UNIVERSITY OF CAMBRIDGE

p-wave superconductivity in the itinerant ferromagnet

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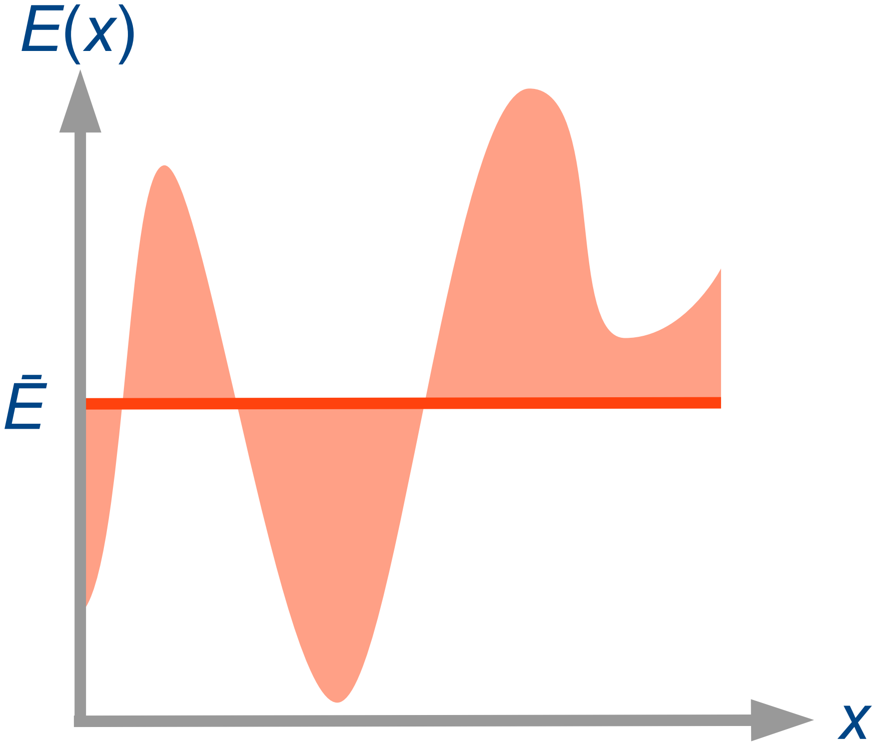
Pseudopotentials

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

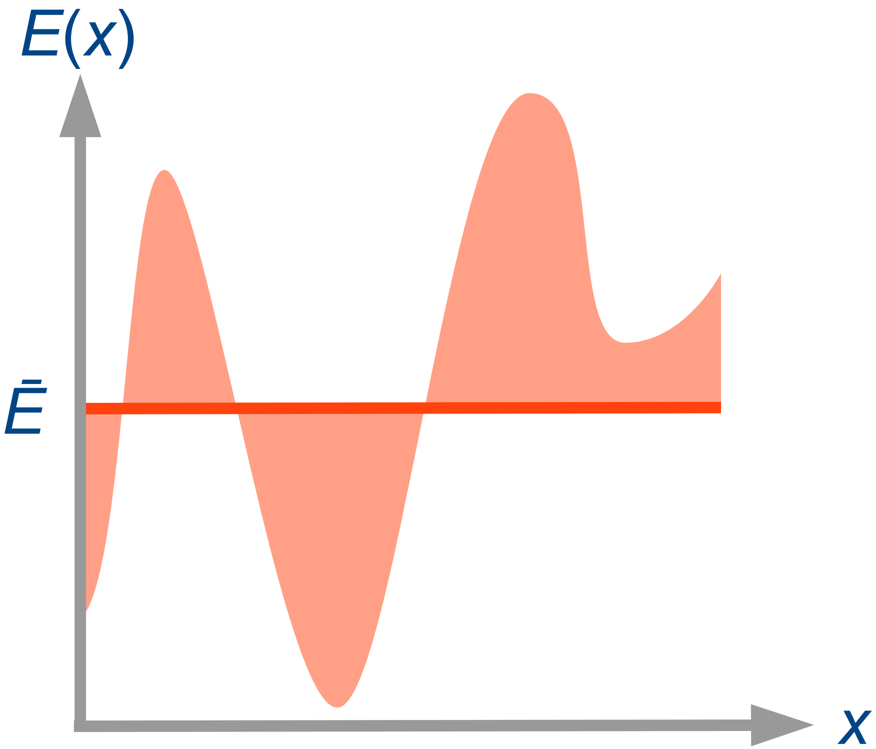
$$\bar{\bar{E}} = \frac{\int \bar{\psi} \hat{H} \psi \, d\boldsymbol{r}}{\int \bar{\psi} \psi \, d\boldsymbol{r}} = \int_{\bar{\psi}\psi} \bar{\psi}^{-1} \hat{H} \psi \, d\boldsymbol{r}$$

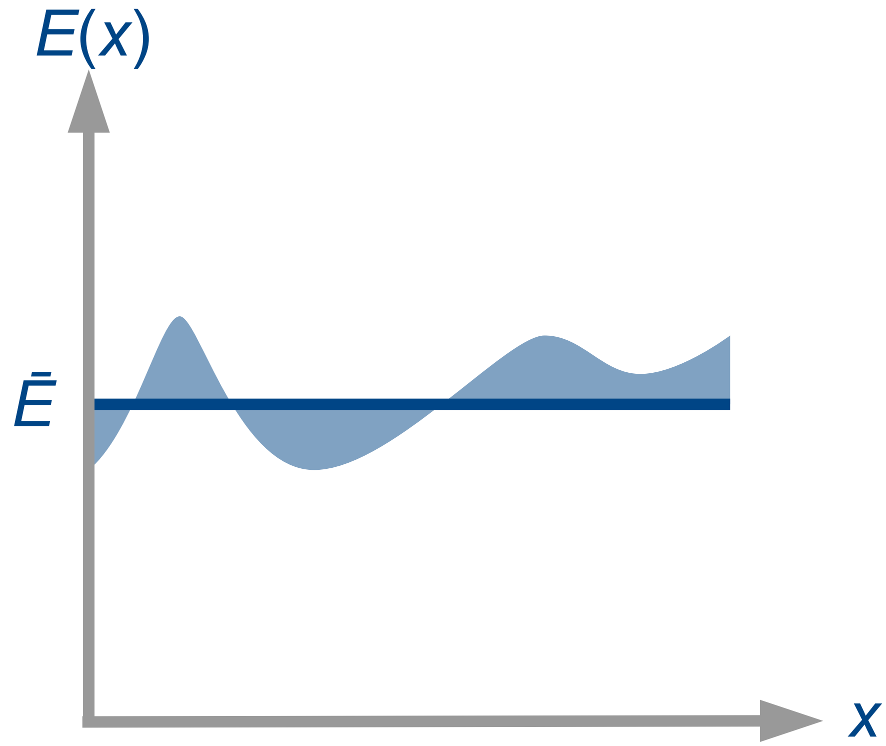
Pseudopotentials

Standard



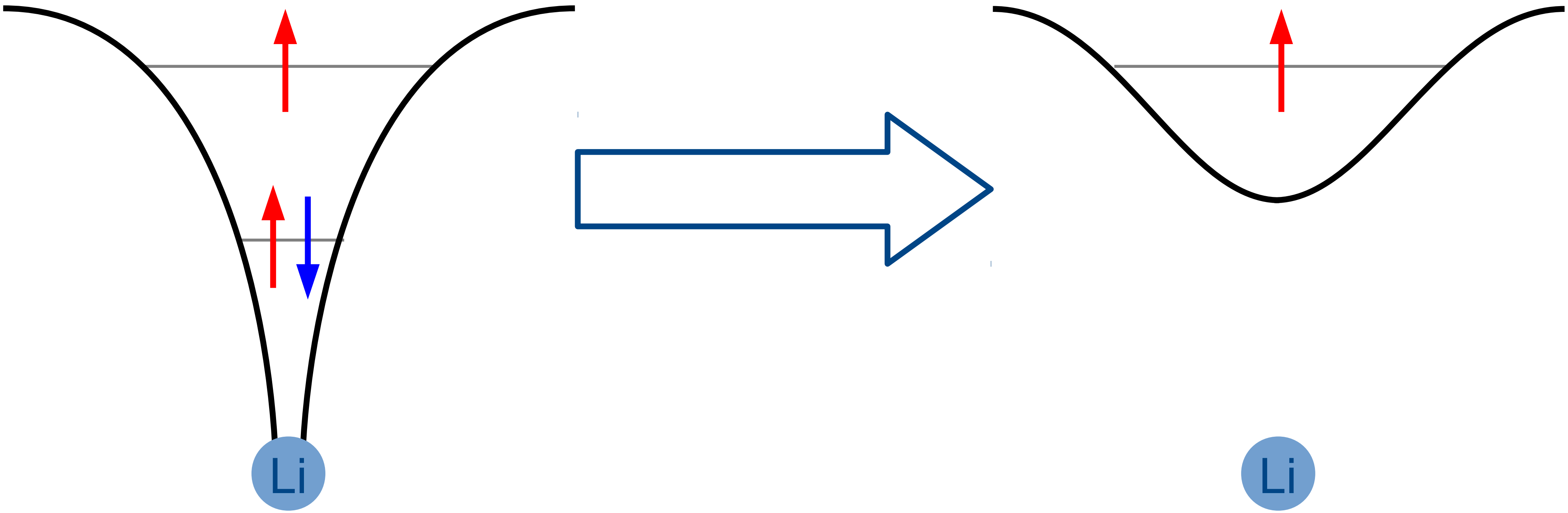
Pseudopotentials





Pseudopotentials

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

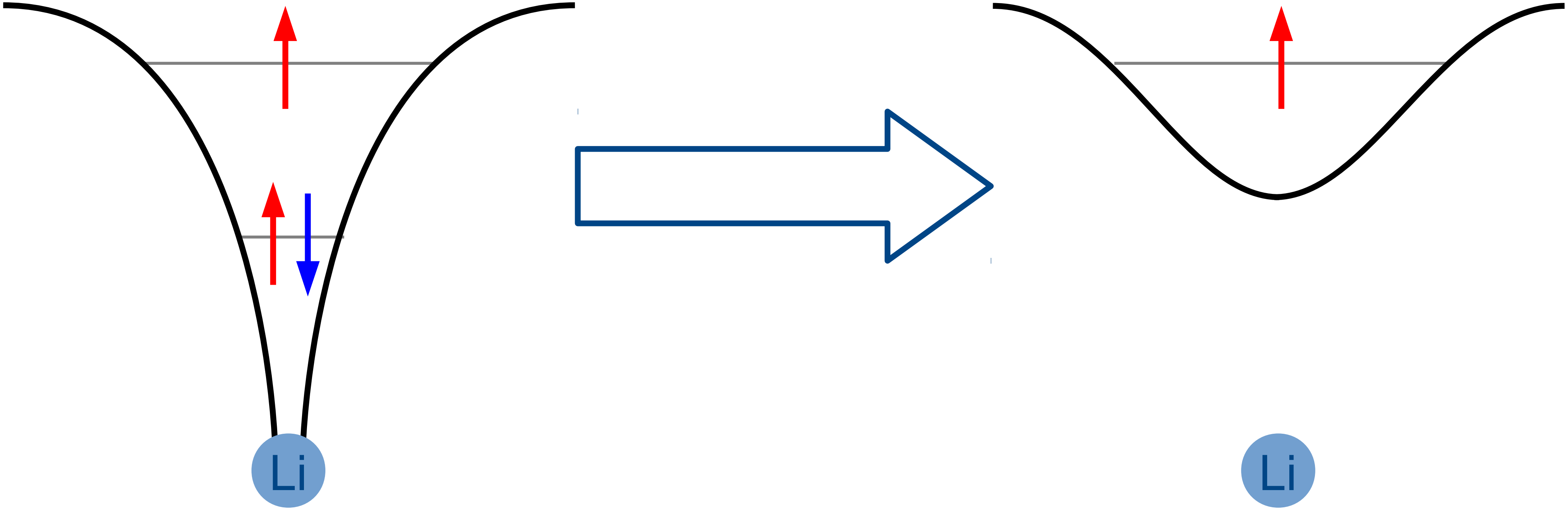


Pseudopotentials

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

Smooth background

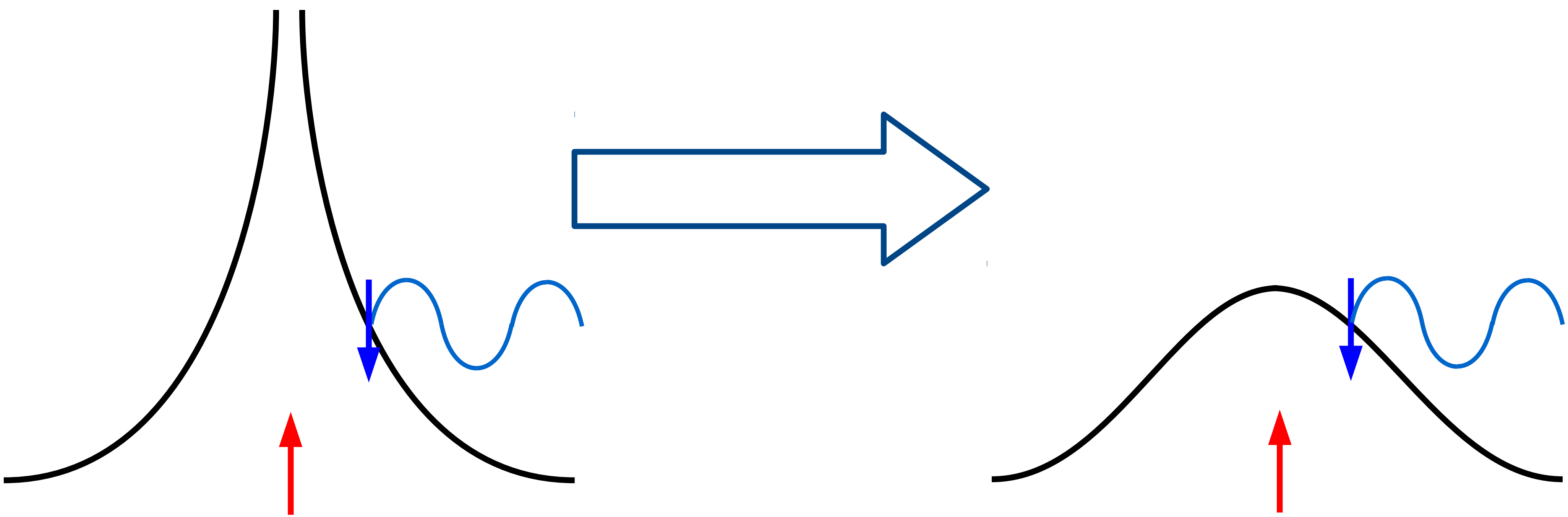
Fewer electrons



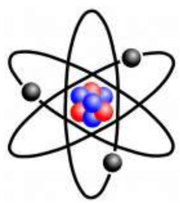
Pseudopotentials

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

Smooth background

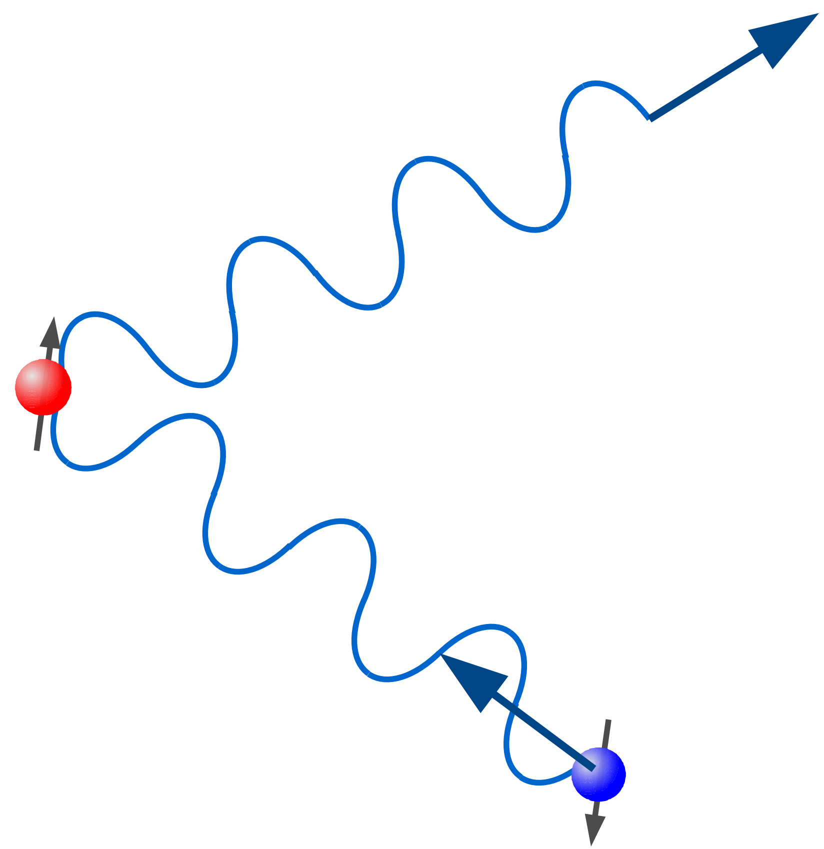


Scattering in ultracold atom gases



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

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



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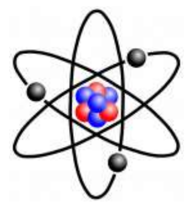
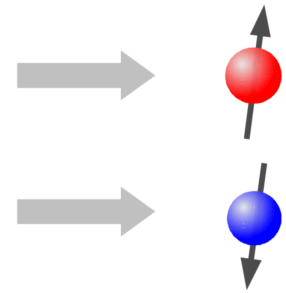


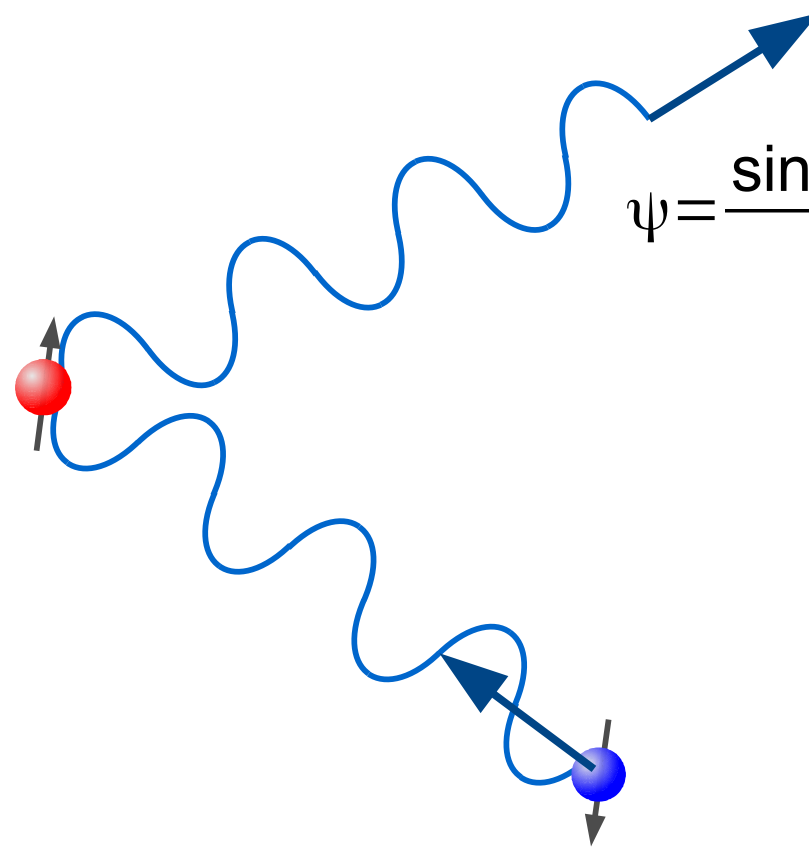
^{6}Li atom

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

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



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

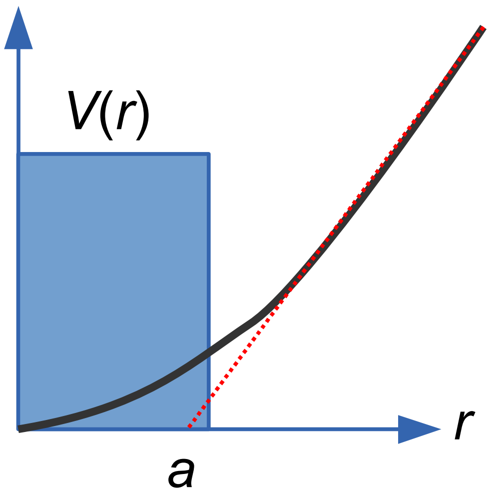


$$\psi = \frac{\sin(kr+\delta)}{kr}$$

Scattering potentials

Underlying repulsive

Effective repulsive



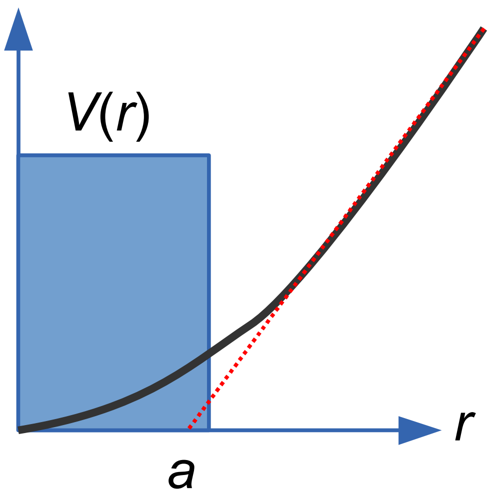
Scattering potentials

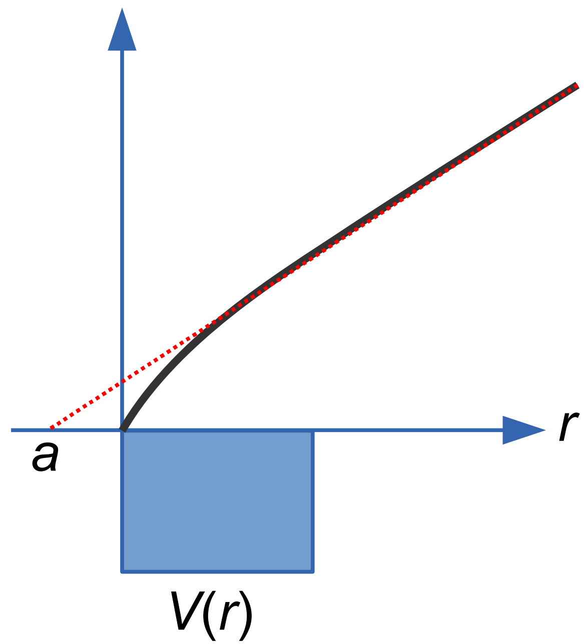
Underlying repulsive

Effective repulsive

Underlying attractive

Effective attractive





Scattering potentials

Underlying repulsive

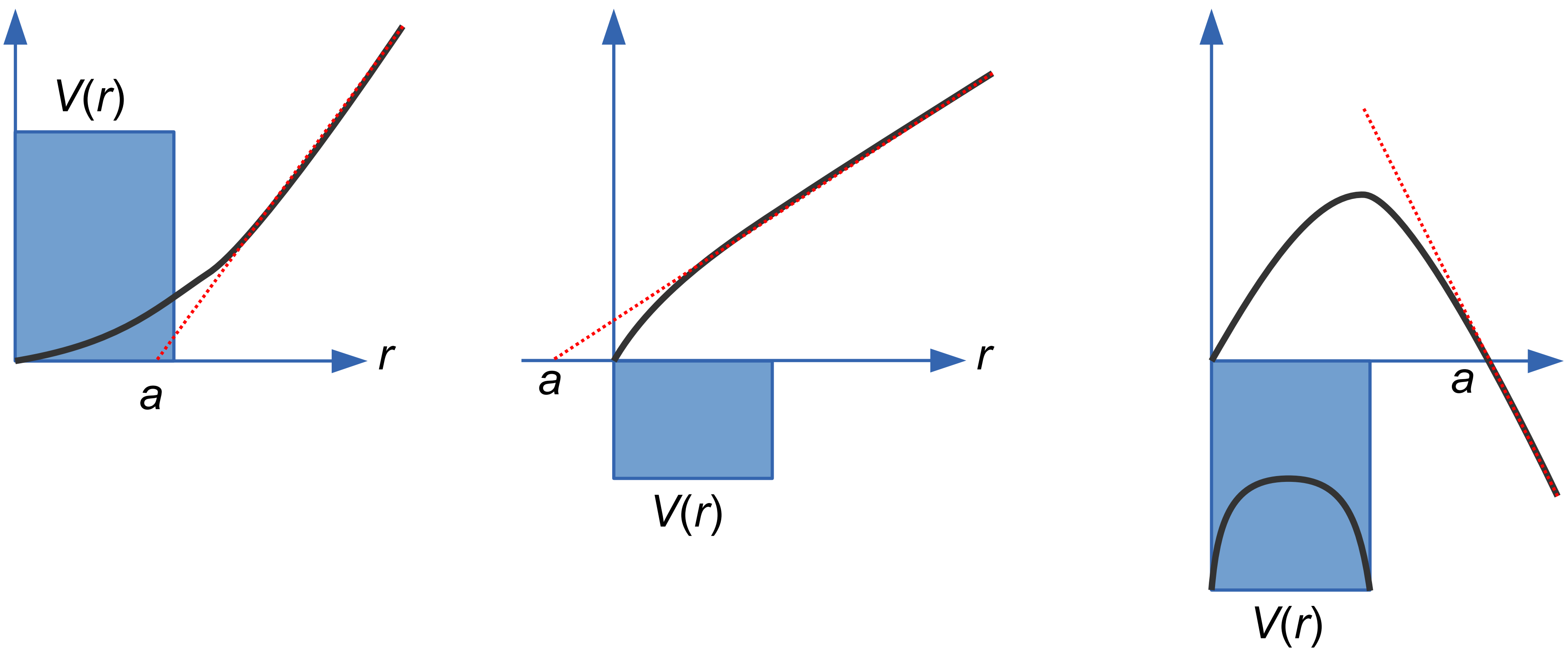
Effective repulsive

Underlying attractive

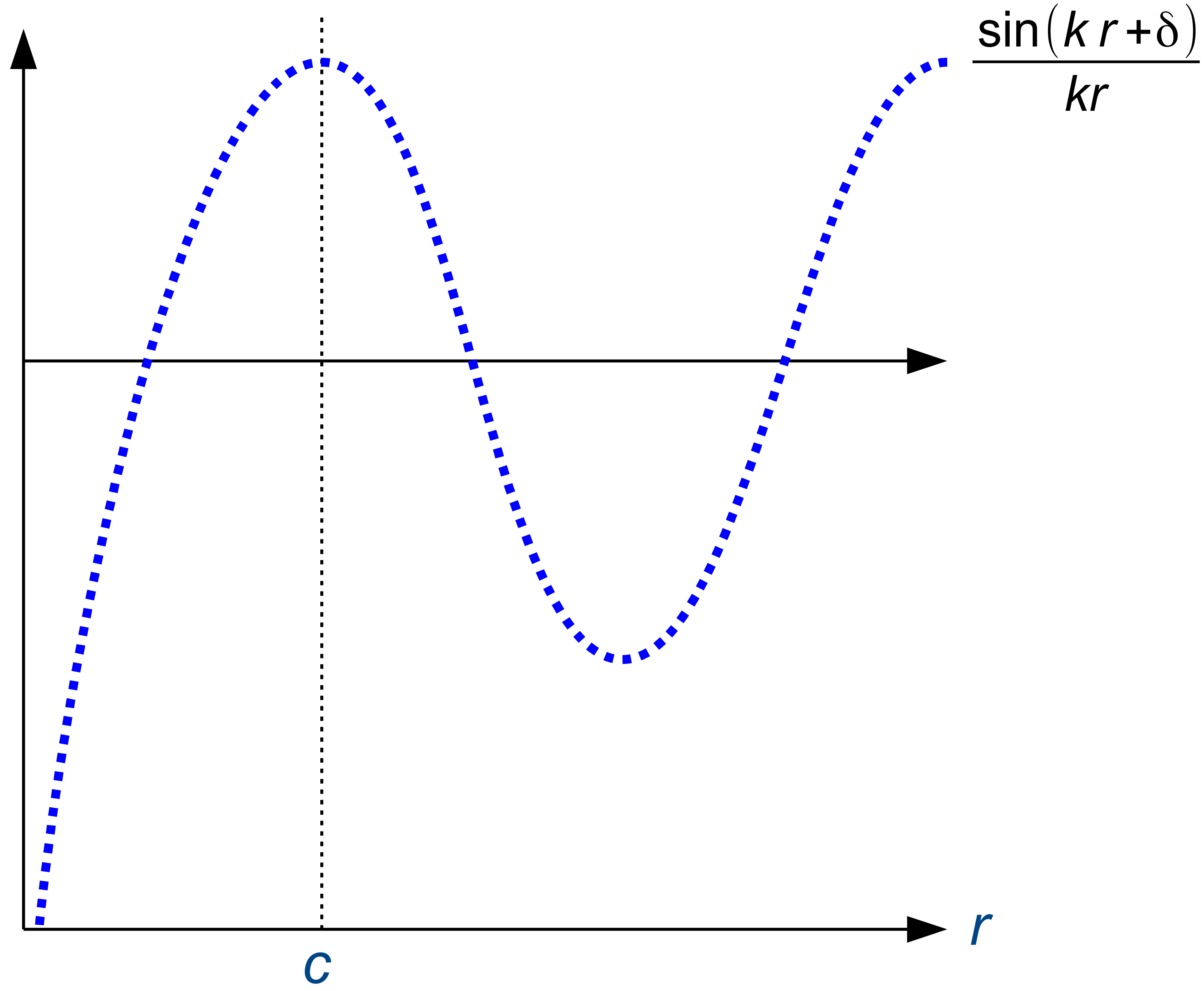
Effective attractive

Underlying attractive

Effective repulsive



Construction of a pseudopotential



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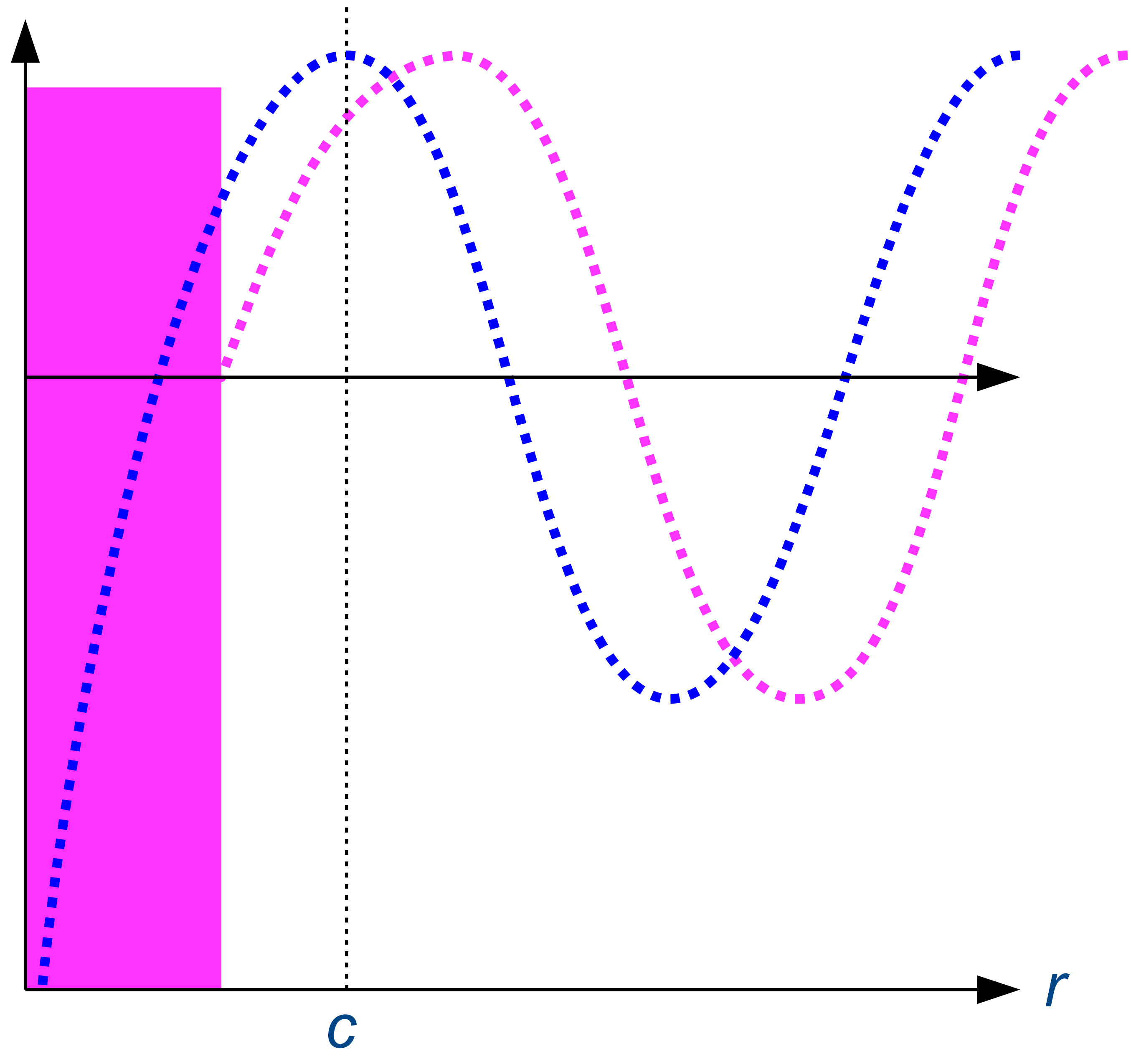
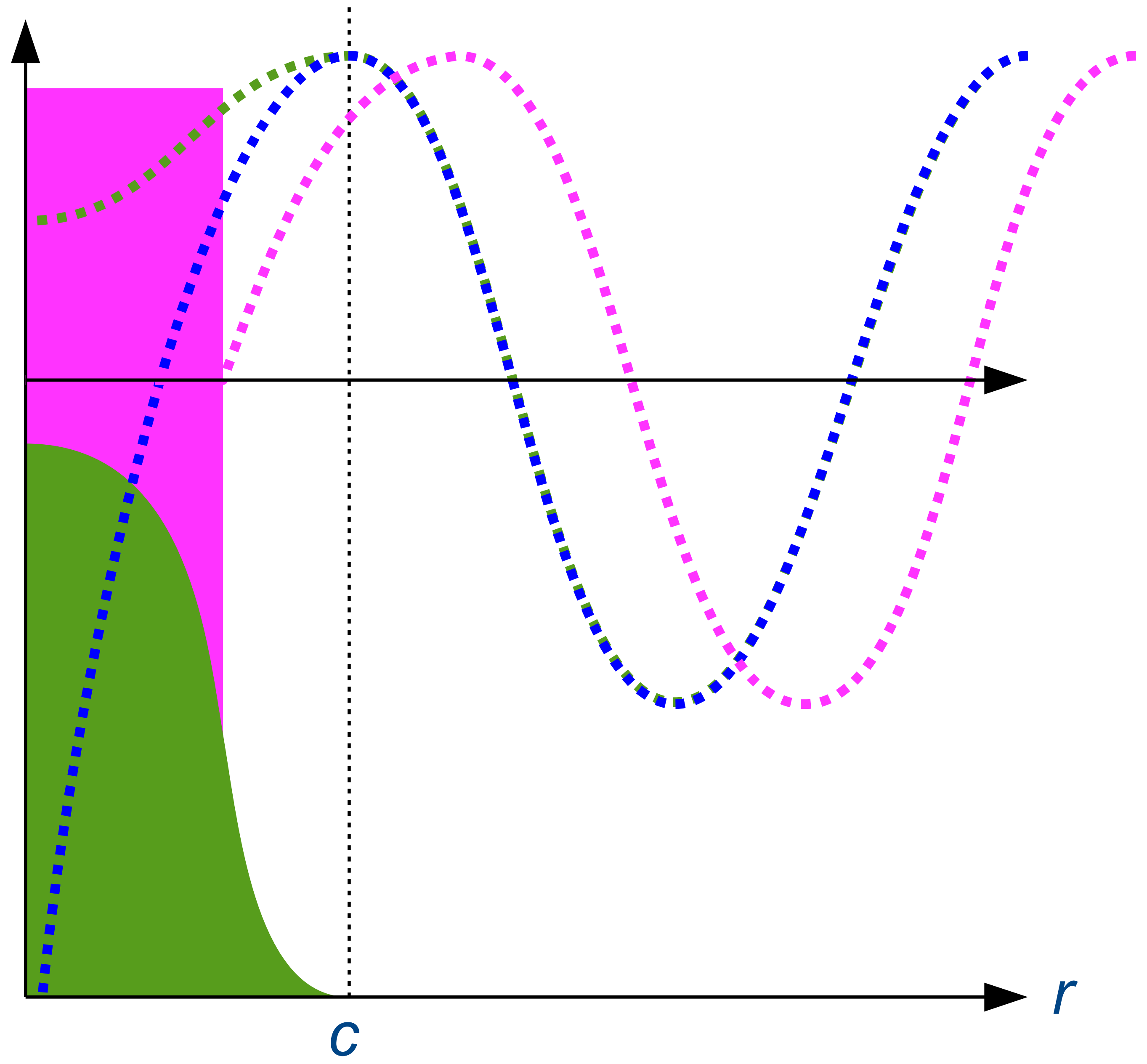


Construction of a pseudopotential



Trial form for the pseudopotential

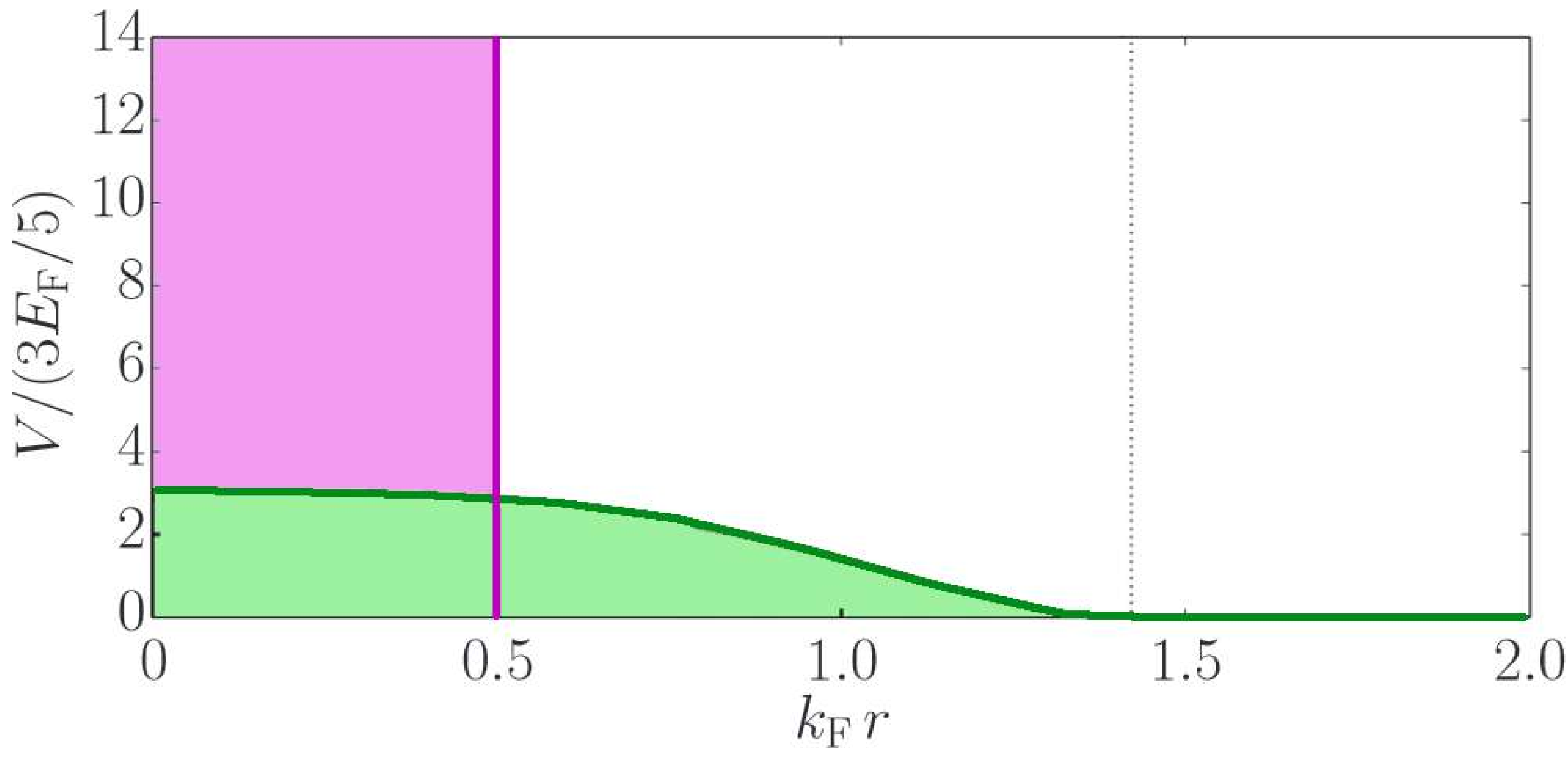
$$V_{\mathrm{PP}}(r)=\begin{cases}\left(1-\dfrac{r}{c}\right)^{2}\left[v_1\left(\dfrac{1}{2}+\dfrac{r}{c}\right)+\sum_{i=2}^{N_{\mathrm{v}}} v_i\left(\dfrac{r}{c}\right)^{i}\right] & r<c\\ 0 & r>c\end{cases}$$

Trial form for the pseudopotential

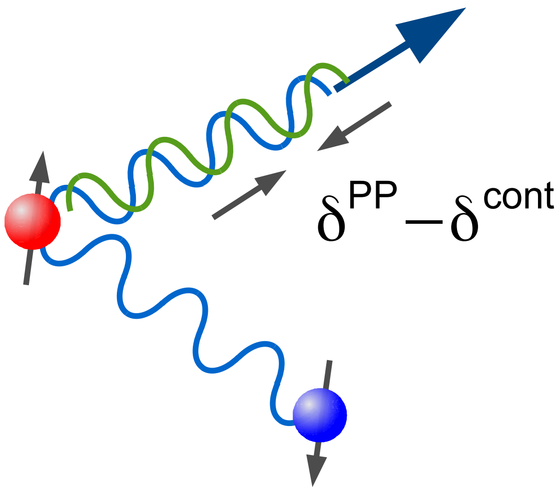
$$V_{\mathrm{PP}}(r)=\begin{cases}\left(1-\frac{r}{c}\right)^2\left[v_1\left(\frac{1}{2}+\frac{r}{c}\right)+\sum_{i=2}^{N_v} v_i\left(\frac{r}{c}\right)^i\right] & r<c\\ 0 & r>c\end{cases}$$

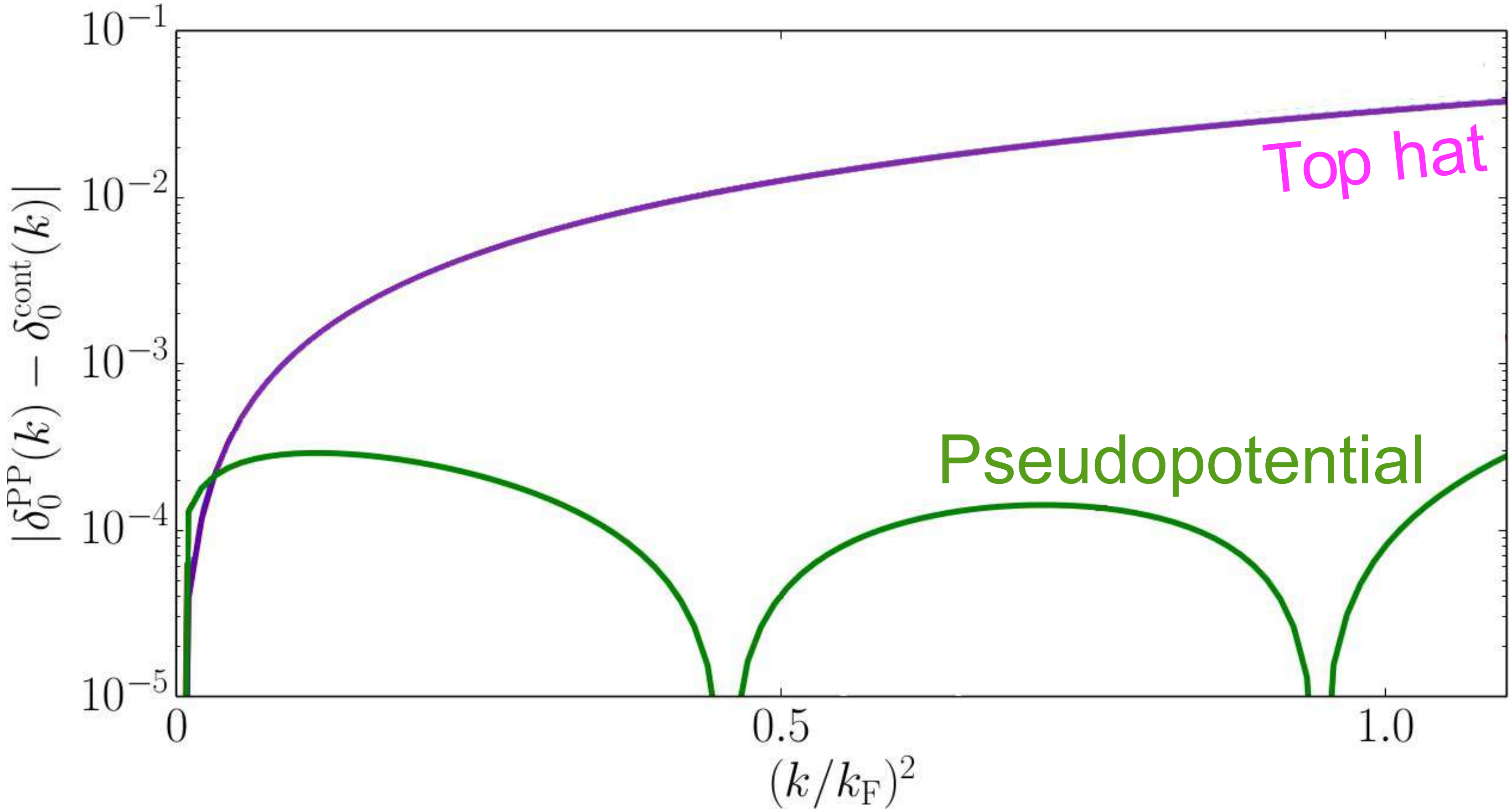
$$\langle\Delta\delta^2\rangle=\sum_{l=0}^{l_{\max}}\int_0^{k_F}\left[\left.\frac{\mathrm{d}\ln\psi_{\mathrm{PP}}(k,l)}{\mathrm{d}r}\right|_c-\left.\frac{\mathrm{d}\ln\psi_{\mathrm{cont}}(k,l)}{\mathrm{d}r}\right|_c\right]^2\mathrm{d}k$$

Optimal pseudopotential

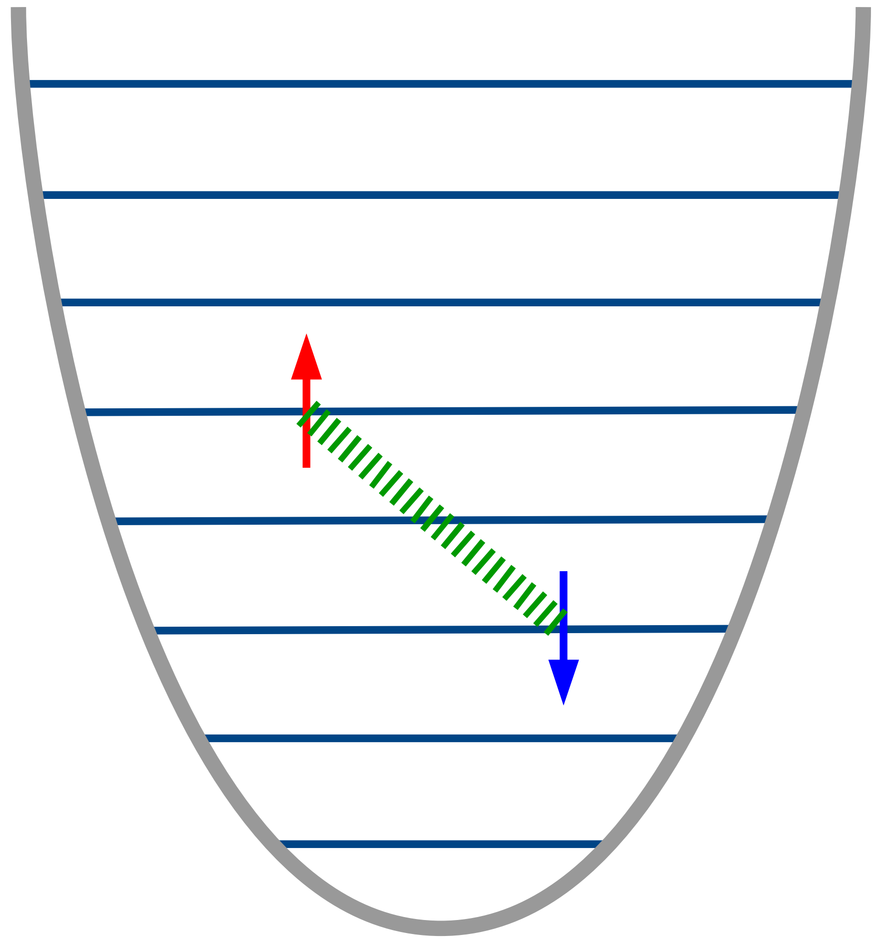


Pseudopotential: scattering phase shift





Pseudopotential: two atoms in a trap



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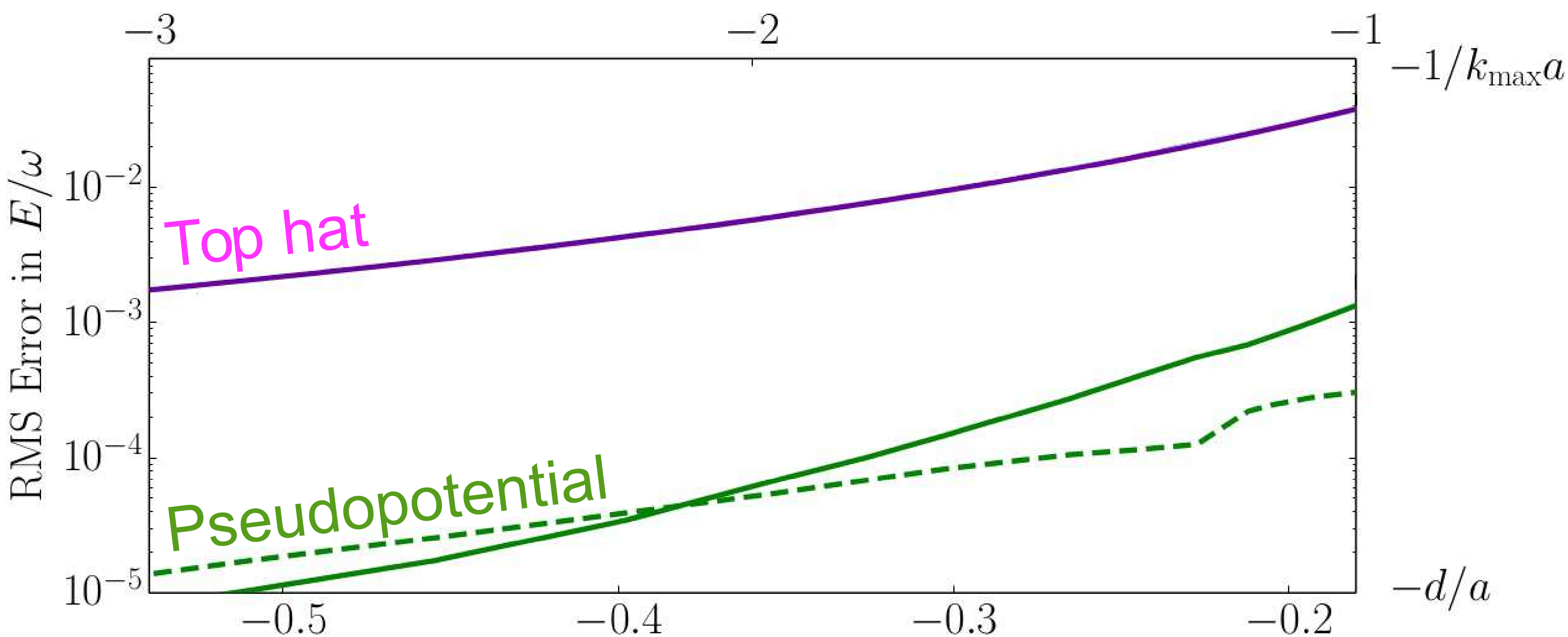


Pseudopotentials summary

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

Bound state: 1000 times more accurate, 1000 times faster

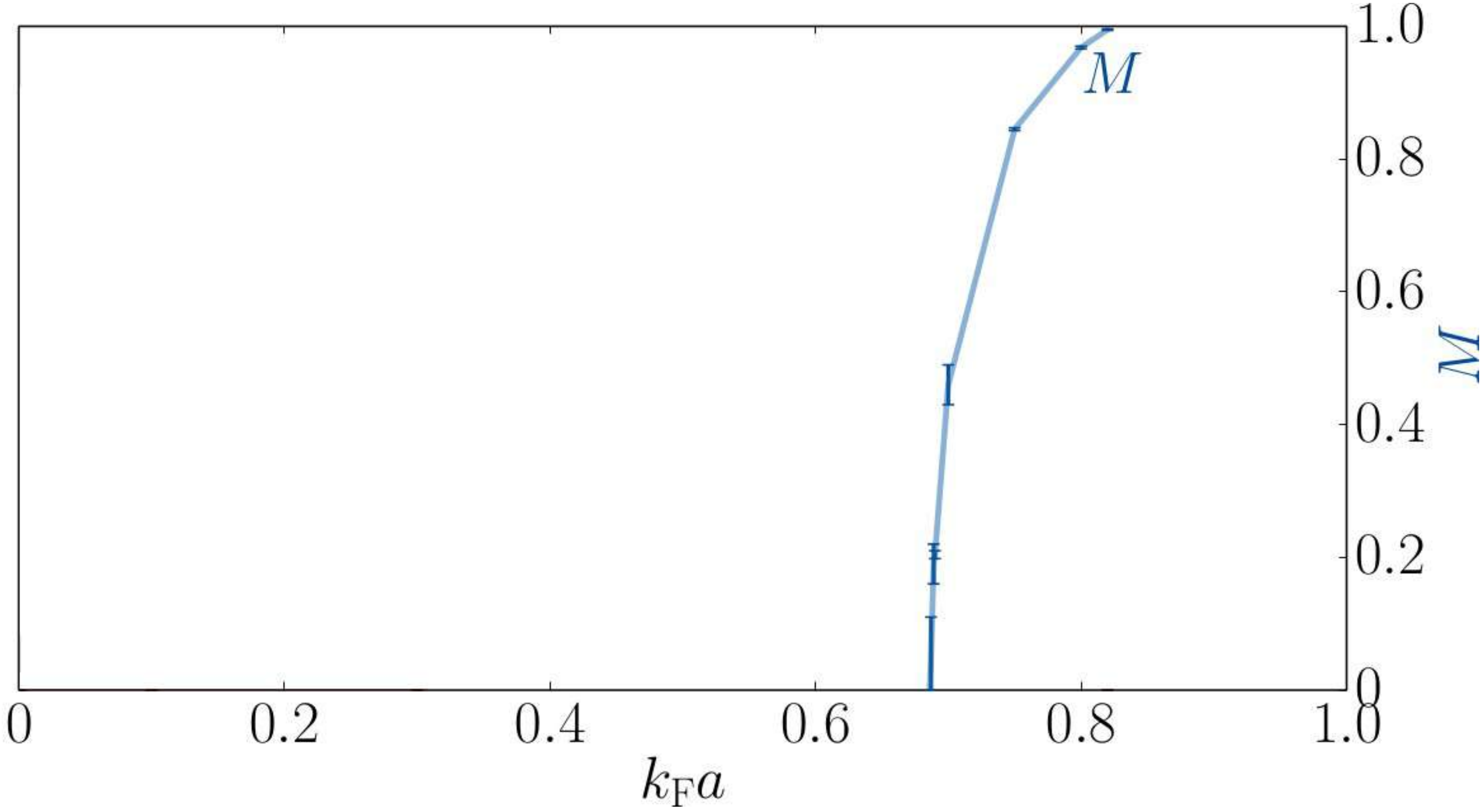
Stoner Hamiltonian

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

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 top hat	First order	$k_F a$=0.81(2)
Hartree Fock MC	First order	$k_F a$=0.83(2)

Stoner Hamiltonian ground state magnetization

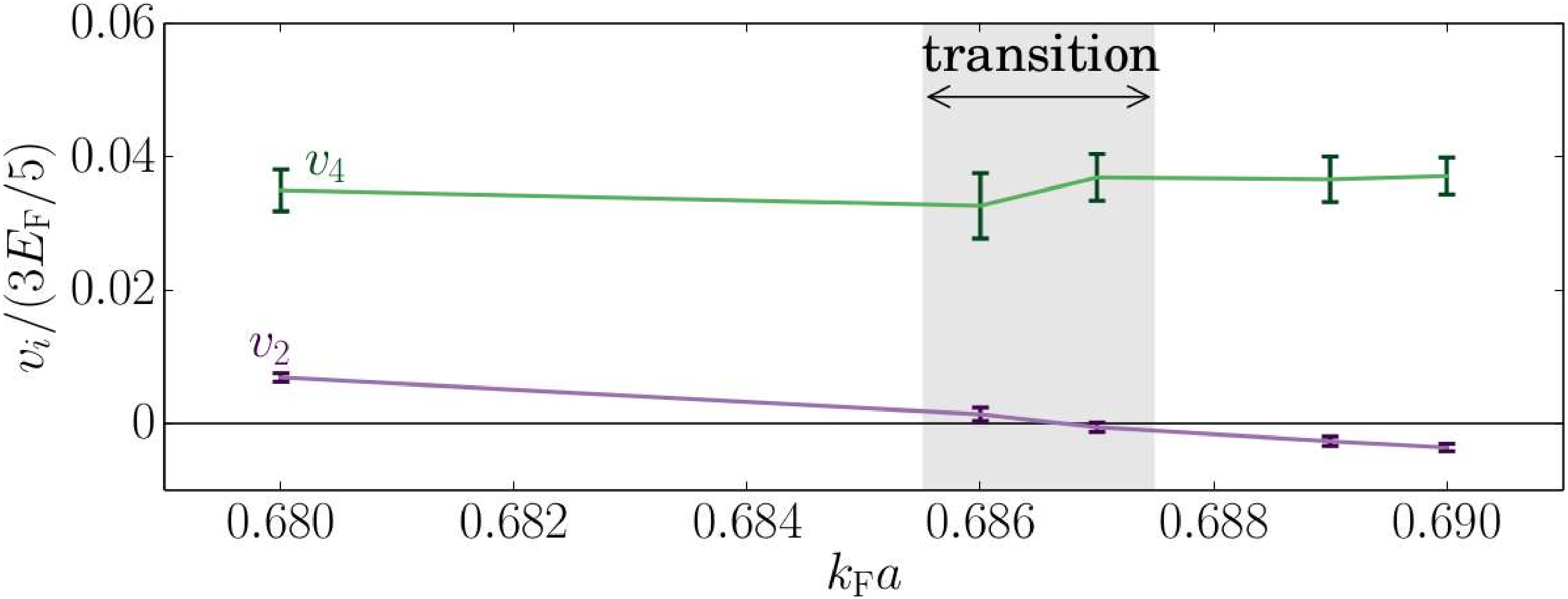


Landau expansion

$$F(M)=F(0)+v_2 M^2+v_4 M^4+v_6 M^6$$

Landau expansion

$$F(M) = F(0) + v_2 M^2 + v_4 M^4 + v_6 M^6$$



Theories of ferromagnetism

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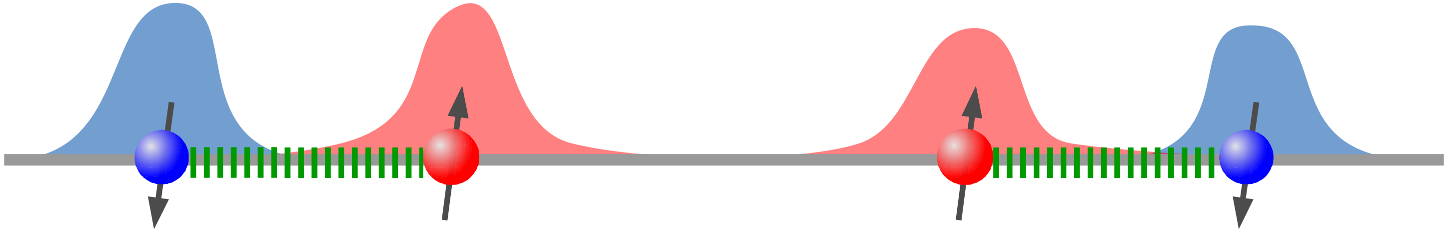
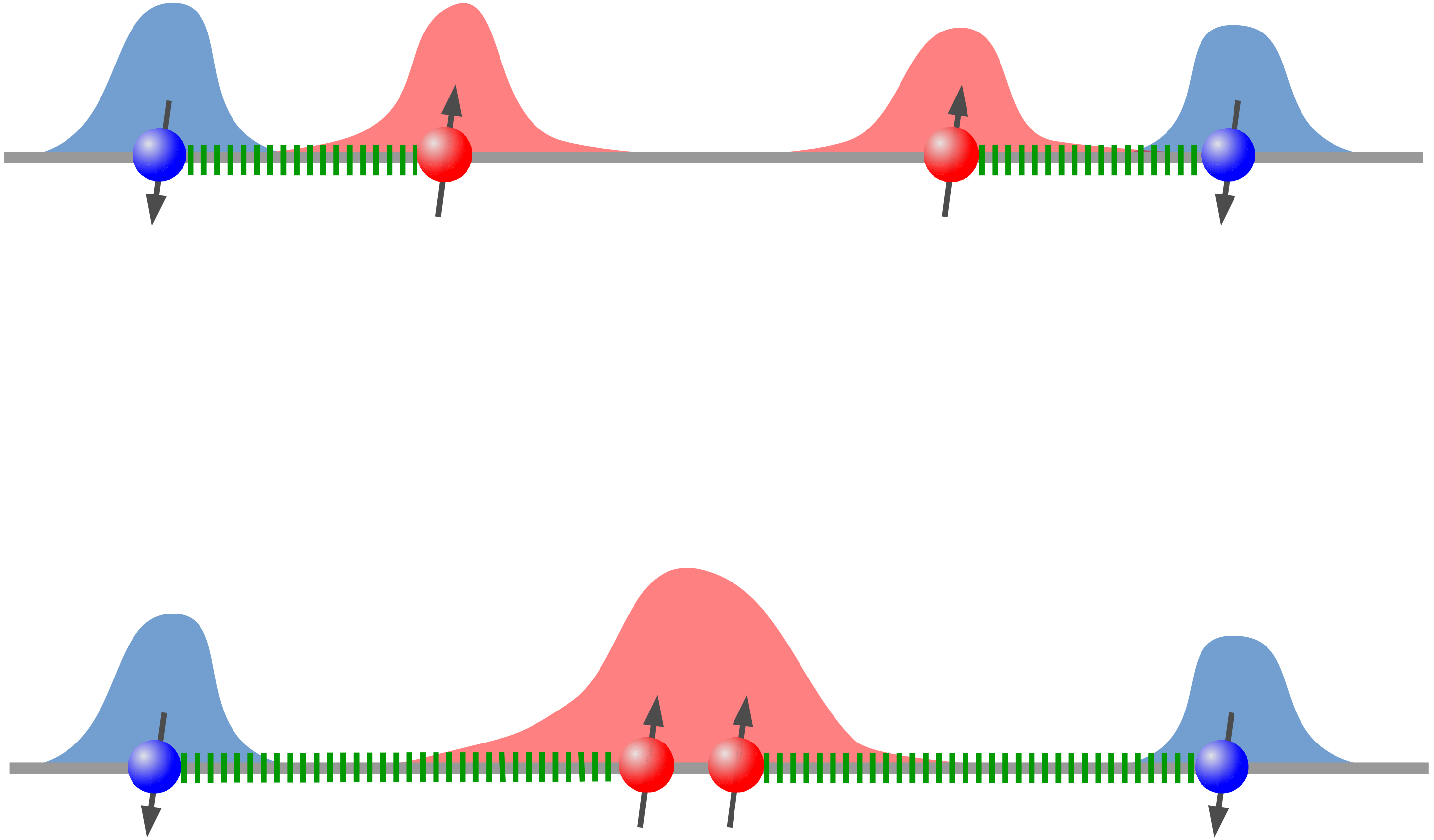
DMC top hat	First order	$k_F a=0.81(2)$
Hartree Fock MC	First order	$k_F a=0.83(2)$
DMC pseudopotential	Second order	$k_F a=0.683(1)$

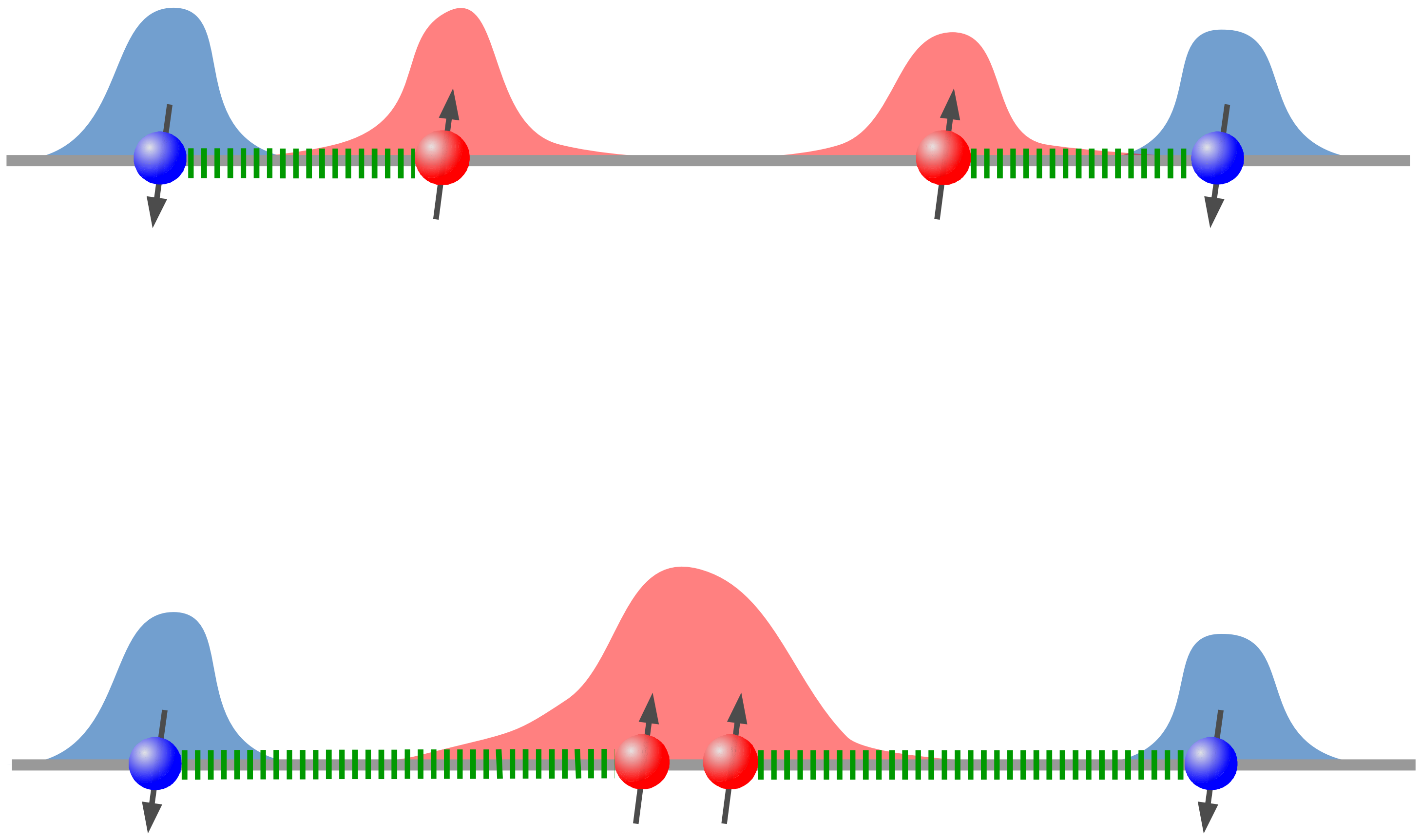
Fluctuation contributions



Fluctuation contributions drive pairing

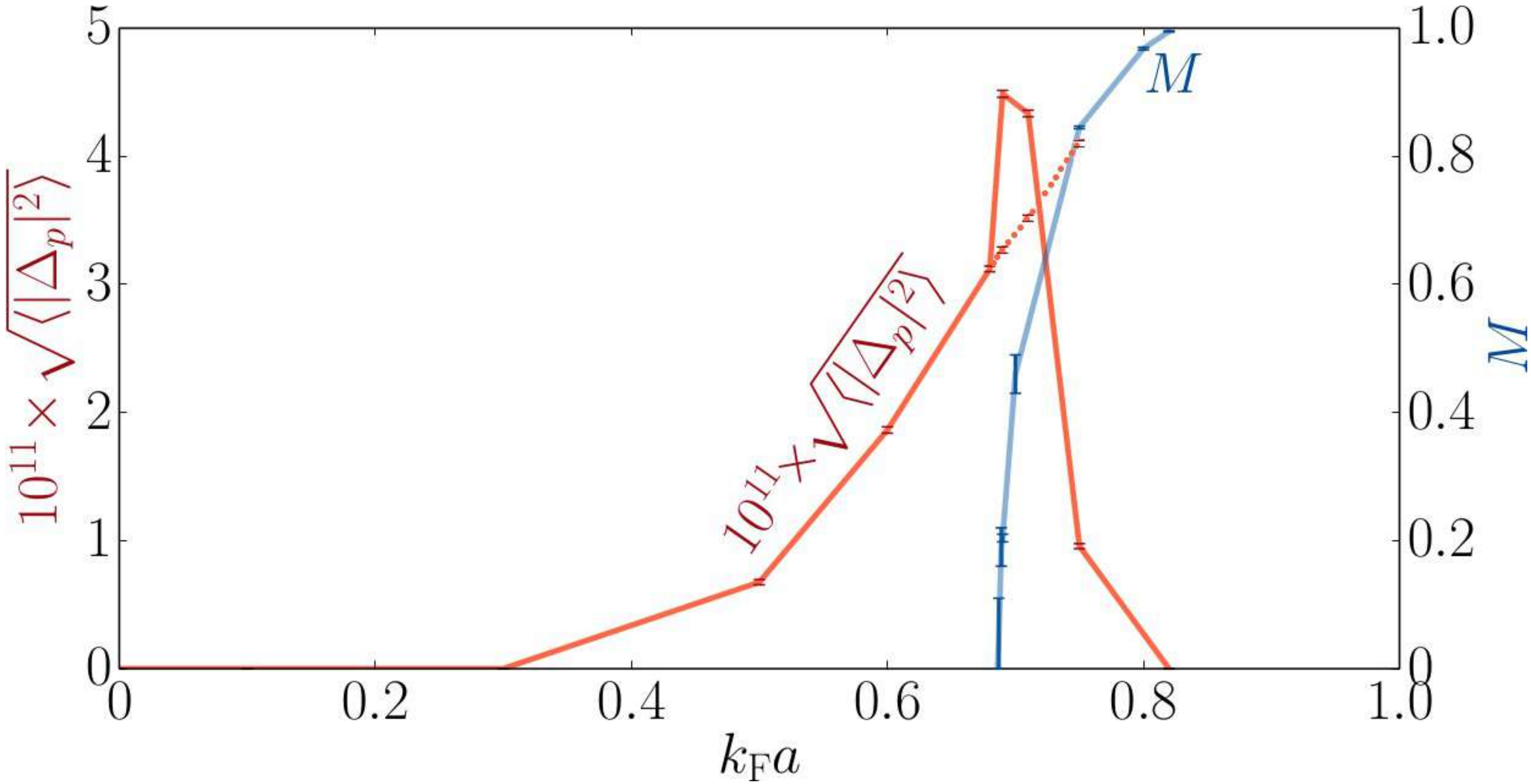


Fluctuation contributions drive pairing

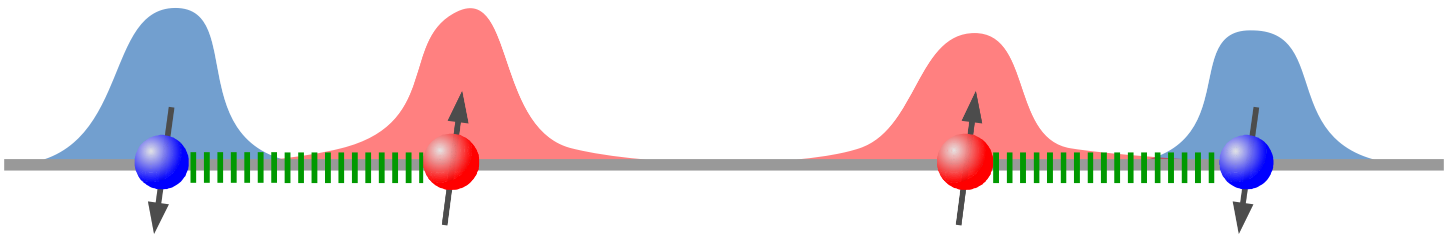


UGe_2, URhGe, UCoGe, $ZrZn_2$, Sr_2RuO_4, $LaNiGa_2$, $LaNiC_2$

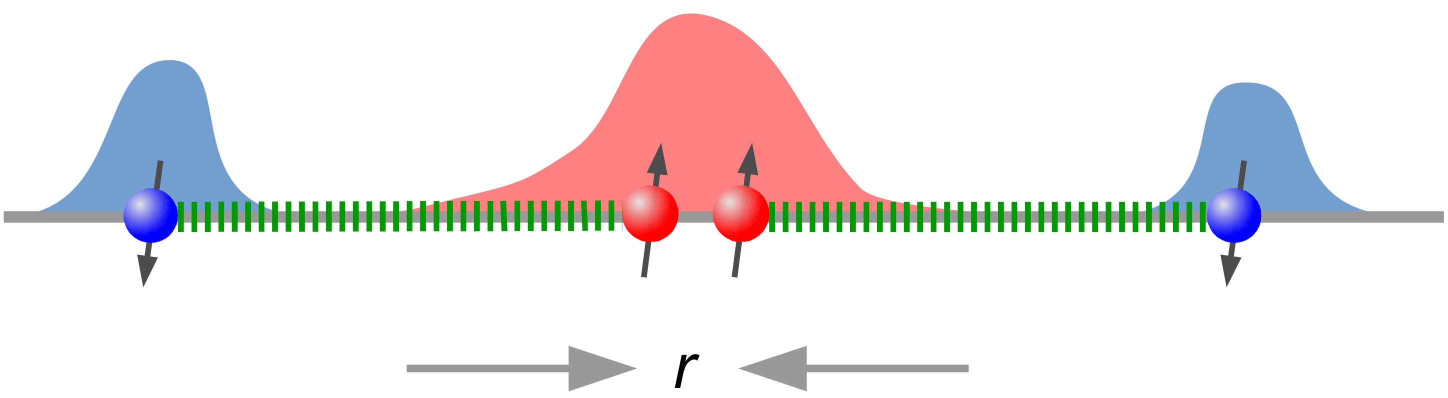
Emergence of superconducting order



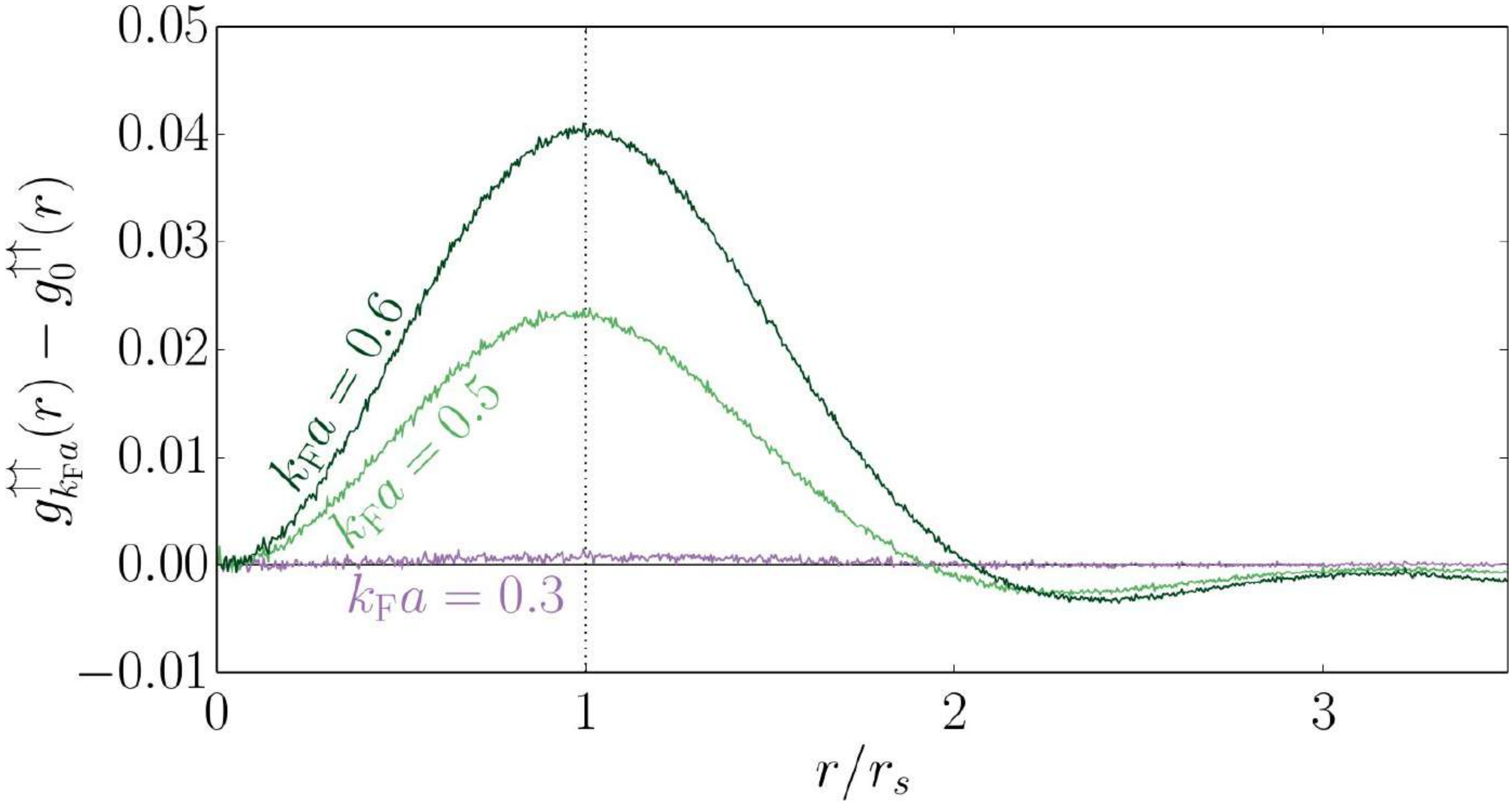
Fluctuation contributions: pair correlation function



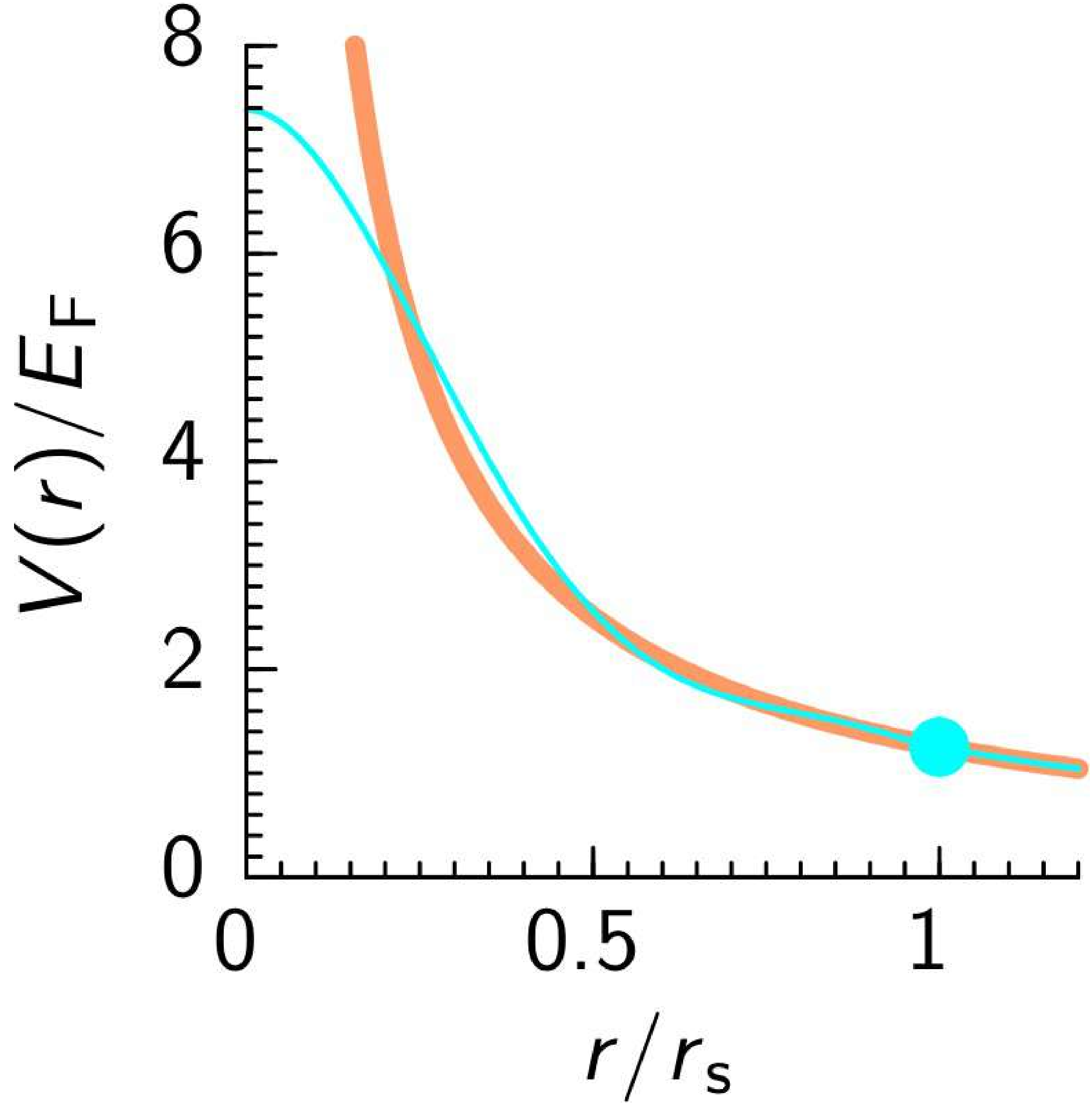
$$g(r) = \langle n_{\uparrow}(\boldsymbol{r}+\boldsymbol{r}')\, n_{\uparrow}(\boldsymbol{r}') \rangle$$



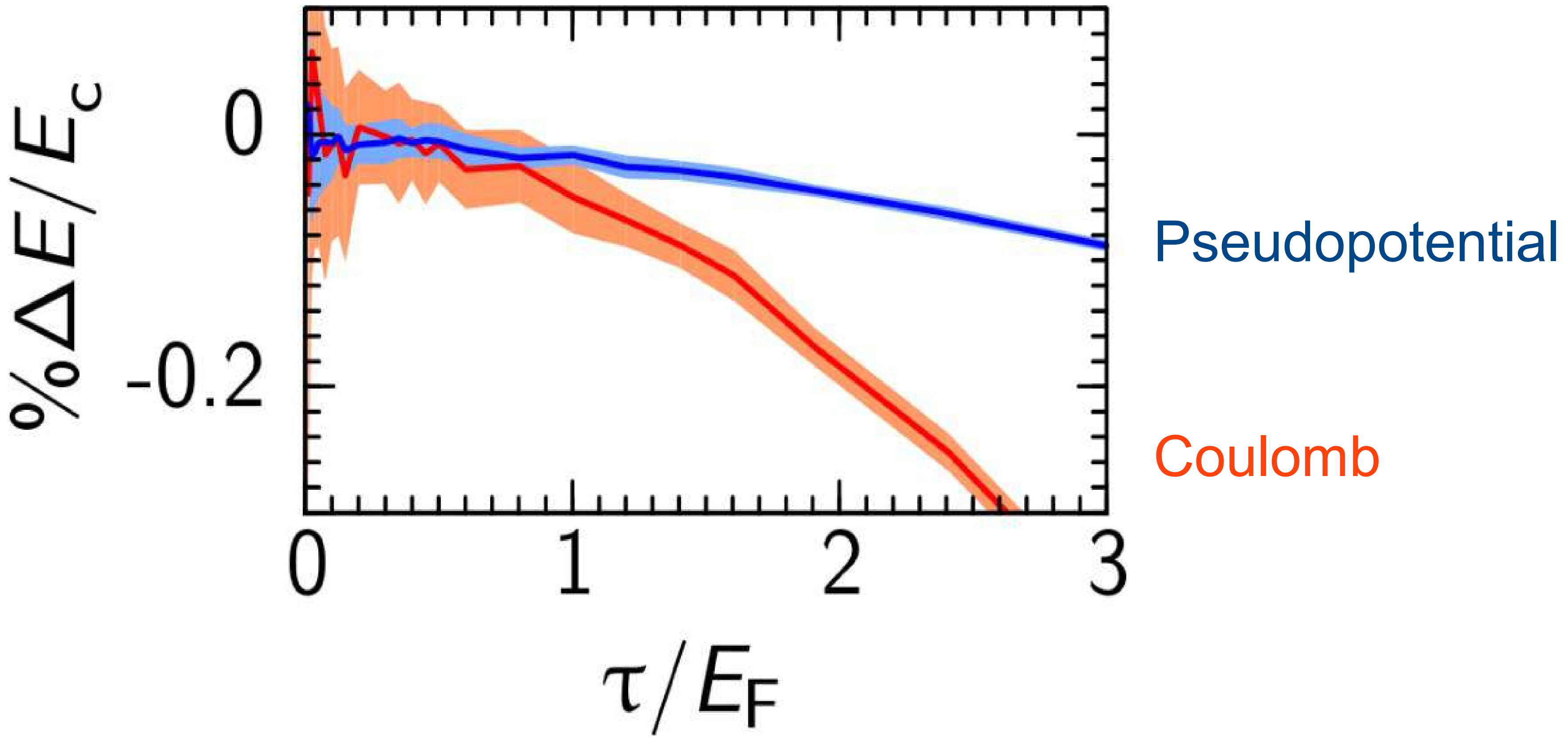
Pair correlation function



Coulomb pseudopotential

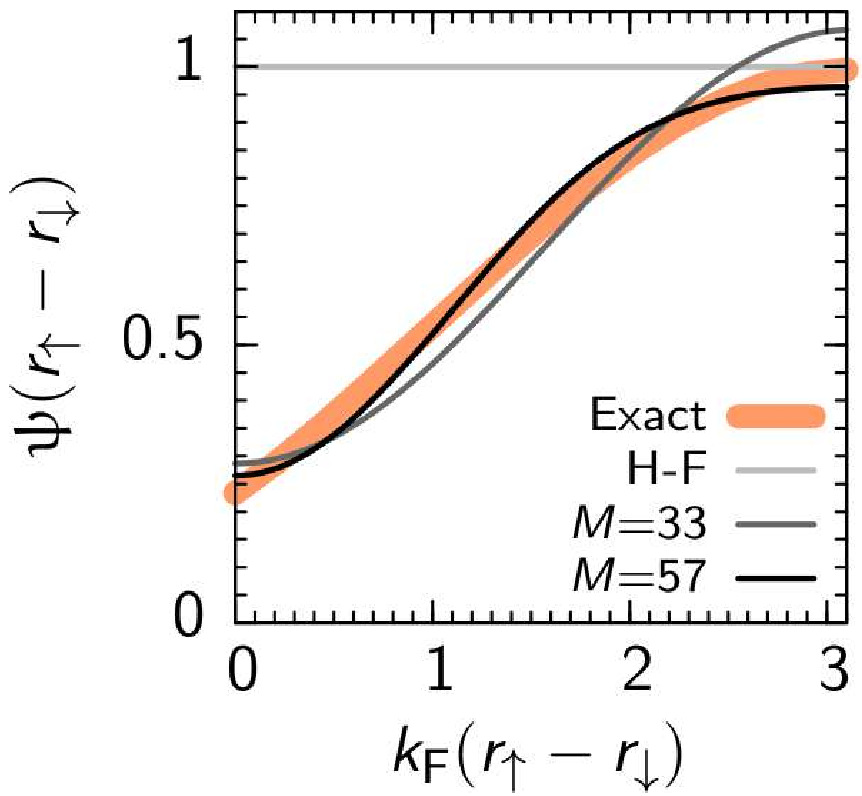


Monte Carlo error with Coulomb pseudopotential

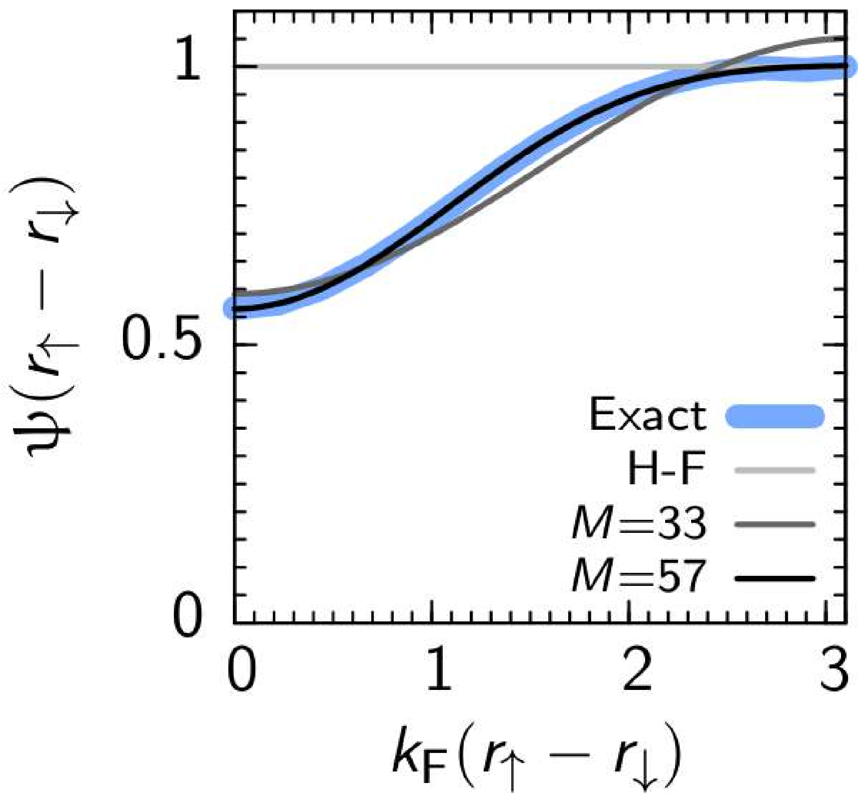


Configuration interaction with Coulomb pseudopotential

Coulomb



Pseudopotential



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