First Order Phase Transition in a Classical 2d Wigner Crystal on a Helium Film

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Using molecular dynamics simulation, we have investigated the melting and freezing transitions in a 2d system consisting of classical electrons over a liquid helium film adsorbed on a substrate. Surface electrons on a thin liquid helium film is an interesting low-dimensional system because one can change the form of the pair interaction from $1/r$ to $1/r^2$ by varying the film thickness and dielectric constant of the substrate. The surface electrons interacte through a screened coulomb potential, the screening being described by the interaction between surface electrons and between surface electrons and it images in a helium film coating a solid substrate. In this simulation, we first investigate the influence of the film thickness on the melting transition, comparing it with available experimetal values through the internal energy calculation as a function of the temperature. Next, we compare the melting points for the bulk case with those obtained using aproximative methods [1].

Keywords: Wigner Cristal; Molecular Dynamics Simulation

I. INTRODUCTION

A two-dimensional (2D) sheet of electrons on thin-helium films forms an interesting system for studying the physics of low-dimensional system and has attracted considerable interest in the last years. Such systems can be used for testing several theoretical phase transitions and also most of them can be realized experimentally. Electrons supported by a bulk surface form a crystal at a temperature [3] $T_m = e^2(\pi n)^{1/2}/\bar{\epsilon}\Gamma_m$, which is much higher than the Fermi temperature, $T_F = \hbar^2\pi n/m$. Therefore, such electrons obey the Classical Boltzmann statistics. Here n is the electron areal densities, $\bar{\epsilon} = (\epsilon+1)^{1/2}$ where ϵ is the dieletric constant of helium. $\Gamma_m = \langle U\rangle/\langle K\rangle$ is the plasma parameter in a melting temperature. The thermodynamic state of a classical coulomb system is determined by the quantity Γ which is a measure of the ratio of mean coulomb potential energy to mean kinetic energy per electrons. From theoretical point of view, for $\Gamma \lesssim 1$ the kinetic energy predominates and the system behaves like an electron gas. At intermediate densities $1 \lesssim \Gamma \lesssim 100$, the electron motion becomes highly correlated or liquidlike. At a high densities $\Gamma \gtrsim 100$ the coulomb potential energy predominates and the electrons are expected to undergo a phase-transition to form a periodic crystalline array. Experimentally the liquid-to-solid transition in the bulk takes place for a value of the coupling constant $\Gamma_m = 137 \pm 15$. Computer simulations indicate a firt-order melting in $\Gamma_m = 118$. In this work, we present a partial study of the melting transition of electrons on a bulk, and a helium film using molecular dynamics.

II. THE SYSTEM AND NUMERICAL APPROACH

The molecular dynamics calculations were performed on a system of 100 electrons immersed on a rigid, uniform, positive charge background. The electrons are distributed in a rectangular box, and arranged in a triangular lattice with periodic boundary condictions. The geometric arrangement of the system is showed in figure 1. The electron-electron interaction potential on a helium film of thicness d is given by [2]

$$\mathbf{V}(r) = e^{*\mathbf{2}}\left[\frac{\mathbf{1}}{r} - \frac{\delta}{\sqrt{r^{\mathbf{2}} + (\mathbf{2}d)^{\mathbf{1/2}}}}\right] \qquad (1)$$

Where $e^* = e/(1+\epsilon)^{1/2}$ is the renormalized electron charge and $\delta = (\epsilon_s - \epsilon)/(\epsilon_s + \epsilon)$, with ϵ and ϵ_s being the dielectric constants of helium and substrate, respectvely. In equation (1), the electron-electron interaction is screened by the presence of the substrate and the heliun film in the second term of this equation. For small interparticle distances ($r \ll d$), the screening is negligible and we obtain the bare potential $\mathbf{V}(r) = e^{*\mathbf{2}}/r$. If, on the other hand, the electrons are far apart ($r \gg d$) we have

$$\mathbf{V}(r) = \frac{(\mathbf{1}-\delta)}{r}e^{*\mathbf{2}} + \frac{\mathbf{2}\delta e^{*\mathbf{2}}d^{\mathbf{2}}}{r^{\mathbf{2}}}. \qquad (2)$$

For the equation (2), the plasma parameter ($\Gamma = \langle U\rangle/\langle K\rangle$) is given by

$$\Gamma = \Gamma c\left[1 - \delta\left(1 + \frac{4d^2}{a^2}\right)\right] \qquad (3)$$

where $\Gamma_c = e^{*2}/K_B Ta$ is the plasma parameter for $1/r$ interaction, $a = (\pi n)^{-1/2}$, n is the electron density, and T is the temperature. The MD simulations were performed for a system of $N = 100$ electrons in a rectangular box for various values of electron densities between $1.477 \times 10^8 e/cm^2$ and $1.7 \times 10^{10} e/cm^2$. We use periodic boundary condictions and employ the Ewald summation to take care of the long range interactions. The dimensions of the MD cell have a ratio of $\sqrt{3/2}$ in order to accomodate a perfect triangular lattice with $4M^2$ where M is an integer.

III. RESULTS

Figure 1 we show a schem of the geometrical arrangement of the electron layer above the helium film coating substrate. The solid-liquid phase transition was studied through the temperature dependence of the total energy per particle and the pair correlation function for a system with diferent film thicknesses.

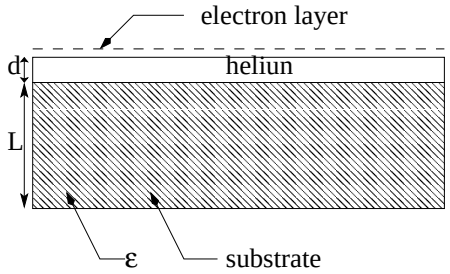

FIG. 1: *Schem of the geometrical arrangement.*

Figure 2 displays the total energy per particle versus temperature for a 100-particle system on a heliun film suported by a glass substrate ($\epsilon_s = 7.3$, $\delta = 0.75$) for $d = 240$Å, the electron density is $1.3 \times 10^{10} e/cm^2$ for this system. The up triangles and the crosses represent the solid and liquid phases respectvely; the vertical dashed line in figure 2 represent the hysteresis region containing the supercooled and superheated phases. In figure 3 we show the pair correlation function for solid phase (red) and liquid phase (blue) for the system of the figure 2.

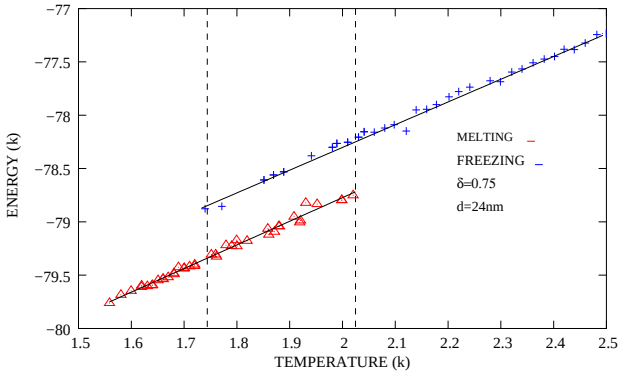

FIG. 2: *Total energy per particle versus temperature.*

Figure 4 shows the electron density as a function of the melting temperature for a system of electrons over heliun film and figure 5 shows its extrapolation points for real system. The results for T_m using MD method are compared with melting curves [1] and experimental points in figure 4 for $d = 240$, 260, 285 and 305Å. Our results showed in figure 4 are in reasonable agreemment with those obtained both theoretycally and experimentally [4]

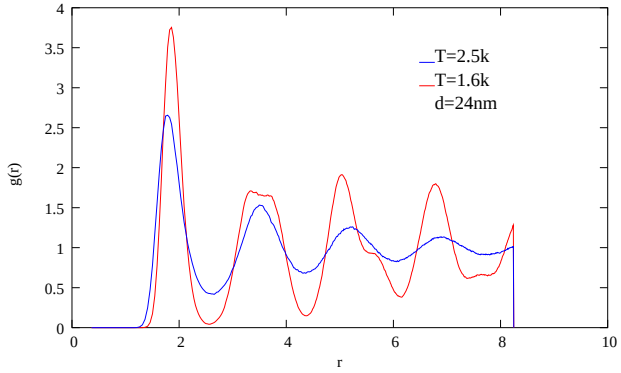

FIG. 3: *Pair correlation function.*

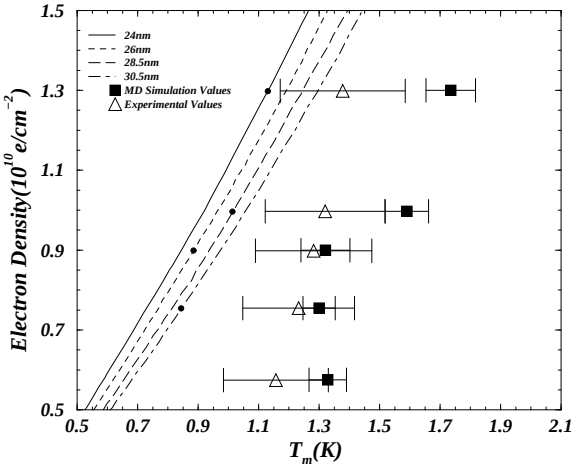

FIG. 4: *Electron density as a funtion of Melting temperature.*

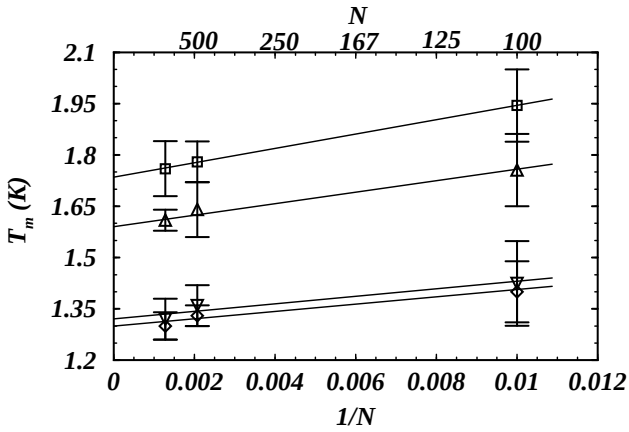

FIG. 5: *Extrapolation points for real system.*

IV. CONCLUSIONS

In this work, we report the study of the melting and freezing transitions in a system formed by classical electrons deposited over a helium liquid film adsorbed on a

substrate. On the basis of the MD results, we confirm that the melting of the system is a first-order transition, as well as other 2D charge classical system. We compare our results for the melting transition with available teoretical and experimental values and find a good agreemment [1,3-4].

Acknowledgments

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