Fourier Monte Carlo Simulation of Hexatic Membranes

A. Tröster

Vienna University of Technology, Wiedner Hauptstrasse 8-10/136, A-1040 Wien, Austria

E-mail: andreas.troester@tuwien.ac.at

Abstract. Hexatic membranes are extremely difficult to study both in theory as well as in simulations based on conventional real space algorithms. We present new results for the flat phase of hexatic membranes using a unique simulation approach based on an recently developed optimization [1] of our Fourier Monte Carlo algorithm [2, 3]. In our present treatment, the case of hexatic membranes is found to closely resemble that of solid membranes for which our algorithm has already proven to be quite successful [1]. This success is based on tuning the Monte Carlo acceptance rates separately for each wavevector, which enables us to drastically reduce critical slowing down and thus observe critical behavior with excellent statistical accuracy. The resulting simulation scheme provides a new tailor-made approach to study critical behavior of systems with long-range interactions.

In detail, we calculate correlation function $< |f(q)| >^2 = G(q)$ and the related mean squared displacement $< (\Delta f)^2 >$ of the membrane's out-of-plane deformations in the Monge parametrization and give a detailed finite size scaling analysis of these data. For hexatic membranes, our simulations yield evidence for a logarithmic singularity of the critical exponent $\eta = 0_{\log}$. For the solid case, our numerical estimate for η is markedly smaller than that derived from other recent simulations [4], and we find clear evidence against "intrinsic ripples", whose existence has recently been claimed in the graphene-related literature [5].

[1] A. Tröster, Phys. Rev. B **87**, 104112 (2013).
[2] A. Tröster, Phys. Rev. B **76**, 012402 (2007).
[3] A. Tröster, Phys. Rev. Lett. **100**, 140602 (2008).
[4] J. H. Los, M. I. Katsnelson, O. V. Yazyev, K. V. Zakharchenko, and A. Fasolino, Phys. Rev. B **80**, 121405 (2009).
[5] A. Fasolino, J. Los, and M. I. Katsnelson, Nature Materials **6**, 858 (2007).