Final projects

1 Coulomb clusters in a trap

2 Lennard-Jones droplet

3 Two quantum particles in harmonic oscillator

4 Soliton

5 Wigner-crystal --- gas phase transition

6 He - Li clusters

7 Simulation of superfluid 4He

8 Wigner Crystal of N charges in a 2D Harmonic trap

9 N particles with short range interaction in a 1D Harmonic trap

10 Coulomb charges on a sphere

Presentation.

The presentation should contain:

1) Title
2) Introduction, why the present problem is interesting?
3) The problem under study, model, Hamiltonian, dimensionless units, etc
4) Methods (numerical algorithms used, convergence)
5) Results: figures and interpretation
6) Conclusions

-Introduction should contain the literature overview, in our case it might be omitted.
-The largest section is the Results part. All figures should have units (both axes).
- Conclusions (written in a scientific way, which relevant information/properties was obtained in the study)

1 Coulomb clusters in a trap

Consider N coulomb charges in a harmonic trap.

Using annealing procedure, find equilibrium positions for different number of particles, so that (1,2,3,4) shells are formed in equilibrium positio

Show the radial distribution function

Study how the shells are melted with temperature, show the radial distribution function for small and high temperatures

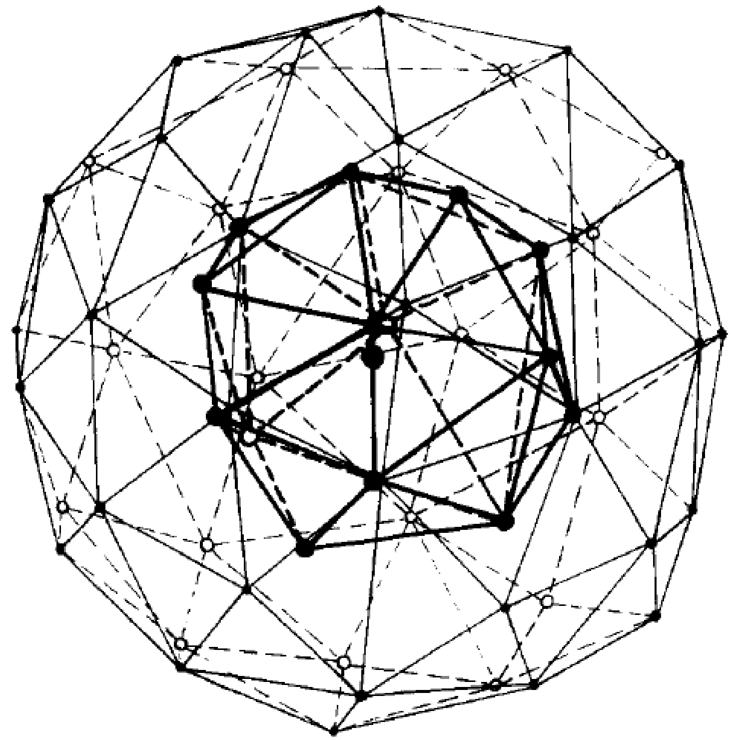


Fig. 1. The instant picture of a 3D cluster of 67 particles. The 1st, 2nd, 3rd shells consist of 1, 15, 21 particles respectively.

COULOMB CLUSTERS IN A TRAP
Yu.E. LOZOVIK and V.A. MANDELSHTAM

2 Lennard-Jones droplet

Consider N particles interacting via (6-12) Lennard-Jones potential which has repulsion at short distances and attraction at large distances. Equilibrium probability distribution at temperature T is given by the Boltzmann formula.

Average quantities can be conveniently calculated using Monte Carlo method. Calculate energy and radial distribution function.

For a given temperature calculate how the system energy depends on the number of particles. Extract the volume energy E_v (energy of bulk equilibrium liquid), surface and curvature energy

$$E/N = E_v + E_s N^{-1/3} + E_c N^{-2/3}$$

calculate the surface tension $t = E_t/(3\pi r_0^2)$ where the unit radius is such that $(4/3)\pi r_0^3 = 1$

3 Two quantum particles in harmonic oscillator

Consider a system composed of 2 particles interacting via with a repulsive delta-pseudopotential in 3D or 1D geometry. Delta-interaction potential results into a boundary condition on the two-body Jastrow term

$f_2(r_{ij}) = 1 - a_s / r_{ij}$ in 3D
$f_2(r_{ij}) = r_{ij} - a_s$ in 1D

The one-body term can be taken in the shape of a Gaussian
$f_1(r)=\exp(-\alpha r^2)$
Where α is a variational parameter.
Calculate energy and correlation functions (radial density profile and pair correlation function).
Compare the variational energy with the exact analytical solution

T. Busch, B.-G. Englert, K. Rzążewski, and M. Wilkens, Two Cold Atoms in a Harmonic Trap, Found. Phys. 28, 549 (1998)

4 Soliton

Consider a system composed of N particles interacting via with a delta-pseudopotential in 1D geometry. Delta-interaction potential results into a boundary condition on the derivatives with respect to pair distances in the wave function.

$$f_2(x_{ij}) = \exp(- |x_{ij}| / a_s)$$

Calculate energy and correlation functions (radial density profile and pair correlation function).

In one-dimensional system compare the energy with McGuire solution.

J. B. McGuire Study of Exactly Soluble One-Dimensional N-Body Problems J. Math. Phys. 5, 622 (1964)

Compare the density profile with the (approximate) solution for a soliton $n(x) = \text{const} / \cosh(c2\, x)^2$

5 Lennard-Jones, solid --- gas phase transition in 3D

Consider N particles of mass m and charge Q interacting via Lennard-Jones potential in a L^3 box with periodic boundary conditions. Equilibrium probability distribution at temperature T is given by the Boltzmann formula. For a fixed density, $n=N/L^3$, a Wigner crystal is formed at small temperature while the gas state is realized at high temperature.

Average quantities can be conveniently calculated using Monte Carlo method. Calculate energy and pair-distribution distribution function.

Show how the structural properties strongly differ in gas and crystal state (high peaks in the pair-distribution function in a crystal)

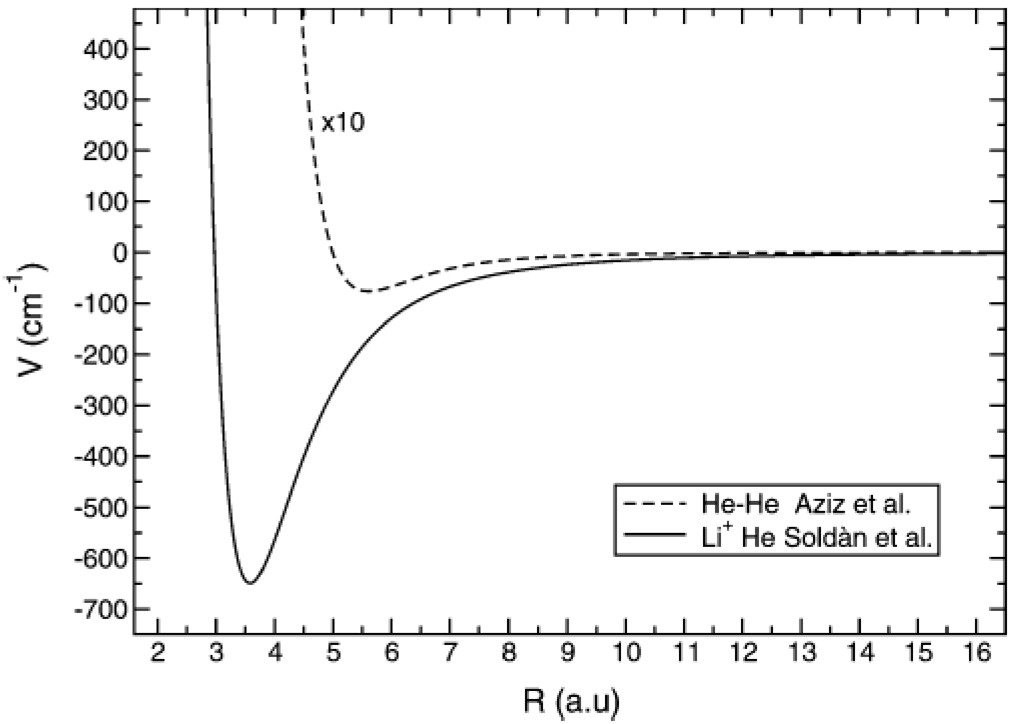
Study how the phase transition depends on the density. Draw (qualitatively) the phase diagram.

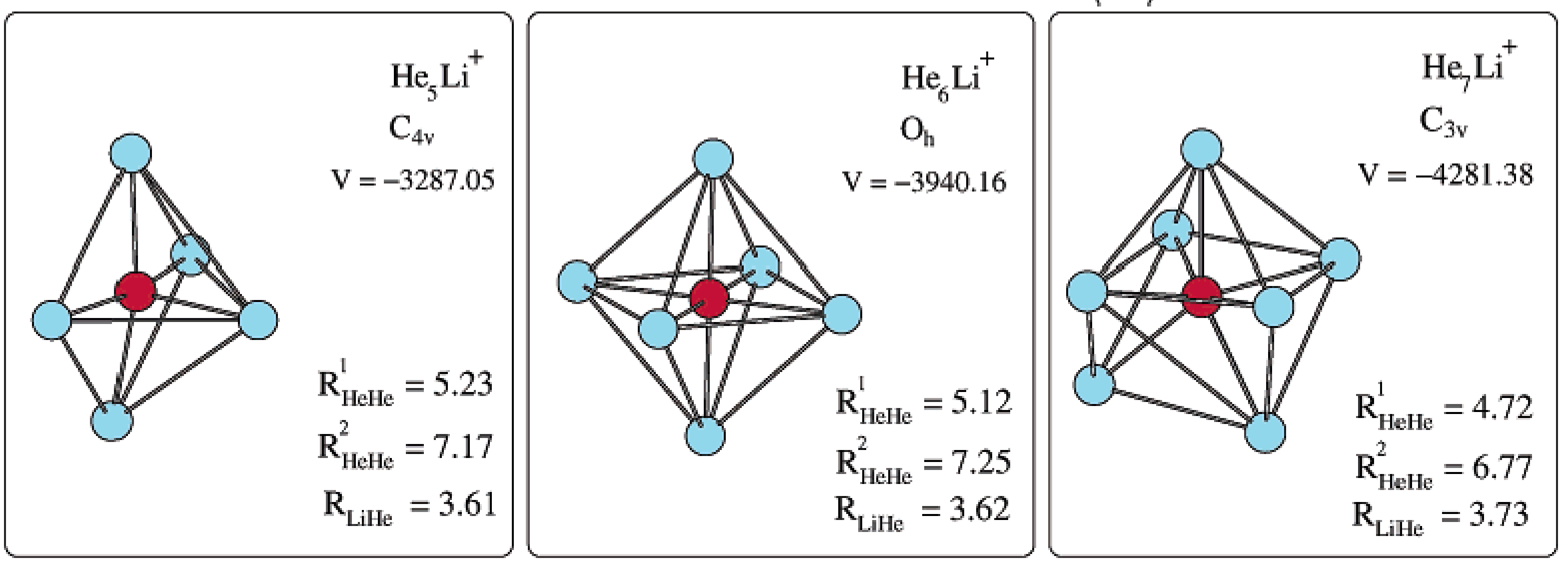
6 He - Li clusters

1046 *J. Chem. Theory Comput.*, Vol. 1, No. 5, 2005

Consider a cluster consisting of N helium atoms and a single lithium atom. Interaction potential has a Lennard-Jones form (see Fig).

Calculate the energy and structure of small clusters (with $N < 10$ helium atoms) at small temperature.





7 Simulation of superfluid 4He

Use Aziz II potential for describing interactions between helium atoms. The homogeneous system is modelled in a box with periodic boundary conditions.

Use the following ansatz for the Jastrow terms

$$f_2(r_{ij}) = \exp(- \alpha / |r_{ij}|^{\beta})$$

wher α and β are variational parameter.

Calculate the ground-state energy and pair distribution functions for the superfluid helium at equilibrium.

8 Wigner Crystal of N charges in a 2D Harmonic trap

Diffusion Monte Carlo method has to be implemented in order to find the ground-state energy exactly.

The system is composed of N charges interacting via Coulomb charges which are confined by a harmonic trap.

https://en.wikipedia.org/wiki/Diffusion_Monte_Carlo

9 N particles with short range interaction in a 1D Harmonic trap

Diffusion Monte Carlo method has to be implemented in order to find the ground-state energy exactly.

The system is composed of N particles interacting with zero-range pseudopotential. The particles are confined by a harmonic trap. The interaction potential imposes a certain boundary condition on the two-body Jastrow terms.

https://en.wikipedia.org/wiki/Diffusion_Monte_Carlo

10 Coulomb charges on a sphere

Consider N coulomb charges with their movement restricted to a unit sphere.

Using annealing procedure, find optimal positions for different number of particles.

Spherical coordinates can be used in order to generate valid displacements
$r=(x,y,z)=(\rho, \theta, \varphi) \to r'=(\rho, \theta', \varphi')=(x',y',z')$
so that angles θ and φ are changed while ρ is kept fixed.

Report:
- optimal configuration
- optimal energy
- the radial distribution function

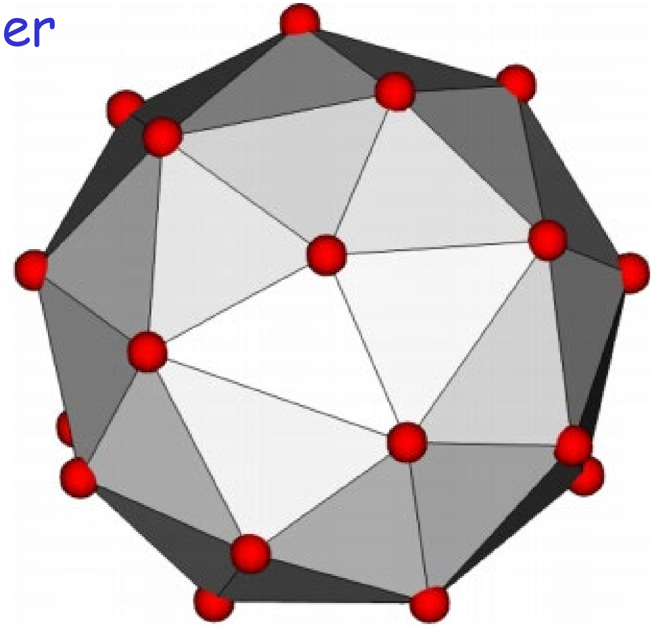


FIG. 1. Solution to the Thomson Problem for $N = 25$ in which point charges (shown in red) are uniformly distributed on the unit sphere.