Rippled and buckled phases in a rotationally-invariant spin-string model

Gregorio García-Valladares[1], Antonio Prados[1], and Carlos A. Plata[1]
[1]Física Teórica, Universidad de Sevilla, Apartado de Correos 1065, E-41080 Seville, Spain

The study of rippled and buckled phases in low-dimensional system like graphene is an active research field [1, 2]. When the system is heated in STM experiments [3], there appear transitions from a rippled to a buckled state that have been qualitatively described by spin-string (in the one-dimensional case) [4] or spin-membrane (in the two-dimensional case) [5, 6] models. However, these latter models are not consistent with the classical theory of elasticity [7]—they break rotational symmetry, even though there are not any external forces.

We propose a variant of the models in Refs. [4, 5] that preserves rotational invariance. Interestingly, the phase diagram of the rotationally-invariant model has strong similarities with that found in [4]. Buckled phases emerge for low enough temperature. Their relative stability to the rippled (flat) phase depends on the strength of the antiferromagnetic interaction between the pseudospins—in the case of graphene, this mimics the electrostatic repulsion between out-of-plane electrons.

In our model, the interactions involve exclusively the curvature of the string and the internal, pseudospin, degrees of freedom. In the continuum limit, the equilibrium probability density of finding the system with a string profile $u(x)$ at temperature T can be written as $\mathcal{P}[u'';\theta,\kappa] \propto \exp\left(-F[u'';\theta,\kappa]/\theta\right)$, where θ and κ are the dimensionless temperature and coupling constant, respectively. The functional

$$F[u'';\theta,\kappa] = N\int_0^1 \mathrm{d}x\; f(u'';\kappa,\theta) \tag{1}$$

is the free energy of the string, and its minimisation provides us with its most probable configuration. Thus, the equilibrium profile obeys the Euler-Lagrange equation

$$\partial_{xx}\left(\frac{\partial f}{\partial u''}\right) = 0, \tag{2}$$

which is complemented with suitable boundary conditions.

This spin-string system exhibits different kinds of phase transitions between flat and buckled profiles. The profiles have been computed solving Eq. (2) both analytically, using bifurcation theory and the Landau theory of phase transitions, and numerically. Our study allows us to obtain the complete phase diagram, see Figure 1, where the free energy of the most stable buckled profile with respect to the flat profile is shown. (If only the flat profile exists, we set $\Delta F = 0$.) Above the tricritical point K, the black solid curve defines a second order transition line. Below the tricritical point, the order of the transition changes to first order, with the dotted line marking the change of stability between the flat and the locally stable buckled phase—there is also a unstable buckled phase. The dashed line to its right (solid line to its left) marks where the buckled phase (flat phase) disappears.

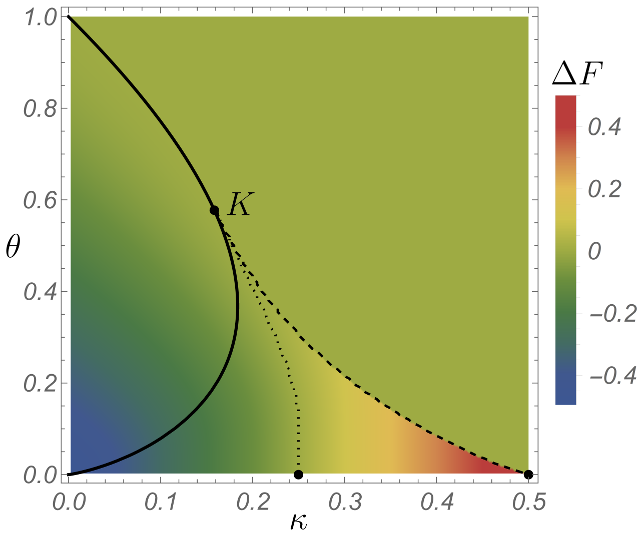

Fig. 1. Density plot of the free energy difference ΔF of the locally stable buckled state respect to the flat profile. The lines represent different kinds of phase transitions and the point where all of them intersect is the tricritical point K.

[1] P. Z. Hanakata, S. S. Bhabesh, M. J. Bowick, D. R. Nelson and D. Yllanes, Extreme Mech. Lett. **44**, 101270 (2021).

[2] A. Morshedifard, M. Ruiz-García, M. Javad and A. Komrlj, J. Mech. Phys. Solids **149**, 104296 (2021).

[3] J. Schoelz, P. Xu, V. Meunier, P. Kumar, M. Neek-Amal, P. Thibado and F. Peeters, Phys. Rev. B. **91**, 045413 (2015).

[4] M. Ruiz-García, L. L. Bonilla, and A. Prados, Phys. Rev. E. **94**, 062147 (2017).

[5] M. Ruiz-García, L. L. Bonilla, and A. Prados, J. Stat. Mech. P05015 (2015).

[6] M. Ruiz-García, L. L. Bonilla, and A. Prados, Phys. Rev. B. **94**, 205404 (2016).

[7] L. Landau and E. B. Lifshitz, *Course of Theoretical Physics Volume 7* (Butterworth-Heinemann, Oxford, 1986).