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Modelling of quasi-1D Wigner solid melting in a parabolic confinement

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Phase transitions in two dimensional (2D) crystal has a special importance in condensed matter physics, which includes Wigner crystallization and melting in a strongly correlated systems [1, 2]. To study this phenomena different theoretical approaches based on topological defects [3], displacement of particles [4, 5] and correlation between them [6, 7] were applied. This work was inspired by recent experimental studies of a q1D electron crystal in confined geometry [8–10].

The aim of this work is to build a computer model to simulate processes investigated experimentally, obtain critical temperature at the phase transition using different melting criteria (Lindemann parameter, structure factor, translational correlation function [11, 12, 15]). In this work a q1D electron system with unscreened Coulomb interaction was considered. Quantum effects are not significant in this case due to low density of electrons in the system with typical interelectron distance $\sim 0.5\,\mu$m.

The system has periodic boundary conditions in x direction and parabolic potential in transversal y direction. The total energy can be written as

$$E_V = \sum_{i,j} \frac{1}{4\pi\varepsilon_0} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{k}{2} \sum_i y_i^2, \qquad (1)$$

where $\mathbf{r}_i$ is coordinate of particles, ε_0 – vacuum permittivity, e – charge of electron, $k = m\omega_y^2$ is the parameter of the parabolic potential with m being mass of electron and ω_y – angular frequency describing confinement. In computer realisation of this model dimensionless parameters were used. A ground state configuration of particles with the lowest total energy was obtained as a first step in the computation. Particles were randomly distributed in the cell and energy minimisation procedure based on gradient descent method was applied to find the ground state configuration. In the second step thermal motion was introduced to the system. Thermal motion was introduced by 500 steps of Molecular Dynamics (MD) to avoid local extremum of the energy. The algorithm was repeated until convergence was achieved. The whole procedure was repeated several times and system with the lowest energy was chosen. Energy of the system was calculated using Ewald summation technique [13]. MD simulations are based on Verlet integration, temperature was introduced using Langevin Brunger–Brooks–Karplus (LBBK) method using NVT ensemble [14, 15]. In this work we investigate only intrinsic properties of the electron system and do not take into account interaction of electrons with ripplons (quantized capillary waves of helium surface) and helium vapour atoms. Time step Δt was chosen with respect to the characteristic time of electron-electron interaction in 2D system which is defined by short- wavelength plasma frequency $\omega_p = (e^2 n_s^{3/2}/2m\varepsilon_0)^{1/2} \approx 500\tau_0^{-1}$ for the typical electron densities, $\Delta t = (2\pi/\omega_p)/100 = 10^{-4}\tau_0$.

Critical temperature was obtained using melting criteria based on modified Lindemann parameter, structure factor, pair correlation function, translation correlation function, and density of particles with a non-typical number of neighbours.

Computer simulation of melting of a quasi-1D crystal was tested in the system with four electron chains. The ground state configuration of this system is free from defects [16]. Total number of electrons in the simulation cell was chosen $N = 160$ and parameter of confinement $\tilde{\kappa} = 2 \times 10^5$.

The temperature dependence of the modified Lindemann parameter is presented in Fig. 1. Two different regions were identified at low and high temperatures and attributed to solid and liquid phases of q1D system respectfully. Generally melting point is determined when Lindemann parameter reaches the threshold value (0.1–0.2) [12]. In our analysis melting point was identified differently. At small temperatures $L_p(T)$ grows linearly and above the critical temperature have rapid increase. These two regions of $L_p(T)$ were approximated with linear functions independently, melting temperature $T_m \approx 0.55$ was obtained at the crossing point of two lines (solid red lines in Fig. 1). Temperature depen-

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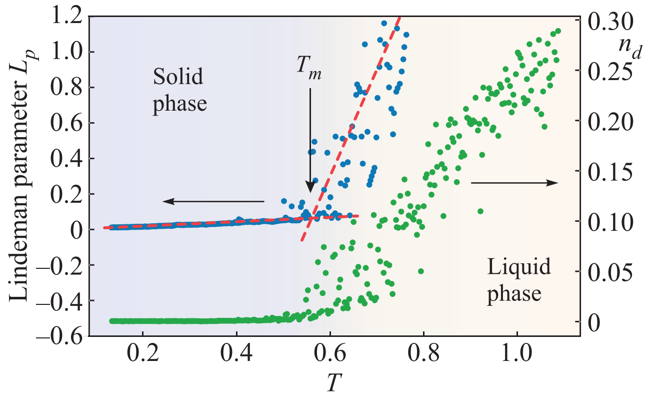

Fig. 1. (Color online) Temperature dependence of L_p (black) and density of particles with a wrong number of neighbours n_d (blue) in the system with $N = 160$. Red lines represent linear approximation of the two temperature regions, related to solid and liquid phases

dence of the density of particles with a wrong number of neighbours (not 6 for bulk particles and not 4 for edge particles) n_d is also presented in Fig. 1. The temperature dependence $n_d(T)$ is similar to $L_p(T)$ and the critical temperature is located at the same place. At low temperatures there are almost no defects, above T_m the number of defects grows rapidly with temperature.

Structure factor $S(q)$ was calculated using coordinates of particles obtained in MD simulations. The intensity of peaks decreases with temperature, which indicates loss of the translational order in the system. The system is finally disordered at $T_m \approx 0.65$ – in a good agreement with melting temperature obtained from temperature dependence of modified Lindemann parameter.

We calculated translation correlation function $g_G(r)$, at low temperatures translational correlation function decreases with the power law dependence $g_G(r) \propto r^{-\eta_G}$, at high temperatures $g_G(r) \propto e^{-r/\xi}$, where ξ is the correlation length. Close to the phase transition point correlation length ξ diverges. Joint analysis of two $\eta_G(T)$ and $\xi(T)$ dependences gives us value for critical temperature $T_m \approx 0.6$, which is in agreement with previous estimations.

Recently an experimental study of phase transitions in the system of electrons on the surface of liquid helium in a quasi-1D microchannels was reported [8]. These experiments demonstrated a good control over the number of electron rows formed in the microchannel, ranging from $1 < N_y < 25$. This gives $T_0 = 0.7$ K, therefore the melting temperature $T_m^{\mathrm{MD}} = 0.42$ K presented in this work is in a good agreement to the experimental value $T_m^{\mathrm{exp}} = 0.6$ K. It should be noted, that the corresponding plasma parameter $\Gamma = 94 \pm 10$ at the melting point is lower that the 2D melting criteria. The explanation of this behaviour will be described elsewhere.

In conclusion we studied melting process in the quasi-1D electron crystal in the harmonic potential using molecular dynamics. All methods gave similar critical temperatures $T_m \approx 0.6$. We found that the phase transition is more pronounced in temperature dependence of modified Lindemann parameter. The value of the critical temperature $T_m = 0.42$ K obtained from calculations is in good agreement with the experimental value $T_m^{\mathrm{exp}} = 0.6$ K.

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1. K. J. Strandburg, Rev. Mod. Phys. **60**, 161 (1988).
2. E. Wigner, Phys. Rev. **46**, 1002 (1934).
3. D. R. Nelson, *Defects and Geometry in Condensed Matter Physics*, Cambridge University Press, N.Y. (2002).
4. F. A. Lindemann, Phys. Z. **11**, 609 (1910).
5. G. Piacente, I. Schweigert, J. J. Betouras, and F. M. Peeters, Phys. Rev. B **69**, 045324 (2004).
6. K. Zakh and G. Maret, Phys. Rev. Lett. **85**, 3656 (2000).
7. P. Dillmann, I. Schweigert, P. Keim, and F. M. Peeters, J. Phys. Condens. Matter **24**, 464118 (2012).
8. D. G. Rees, N. R. Beysengulov, Y. Teranishi, C. S. Tsao, S. S. Yeh, S. P. Chiu, Y. H. Lin, D. A. Tayurskii, J. J. Lin, and K. Kono, Phys. Rev. B **94**, 045139 (2016).
9. N. R. Beysengulov, D. G. Rees, Y. Lysogorskiy, N. K. Galiullin, A. S. Vazjukov, D. A. Tayurskii, and K. Kono, J. Low Temp. Phys. **182**, 28 (2016).
10. D. G. Rees, N. R. Beysengulov, J. J. Lin, and K. Kono, Phys. Rev. Lett. **116**, 206801 (2016).
11. F. M. Peeters, Phys. Rev. B **30**, 159 (1984).
12. A. Brodin, A. Nych, U. Ognysta, B. Lev, V. Nazarenko, M. Škarabot, and I. Muševič, Cond. Matt. Phys. **13**, 33601 (2010).
13. P. P. Ewald, Ann. Phys. (Leipzig) **64**, 253 (1921).
14. L. Verlet, Phys. Rev. **159**, 98 (1967).
15. P. Langevin, C. R. Acad. Sci. Paris. **146**, 530 (1908).
16. A. D. Klironomos and J. S. Meyer, Phys. Rev. B **84**, 0241173 (2011).