Monte-Carlo project: Computational physics

Recently, there has been considerable theoretical and experimental progress in the study of mesoscopic systems consisting of a finite number of charged particles which are confined into an artificial circular symmetric potential. In 1934, Wigner suggested that a liquid to solid phase transition should occur in a three-dimensional (3D) Fermi system at low densities[1]. Typical experimental model systems for the study of this system are electrons on the surface of liquid helium[2], electrons in quantum dots[3], colloidal suspensions[4] and in confined plasma crystals[5]. On the other hand, various similar systems, like the vortex clusters in an isotropic superfluid[6], vortices in superfluid He^4[7], vortices in a Bose-Einstein condensate stirred with a laser beam[8] and in mesoscopic superconducting disks[9] have many common features with those of 2D charged particles. Colloidal particles dissolved in water[10] are another example of an experimental system where classical particles exhibit Wigner crystallization. Recently, macroscopic 2D Wigner islands, consisting of charged metallic balls above a plane conductor were studied and ground state, metastable states and saddle point configurations were found experimentally[11]. You will study such a system with a finite number of particles, and construct a Mendeleev-type of table which gives the distribution of those particles. You will observe and discuss the configurations of the ground state (lowest energy) and the metastable states (higher energy), and that for a Coulomb, Yukawa, and dipolar interparticle interactions between particles in a parabolic confinement. The defect structure in crystals is of paramount importance for the stability and the strength of materials. Therefore, you will investigate the topological defects in Wigner clusters and their effect on melting. As a hint - it is well known that the Kosterlitz-Thouless-Halperin-Nelson-Young scenario describes 2D melting as a defect-mediated phenomenon. The melting properties of the present system have been also studied experimentally[10,12].

The Monte-Carlo (MC) simulation technique is relatively simple and rapidly convergent and it provides a reliable estimation of the total energy of the system in cases when relatively small number of Metropolis steps is sufficient. Note however that the accuracy of this method in calculating the explicit states is poor for systems with a large number of particles, which have significantly more metastable states, and you will have to manage your way numerically through the energy landscape (as shown in the course). The structure and potential energy of the system at $T \neq 0$ can be found by the standard Metropolis algorithm[13] in which at some temperature the next simulation state of the system is obtained by a random displacement of one of the particles. We allow the system to approach its equilibrium state at some temperature T, after executing enough MC steps. Each MC step is formed by a random displacement of all particles. If the new configuration has a smaller energy it is accepted, but if the new energy is larger the configuration is accepted with a temperature dependent probability.

The tasks

The final report should be organized around following tasks:

1) Testing and comments on the behavior of the given random number generator.
2) Implementing correctly (the temperature in) the Metropolis algorithm.
3) Analyze the cluster formation and the ground and metastable states of the Coulomb clusters in parabolic confinement (for number of particles $N < 200$, in comparison with Ref.[14]).
4) Briefly discuss the influence of the strength of the confinement and the choice of the inter-particle interaction on the cluster configurations.
5) Discuss the influence of the initial conditions, the number of MC steps, and the chosen maximal displacement in each MC step on the final results.
6) Identify the structural defects in the clusters.
7) Increase the temperature and describe the melting, where it starts and why. Plot the particle trajectories during melting. Adopt the criterion for melting of the cluster in accordance with Ref.[14].

For a publishable bonus, choose one topic from below:

*) Implement Lennard-Jones inter-particle potential instead of the Coulomb one. Study configurations and melting with and without confinement in 2D or 3D.

*) Consider magnetic particles - dipole-dipole inter-particle potential instead of the Coulomb one. Study configurations and melting with and without confinement in 2D or 3D.

---

* Electronic address: milorad.milosevic@uantwerpen.be

[1] E. Wigner, Phys. Rev. **46**, 1002 (1934).
[2] C. C. Grimes and G. Adams, Phys. Rev. Lett. **42**, 795 (1979).
[3] R. C. Ashoori, Nature (London) **379**, 413 (1996).
[4] S. Neser, C. Bechinger, P. Leiderer, and T. Palberg, Phys. Rev. Lett. **79**, 2931 (1997).
[5] J. H. Chu and L. I, Phys. Rev. Lett. **72**, 4009 (1994).
[6] Y. Kondo, J.S. Korhonen, M. Krusius, V. V. Dmitriev, E. V. Thuneberg, and G. E. Volovik, Phys. Rev. Lett. **68**, 3331 (1992).
[7] W. I. Galberson and K. W. Schwarz, Physics Today **40** (2), 54 (1987).
[8] F. Chevy, K. W. Madison, and J. Dalibard, Phys. Rev. Lett. **85**, 2223 (2000).
[9] V. A. Schweigert, F. M. Peeters, and P. S. Deo, Phys. Rev. Lett. **81**, 2783 (1998).
[10] R. Bubeck, C. Bechinger, S. Neser, and P. Leiderer, Phys. Rev. Lett. **82**, 3364 (1999).
[11] M. Saint Jean, C. Even, and C. Guthmann, Europhys. Lett. **55**, 45 (2001).
[12] K. Zahn, R. Lenke, and G. Maret, Phys. Rev. Lett. **82**, 2721 (1999).
[13] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. M. Teller, and E. Teller, J. Chem. Phys. **21**, 1087 (1953).
[14] V. M. Bedanov and F. M. Peeters, Phys. Rev. B **49**, 2667 (1994).