Pseudopotentials for an ultracold dipolar gas

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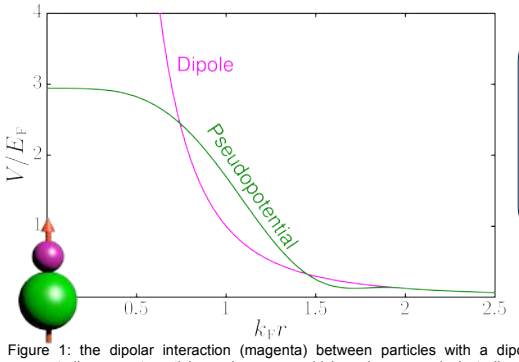


Figure 1: the dipolar interaction (magenta) between particles with a dipole moment diverges at particle coalescence, which makes numerical studies of particles interacting in this way inefficient. In order to remedy this we propose a smooth new pseudopotential (green).

Experimental background

Ultracold molecular gases combine many-body effects with fine control over interactions. They present a cleaner system than the solid state, allowing access to effects due to the combination of many-body interactions and quantum mechanics.

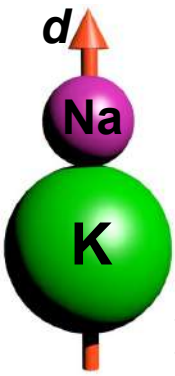
Experiments now allow the condensation of molecules that carry dipole moments, which interact via the long-range anisotropic dipolar interaction. For example, the Zwierlein group [2] uses fermionic $^{23}Na^{40}K$ molecules with a large tunable electric dipole moment ***d***.

A particularly appealing geometry is a single component quantum-degenerate gas in 2D, with all the dipole moments aligned normal to the 2D plane. This arrangement is now within experimental reach [2,3].

Theoretical problems

Analytical models of this isotropic 2D dipolar gas have predicted a rich phase diagram, including an inhomogeneous density wave phase [4]. However, numerical studies of the system do not observe such a stable stripe phase [5].

In order to resolve this disagreement we improve the modelling of the dipolar potential, to increase the accuracy of numerical simulations. We propose the pseudopotential [6] shown in Figure 1, which captures the essential physics of the real dipolar interaction, as well as being easier to work with numerically [1]. The smoother pseudopotential means we can run simulations of the dipolar gas >450 times quicker than using the real dipolar potential, as shown in Figure 2.



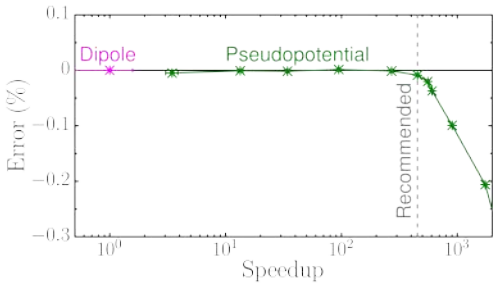
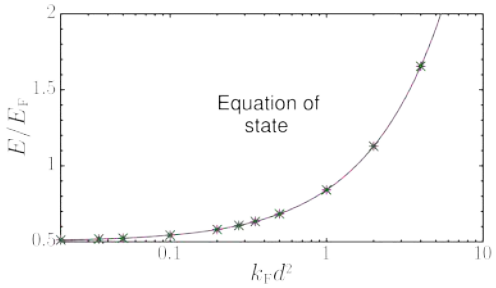


Figure 2: the accuracy of the pseudopotential against the speedup in simulations, as found by varying the cutoff radius at which the pseudopotential joins onto the real dipolar potential. The recommended cutoff gives accuracy of order 0.02% and a speedup of ~450 times when compared to a simple simulation using the dipolar interaction. This can be increased further by taking advantage of the improved scaling properties with diffusion Monte Carlo timestep.



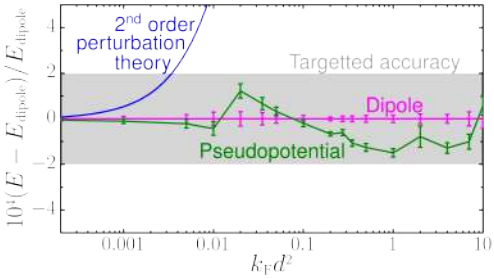


Figure 3: the equation of state of the Fermi liquid phase of the isotropic 2D dipolar gas, as calculated using diffusion Monte Carlo [7] using the dipolar interaction (magenta) and pseudopotential (green), and the accuracy of the pseudopotential at capturing the equation of state. The targetted 0.02% accuracy is that used in [4].

Conclusions

- Accurate pseudopotential for dipolar interaction
- >450 times speed up

Results

In Figure 3 we show the equation of state calculated using our pseudopotential and using the real dipolar potential, demonstrating high agreement between the simulations. The pseudopotential formalism developed here is now being used to investigate the stripe phase, and could be used for the rest of the dipolar gas phase diagram.

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Tilted dipoles

If the dipoles are tilted away from vertical the dipolar interaction becomes anisotropic. This means that angular momentum is no longer a good quantum number and the scattering problem is more difficult to solve, making the use of pseudopotentials to accelerate numerical calculations even more beneficial in the anisotropic part of the phase diagram.

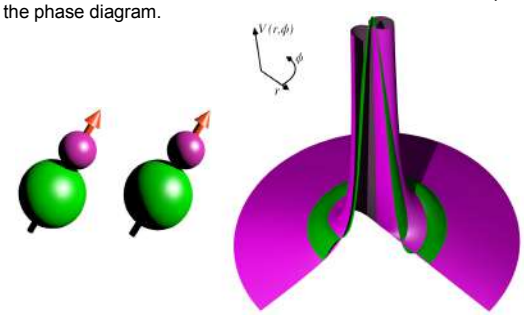

Figure 4: when the dipoles are tilted away from vertical the inter-particle potential is anisotropic. The pseudopotential formalism can be used to create pseudopotentials like that shown in green, which are smoother both radially and azimuthally than the dipolar interaction.