Melting temperature of screened Wigner crystal on helium films by molecular dynamics

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Using molecular dynamics (MD) simulation, we have calculated the melting temperature of two-dimensional electron systems on 240Å-500Å helium films supported by substrates of dielectric constants $\epsilon_s = 2.2 - 11.9$ at areal densities $n$ varying from $3 \times 10^9$ cm$^{-2}$ to $1.3 \times 10^{10}$ cm$^{-2}$. Our results are in good agreement with the available theoretical and experimental results.

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At sufficiently low densities and temperatures, an electron gas is expected to undergo a phase transition to a lattice (because of the domination of the Coulomb interaction energy over the kinetic energy) which has received the name Wigner crystal. The two-dimensional (2d) Wigner crystal is well-established and experimentally it was first observed on liquid helium surface and more recently in semiconductors structures like MOS-FET’s and heterojunctions. These systems can be used for testing several theoretical predictions in many-body theory, such as phase-transitions of the electron system, metal-insulator transition and now electrons on helium surface are being proposed as a set of strongly interacting quantum bits for quantum computers. Electrons on the surface of bulk helium form a crystal at a temperature $T_m = 2\epsilon^2(\pi n)^{1/2}/(\epsilon_{He} + 1)\Gamma_m$, which is much higher than the Fermi temperature, $T_F = \pi n\hbar^2/m$ in a density range of $10^5 - 10^9$ cm$^{-2}$ (where $n$ is the electron areal density, $\epsilon_{He}$ is the dielectric constant of helium and $\Gamma_m$ is the plasma parameter in the melting temperature defined as the ratio of potential to kinetic energy). Therefore, such electrons in this regime obey the classical Boltzmann statistics. Experimentally the liquid to solid transition in the bulk takes place for a value of the dielectric constant $\epsilon_{He}$ higher than the Fermi temperature, $T = \pi n\hbar^2/m$.

In this paper, we present an accurate MD calculation for the melting temperature for an electron system over a helium film adsorbed on a dielectric substrate. In Fig. 1 we show schematically the geometrical arrangement of the system considered. The obtained results are directly compared with the available experimental data, of Mistura et al. and Jiang et al., and the theoretical results of Peeters and Saitoh.

We consider a two-dimensional system of electrons on a helium film of thickness $d$ adsorbed on a substrate of dielectric constant $\epsilon_s$ interacting through a screening Coulomb potential. The electron system is immersed in a rigid, uniform, positively charged background to make a neutral charged system. The Hamiltonian for such a system is given by

$$H = \frac{1}{2}m \sum_i v_i^2 + \sum_{i>j} \epsilon^2 \left[ \frac{1}{r_{ij}} - \frac{\delta}{r_{ij}^2 + (2d)^2} \right] + U_b, \quad (1)$$

where $\delta = (\epsilon_s - 1)/(\epsilon_s + 1)$ with the dielectric constant of helium approximated by 1 ($\epsilon_{He} = 1.057$) and $U_b$ is the interaction of electrons with the uniform positively charged background.

In this work most of the molecular dynamics calculations were performed on a system of 100 electrons with a few runs of 484 and 784 electrons to study size effect. The finite size effect is investigated by changing the system size and the thermodynamical behavior in an infinite system is derived from their extrapolation. The initial position of the electrons is a triangular lattice which is accommodated in a rectangular box with periodic boundary conditions to eliminate the surface effects. Because of the long range nature of the electron-electron interaction energy over the kinetic energy which has received the name Wigner crystal.
and electron-background interacting potential we are employing Ewald summation which splits the potential into a long-range and a short-range part. The long-range part is handled in the k-space, while the short range part in the real space. We have used the fifth-order predictor-corrector algorithm to integrate the Newton’s equation of motion with the MD time step varying from $10^{-12}$ to $10^{-15}$ sec, since it has some scale dependence on the electron densities. The optimum time step leads to a conservation of the total energy of 1 part in $10^4$ after several thousand time step runs. The time average of the physical quantities were obtained over 120 000 time steps after the system has reached equilibrium.

In Fig. 2 we present the results for the total energy per electron versus temperature to illustrate the general feature of the melting transition in this system. The solid squares in the figure represent the results for the electron liquid which has been monotonically cooled from a higher temperature. The open circles are the results for the electron solid which has been monotonically heated from a lattice at very low temperatures. It means that our simulations were performed in cascade, i.e., an equilibrated configuration obtained for a given higher (lower) temperature was used as an input to reach another configuration at lower (higher) temperature. As one can see the electron system shows hysteresis and latent heat on melting, which characterize a first order transition as other 2d classical systems. The melting temperature range is 1.83 K $< T < 2.05$ K defined from the vertical dashed lines in Fig. 2 representing the hysteresis region. Thus, we would define the melting temperature, $T_m$, as exactly the mean point in the temperature width of the hysteresis $\Delta T$, i.e., $T_m = (1.94 \pm 0.11)$ K with the error bar giving by half the temperature width of the hysteresis. The value of the latent heat per particle and the change in the entropy on melting are found to be 0.40 K and 0.21 k$_B$, respectively. We also find our MD results for the melting temperature is in agreement with those of Kalia et al. for the bulk limit. Fig. 3 shows size dependences of the transition temperature $T_m$ for different electron densities. The error bars on $T_m$ indicate the hysteresis width. When electron number becomes larger, $T_m$ decreases because the periodic boundary conditions favors the solid phase. The transition temperature, however, seems to follow a linear decrease as a function of 1/N. Therefore the melting point in the thermodynamic limit can be obtained definitely by extrapolating the finite size data.

The extrapolated melting temperature is exhibited in Fig. 4 as a function of the electron density (top), film thickness (middle) and dielectric constant of the substrate (bottom). We roughly estimated the error bar on the experimental values for the melting temperature to indicate the uncertainty of about 15% – 20% on the experimental measurement of the electron density. As is shown in Fig. 4, our results are in good agreement with those obtained experimentally in Ref. [10]. The top panel
shows that the melting temperature increases with increasing the electron density (for fixed \( \varepsilon_s \) and \( d \)) due to the the fact that the screening becomes weaker and, consequently, the electron-electron interaction is enhanced. The middle panel also shows a shift in the melting transition to higher temperature with increasing the film thickness (for fixed \( n \) and \( \varepsilon_s \)), which is a consequence of decreasing in the screening resulting in a stronger electron-electron interaction. In the bottom panel, the melting temperature decreases as the dielectric constant of the substrate increases at fixed \( d \) and \( n \). A larger dielectric constant of the substrate leads to a more polarizable system with stronger screening. As a consequence, the melting temperature goes down.

In table I, we show a comparison of our MD simulation results of the melting temperature with the available theoretical and experimental results for electron systems on a thin helium film surface. For densities below \( 1.0 \times 10^{10} \text{ cm}^{-2} \) one can see that our MD calculations are in agreement with both Jiang et al. \[9\] and Mistura et al. \[10\] experimental measurements. They are also in agreement with Saitoh’s theoretical results \[7\] in the range of the densities studied. However, we got some discrepancies with Peeters’s results \[6\] that can be justified, as pointed out by Saitoh \[7\], as a possible double counting on \( T_m \). For densities larger than \( 1.0 \times 10^{10} \text{ cm}^{-2} \), our MD simulation melting temperatures are higher than the experimental ones, though the differences are almost within the uncertainty of the experimental results. A possible explanation for this discrepancy is that the quantum effect can be important at such densities. Besides, we note that the change in entropy on melting decreases as the density or the dielectric constant of the substrate (the film thickness) increases (decreases). This might imply that transition becomes continuous at high densities.

In conclusion, we have shown that the MD is able to reproduce the experimental measurements of the melting temperature in the two-dimensional electrons on thin liquid He films. Our results are in good agreement with those obtained by Mistura et al. \[10\] and Jiang et al. \[9\]. These results in the classical regime (\( \varepsilon < 1.0 \times 10^{10} \text{ cm}^{-2} \)) should be useful to the experimental and theoretical investigation of the melting transition in this system. For larger densities (\( n > 1.0 \times 10^{10} \text{ cm}^{-2} \) and \( \varepsilon_s > 2.2 \)), the results might be beyond the applicability of the present method.

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TABLE I: Data of melting temperature $T_m$ for different thicknesses $d$, dielectric constant of the substrates $\epsilon_s$ and electron densities $n$. The experimental uncertainty in the absolute value of the electron density is about 15% – 20% in Refs. [9] and [10]. Quantities in ( ) are the estimated error on $T_m$ defined as half of temperature width of the hysteresis, in the last decimal place.

| $\epsilon_s$ | $d$ (Å) | $n$ ($10^{10}$ cm$^{-2}$) | Mistura et al. [10] | Jiang et al. [9] | Peeters [6] | Saitoh [7] | MD - this work |
|-------------|---------|--------------------------|---------------------|-----------------|------------|----------|--------------|
| 2.2         | 300     | 0.42                     | 1.16                | –               | –          | 1.08     | 1.16(6)      |
| 2.2         | 300     | 0.53                     | 1.43                | –               | –          | 1.21     | 1.26(7)      |
| 2.2         | 300     | 0.57                     | 1.50                | –               | –          | 1.26     | 1.33(6)      |
| 2.2         | 500     | 0.32                     | 1.15                | –               | –          | 1.05     | 1.05(4)      |
| 2.2         | 500     | 0.40                     | 1.39                | –               | –          | 1.17     | 1.31(5)      |
| 2.2         | 500     | 0.50                     | 1.60                | –               | –          | 1.29     | 1.37(7)      |
| 3.9         | 237     | 1.05                     | 1.16                | –               | –          | –        | 1.64(9)      |
| 7.3         | 305     | 0.75                     | –                   | 1.23            | 0.85       | 1.24     | 1.29(5)      |
| 7.3         | 260     | 0.90                     | –                   | 1.28            | 0.89       | 1.31     | 1.32(8)      |
| 7.3         | 285     | 1.00                     | –                   | 1.32            | 1.02       | 1.54     | 1.59(7)      |
| 7.3         | 240     | 1.30                     | –                   | 1.38            | 1.14       | 1.62     | 1.73(8)      |

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