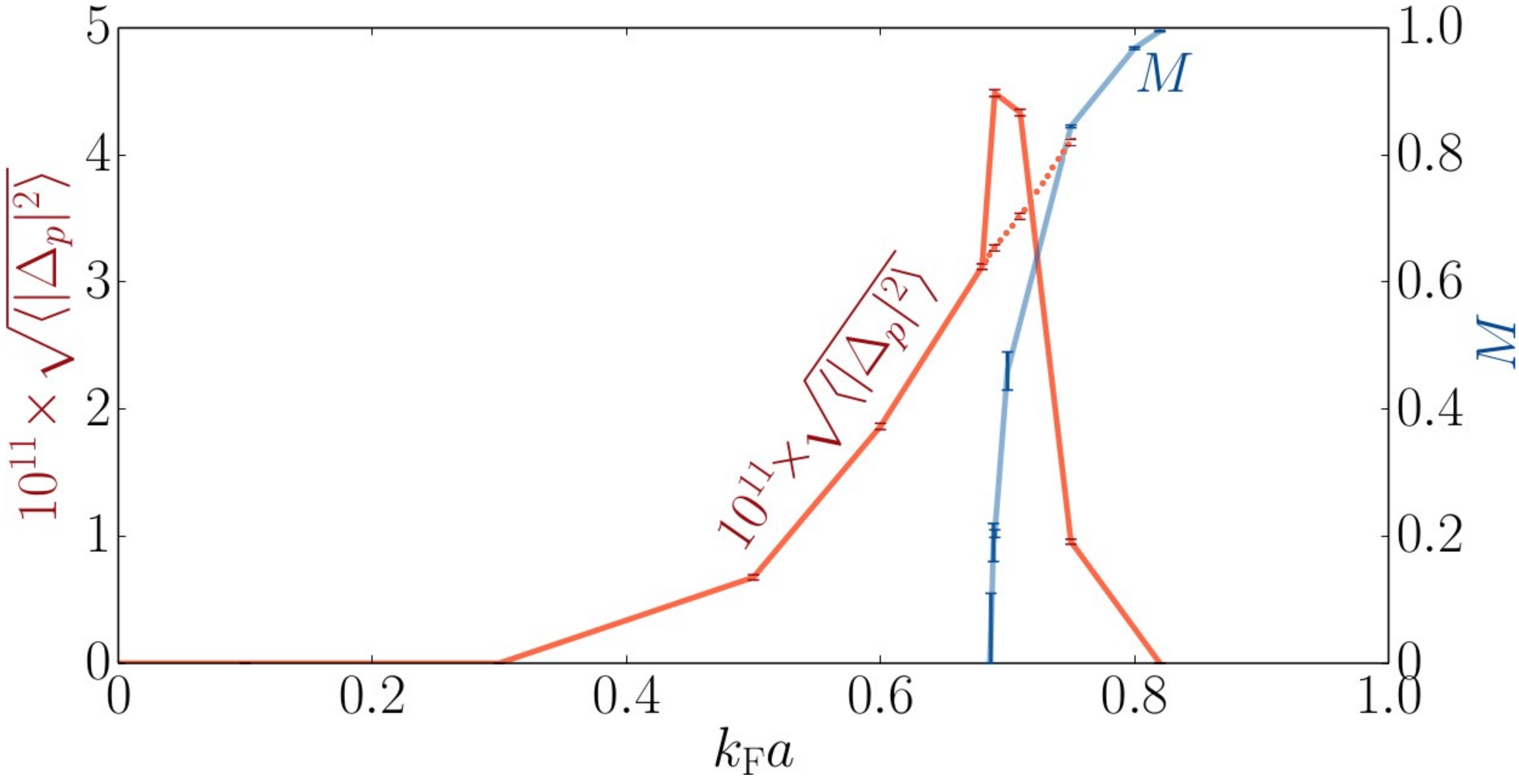
Fluctuation contributions



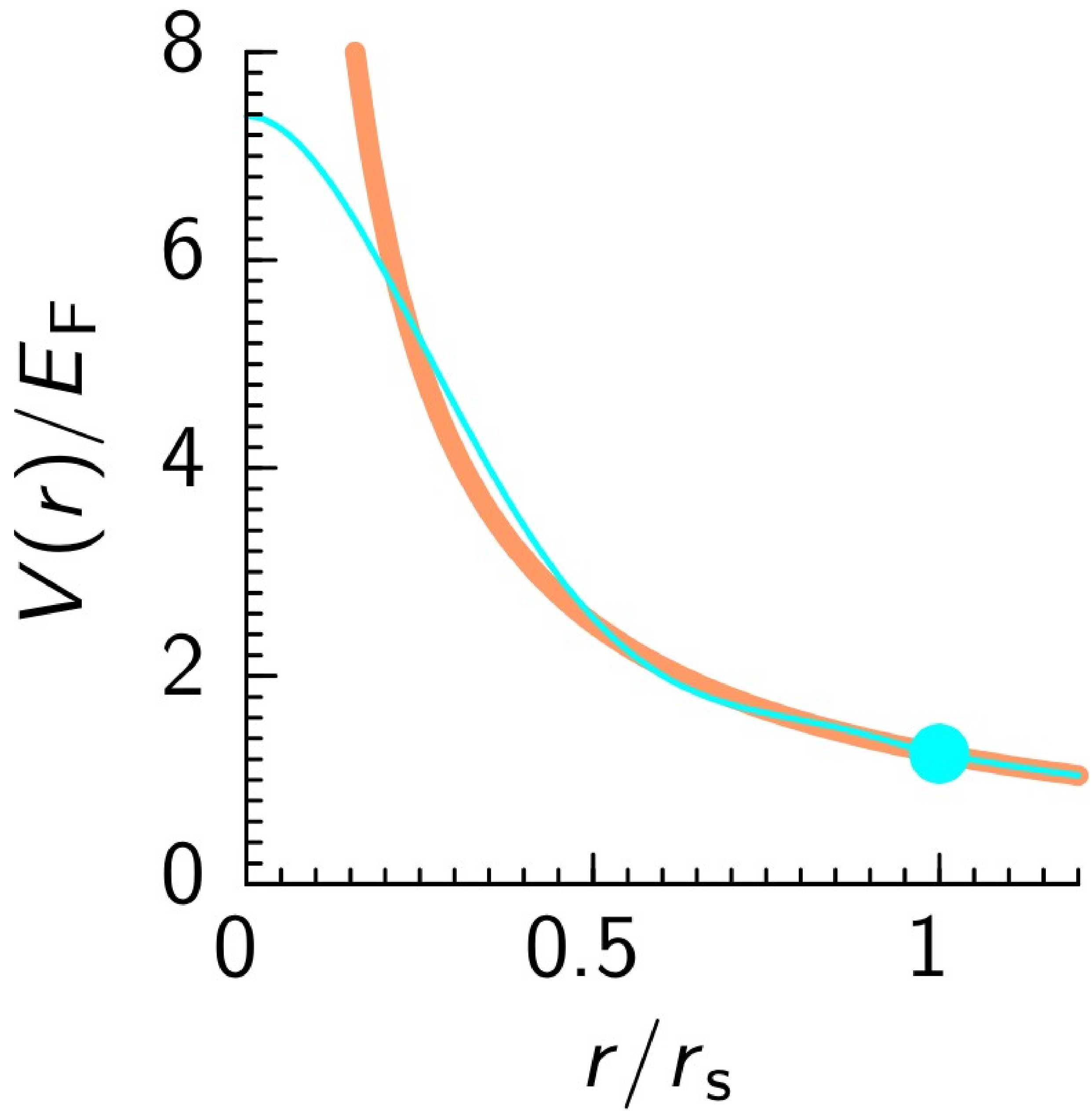
Fluctuation contributions



Stoner Hamiltonian



Coulomb pseudopotential



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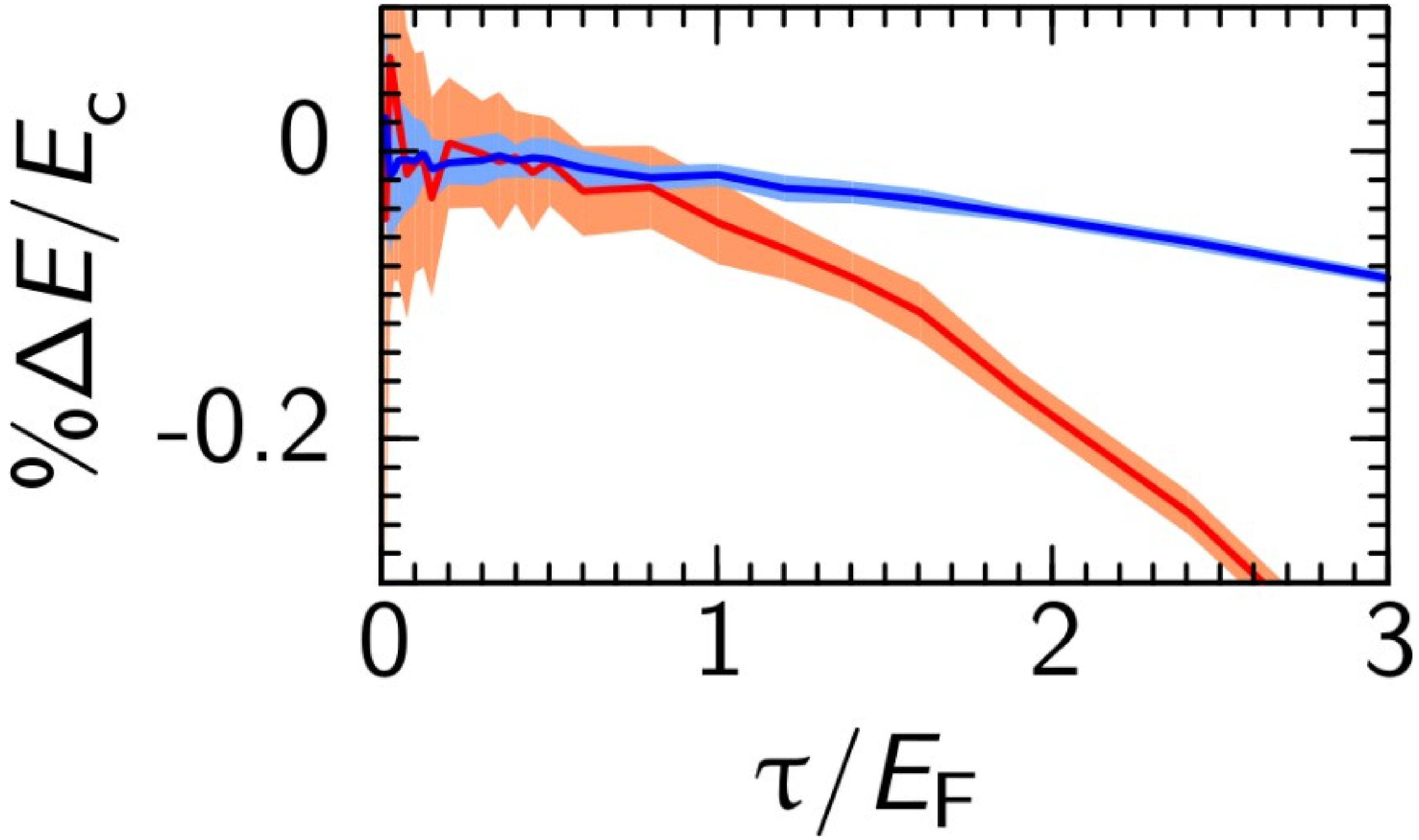
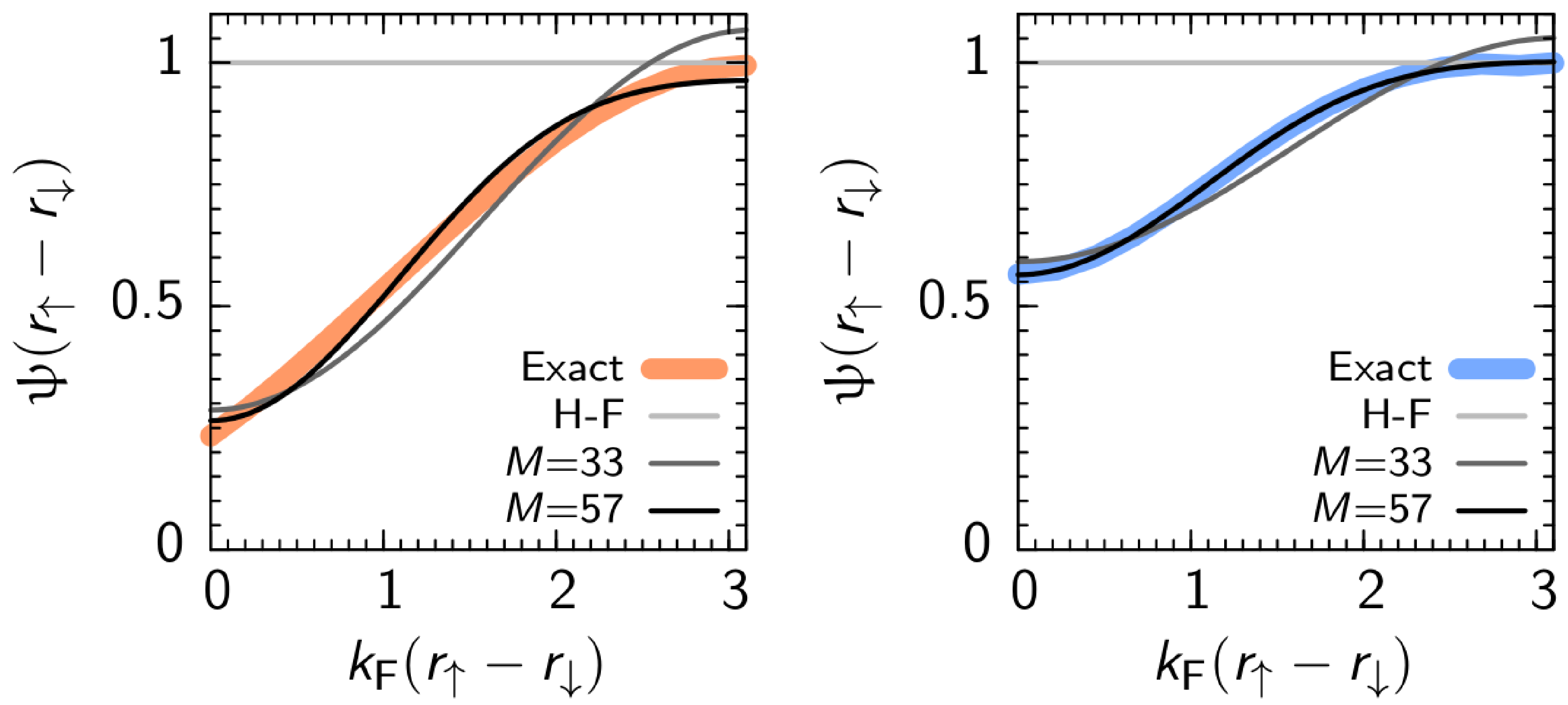


Coulomb pseudopotential



Pseudopotentials summary

Created a pseudopotential for the contact interaction that is 100 times more accurate, 1000 times faster

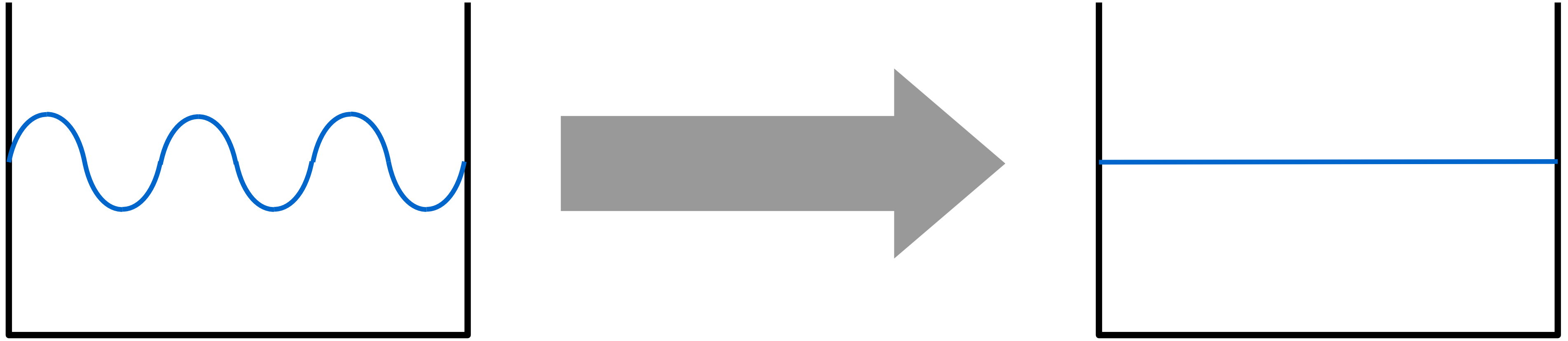
Stoner Hamiltonian displays second order ferromagnetic phase transition and p-wave ordering

Created a pseudopotential for the Coulomb interaction that is 30 times faster

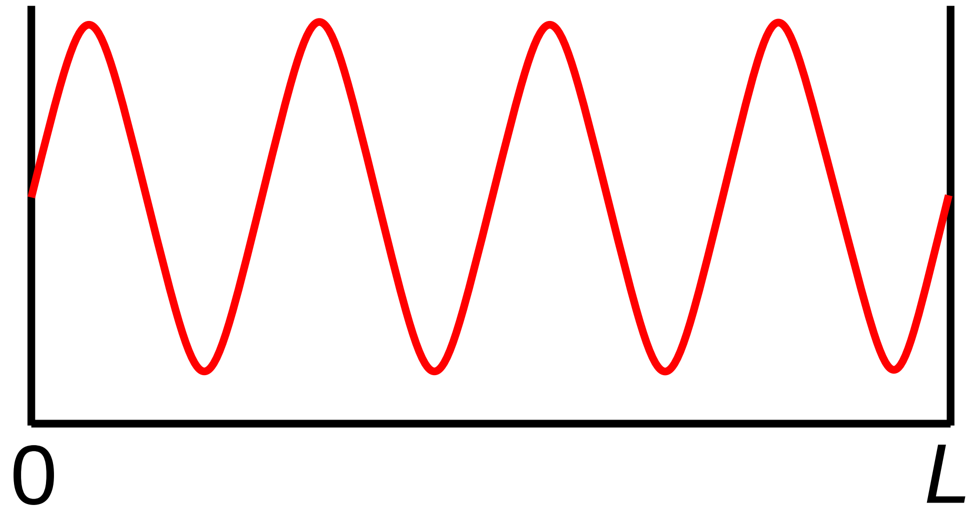
Pseudopotentials

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

Smooth integrand



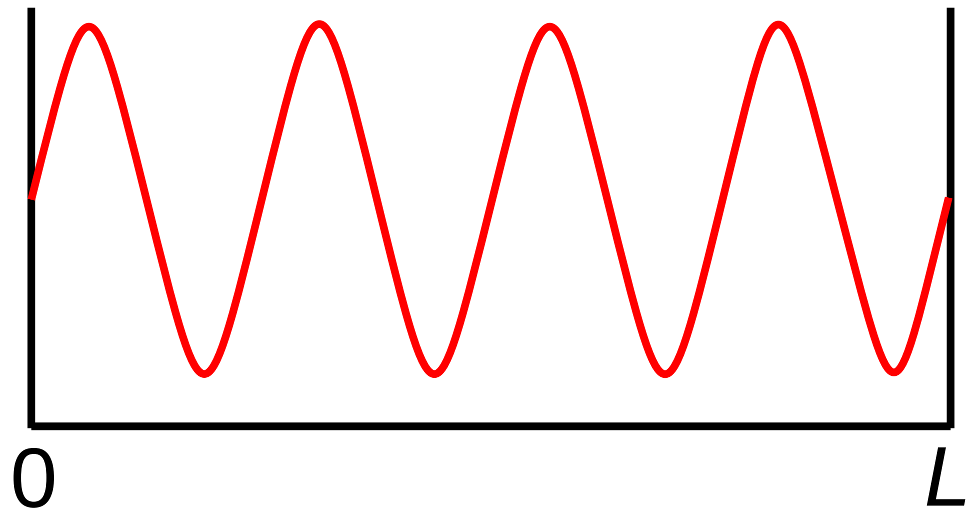
Particle in a box



$$\psi = A\sin\left(8\pi\frac{x}{L}\right)$$

$$E = -\int \bar{\psi}\frac{\nabla^2}{2}\psi\,dx$$

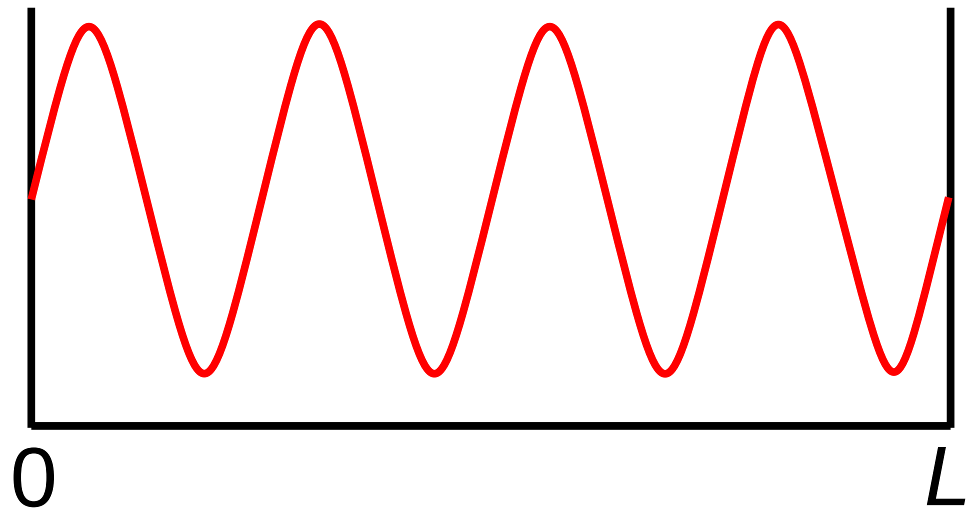
Particle in a box



$$\psi = A \sin\left(8\pi \frac{x}{L}\right)$$

$$E = -\int \bar{\psi} \frac{\nabla^2}{2} \psi \, dx$$
$$= \frac{32\pi^2 A^2}{L^2} \int \sin^2\left(8\pi \frac{x}{L}\right) dx$$

Particle in a box



$$\psi = A \sin\left(8\pi \frac{x}{L}\right)$$

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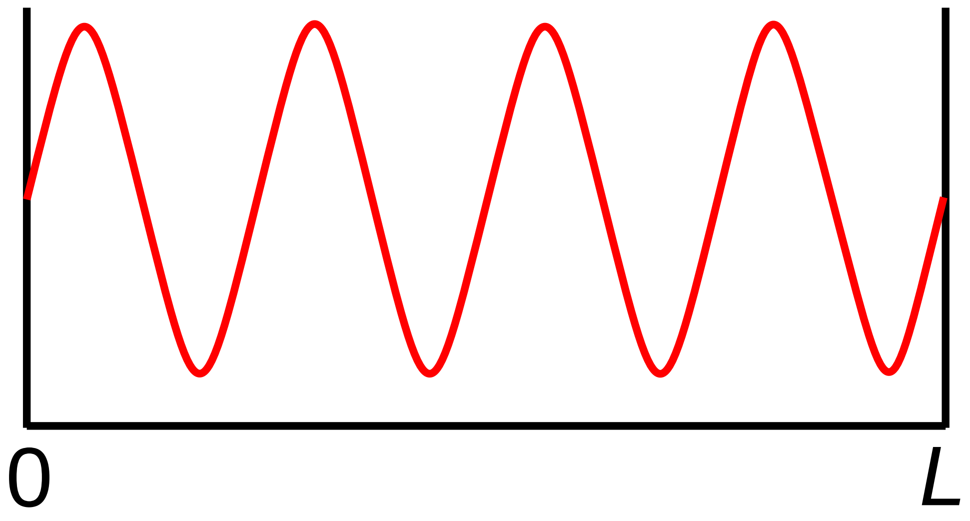
$$= \frac{32\pi^2 A^2}{L^2} \int \sin^2\left(8\pi \frac{x}{L}\right) \mathrm{d}x$$

$$\langle \sin^2 \rangle = \frac{1}{2}$$

Particle in a box



$$\psi = A \sin\left(8\pi \frac{x}{L}\right)$$

$$E = -\int \bar{\psi} \frac{\nabla^2}{2} \psi \, dx$$

$$= \frac{32\pi^2 A^2}{L^2} \int \sin^2\left(8\pi \frac{x}{L}\right) dx$$

$$= \frac{16\pi^2 A^2}{L}$$

Particle in a box

$$E = \langle \sin^2 \rangle$$

$$\langle \sin^2 \rangle = \frac{1}{2}$$

Particle in a box

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$$\cos^2 + \sin^2 = 1$$

Particle in a box

$$E = \langle \sin^2 \rangle$$

$$\langle \sin^2 \rangle = \frac{1}{2}$$

$$\cos^2 + \sin^2 = 1$$

$$\frac{d}{dx} \sin x = \cos x$$

Particle in a box

$$-\bar{\psi}\frac{\nabla^2}{2}\psi \quad \rightarrow \quad \frac{k^2}{2}A^2\sin^2(kx)$$

$$\frac{(\nabla\bar{\psi})(\nabla\psi)}{2} \quad \rightarrow \quad \frac{k^2}{2}A^2\cos^2(kx)$$

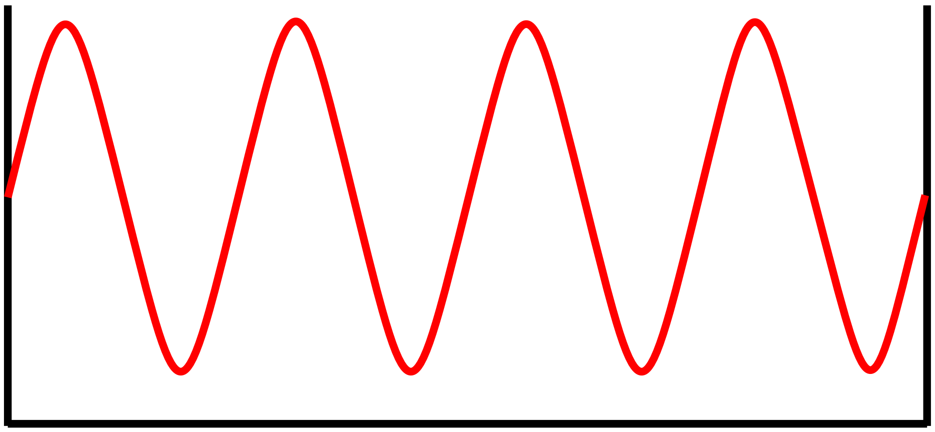
Particle in a box

$$-\bar{\psi}\frac{\nabla^2}{2}\psi \rightarrow \frac{k^2}{2}A^2\sin^2(kx)$$

$$\frac{(\nabla\bar{\psi})(\nabla\psi)}{2} \rightarrow \frac{k^2}{2}A^2\cos^2(kx)$$

$$E=\frac{1}{2}\int -\bar{\psi}\nabla^2\psi\,\mathrm{d}x \rightarrow \frac{1}{4}\int (\nabla\bar{\psi})(\nabla\psi)-\bar{\psi}\nabla^2\psi\,\mathrm{d}x$$

Particle in a box



$$\psi = A\sin\left(8\pi\frac{x}{L}\right)$$

$$E = \frac{1}{4}\int(\nabla\bar{\psi})(\nabla\psi) - \bar{\psi}\nabla^2\psi\,\mathrm{d}x$$

$$= \frac{16\pi^2 A^2}{L^2}\int\cos^2\left(8\pi\frac{x}{L}\right) + \sin^2\left(8\pi\frac{x}{L}\right)\mathrm{d}x$$

$$= \frac{16\pi^2 A^2}{L}$$

Wave function normalization

$$N = \int \bar{\psi}\psi \, \mathrm{d}x \rightarrow \frac{1}{2}\int \bar{\psi}\psi + \frac{(\nabla\bar{\psi})(\nabla\psi)}{k^2} \, \mathrm{d}x$$

$$k^2 = \frac{-\nabla^2\psi}{\psi}$$

Pseudizing the Hamiltonian

$$E = \int \hat{KE}\, \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}}$$

$$+ V_{\text{e-i}}\left(\vec{r} - \vec{r}\,'\right) n_{\vec{r}\,'}\, \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}}$$

$$+ V_{\text{e-e}}\left(\vec{r} - \vec{r}\,'\right) \bar{\psi}_{\vec{r}}\, \bar{\psi}_{\vec{r}\,'}\, \psi_{\vec{r}\,'}\, \psi_{\vec{r}}$$

$$N = \int \bar{\psi}_{\vec{r}}\, \psi_{\vec{r}}$$

Pseudizing the Hamiltonian

$$E=\frac{\int \frac{-\bar{\psi}\nabla^2\psi+(\nabla\bar{\psi})(\nabla\psi)}{2}+V\left(\bar{\psi}\psi+\frac{(\nabla\bar{\psi})(\nabla\psi)}{-\nabla^2\psi/\psi}\right)\mathrm{d}r}{\int \bar{\psi}\psi+\frac{(\nabla\bar{\psi})(\nabla\psi)}{-\nabla^2\psi/\psi}\mathrm{d}r}$$

$$E=\frac{\int \left(\frac{-\bar{\psi}\nabla^2\psi}{2}+V\bar{\psi}\psi\right)\left(1+\frac{(\nabla\bar{\psi})(\nabla\psi)}{\bar{\psi}\nabla^2\psi}\right)\mathrm{d}r}{\int \bar{\psi}\psi\left(1+\frac{(\nabla\bar{\psi})(\nabla\psi)}{\bar{\psi}\nabla^2\psi}\right)\mathrm{d}r}$$

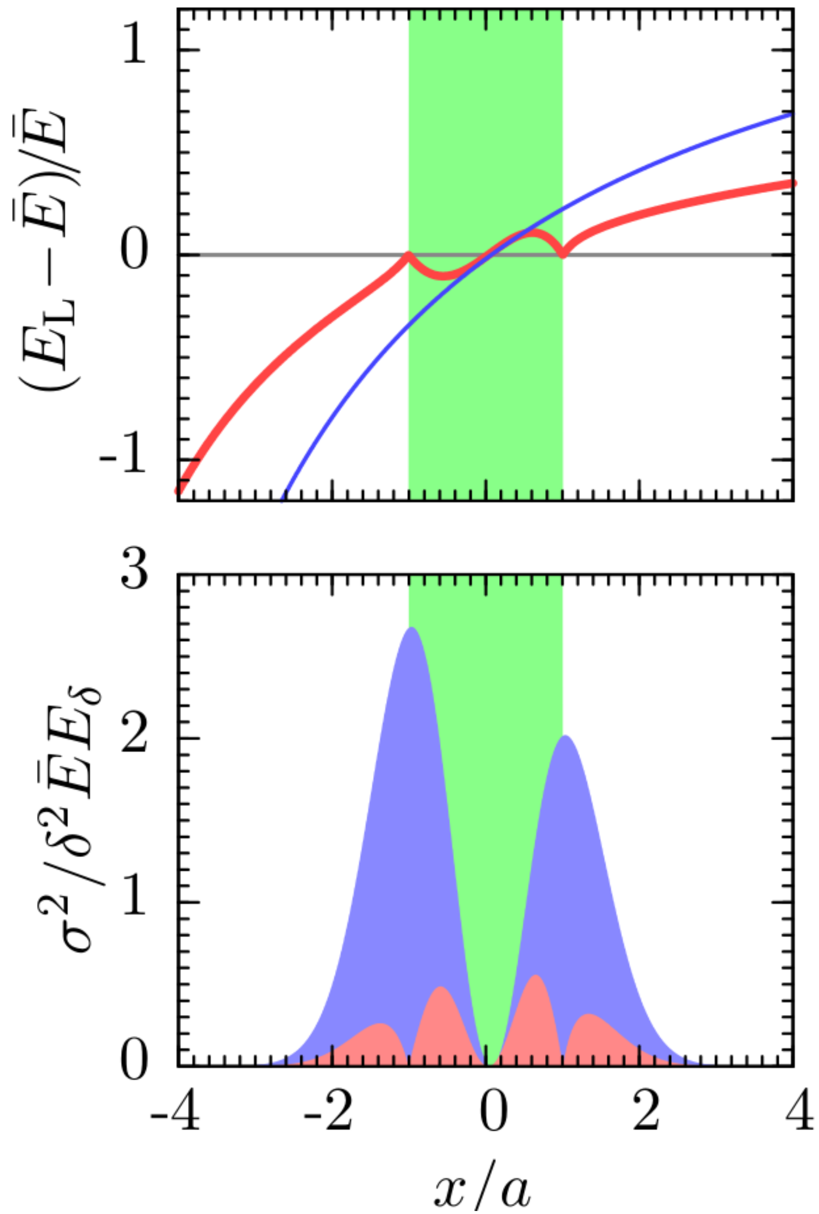
$$E=\frac{\int E\bar{\psi}\psi\left(1+\frac{(\nabla\bar{\psi})(\nabla\psi)}{\bar{\psi}\nabla^2\psi}\right)\mathrm{d}r}{\int \bar{\psi}\psi\left(1+\frac{(\nabla\bar{\psi})(\nabla\psi)}{\bar{\psi}\nabla^2\psi}\right)\mathrm{d}r}=E$$

Pseudizing the Hamiltonian

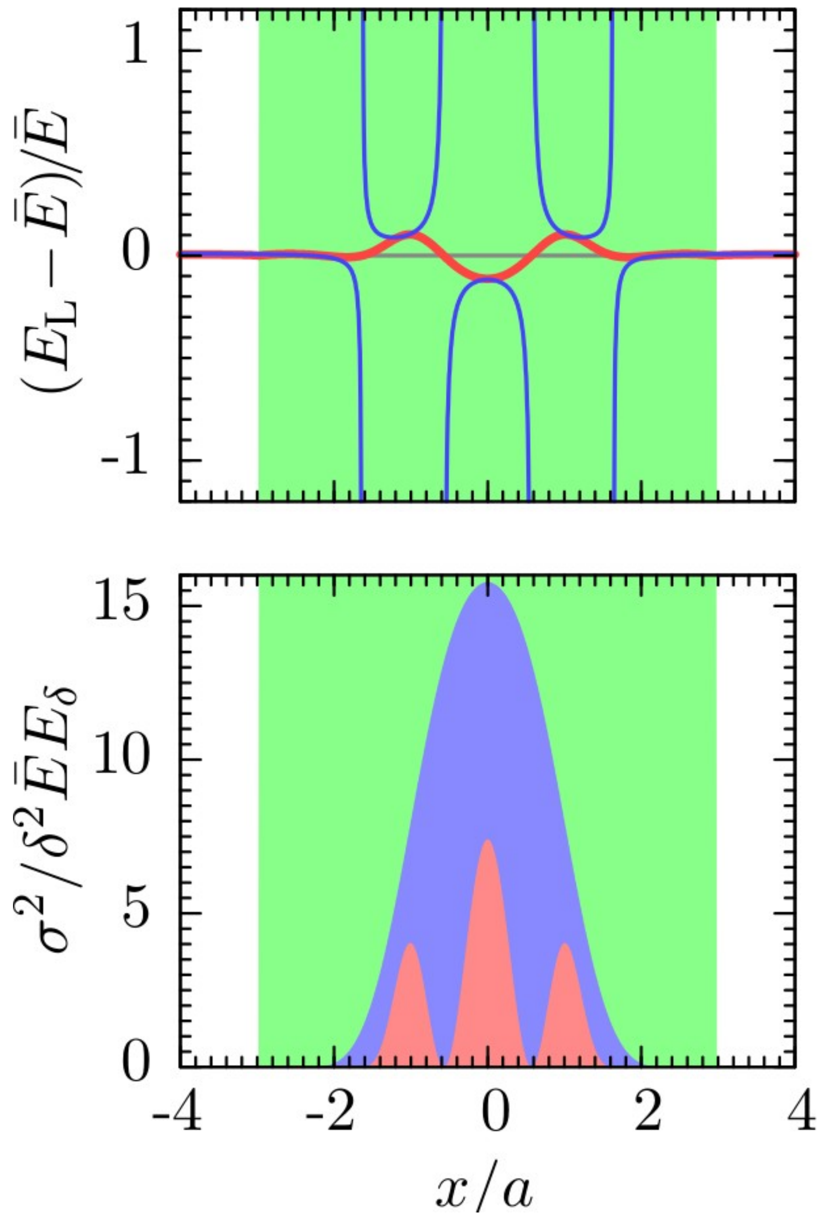
$$E = \frac{\int \bar{\psi} \hat{H} \psi \, \mathrm{d}r}{\int \bar{\psi} \psi \, \mathrm{d}r} = \int_{\bar{\psi}\psi} \frac{\bar{\psi} \hat{H} \psi}{\bar{\psi} \psi} \, \mathrm{d}r$$

$$\frac{\sigma^2_{\mathrm{PP}}}{\sigma^2_{\mathrm{std}}} = \frac{1}{4}$$

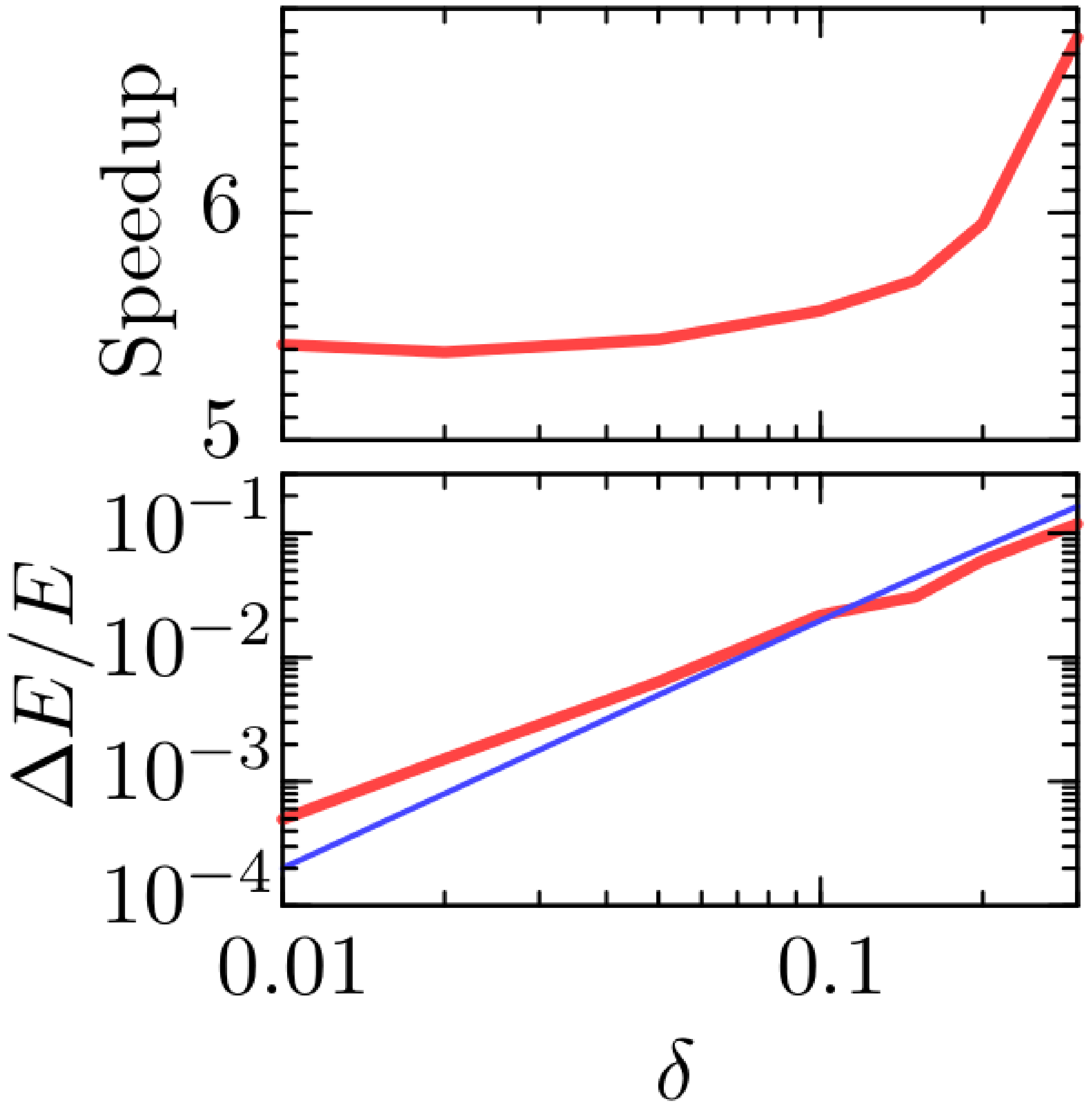
Results: $\Psi_0 + 0.1\Psi_1$



Results: $\Psi_4 + 0.1\Psi_0$



Results: $\Psi_0+\delta\ \Psi_1$



Summary

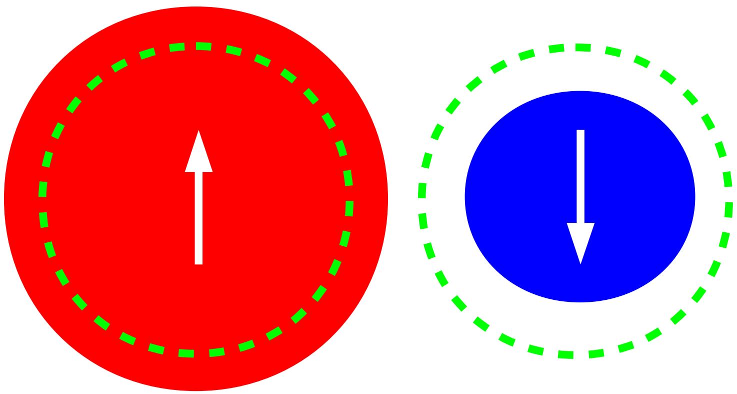
Developed a pseudopotential for the contact and Coulomb interactions

Stoner Hamiltonian displays second order ferromagnetic phase transition, and p-wave ordering

Proposed the formalism to pseudize the kinetic energy and wave function

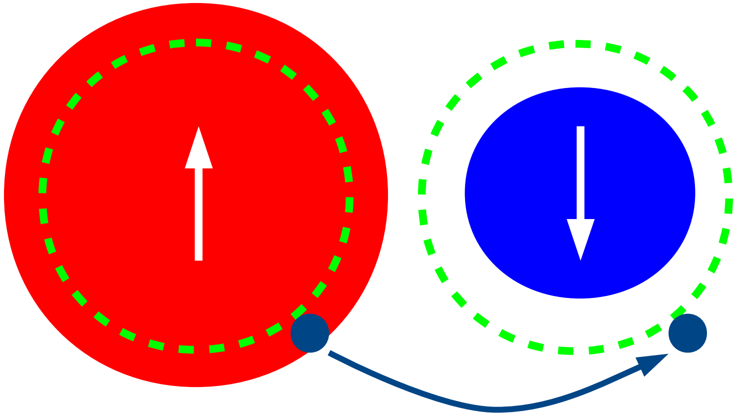
Fluctuation contributions

Ferromagnetic



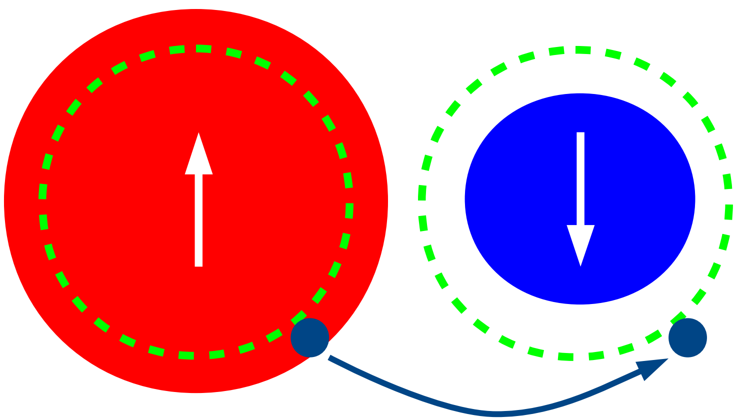
Fluctuation contributions

Ferromagnetic

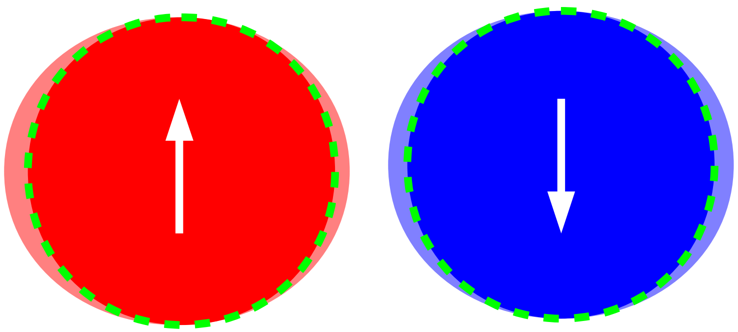


Fluctuation contributions

Ferromagnetic



Superconducting



Pseudoψence

$$E = \frac{\int \bar{\psi} \hat{H} \psi \, dr}{\int \bar{\psi} \psi} = \int_{\bar{\psi}\psi} \frac{\bar{\psi} \hat{H} \psi}{\bar{\psi} \psi} dr$$

$$\psi = A \sin\left(8\pi \frac{x}{L}\right)$$

$$E = \int_{\bar{\psi}\psi} \frac{32\pi^2}{L^2} dx$$

Pseudoψence

$$\sigma^2 = \int \left(\frac{\bar{\psi} H \psi}{\bar{\psi} \psi} - E \right)^2 \bar{\psi} \psi \, dx$$

$$\psi = A \sin\left(\sqrt{2 E_T}\, x\right)$$

Pseudoψence

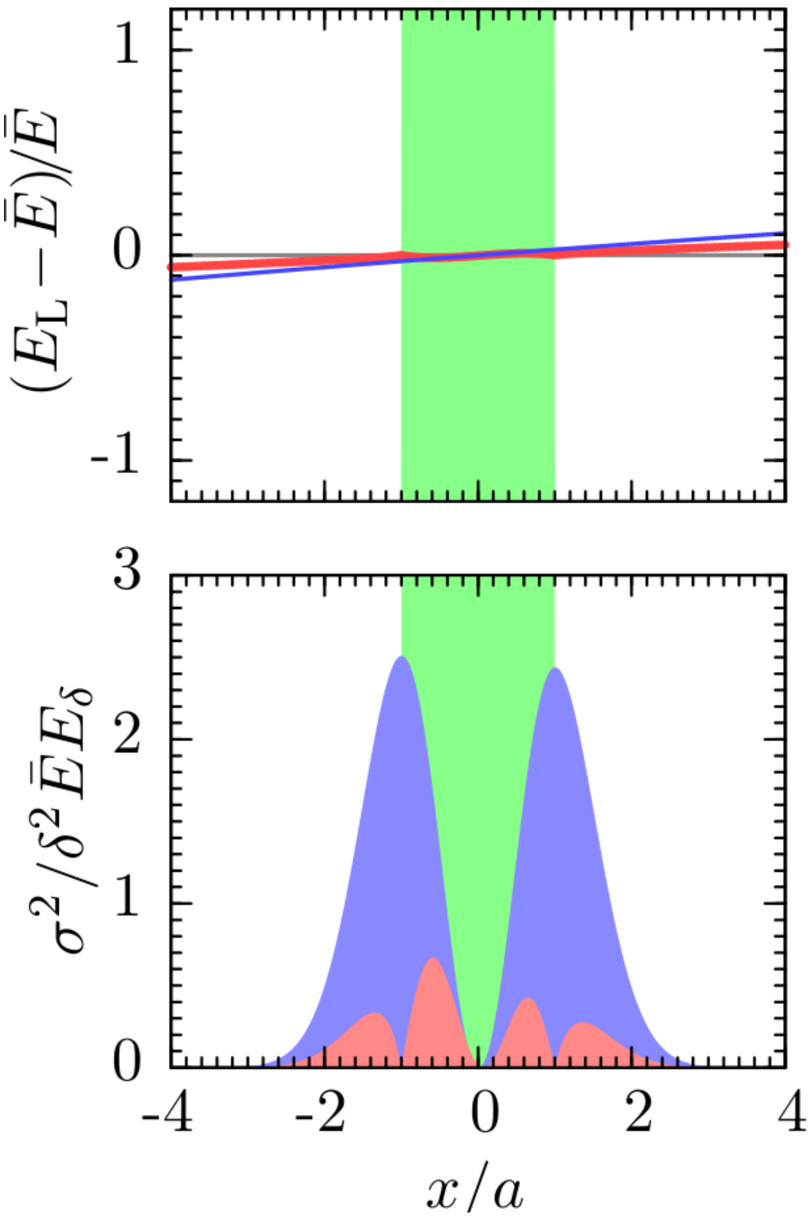
$$\sigma^2 = \int \left(\frac{\psi^* H \psi}{\psi^* \psi} - E \right)^2 \psi^* \psi \, dx$$

$$\psi = A \sin\left(\sqrt{2 E_T} x \right)$$

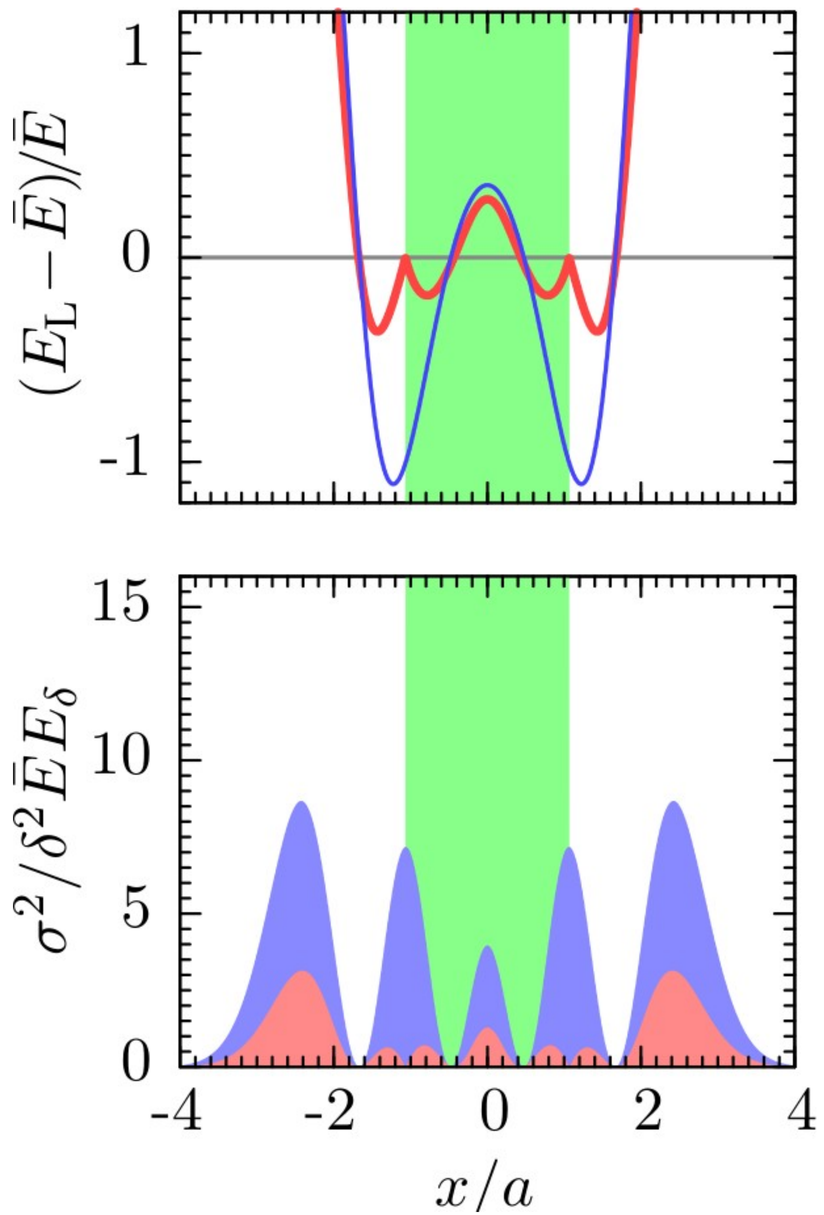
$$\sigma^2(\chi) = \left(\frac{E_T}{1 - \chi + \chi E_T / E} - E \right)^2 \left(1 - \chi + \chi E_T / E \right)$$

$$\frac{\sigma^2(1/2)}{\sigma^2(0)} = \frac{1}{4}$$

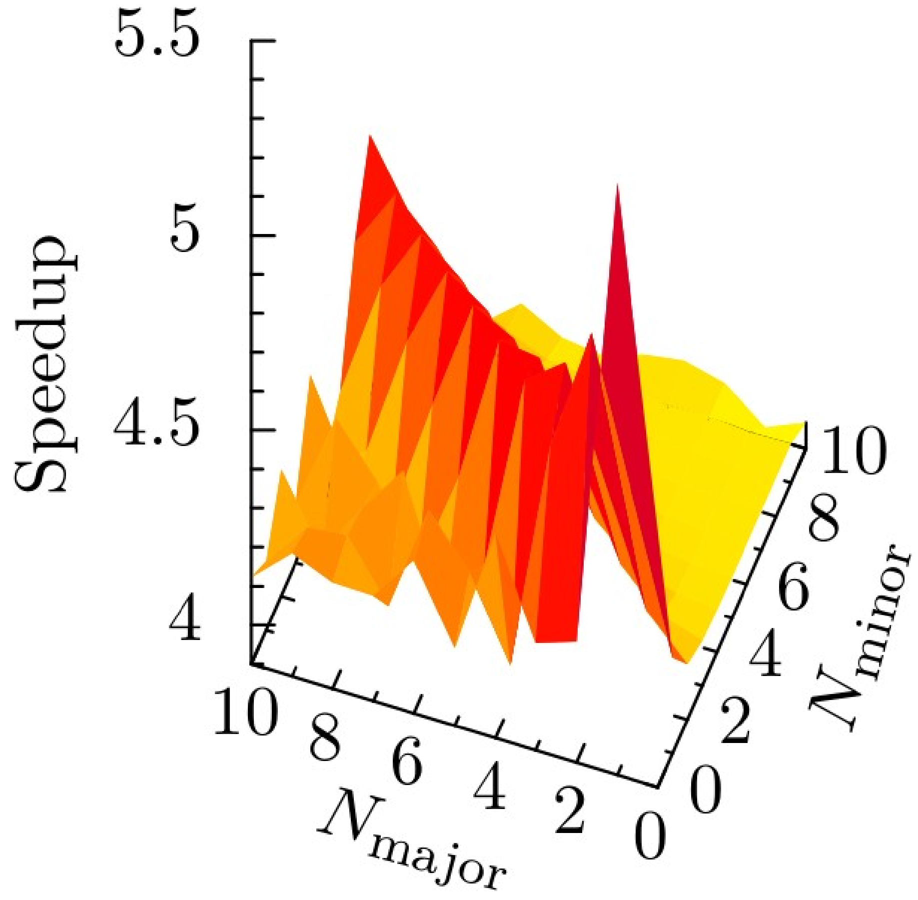
Results: $\Psi_0+0.01\Psi_1$



Results: Ψ_0+0.1Ψ_4



Results: $\Psi_{Nmajor} + \delta\ \Psi_{Nminor}$



Solid hydrogen