

Phase diagram of the 2D ^4He in the density-temperature plane

F. V. Kusmartsev^a and M. Saarela^b; ^aNordita, Blegdamsvej 17, Copenhagen, Denmark

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Abstract

Thin ^4He films adsorbed to weakly attractive substrates form nearly 2D layers. We describe the vortices in 2D superfluid ^4He like quasiparticles. With the aid of a variational many-body calculation we estimate their inertial mass and describe their interactions with the ^4He particles and other vortices. Third sound measurements revealed anomalous behavior below the BKT-phase transition temperature. We ascribe this to the sound mode traveling in the fluid of vortex-antivortex pairs. These pairs form a crystal (or liquid crystal) when the film thickness increases, the third sound mode splits into two separate modes as seen in experiments. Our many-body calculation predicts the critical density, at which the phase transition into the vortex-antivortex state at zero temperature occurs. We also describe the phase diagram of thin ^4He films.

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In thin ^4He films the superfluidity is destroyed by the creation of free vortices at finite temperature. Vortices appear from the dissociation of bound vortex-antivortex (V-A) pairs [1] in the Beresinski-Kosterlitz-Thouless (BKT) phase transition. The interaction between classical vortex and antivortex is attractive and logarithmic leading to annihilation at zero separation distance. The (V-A) pair may exist in motion when the logarithmic attraction is balanced by a repulsion due to the Magnus force.

Recently a new transverse third sound mode in the superfluid ^4He film was observed [2] suggesting the formation of a crystal phase in the region near the BKT phase transition. The authors removed the possibility of substrate corrugation effects and state that the new phase is observable from zero temperature upto the BKT-transition temperature at densities below 0.6 ± 0.1 layers of ^4He adsorbed on the solid hydrogen substrate.

Zhang [3] considered the thermodynamics of vortices and antivortices by mapping them into a classical two-dimensional (2D) Coulomb gas and proposed a phase diagram with two new phases; the square and hexatic V-A lattice. Wagner and Ceperley [4] made a path integral Monte Carlo study of the film and found no new crystal phases in their simulations.

We have proposed a quantum mechanical approach for the description of vortices as quasiparticles having an inertial mass [5]. In that variational many-body formalism vortices and antivortices are included in the superfluid ^4He through the phase factor of the many-body wave function,

$$\begin{aligned} \Psi(\mathbf{r}_v, \mathbf{r}_a, \mathbf{r}_1, \dots, \mathbf{r}_N) &= e^{i \sum_{j=1}^N \phi(\mathbf{r}_v, \mathbf{r}_j) - \phi(\mathbf{r}_a, \mathbf{r}_j)} \\ &\times \psi_0(\mathbf{r}_v, \mathbf{r}_a, \mathbf{r}_1, \dots, \mathbf{r}_N). \end{aligned} \quad (1)$$

The coordinates $\mathbf{r}_1, \dots, \mathbf{r}_N$ refer to the superfluid particles and \mathbf{r}_v and \mathbf{r}_a to the vortex and antivortex cores respectively. The modulus, ψ_0 , is expanded in terms of the Jastrow type correlation functions.

The quasiparticle nature of the vortex implies two assumptions: (1) Vortices carry the *inertial mass*, which we set equal to the mass of the expelled superfluid and calculate self-consistently from the long wave length limit of the vortex-background structure function. (2) The effective interaction between a vortex and background particles and vortices themselves is determined by the phase factor of the many body wave functions plus the induced interaction caused by the polarization of the medium due to the presence of the vortices.

Table 1: The vortex mass and the binding energy of the vortex-antivortex pair, μ^{va} , as a function of density.

density \AA^{-2}	mass (amu)	$\mu^{va}(K)$
0.035	16.67	-0.57
0.040	8.52	0.73
0.045	5.27	2.21
0.050	3.59	3.84
0.055	2.60	5.66
0.060	1.96	7.46
0.065	1.53	9.39

These assumption define the effective Hamiltonian. We calculate the variational upper bound of its expectation value i.e. the energy required to create one V-A pair at zero temperature by minimizing the vortex-background and vortex-antivortex correlation functions in ψ_0 . The locations of the vortex and antivortex cores are translationally invariant, and thus the average density of the superfluid remains constant. The solutions of the optimizing Euler equations give then the probability of finding a ^4He particle at a given distance away from the vortex core and the probability distribution of the V-A pair at the zero temperature.

As a consequence the distance between the vortex and antivortex is determined by the balance between their kinetic energies and effective interaction giving rise to a bound quantum vortex-antivortex state. For an illustration the V-A pairs can be thought as an equivalent to excitons in solids. The breaking up of V-A pairs in 2D ^4He is similar to the decay of excitons in Coulomb plasma into positive and negative charges (i.e. electron-hole liquid), when the density ρ_{VA} increases. When the radius of the Debye screening $\sim 1/\rho_{\text{VA}}$ decreases, the vortex-antivortex interaction decreases, too, letting single vortices move independently.

In the careful analysis of the structure of thin films [6] one can show that below the density 0.031\AA^{-2} the film becomes unstable against cluster formation, which is the spinodal instability. Above the density 0.068\AA^{-2} 2D ^4He crystalizes, but the solid hydrogen substrate potential is so weak that atoms jump to a new layer before the first layer solidifies. This new layer again consists of clusters before the density is high enough to form a uniform superfluid layer and the procedure is repeated for thicker films.

In Table I we give results for the liquid densities of 2D ^4He using the Aziz potential between ^4He atoms and setting the vorticity equal to one. The V-A pair is assumed to be in the relative s-state. We find that at densities less than 0.037 \AA^{-2} the chemical potential for creation of V-A pair becomes negative. This signals a new kind of an instability in the system, where the quantum pairs are spontaneously created.

We argue that by increasing the fugacity of the pair y_{VA} (but not of a single vortex as argued by Zhang [3]) at a fixed low temperature (which can be done by decreasing the ^4He density), the density of V-A pairs increases and then it is preferable for the pairs to form a lattice before they break due to Debye screening. Because of the anisotropy of the V-A excitons a liquid crystal may be created as well. Our estimate of the critical density at $T = 0$, $\rho_c \sim 0.5$ layers agrees well with experiments[2]. Thus our approach explains the experiments in the whole temperature as well as the coverage range and gives the phase diagram shown in Fig. 1. The phase diagram of a thin ^4He film.

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