

➤ Lévy Flights in Freestanding Monolayers (E, Thibado)

Current membrane theory extends beyond elasticity theory by including stochastic effects via Langevin's equation. One critical prediction arising from Langevin's equation is a Gaussian velocity distribution for the local fluctuations of the membrane. However, no direct experimental observation of the Gaussian distribution for a membrane has been made. In contrast, our recent experimental results show a substantial deviation from the Gaussian distribution. In fact, the measured distribution favors much higher velocities than would ever be predicted using a Normal distribution, and are more consistent with the long-excursions found in the theory of Lévy flights. This finding highlights shortcomings in the current state-of-the-art in membrane theory, which this project seeks to address and remedy.

The transformative idea about freestanding monolayers, is that they self-compress to form a rippled morphology [1]. This subtle point is key to understanding why monolayer mechanical properties fundamentally deviate from classical membrane theory. When a 2D material is placed over a picture frame to make it freestanding, the material will wrap around the frame due to the strong van der Waals interaction. The wrapping will continue until a specific tension in the freestanding monolayer is reached, in a process known as self-tensioning [2]. Interestingly, the final morphology is not stretched flat, but instead is a bumpy, rippled surface morphology more like an egg carton.

High-Velocity Movement of 2D Materials

From our STM height-time measurements, we can calculate the instantaneous velocity of the freestanding monolayer. The calculated velocity from our STM data is shown in the inset of Fig. 1(a). Note the spiky, highly irregular behavior (characteristic of a short-memory statistical process) with velocities up to 500 nm/s. The velocity autocorrelation function (VACF), where $VACF(\tau) \equiv \langle v(t) v(t+\tau) \rangle$, is shown in the main section of Fig. 1(a). The VACF decreases rapidly and becomes negative around 0.1 s, indicative of a liquid-like behavior, before finally decaying to zero within 0.5 s of our 10,000 s measurement. This data proves that the equilibrium properties of 2D membranes can be measured using our STM technique.

The membrane velocity probability distribution function (VPDF), fundamental to this project, will also be calculated. An example VPDF is shown in Fig. 1(b). This shows the probability of a particular velocity occurring as a function of all possible velocities, with the area under the curve normalized at 100%. The blue circles are STM-derived data points, while the solid green line is a best-fit Cauchy-Lorentz distribution. The velocity distribution peaks at zero and is symmetric about it, consistent with an equal likelihood of the membrane moving up or down. This demonstrates that 2D materials display balanced movement in the presence of the STM tip, and indicates that our results are within the elastic limit for our tunneling conditions.

The black dashed curve in Fig. 1(b) is the best-fit Gaussian distribution for the data. Our STM data clearly follow the Cauchy-Lorentz distribution more closely than a Gaussian, especially for speeds greater than 5 nm/s. This is a significant discovery and a key element of our recent publication in Physical Review Letters (PRL) [3]. The distribution shows that the 2D membrane favors higher velocity values than one would predict using a Normal distribution. *We believe this is fundamental property of 2D membranes that makes them excellent candidates for studying Lévy flights.*

Project A:

Measurements will be made of the intrinsic constant motion of freestanding TMDC monolayers (MoS_2 , MoSe_2 , WS_2 , WSe_2 , ReS_2 , and ReSe_2) using a new, statistically significant scanning tunneling microscopy (STM) method. With this technique, the vibration of the 2D materials will be continuously monitored in ultra-high vacuum while recording 8,000,000 data points at a rate of 800 Hz. The STM equipment is a state-of-the-art customized Omicron LT system. The mean squared displacement (MSD) and velocity probability distribution function (VPDF) for each material type, substrate temperature, and membrane size (key kinetic power parameters) will be determined.

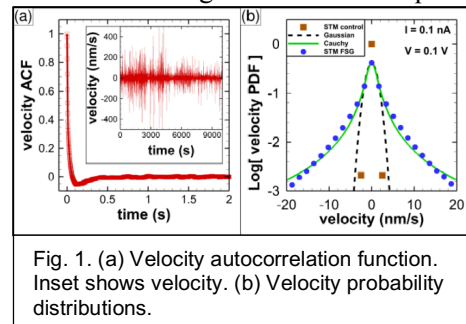


Fig. 1. (a) Velocity autocorrelation function. Inset shows velocity. (b) Velocity probability distributions.

Project B:

Molecular dynamics simulations for the freestanding 2D TMDC monolayers will be performed to provide support for the experimental results using the free, executable version of the program large-scale atomic/molecular massively parallel simulator (LAMMPS), produced by Sandia National Laboratories [4]. This software is installed on a Dell Precision T3610 mid-range workstation in the PI's laboratory. It has an Intel Xeon processor with four cores running at 3 GHz and 16 GB of RAM. The LAMMPS software was easily installed, executes on Windows (no need to compile the code), and allows four simulations to be run in parallel. The MD simulations published in our recent PRL were carried out by the PI on this computer. Temperature accelerated dynamics (TAD) will be used to expand the simulation time from nanoseconds to seconds [5]. Simulation output will report the atomic height of the membrane as a function of the simulation time step. This data mirrors the STM data and will be similarly processed to determine the MSD and VPDF for each material type, substrate temperature, and membrane size.

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