

## Persistence of vibrational modes in a classical two-dimensional electron liquid

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## LETTER TO THE EDITOR

**Persistence of vibrational modes in a classical two-dimensional electron liquid**

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**Abstract.** Vibrational density of states of a classical two-dimensional electron system obtained with a molecular-dynamics simulation is shown to have a peak in both solid and liquid phases. From an exact diagonalization of the dynamical matrix, the peak is identified to be vibrational modes having wavelengths of the order of the electron spacing, and the result is interpreted as persistent vibrational modes with short wavelengths in a liquid.

It is an interesting question to ask to what extent vibrational modes remain well defined in liquid states. A typical system that is known to have a solid–liquid transition is the classical two-dimensional electron system (2DES; electrons interacting with the Coulomb repulsion in a uniform neutralizing positive background), which has attracted a great deal of experimental and theoretical interests, especially in the context of melting in two dimensions (see references cited in [1]). A classical 2DES can be realized on a liquid–helium surface [2], where electrons obey classical statistics since the Fermi energy is much smaller than the thermal energy. Both experimental and numerical studies, including a recent one [1], show that the solid–liquid transition occurs around the plasma parameter

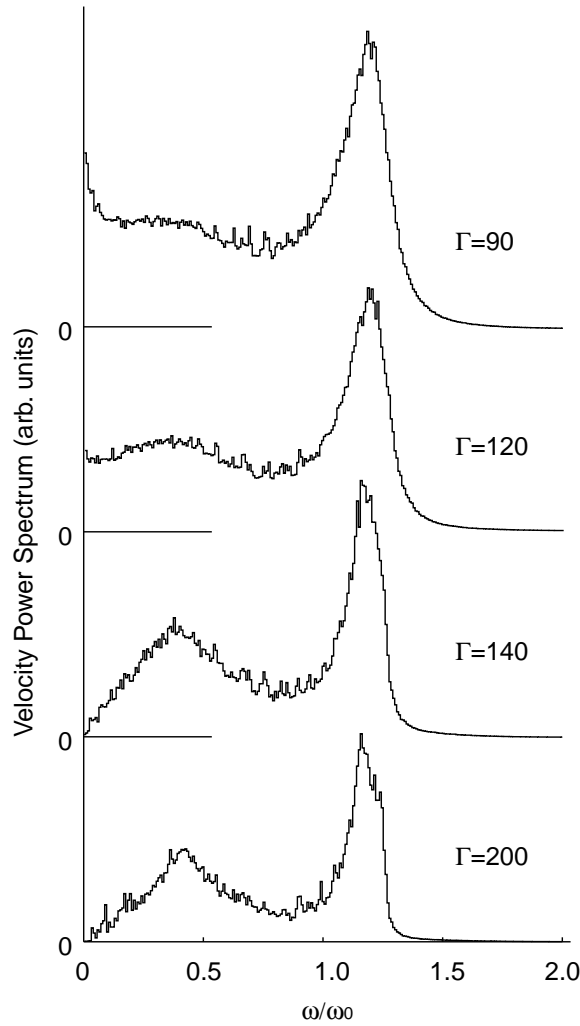
$$\Gamma \equiv (e^2/4\pi\epsilon a)/k_B T \simeq 130 \quad (1)$$

where  $a = (\pi n)^{-1/2}$  is the mean electron separation with  $n$  being the density of electrons.

Numerical simulations have been extensively done for the classical 2DES. In some of the early studies with the molecular-dynamics (MD) method, which allows one to calculate dynamical quantities as well as thermodynamic quantities, an oscillation is observed in the velocity autocorrelation function  $Z(t) \equiv \langle \sum_i \mathbf{v}_i(t) \cdot \mathbf{v}_i(0) \rangle / \langle \sum_i v_i^2(0) \rangle$ , whose period is almost independent of temperature [3, 4]. That is, the oscillation in  $Z(t)$  persists for large  $t$  even in the liquid phase. These authors, however, do not give physical interpretations, and this has motivated us to look into the problem in more detail.

We use the canonical MD method developed by Nosé [6] and Hoover [7] for 900 electrons to investigate dynamical properties of a classical 2DES, while the previous simulations were done for microcanonical ensembles for smaller systems. The aspect ratio of the unit cell is taken to be  $L_y/L_x = 2/\sqrt{3}$ , which can accommodate a perfect triangular lattice [5] with  $N = 4M^2$  ( $M$ : an integer) electrons. We impose periodic boundary conditions and use the Ewald sum to take care of the long-range nature of the Coulomb interaction.

First, we present the velocity power spectrum (vibrational density of states) in figure 1, which corresponds to Fourier transform of the velocity autocorrelation (Wiener-Khinchin's theorem). The result shows that the spectrum at zero frequency, which is proportional to the diffusion constant, is vanishingly small in the solid phase while finite in the liquid phase, in agreement with the conventional view that diffusion distinguishes solids from liquids. As the

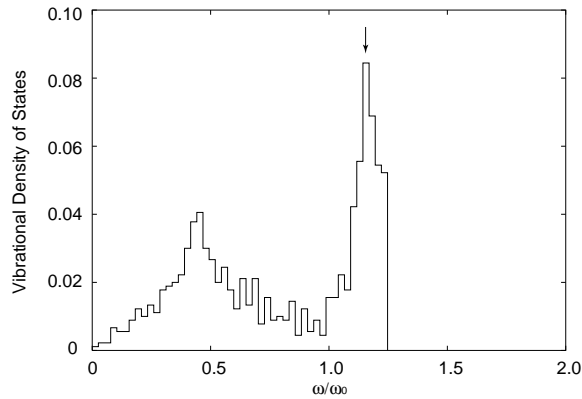


**Figure 1.** MD result for the velocity power spectrum for various temperatures ( $\propto 1/\Gamma$ ). Each spectrum is shown with an offset in the vertical axis. The result is obtained by heating the system from a solid to a liquid. The solid–liquid transition occurs at about  $\Gamma = 130$ .

temperature increases (i.e., as  $\Gamma$  decreases), the low-frequency components grow in the liquid phase, indicating larger diffusion at higher temperatures.

Remarkably, we find a peak around  $\omega \approx 1.2\omega_0$  that persists when  $\Gamma$  is decreased to the liquid regime. Here the frequency is normalized by  $\omega_0 \equiv (e^2/\sqrt{3}\epsilon md^3)^{1/2}$ , where  $d = (\sqrt{3}n/2)^{-1/2}$  is the triangular lattice constant.  $\omega_0$  is defined in such a way that the longitudinal (plasma) mode has  $\omega(q) = \omega_0(qd)^{1/2}$  in the long wavelength limit [5]. For a typical electron density on a liquid–helium surface,  $n = 10^{12} \text{ m}^{-2}$ ,  $\omega_0 \sim 4 \times 10^{10} \text{ Hz}$ . The peak corresponds to the temporal oscillation in the velocity autocorrelation first observed in [3,4]. We have checked that the overall shape of the spectrum does not change significantly with the sample size.

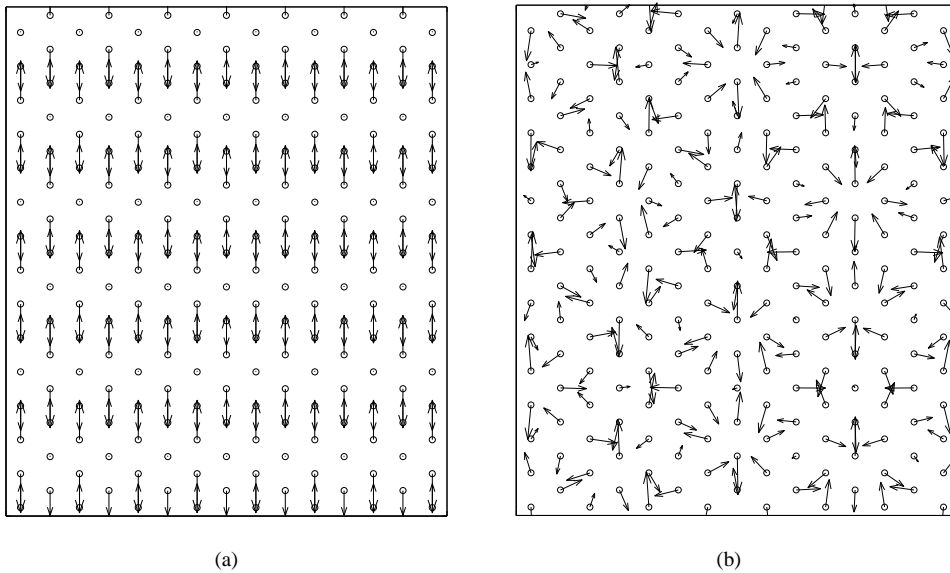
In order to identify the origin of the peak, we have exactly diagonalized the dynamical matrix for the finite-size triangular electron solid, from which we obtain eigenfrequencies and



**Figure 2.** Vibrational density of states for the triangular electron solid, obtained from an exact diagonalization of the dynamical matrix.

eigenmodes. We find that the vibrational density of states (figure 2) qualitatively reproduces the velocity power spectrum for the solid phase.

Typical vibrational modes around the high-frequency peak turn out to be those which vibrate almost out of phase between nearest-neighbour particles with the wavelength  $\sim d$ , as are typically depicted in figure 3. The fact that the peak persists in the liquid phase is considered to imply that the liquid has, despite the absence of the long-range order, well defined local configurations that can sustain large wave-number vibrations in finite spatial and temporal domains.



**Figure 3.** Typical vibrational modes around the high-frequency peak (indicated by an arrow in figure 2) in the vibrational density of states. (a) and (b) have almost the same frequency (1.153 626 (a) and 1.156 830 (b) in units of  $\omega_0$ ) but different wave vectors. A part of the triangular electron solid is shown in either frame.

Our calculation is done for the long-ranged Coulomb potential. It would be interesting to compare the result with those for short-range potentials.

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