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Thermal Fluctuations and Effective Bending Stiffness of Elastic Thin Sheets and Graphene: A Nonlinear Analysis

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Abstract

The study of statistical mechanics of thermal fluctuations of graphene—the prototypical two-dimensional material—is rendered rather complicated due to the necessity of accounting for geometric deformation nonlinearity. Unlike fluid membranes such as lipid bilayers, coupling of stretching and flexural modes in solid membranes like graphene leads to a highly anharmonic elastic Hamiltonian. Existing treatments draw heavily on analogies in the high-energy physics literature and are hard to extend or modify in the typical contexts that permeate materials, mechanics and some of the condensed matter physics literature. In this study, using a variational perturbation method, we present a "mechanics-oriented" treatment of the thermal fluctuations of elastic sheets such as graphene and evaluate their effect on the effective bending stiffness at finite temperatures. In particular, we explore the size, pre-strain and temperature dependency of the out-of-plane fluctuations, and demonstrate how an elastic sheet becomes effectively stiffer at larger sizes. Our derivations provide a transparent approach that can be extended to include multi-field couplings and anisotropy for other 2D materials. To reconcile our analytical results with atomistic considerations, we also perform molecular dynamics simulations on graphene and contrast the obtained results and physical insights with those in the literature.

Keywords:
Graphene, thermal fluctuations, nonlinear elasticity, variational perturbation method

1. Introduction

Just over a decade ago, the first atomically thin crystalline material, graphene, was discovered[1]. An entirely new field of research centered around the so-called 2D materials has emerged since then [2, 3, 4]. Beyond graphene, other examples of 2D materials that have now been made in the laboratories include molybdenum disulphide, phosphorene, boron nitride and many others. Their geometrical and mechanical characteristics along with other associated physical properties have opened up fascinating new application avenues ranging from electronics, energy harvesting, biological systems, structural composites

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