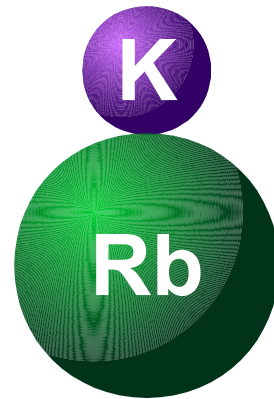


# Pseudopotentials for a dipolar ultracold atomic gas

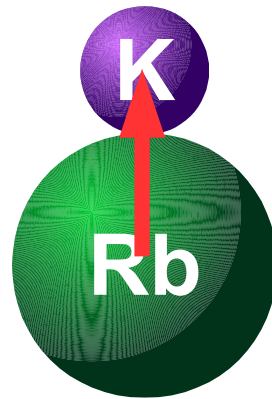
Thomas Whitehead  
Gareth Conduit

TCM Group, Department of Physics

# Dipolar molecule

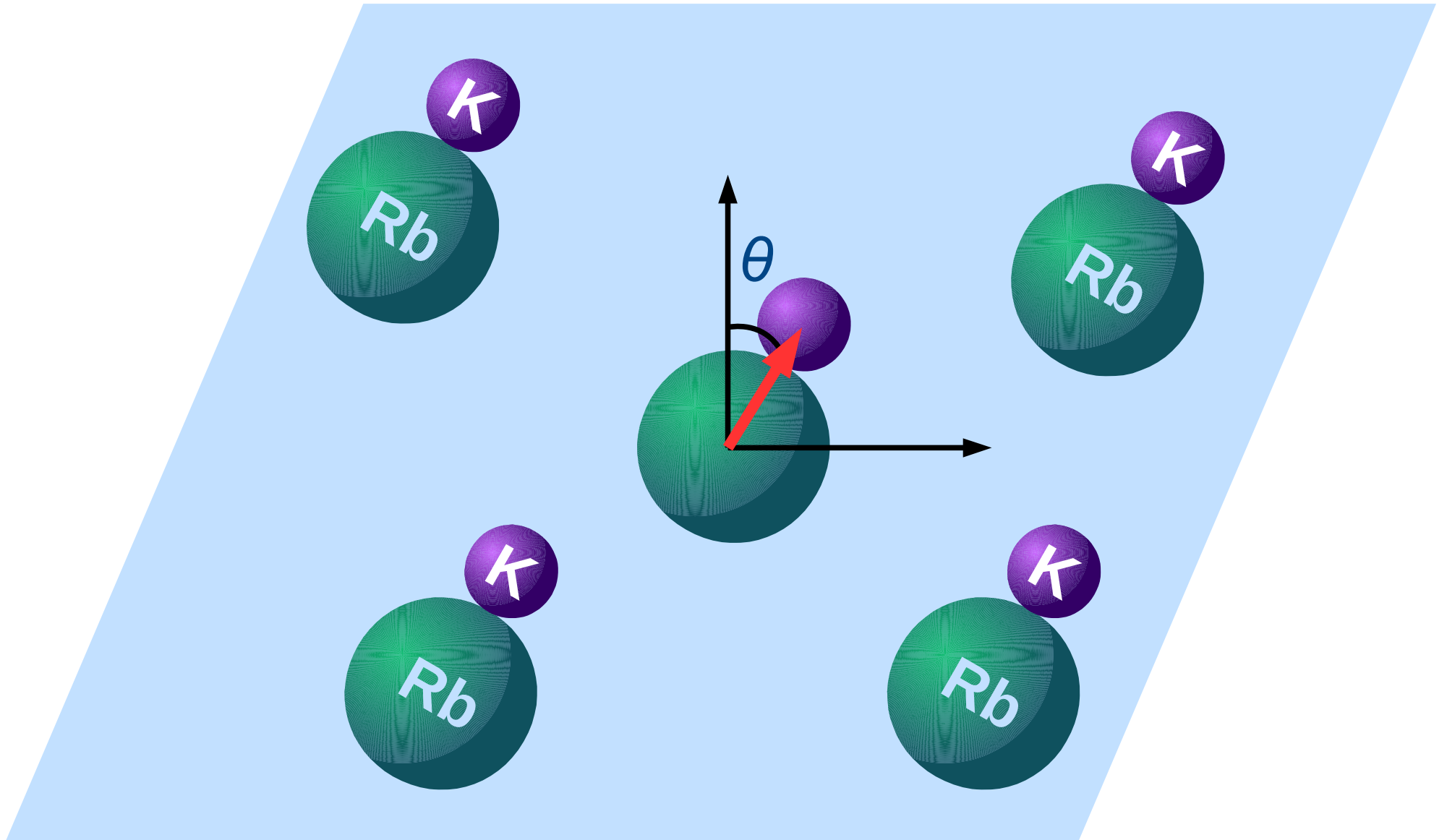


# Dipole moment



$d \sim 0.5$  Debye

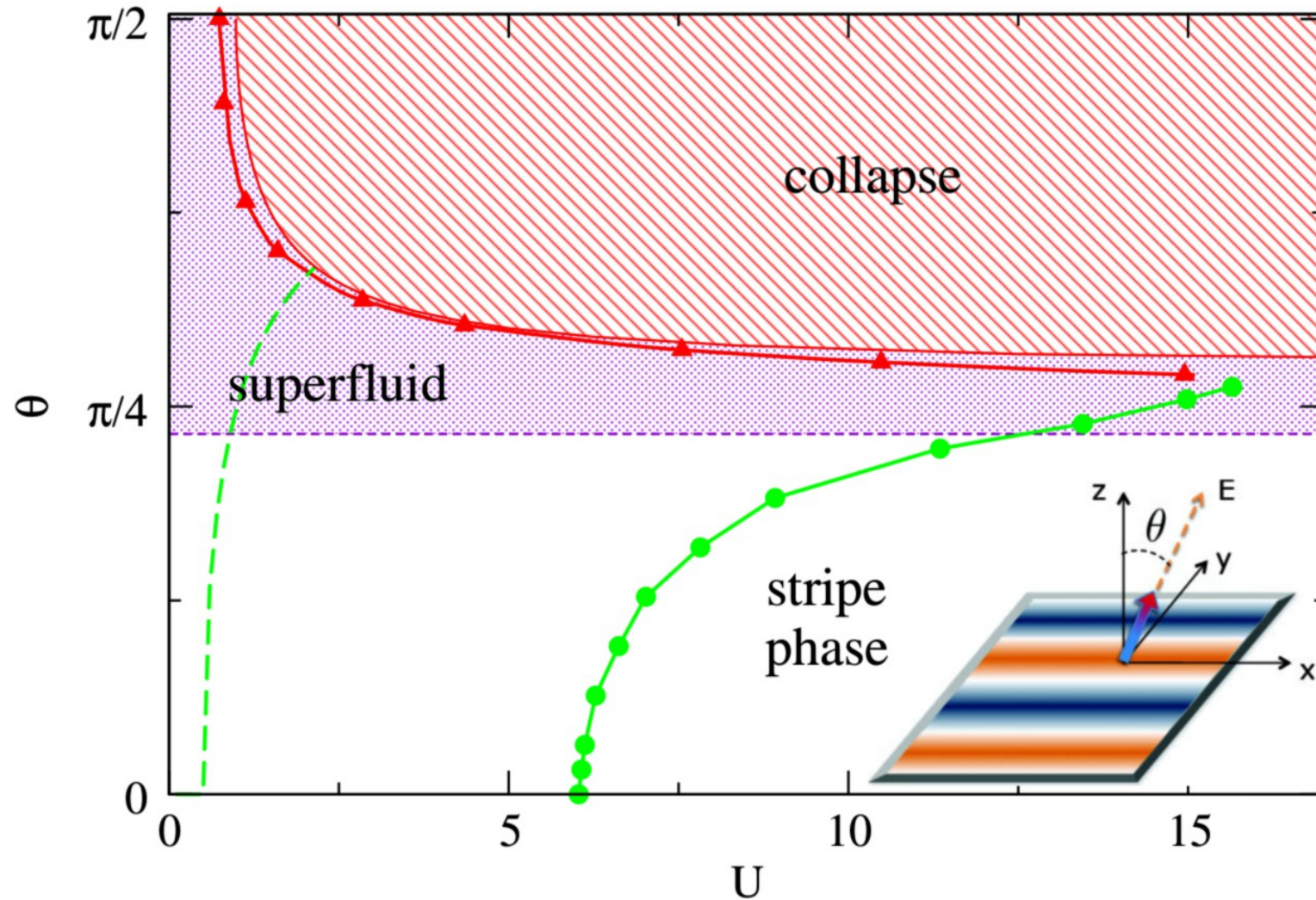
# A 2D dipolar gas



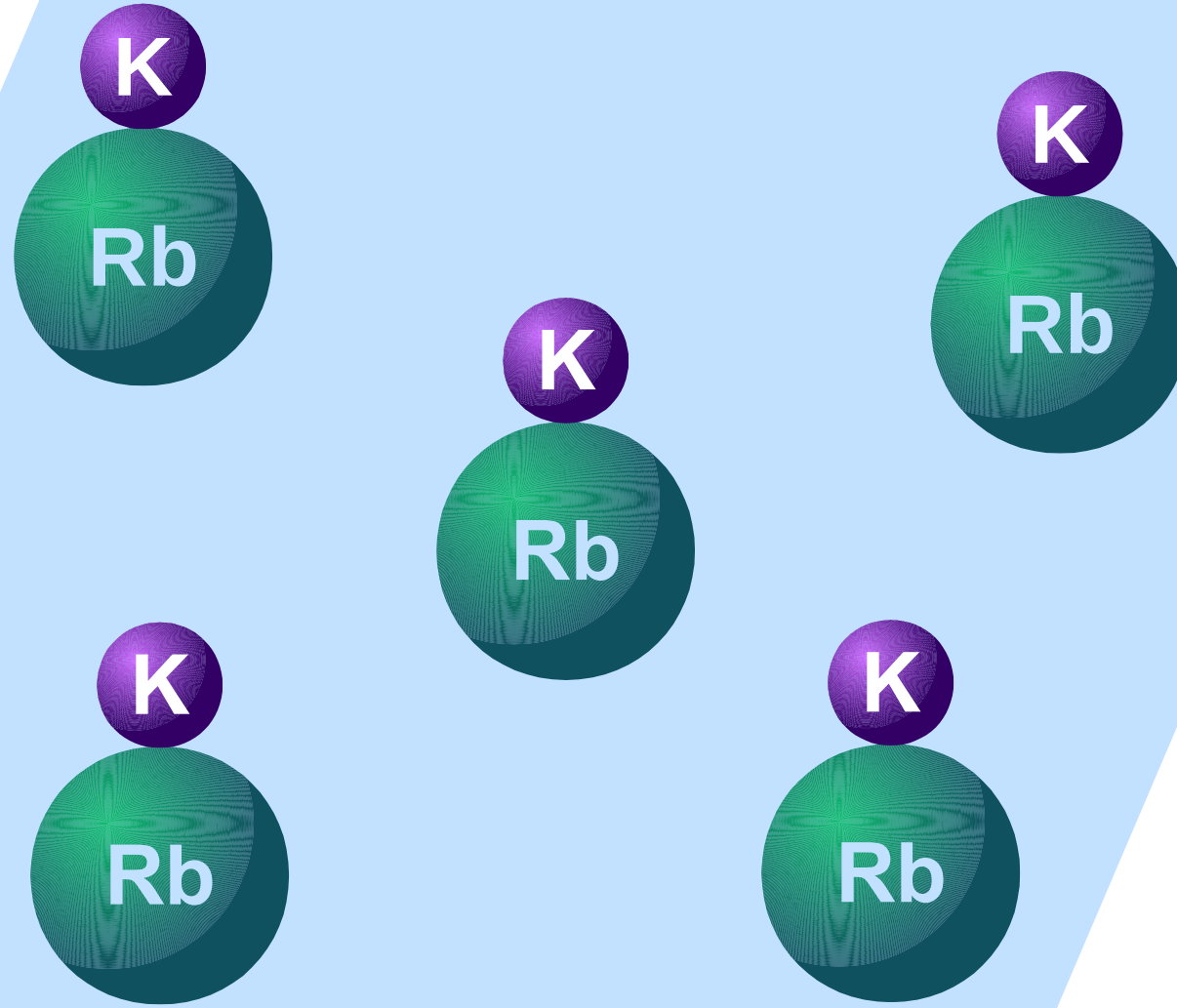
# Reasons for interest

- ~ Control of ultracold chemical reactions
- ~ Quantum information processing
- ~ Novel strongly correlated phases

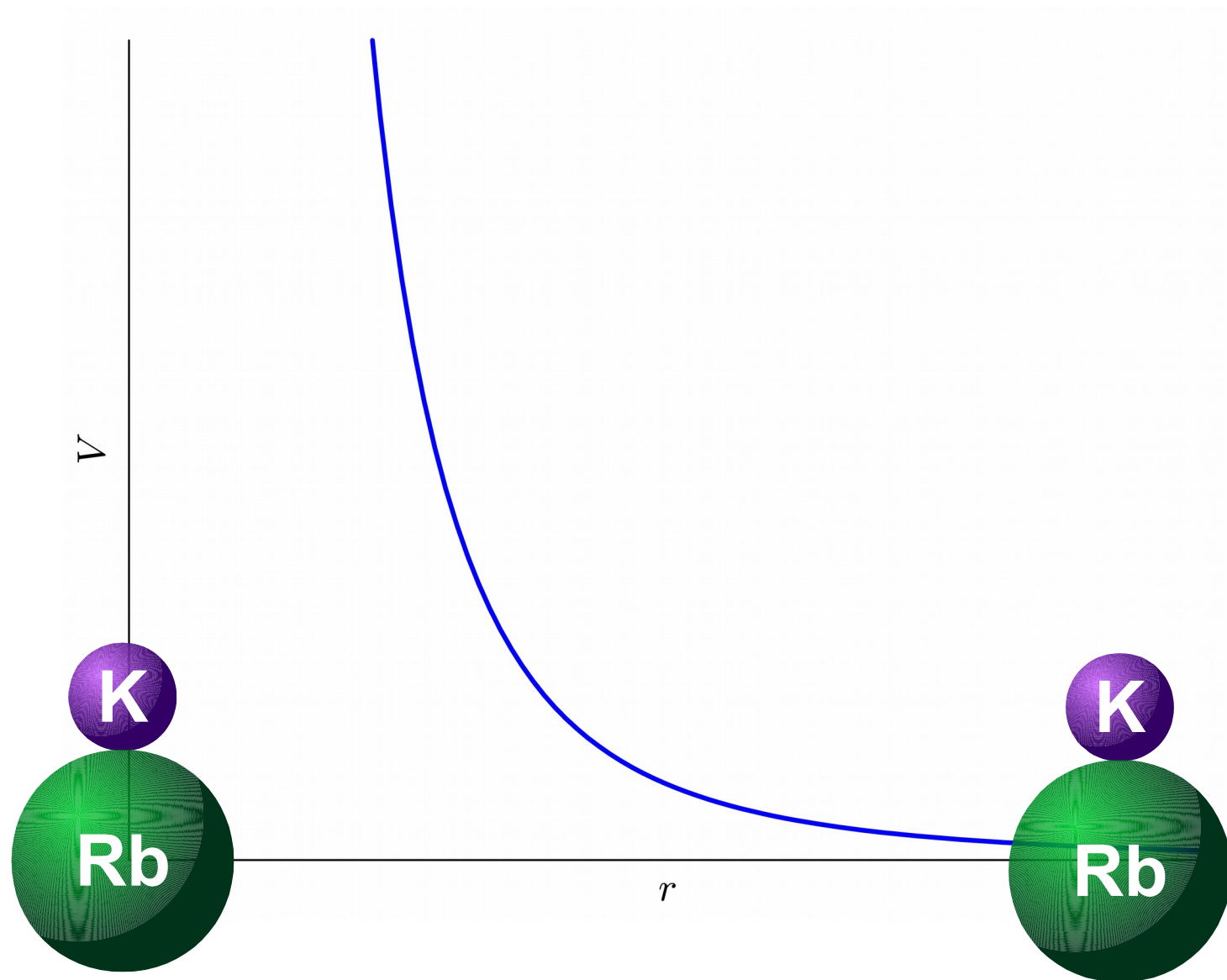
# Phase diagram



$\theta = 0$  case

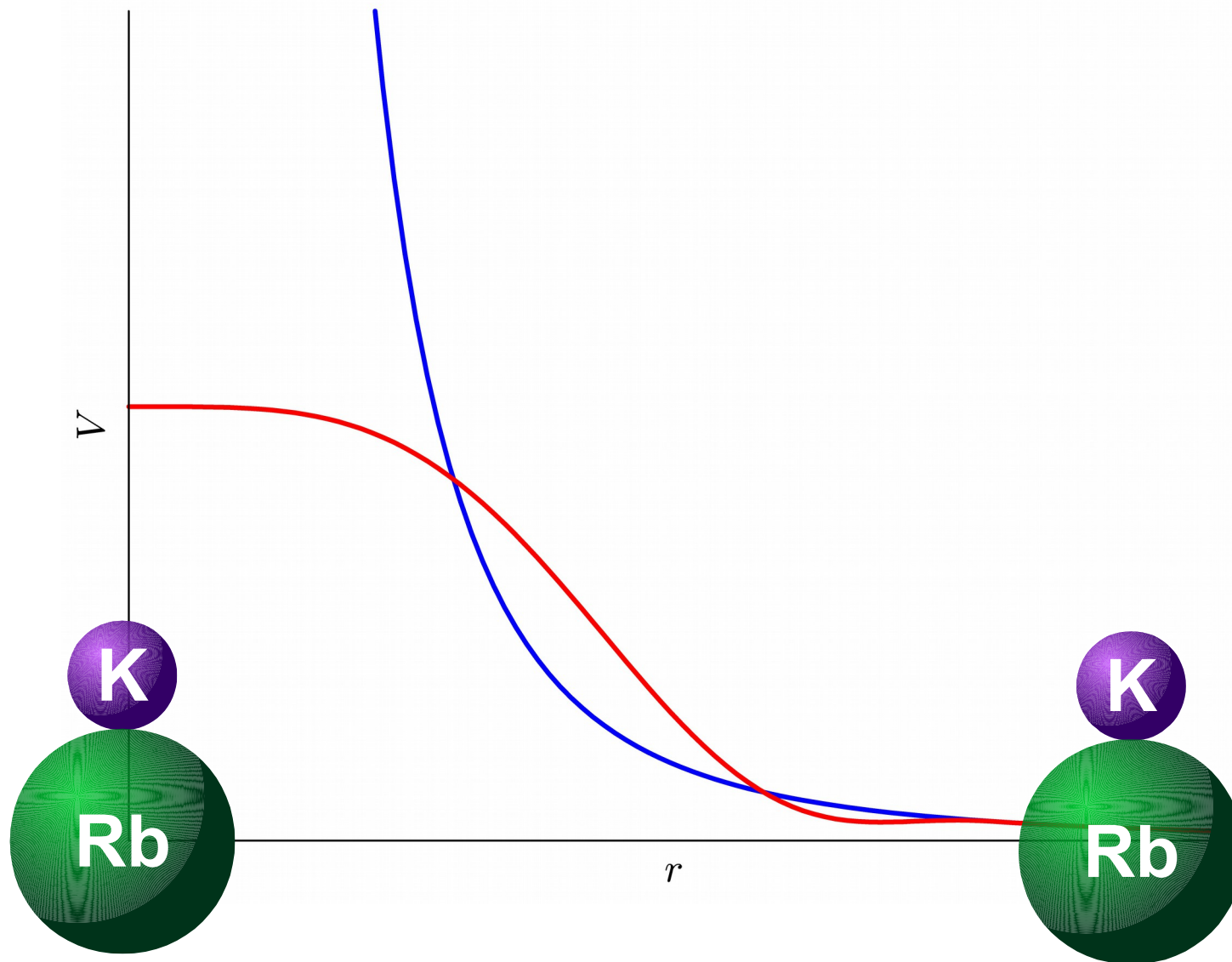


# Two interacting dipoles

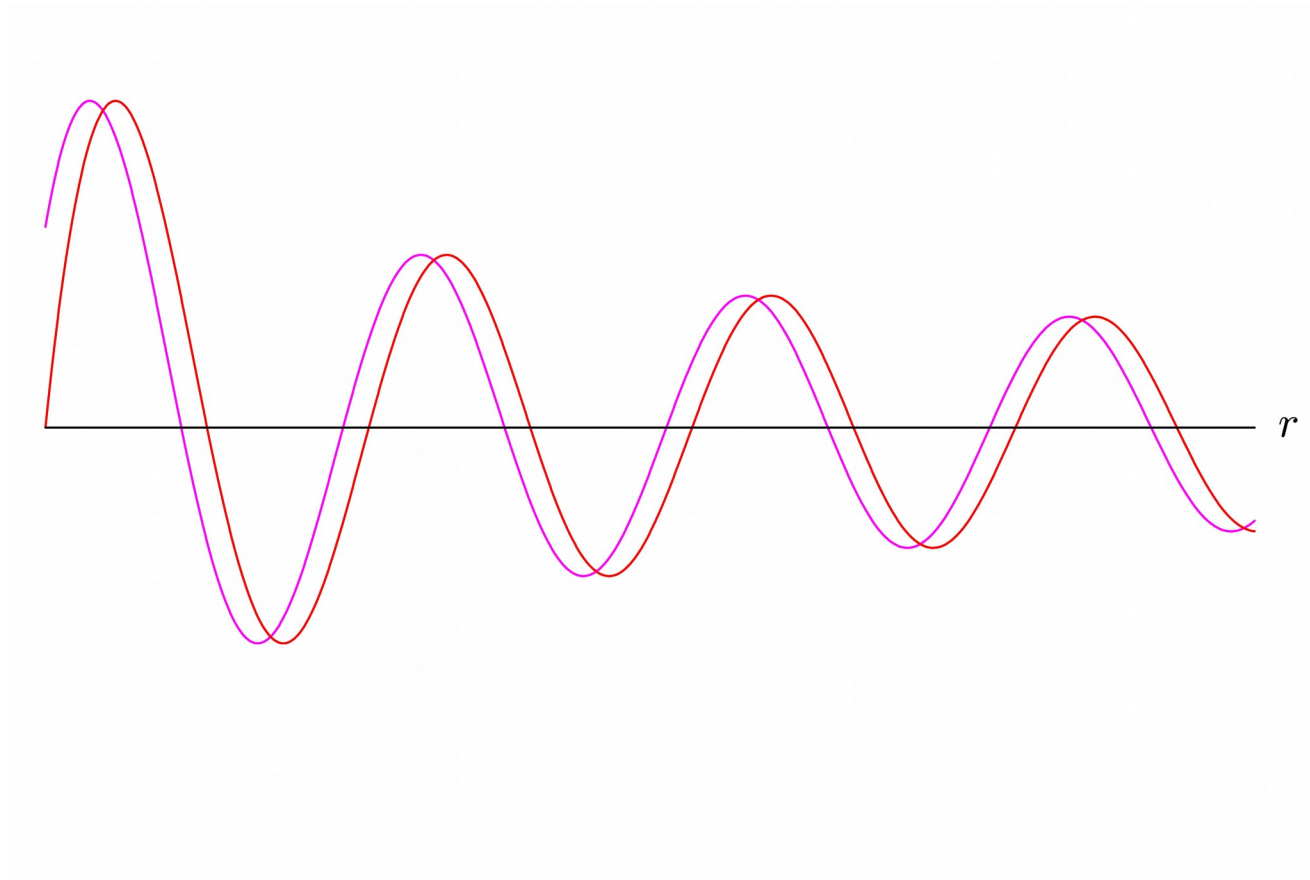




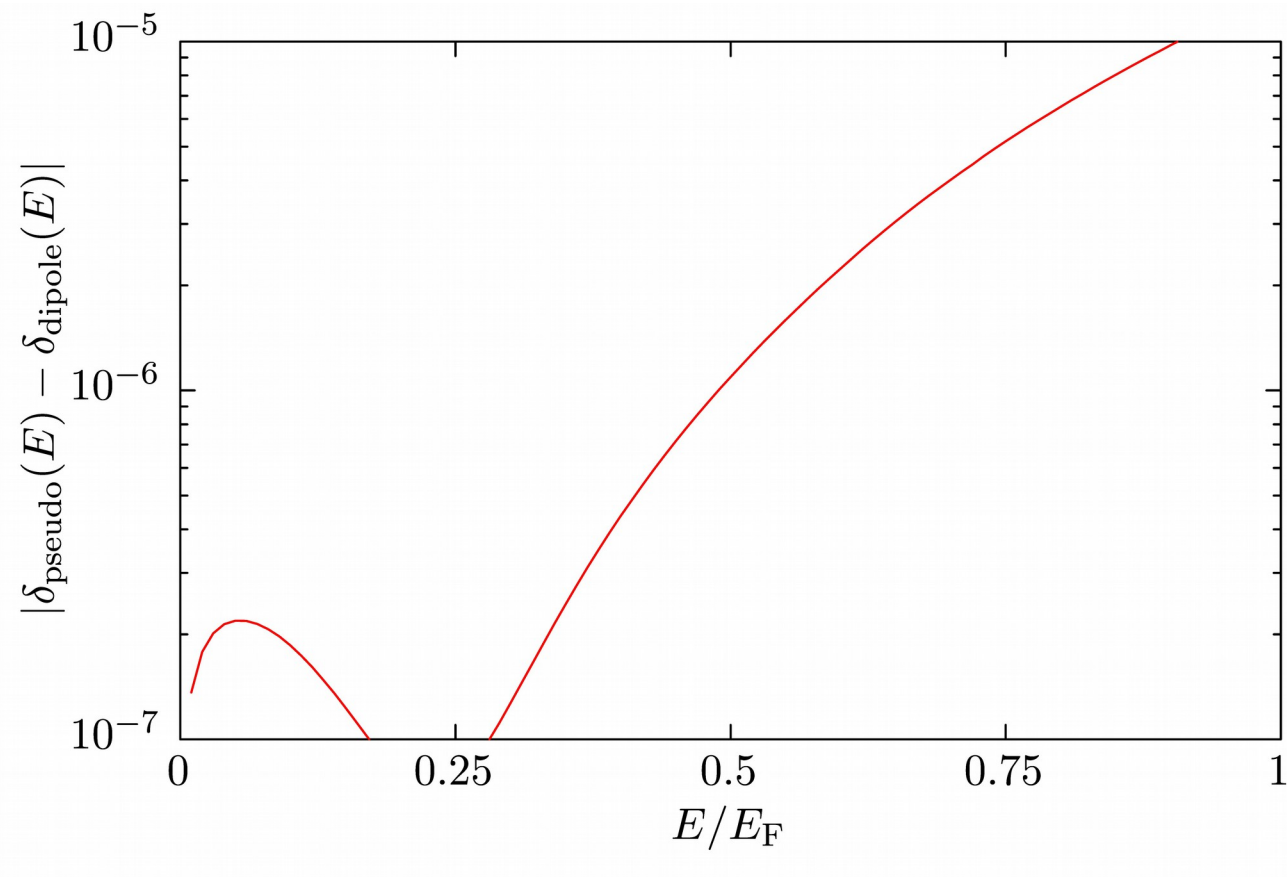
# Two interacting dipoles



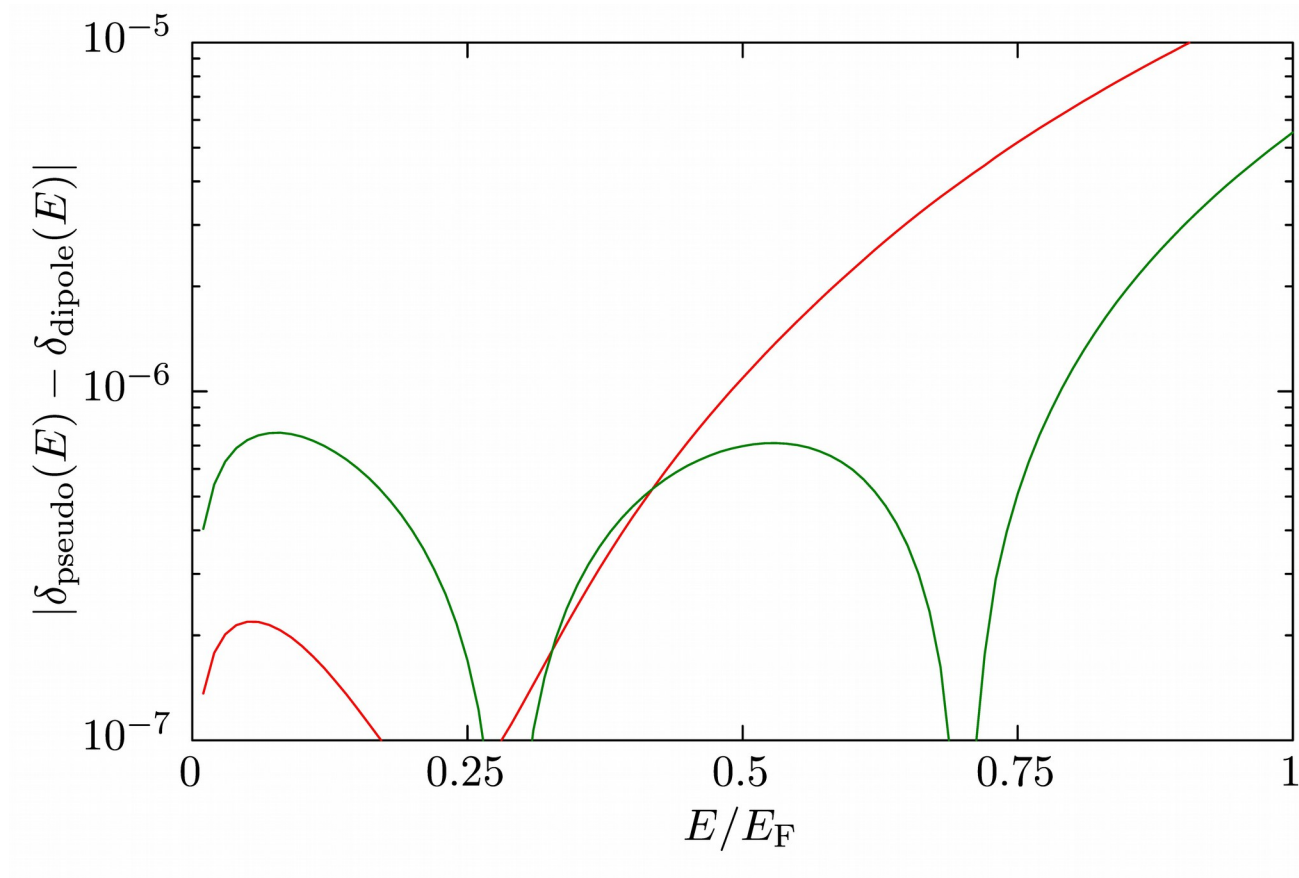
# Phase shift error



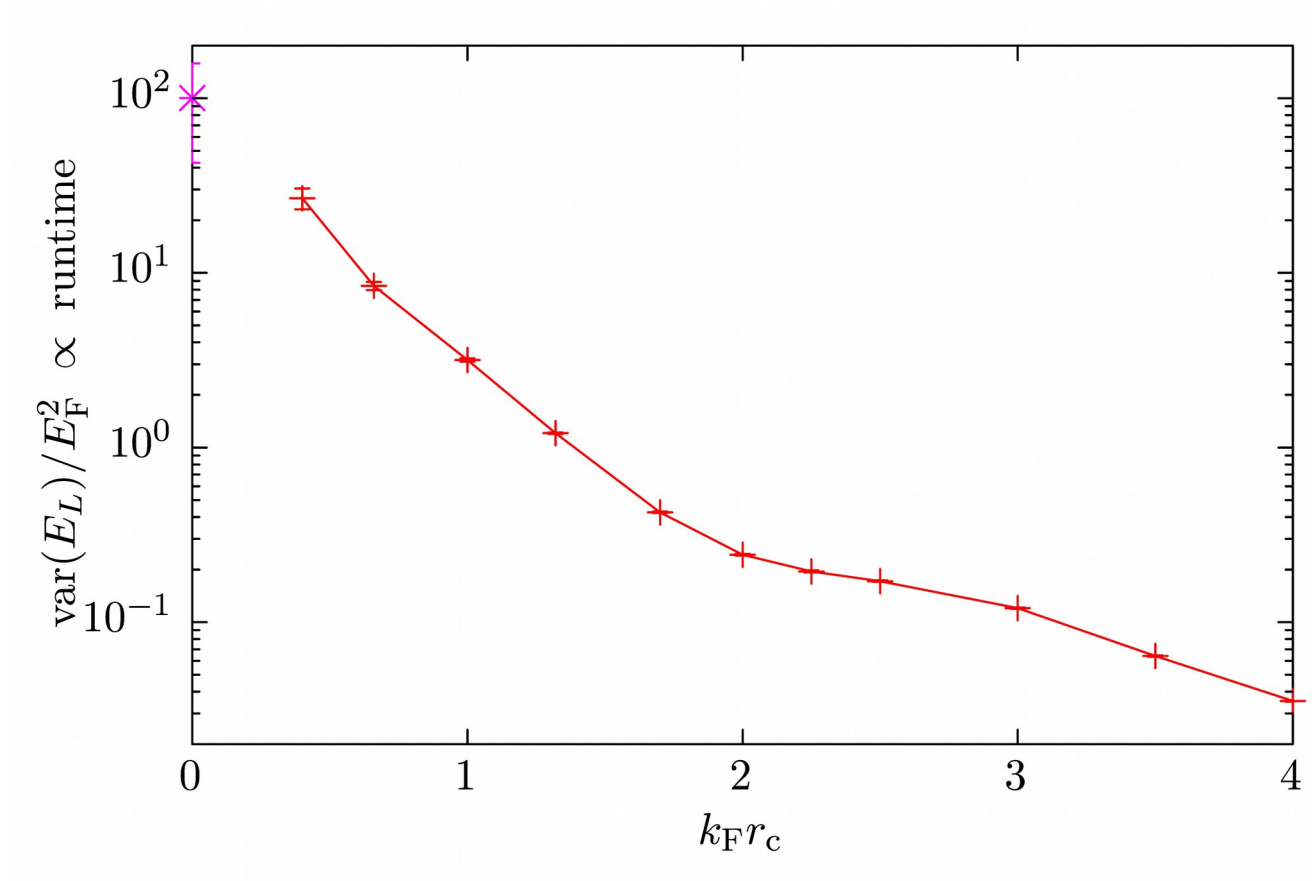
# Phase shift error



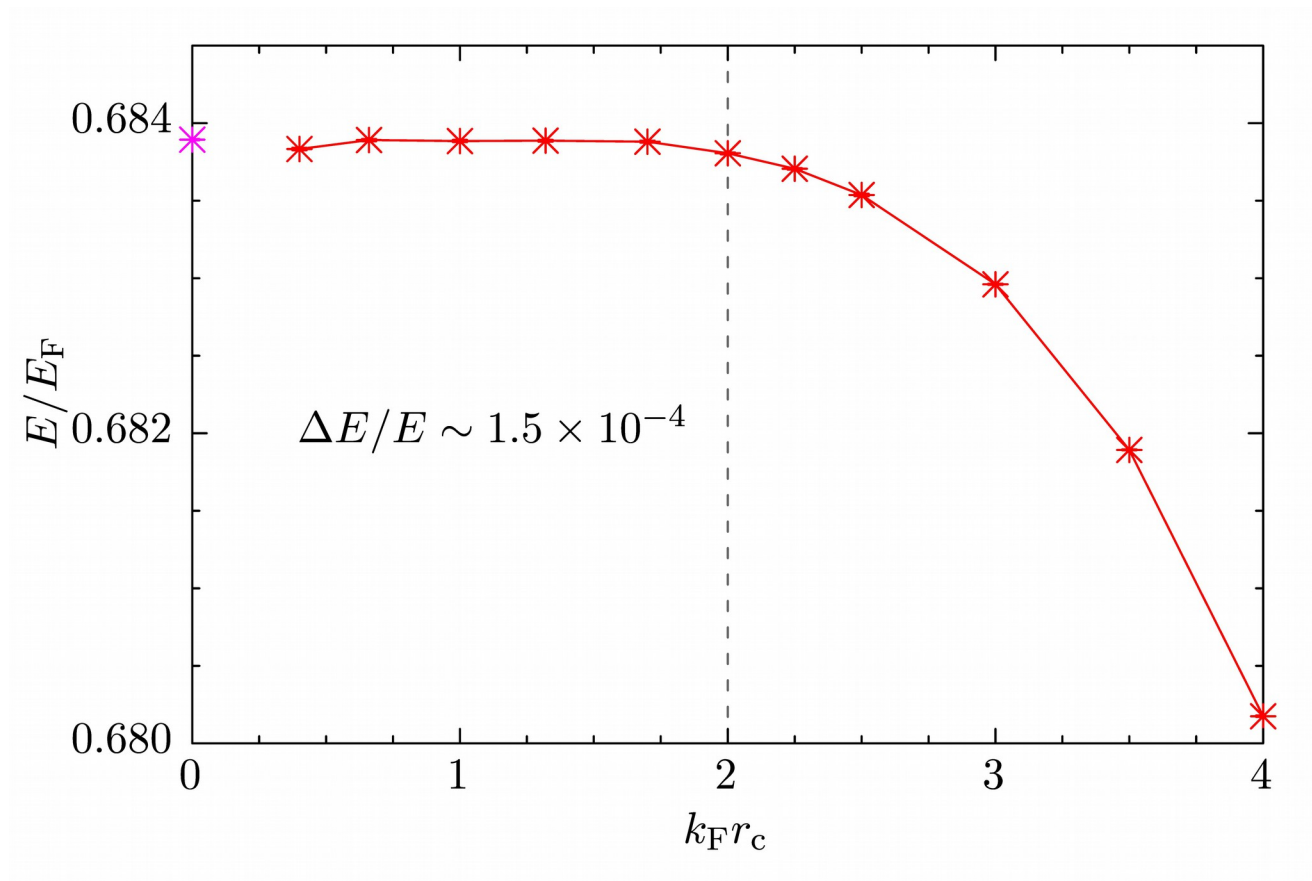
# The ultratransferable pseudopotential



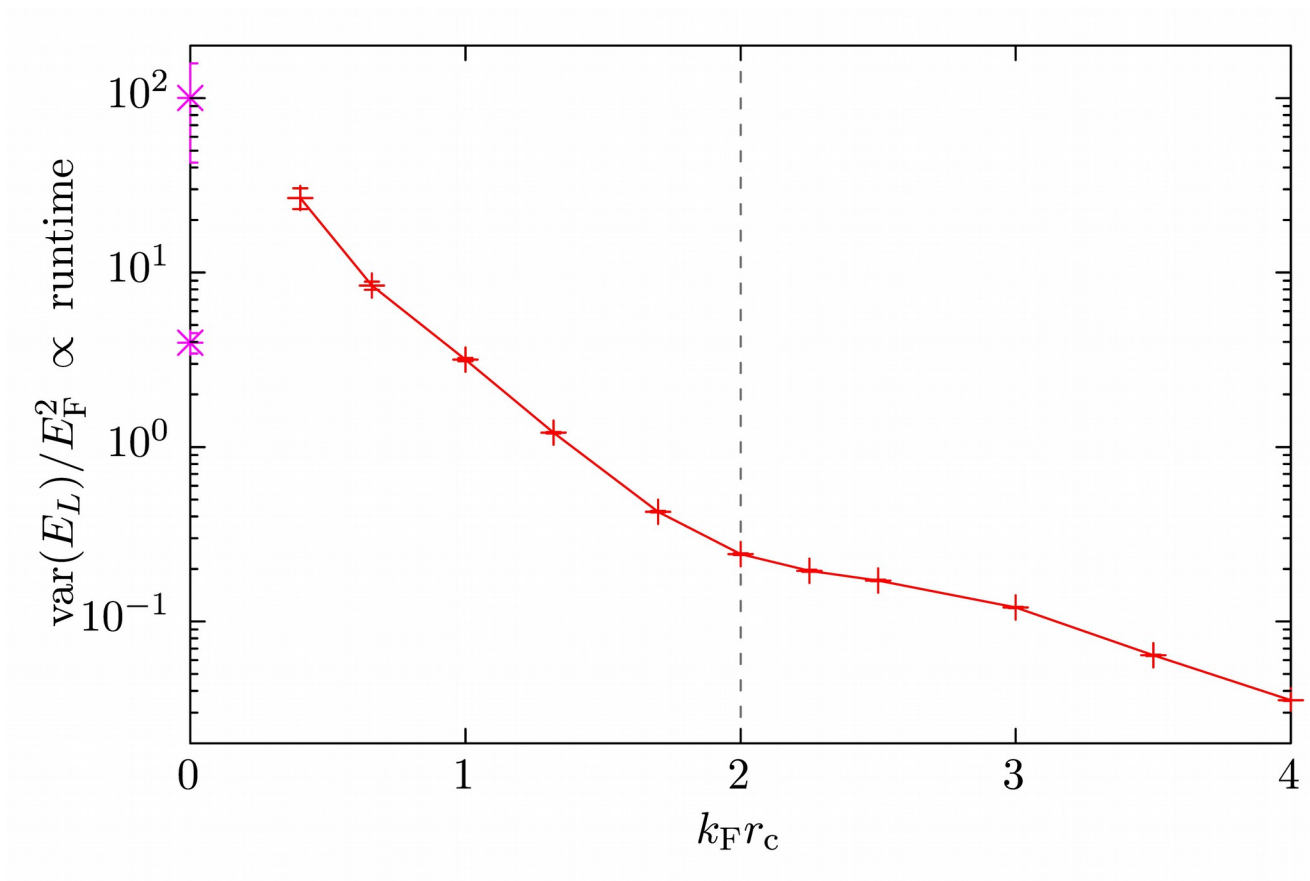
# Runtime speed-up



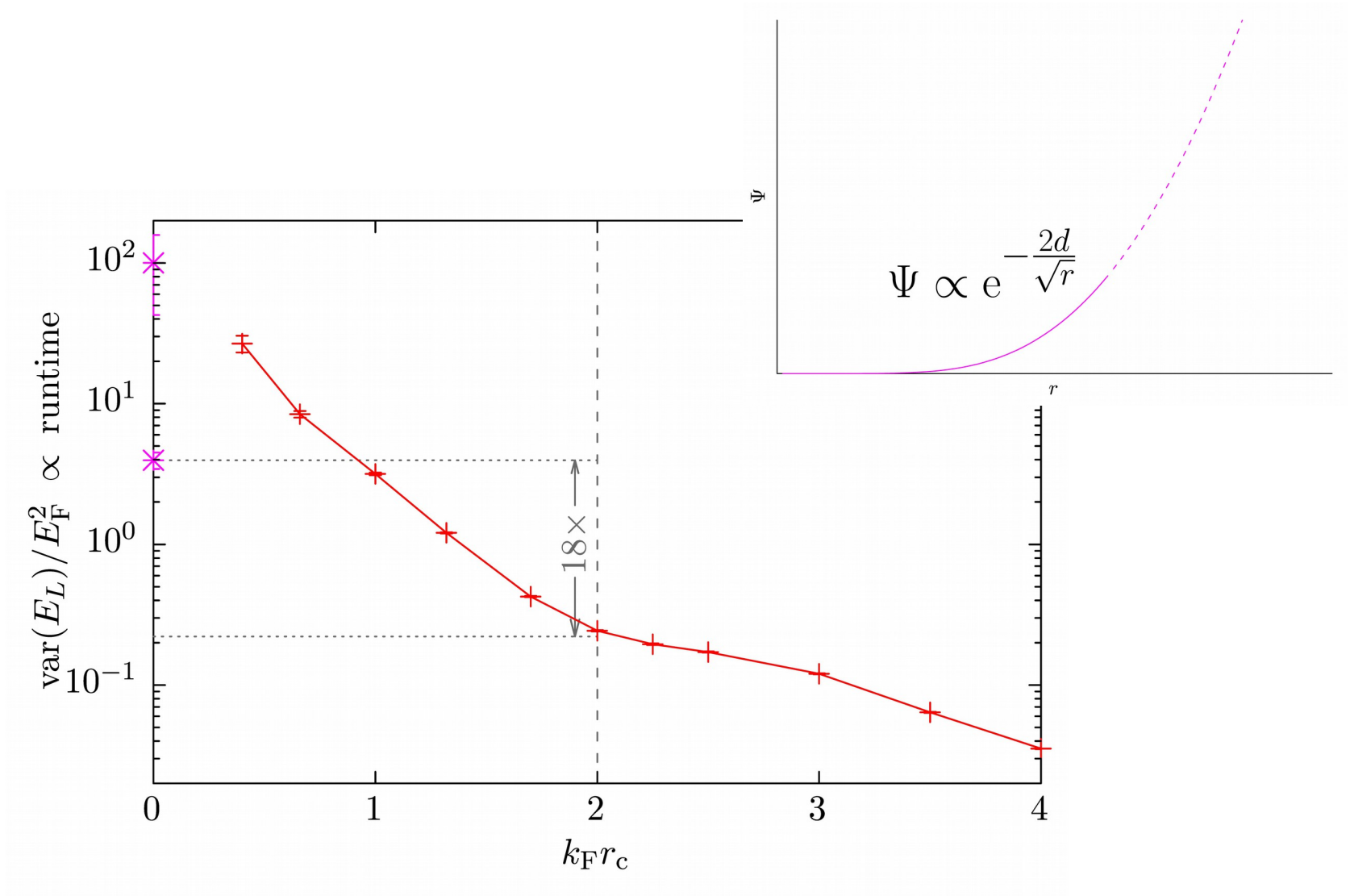
# Change in energy with cutoff radius



# Runtime speed-up

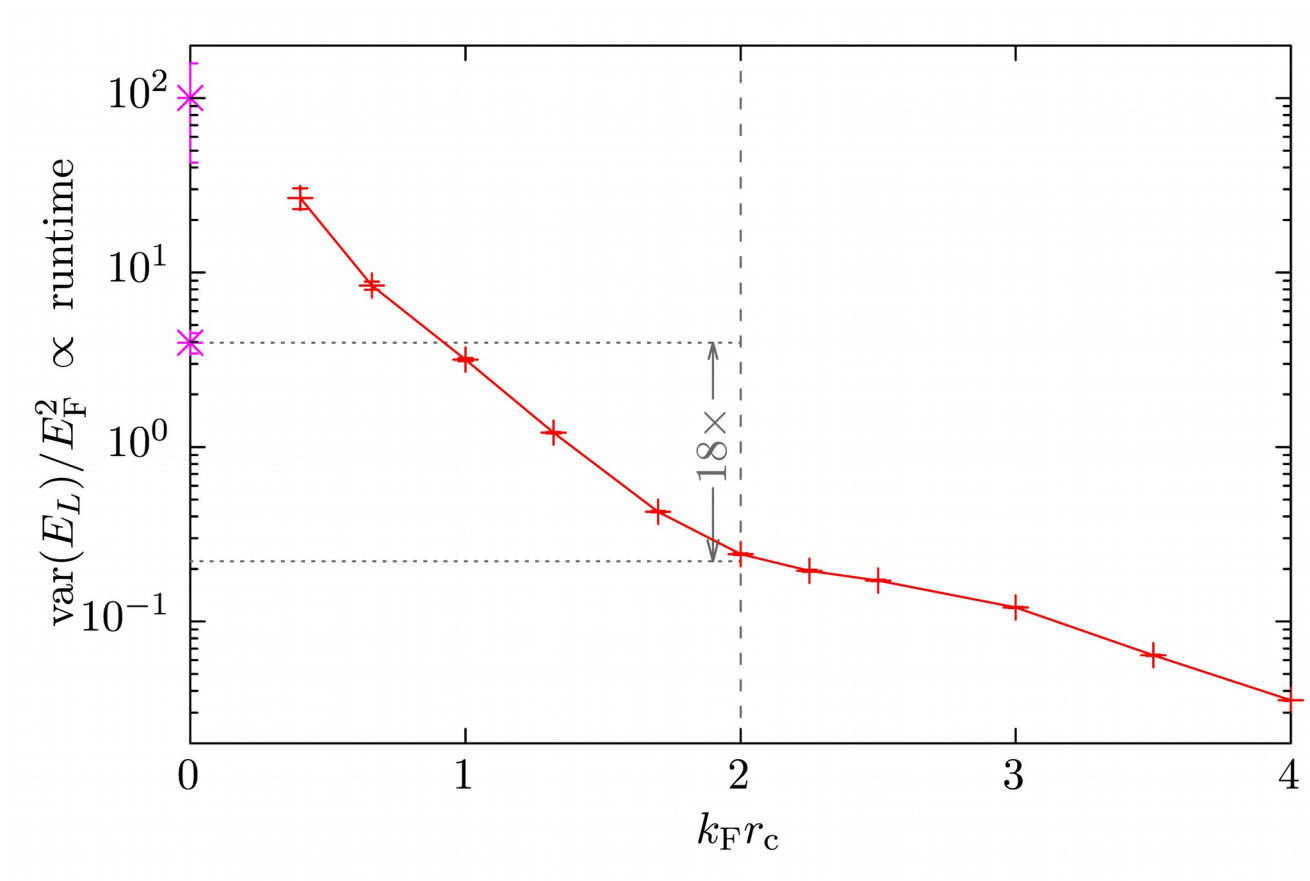


# Runtime speed-up

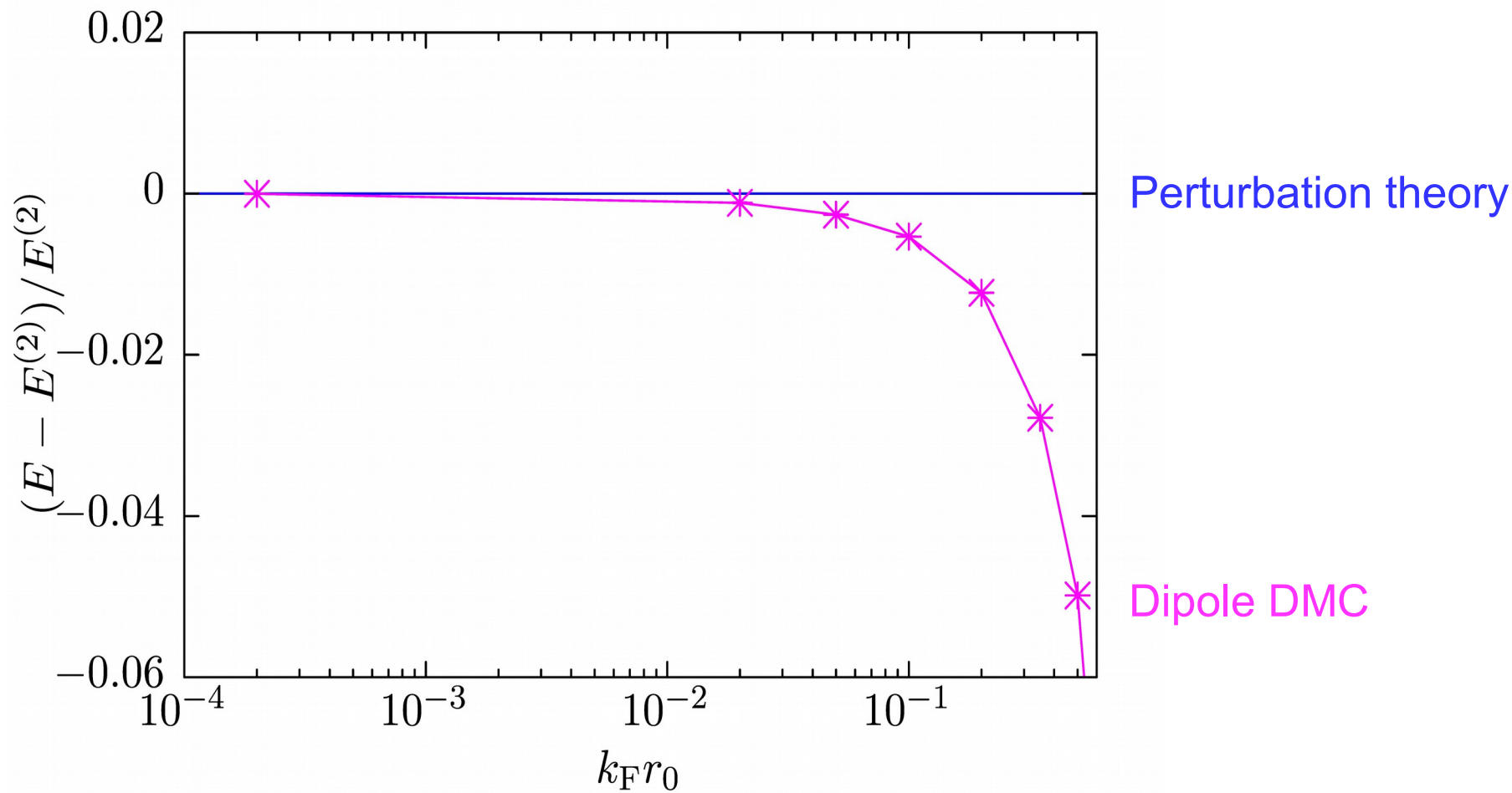




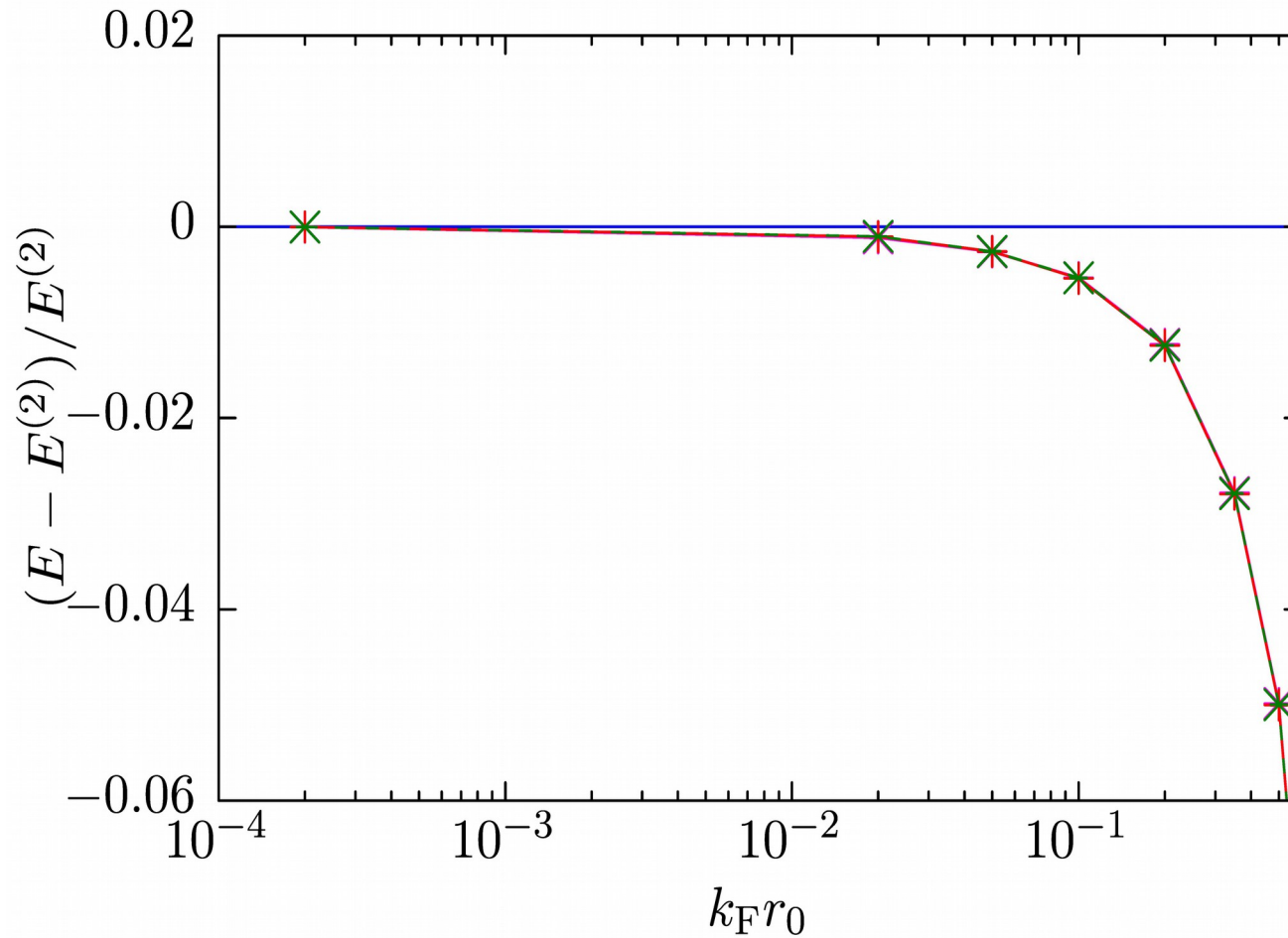
# Runtime speed-up



# Equation of State



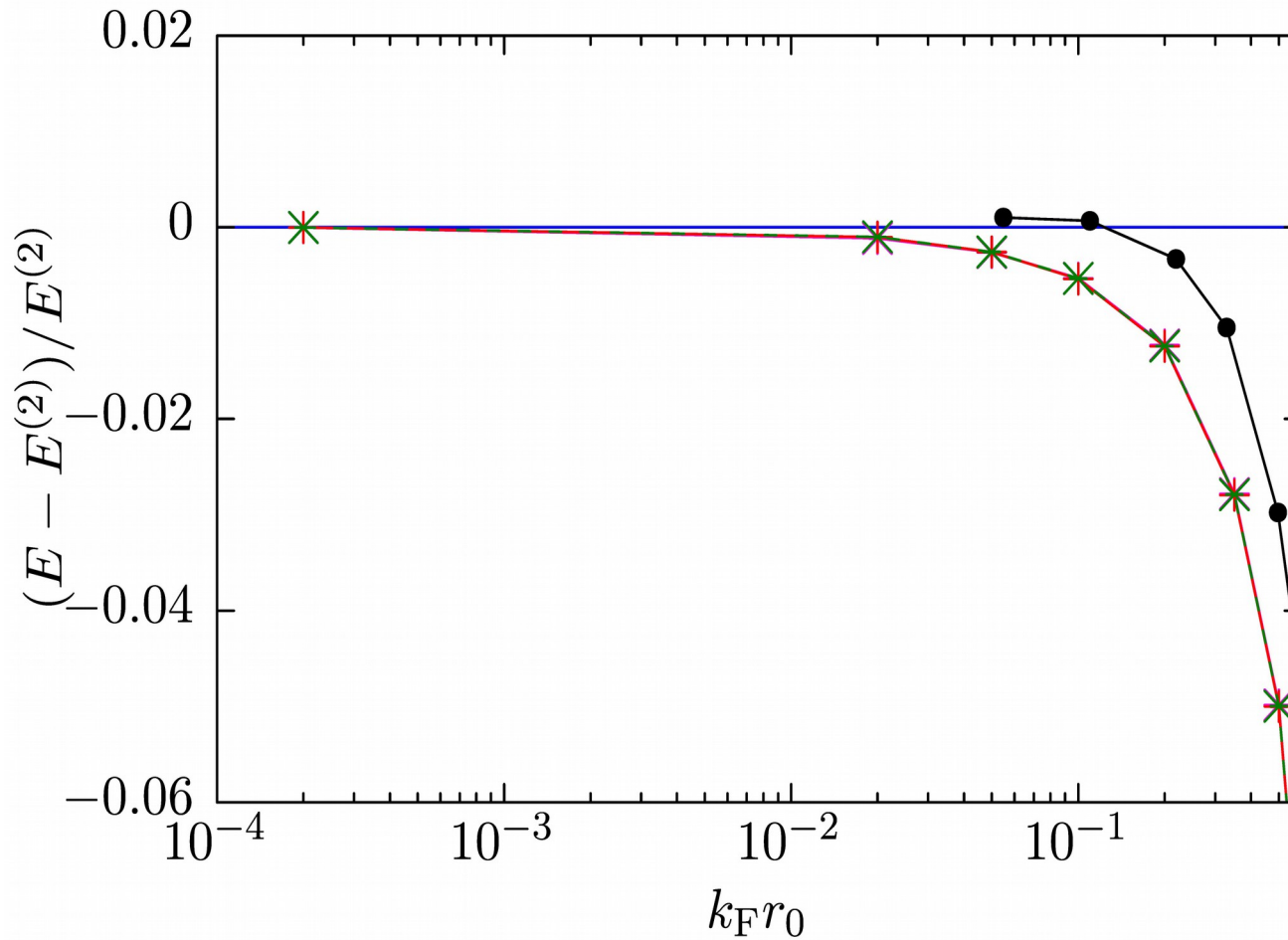
# Equation of State



Perturbation theory

Dipole DMC,  
Troullier-Martins and  
UTP pseudopotentials

# Equation of State



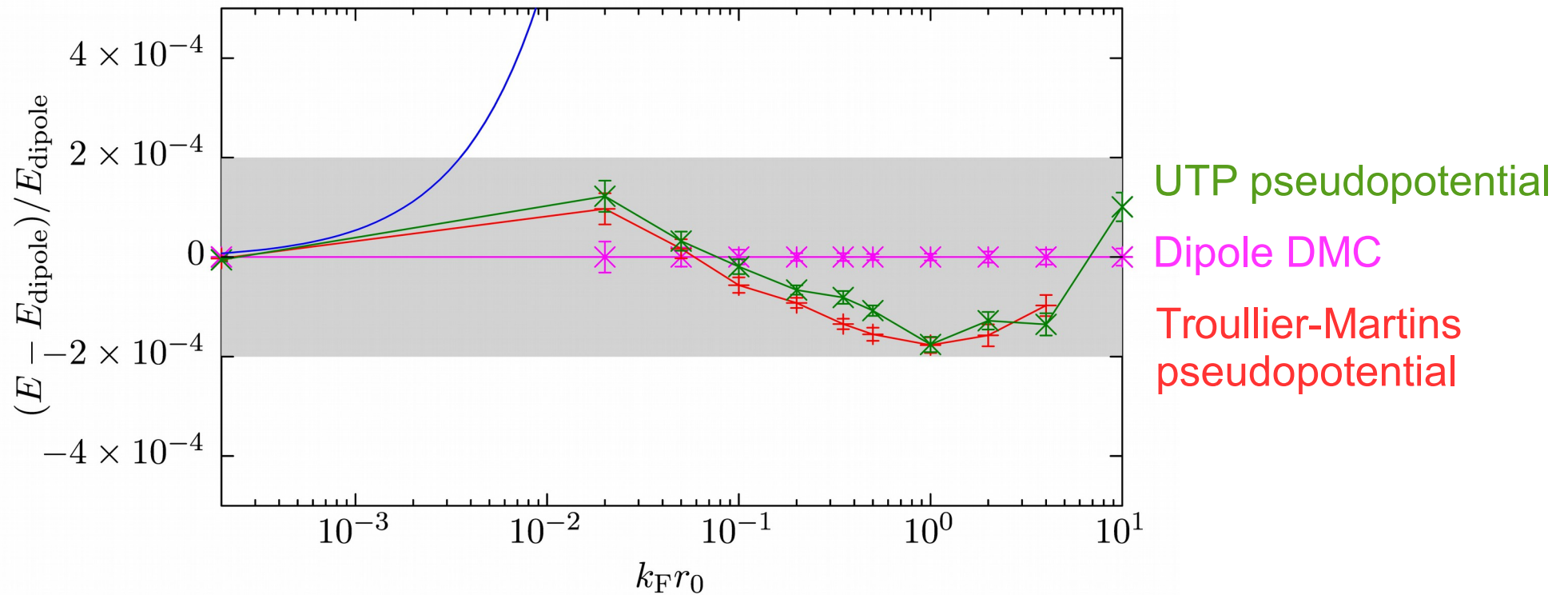
Perturbation theory

Matveeva and Giorgini  
PRL 109, 200401 (2012)

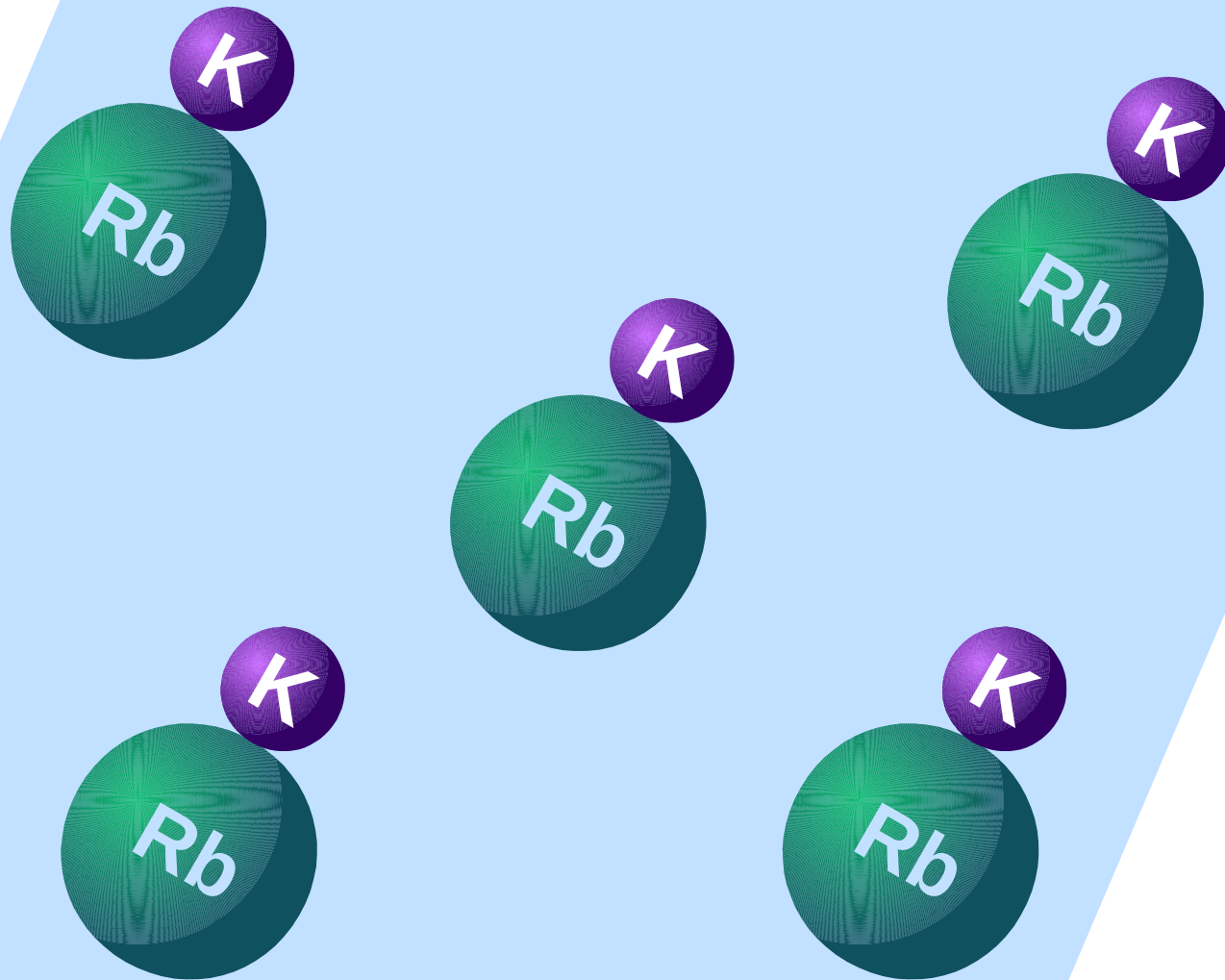
Dipole DMC,  
Troullier-Martins and  
UTP pseudopotentials

# Accuracy of the pseudopotentials

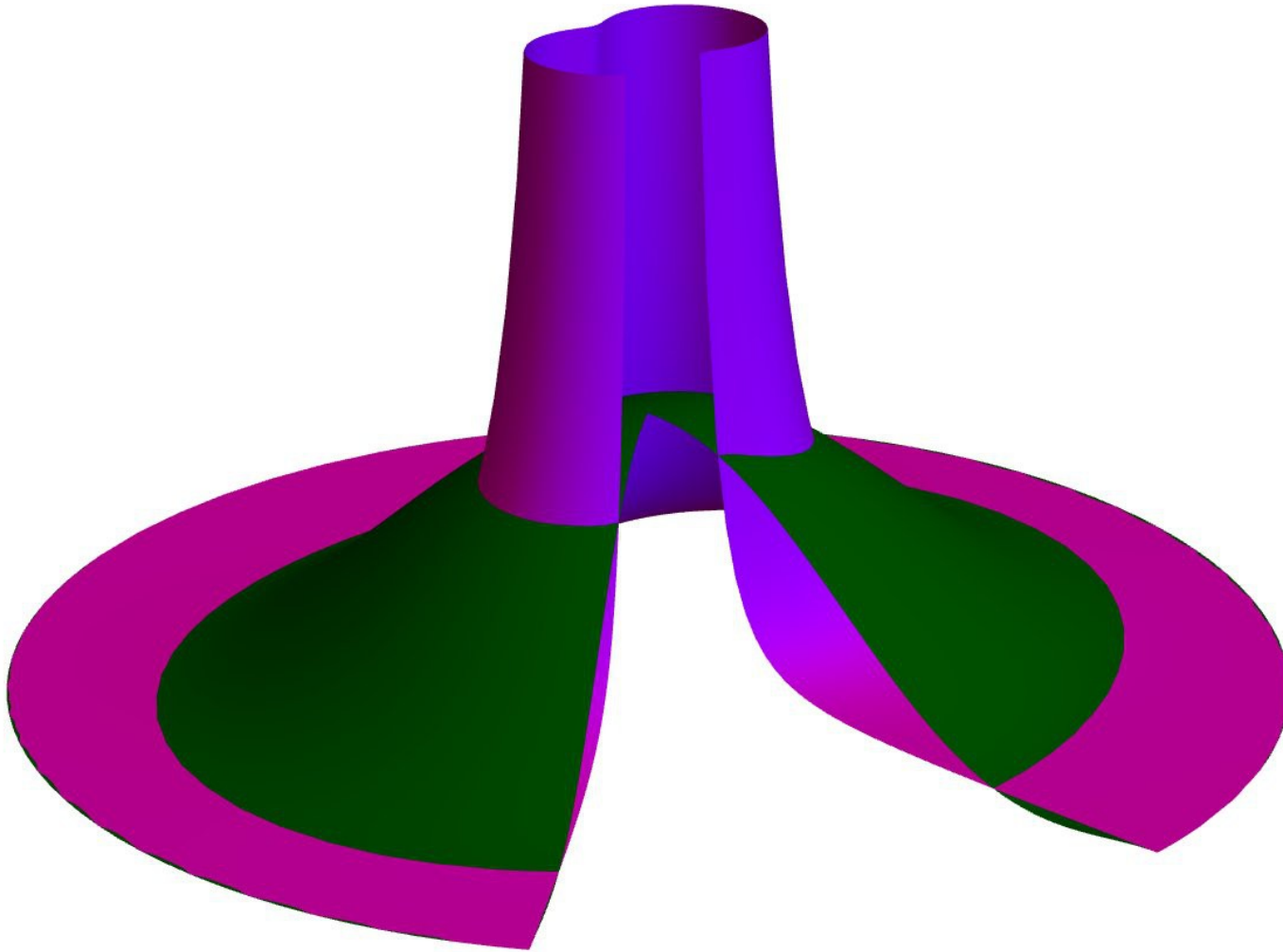
Perturbation theory



# Tilted dipoles



# Tilted pseudopotential



# Future possibilities

- ~ Complete analysis of tilted pseudopotentials
- ~ Investigate stripe phase, Wigner crystal
- ~ Superfluid phase, few particles



# Summary

- ~ Constructed a pseudopotential for the dipolar interaction
- ~  $10^{-4}$  accuracy
- ~ 18x speed-up

# “Kato” cusp conditions

$$E_L = -\frac{1}{r} \frac{\Psi'}{\Psi} - \frac{\Psi''}{\Psi} + \frac{l^2}{r^2} + \frac{d^2}{r^3}$$

$$\Psi \propto r^l e^{J(r)}$$

$$E_L = -\frac{2l+1}{r} J'(r) - J''(r) - (J'(r))^2 + \frac{d^2}{r^3}$$

# “Kato” cusp conditions

