Thermal buckling and symmetry breaking in thin ribbons under compression

Paul Z. Hanakata[a,*], Sourav S. Bhabesh[b,1], Mark J. Bowick[c], David R. Nelson[d], David Yllanes[e,f,c]

[a]*Department of Physics, Harvard University, Cambridge, MA 02138, USA*
[b]*Amazon Web Services (AWS), Washington DC Metro Area, USA*
[c]*Kavli Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106, USA*
[d]*Department of Physics, Lyman Laboratory of Physics and School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA*
[e]*Chan Zuckerberg Biohub, San Francisco, CA 94158, USA*
[f]*Instituto de Biocomputación y Física de Sistemas Complejos (BIFI), 50009 Zaragoza, Spain*

Abstract

Understanding thin sheets, ranging from the macro to the nanoscale, can allow control of mechanical properties such as deformability. Out-of-plane buckling due to in-plane compression can be a key feature in designing new materials. While thin-plate theory can predict critical buckling thresholds for thin frames and nanoribbons at very low temperatures, a unifying framework to describe the effects of thermal fluctuations on buckling at more elevated temperatures presents subtle difficulties. We develop and test a theoretical approach that includes both an in-plane compression and an out-of-plane perturbing field to describe the mechanics of thermalised ribbons above and below the buckling transition. We show that, once the elastic constants are renormalised to take into account the ribbon's width (in units of the thermal length scale), we can map the physics onto a mean-field treatment of buckling, provided the length is short compared to a ribbon persistence length. Our theoretical predictions are checked by extensive molecular dynamics simulations of thin thermalised ribbons under axial compression.

Keywords:

1. Introduction

Thin sheets, possibly with embedded kirigami cuts, have been the object of intense recent study [1]. A careful design allows membranes with cuts to stretch far beyond their pristine limits [2–7], to have non-linear post-buckling behaviours [8, 9], and even to exhibit complex motions such as roll, pitch, yaw, and lift [10]. Many of these novel effects arise due to out-of-plane deflections, i.e., escape into the third dimension. With such mechanical versatility and straightforward actuation, kirigami sheets have been used as building blocks for soft robots, flexible biosensors and artificial muscles [11, 12]. A full theoretical framework for this rich phenomenology must rest on a thorough understanding of the fundamental mechanical effects. In particular, out-of-plane motion in simple kirigami systems (e.g., a sheet with a single slit) have been described as an Euler buckling problem [10]. The buckling of pillars and plates has been studied for centuries, but a unifying theory to understand buckling in nanosystems when thermal fluctuations become important, as in the case of molecularly thin materials such as MoS_2 and graphene [13], is still lacking.

In the classical description, the dimensionless Föppl-von Kármán number $\mathrm{vK} = YW_0L_0/\kappa$, where Y is the 2D Young's modulus, κ is the bending rigidity, W_0 and L_0 are respectively the $T = 0$ width and length of the ribbon, can be used to quantify the ease of buckling a thin sheet out of plane at zero temperature. The picture is more complicated for thermalised membranes [14], where Y and κ become scale dependent and, in particular, the bending rigidity is dramatically enhanced [15–20]. This longstanding theoretical prediction is consistent with an important study of graphene ribbons by Blees et al. [2]. Using a cantilever setup, the effective bending rigidity of micron-size graphene at room temperature was found to increase by a factor of roughly 4000 relative to the zero-temperature microscopic value. Although it is possible that some of this increase may be due to quenched random disorder in the graphene ribbons [21], these room temperature experiments nevertheless demonstrate a striking enhancement over the $T = 0$ density functional theory predictions [22]. When thermal fluctuations are important, classical Euler buckling predictions break down. In fact, in such an entropy-dominated high-temperature setting, some aspects of nanoribbon behaviours have more in common with linear polymers with long persistence length [23].

In this letter, we investigate (i) to what temperature classical Euler buckling still holds, (ii) how we can locate buckling transitions in fluctuating ribbons under compression, and (iii) how these buckling transitions change with temperature and with the ribbon dimensions. To

*Corresponding author.
Email address: paul.hanakata@gmail.com (Paul Z. Hanakata)
[1]Work completed prior to joining AWS.