Pseudopotentials for a dipolar ultracold atomic gas

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Dipolar molecule

Dipole moment

\[ d \sim 0.5 \text{ Debye} \]
A 2D dipolar gas
Reasons for interest

~ Control of ultracold chemical reactions
~ Quantum information processing
~ Novel strongly correlated phases
$\theta = 0$ case
Two interacting dipoles

\[ V \]

\[ r \]
Two interacting dipoles

Phase shift error
Phase shift error
The ultratransferable pseudopotential
Runtime speed-up
Change in energy with cutoff radius

\[ \Delta E/E \sim 1.5 \times 10^{-4} \]
Runtime speed-up

![Graph showing the relationship between \( \frac{\text{var}(E_L)}{E_F^2} \) and \( k_F r_c \). The graph indicates a decrease in the variance of \( E_L \) as \( k_F r_c \) increases.]
Runtime speed-up

\[ \Psi \propto e^{-\frac{2d}{\sqrt{r}}} \]
Runtime speed-up
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

$\frac{E - E_{\text{dipole}}}{E_{\text{dipole}}}$

$k_F r_0$

UTP pseudopotential
Dipole DMC
Troullier-Martins pseudopotential
Tilted dipoles
Tilted pseudopotential
Future possibilities

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

\[
\Psi \propto e^{-\frac{2d}{\sqrt{r}}}
\]