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Melting of the Two-Dimensional Wigner Crystal in the Quantum Region

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The melting transition of two-dimensional electron systems is investigated using a recently developed quantum Monte Carlo method.[1] Our method is based on the Monte Carlo sampling of Feynman's path integral with the higher-order correction of the Trotter's formula.[2,3]

The two-dimensional electron system is represented by the Hamiltonian of the one-component plasma

$$H = H_0 + H_1 \tag{1}$$

with

$$H_0 = -\frac{\hbar^2}{2m} \sum_{i=1}^{N} \frac{\partial^2}{\partial r_i^2} \tag{2}$$

and

$$H_1 = \frac{e^2}{2} \sum_i \sum_{j \neq i} \frac{1}{|r_{ij}|} - V_{k=0} \tag{3}$$

The electron mass and charge are denoted by m and e, respectively. In (3), the term $V_{k=0}$ represents the interaction energy of electrons with uniform compensating positive charge.

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In the path integral, the partition function Z is calculated from

$$\begin{aligned} Z &= \mathrm{Tr}\, e^{-\beta H} \\ &= \lim_{M\to\infty} \mathrm{Tr}[\exp(-\beta H_0/M)\exp(-\beta H_1/M)]^M \\ &= \lim_{M\to\infty} \sum_{l_1}\sum_{l_1'}\sum_{l_2}\sum_{l_2'}\cdots\sum_{l_M'} W(\{l_j\}) \end{aligned} \tag{4}$$

$$W(\{l_j\}) = \prod_{j=1}^{M} \langle l_j|\exp(-\beta H_0/M)|l_j'\rangle\langle l_j'|\exp(-\beta H_1/M)|l_{j+1}\rangle$$

where the summations are over a complete set of states in the coordinate representation. In the Monte Carlo simulation, the summation for the complete set is approximated by the sum of samples generated in the sampling procedure. The number M is taken sufficiently large so as to give correct results. The thermodynamic average of the quantity X is calculated from

$$\langle X\rangle = \sum_{i=1}^{G} X_i \,\mathrm{sign}\, W_i \Big/ \sum_{i=1}^{G} \mathrm{sign}\, W_i \tag{5}$$

where the subscript $i(i=1,\ldots, G)$ denotes a chain of samples.

From the extrapolation of the simulation results in finite size systems, the liquid–solid phase boundary is illustrated by the solid curve in Fig. 1, where the Fermi temperature defined by $T_F \equiv \pi\hbar^2 n_e/(mk_B)$ with the electron density n_e is also plotted as the broken line. The melting is the first-

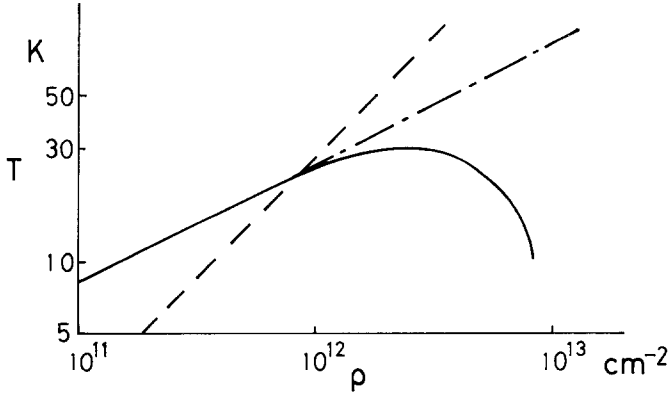

Fig. 1. Solid–liquid phase boundary of the two-dimensional electron system (solid curve) and the fermi temperature (broken curve) in the electron density n_e vs temperature T plane. The dash-dotted line represents the melting line in the classical limit.

order transition at T_c with the hysteresis. Since the hysteresis region ΔT is small ($\Delta T/T_c < 0.05$), we only plotted the midline of the hysteresis region as the melting curve. The melting temperature has the maximum value ~ 30K at the density $\sim 2 \times 10^{12}\,\mathrm{cm}^{-2}$ for two-dimensional electrons with the vacuum dielectric constant and bare mass. Beyond density $7 \times 10^{12}\,\mathrm{cm}^{-2}$ this method has difficulty because the probability of the appearance of the negative sign in W_i approaches 0.5 due to frequent exchange processes, and the convergence in (5) becomes worse. This difficulty becomes serious at lower temperatures and higher density regions than our simulation. The major part of the phase diagram is, however, obtained without such a difficulty, as in Fig. 1.

The Monte Carlo data shows that the quantum effect becomes remarkable for density larger than $10^{12}\,\mathrm{cm}^{-2}$. Although the melting temperature is lower than the fermi temperature, it does not show noticeable quantum effect around $10^{12}\,\mathrm{cm}^{-2}$. This is understood as the suppression of the fermi liquid behavior by the strong interaction, as is well-known in the ^{3}He system. Along the melting line, the mean Coulomb energy is two orders of magnitude larger than the mean kinetic energy. Near the melting temperature, the specific heat is $\sim 2k_B$ per electron and does not depend linearly on the temperature even in the quantum region of our simulation, which also suggests that fully degenerate fermi liquid behavior is strongly suppressed and expected in lower temperature and higher density region than our simulation.

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