Thermal ripples in bilayer graphene

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We study thermal fluctuations of a free-standing bilayer graphene subject to vanishing external tension. Within a phenomenological theory, the system is described as a stack of two continuum crystalline membranes, characterized by finite elastic moduli and a nonzero bending rigidity. A nonlinear rotationally-invariant model guided by elasticity theory is developed to describe interlayer interactions. After neglect of in-plane phonon nonlinearities and anharmonic interactions involving interlayer shear and compression modes, an effective theory for soft flexural fluctuations of the bilayer is constructed. The resulting model has the same form of a well-known effective theory for out-of-plane fluctuations in a single-layer membrane, but with a strongly wave-vector dependent bare bending rigidity. Focusing on AB-stacked bilayer graphene, parameters governing interlayer interactions in the theory are derived by first-principles calculations. Statistical-mechanical properties of interacting flexural fluctuations are then calculated by a numerical iterative solution of field-theory integral equations within the self-consistent screening approximation (SCSA). The bare bending rigidity in the considered model exhibits a crossover between a long-wavelength regime governed by in-plane elastic stress and a short wavelength region controlled by monolayer curvature stiffness. Interactions between flexural fluctuations drive a further crossover between a harmonic and a strong-coupling regime, characterized by anomalous scale invariance. The overlap and interplay between these two crossover behaviors is analyzed at varying temperatures.

I. INTRODUCTION

The statistical properties of thermally-fluctuating two-dimensional (2D) membranes have been the subject of extensive investigations\textsuperscript{1–3}. Crystalline layers, characterized by fixed connectivity between constituent atoms and a subsequent elastic resistance to compression and shear, exhibit a particularly rich thermodynamical behavior, both in clean and disordered realizations\textsuperscript{1–16}. In absence of substrates and without the action of an externally applied tension, fluctuations are only suppressed by elasticity and the bending rigidity of the layer. Although a naive application of the Mermin-Wagner theorem suggests the destruction of spontaneous order at any finite temperature, it has long been recognized that these freely-fluctuating elastic membranes exhibit an orientationally-ordered flat phase at low temperatures\textsuperscript{4,5}. As a result of strong nonlinear coupling between bending and shear deformations, thermal fluctuations in the flat phase present anomalous scale invariance characterized by universal non-integer exponents. In the long-wavelength limit, the scale-dependent effective compression and shear moduli are driven to zero as power laws of the wavevector $q$, while the effective bending rigidity diverges as $\kappa(q) \approx q^{-6–8,10,11,17,18}$. This anomalous infrared behavior sets in at a characteristic ‘Ginzburg scale’ $q^* \approx \sqrt{3YT/(16\pi\kappa^2)}$, where $\kappa$, $Y$ and $T$ are, respectively, the bare bending rigidity, Young modulus and temperature\textsuperscript{4,19}. For shorter wavelengths, $q > q^*$, within the conventional membrane model, fluctuation effects become negligible and the effective elastic moduli approach their bare values.

The first theoretical developments in the statistical mechanics of elastic membranes were driven by the physics of biological layers, polymerized membranes and other surfaces\textsuperscript{1,2,20}. After the isolation of atomically-thin two-dimensional materials, the relevance of statistical mechanical predictions for these extreme membrane realizations has raised vast interest, in both theory\textsuperscript{3,10,12,13,19,21,22} and experiments\textsuperscript{23–27} (see also Refs.\textsuperscript{28–32}).

In the case of atomically-thin 2D membranes, numerical simulations with realistic atomic interactions are accessible\textsuperscript{19,21,22,33–36}, which allows material-specific predictions of the fluctuation behavior. Furthermore, the physics of graphene and other 2D materials stimulated new questions as compared to previously considered membrane realizations.

By exfoliation of graphite, it is possible to controllably extract multilayer membranes composed of $N$ stacked graphene sheets. As in the parent graphite structure, covalently-bonded carbon layers are tied by weaker van der Waals interactions. The large difference between the strengths of covalent and interlayer binding forces generates an intriguing mechanical and statistical behavior, which is attracting vast research interest\textsuperscript{37–42}.

The properties of defect-free multilayers subject to small fluctuations, in the harmonic approximation, is already non-trivial. Mechanical properties are crucially determined by the coupling between interlayer shear deformation and out-of-plane, bending, fluctuations. If layers are free to slide relative to each other at zero energy cost, the bending rigidity of the stack is controlled by the curvature stiffness of individual layers. The dominant contribution to the bending rigidity is thus $N\kappa$, where $N$ is the number of layers and $\kappa$ is the monolayer bare bending stiffness\textsuperscript{39–42}. By contrast, the presence of a nonzero interlayer shear modulus forces layers to compress or dilate in response to curvature. Assuming rigid binding...
between layers, the bending stiffness is then controlled by in-plane elastic moduli and it grows proportionally to $N(N^2 - 1)$ for $N \geq 2$\textsuperscript{43}. For large $N$, the limiting $N^3$ scaling of the bending stiffness\textsuperscript{39-43} is consistent with the continuum theory of thin elastic plates\textsuperscript{3,39,43,44}. In the case of graphene bilayer, the corresponding contribution to the bending rigidity can be written as $(B + \mu)L^2/2$, where $B$ and $\mu$ are compression and shear moduli, and $L$ is the interlayer distance\textsuperscript{39}.

A theory interpolating between these extreme regimes was developed, within a harmonic approximation, in Ref.\textsuperscript{39}. As a modeling framework, the system was described as a stack of continuum two-dimensional elastic media. The energy functional describing coupling between layers was constructed by discretizing the continuum theory of a three-dimensional uniaxial solid. Within this model, coupled and decoupled fluctuation regimes are recovered as limiting cases for long and short wavelengths, connected by a crossover: coupling between flexural and interlayer shear deformations sets in for wavevectors smaller than a characteristic scale $q_c$, determined by elastic stiffnesses\textsuperscript{39}.

Recent experimental measurements of the bending rigidity\textsuperscript{37,40,42,43,46} present a large scatter and indicate smaller values compared to the theoretical prediction for the long-wavelength, rigidly coupled case. In the case of bilayer graphene, different experimental techniques lead to $\kappa = 35.5^{+20.0}_{-15.6}$ eV\textsuperscript{45} and $3.35 \pm 0.43$ eV\textsuperscript{46}, significantly smaller than the elastic contribution $(B + \mu)L^2/2$, which corresponds to a rigidity of the order of 100 eV (theoretical predictions in Ref.\textsuperscript{45} lead to $\kappa \approx 160$ eV). For few-layer membranes with $N \geq 2$, Ref.\textsuperscript{45} reported evidence that the overall bending rigidity scales as $N^2$. More recently, by analyzing pressurized bubbles in multilayer graphene, MoS\textsubscript{2}, and hexagonal BN, Ref.\textsuperscript{40} reported values of $\kappa$ intermediate between the uncoupled limit $N\kappa$ and the continuum prediction, and interpreted the disagreement with continuum theory as the result of interlayer slippage between atomic planes. Finally, Ref.\textsuperscript{45} observed bilayer graphene membranes under varying bending angles. Values of the bending stiffness close to $N\kappa$ were observed for long angles, which was interpreted by a dislocation model of interlayer slippage. Reported results for the interlayer shear modulus in multilayer graphene also exhibit a large dispersion, see e.g.\textsuperscript{37}.

At finite temperatures, statistical properties of fluctuating stacks of crystalline membranes have been long investigated. A rich physics was predicted in early studies motivated by lamellar phases of polymerized membranes. In particular, Ref.\textsuperscript{47} predicted a sharp phase transition between a coupled state and a decoupled phase, in which algebraic decay of crystalline translational order makes interlayer shear coupling irrelevant. Refs.\textsuperscript{48,49} elaborated on the properties of the decoupled state, within a nonlinear three-dimensional continuum theory and determined logarithmic renormalizations due to thermal fluctuations.

In the context of crystalline bilayer and multilayer graphene membranes, finite-temperature anharmonic lattice fluctuations were extensively addressed by numerical simulations (see, e.g.\textsuperscript{34,36,50}).

In this work we study thermal fluctuations of ideal, defect-free bilayer graphene within a phenomenological, elasticity-like model. The theory of Ref.\textsuperscript{39} is assumed as a starting point and generalized to include crucial nonlinearities which control anomalous scaling behavior. An interesting aspect introduced by finite temperatures stems from the interplay of different wavevector scales: characteristic scales marking the onset of coupling between flexural and interlayer shear, and Ginzburg scales $q_c$ controlling the transition from harmonic to strongly nonlinear fluctuations. In order to obtain a global picture of correlation functions at arbitrary wavevector $q$, we derive a numerical solution of Dyson equations within the self-consistent screening approximation (SCSA)\textsuperscript{9,10,51}. In the long wavelength limit, the universal power-law behavior predicted by membrane theory is recovered and the SCSA scaling exponent $\eta = 4/(1 + \sqrt{5})$ is reproduced with high accuracy. The finite-wavelength solution, furthermore, gives access to crossovers in correlation functions and to non-universal properties specific to bilayer graphene. In order to develop material-specific predictions, we combine phenomenology with ab-initio predictions of model parameters focusing on the case of AB-stacked bilayer graphene. The paper is organized as follows: in Sec. II we introduce a phenomenological model which extends the theory of Ref.\textsuperscript{39} with the inclusion of nonlinearities required by rotational invariance. Subsequently, the model is simplified by neglecting all nonlinearities but interactions of the collective out-of-plane displacement field. In II.A, we derive an effective model for flexural fluctuations by successively integrating out all other fields. In Sec. III we discuss model parameters for AB-stacked bilayer graphene and describe first-principle calculations of the interlayer coupling moduli. In Sec. IV correlation functions of the resulting model are calculated at arbitrary wavevector within the SCSA\textsuperscript{9,10,51}; an iterative algorithm is used to determine numerical solutions of SCSA equations. Results are illustrated in Sec. V. Finally, Sec. VI discusses an extension to the theory in which nonlinearities in flexural fields of both layers are taken into account. Sec. VII summarizes and concludes the paper.

II. MODEL

Within a long-wavelength, mesoscopic, description mechanical properties of a graphene layer can be described within two-dimensional elasticity theory. In this framework, configurations of a graphene membrane are specified by the coordinates $\mathbf{r}(\mathbf{x})$ in three-dimensional space of mass points in the layer, identified by an internal two-dimensional coordinate $\mathbf{x}$. A general model for crystalline membranes with isotropic elastic coefficients is given by
the energy functional\textsuperscript{1,6–8,12}

\[ H_0 = \int d^2x \left[ \frac{\kappa}{2} \left( \nabla^2 \mathbf{r} \right)^2 + \frac{\lambda}{2} (U_{\alpha\alpha})^2 + \mu U_{\alpha\beta} U_{\alpha\beta} \right], \]  

where \( \partial_\alpha = \partial/\partial x_\alpha \) denotes differentiation with respect to internal coordinates, and \( U_{\alpha\beta} = \frac{1}{2} (\partial_\alpha \mathbf{r} \cdot \partial_\beta \mathbf{r} - \delta_{\alpha\beta}) \) is the strain tensor, proportional to the local deformation of the metric \( g_{\alpha\beta} = \partial_\alpha \mathbf{r} \cdot \partial_\beta \mathbf{r} \) from the Euclidean metric \( \delta_{\alpha\beta} \). Following a standard choice, mass points are labeled via their coordinates in a configuration of mechanical equilibrium; in the flat phase the crystal fluctuates about a spontaneously selected plane, and reference coordinates \( x_1, x_2 \) are chosen in such way that the state of minimum energy is \( \mathbf{r}(\mathbf{x}) = x_\alpha \mathbf{v}_\alpha = x_1 \mathbf{v}_1 + x_2 \mathbf{v}_2 \), where \( \mathbf{v}_1, \mathbf{v}_2 \) are mutually orthogonal unit vectors spanning the plane. Stiffness of the layer to curvature and metric deformations, expressed by the three terms in Eq. (1), are governed by the bending rigidity \( \kappa \) and the Lamé coefficients \( \lambda \) and \( \mu \), respectively.

Bilayer graphene can be described as a stack of two coupled elastic membranes\textsuperscript{39}. The corresponding energy functional can thus be written as

\[ H = \sum_{i=1}^{2} H_i + H_c, \]  

where

\[ H_i = \int d^2x \left[ \frac{\kappa}{2} \left( \nabla^2 \mathbf{r}_i \right)^2 + \frac{\lambda}{2} U_{i\alpha\alpha}^2 + \mu U_{i\alpha\beta}^2 \right] \]

are single-layer energies, and \( H_c \) represents coupling between membranes. In Eq. (3), \( \mathbf{r}_i \) and \( U_{i\alpha\beta} \) denote the coordinates and the local deformation tensor of the \( i \)-th layer in the stack. To construct interlayer interactions we assume a local coupling truncated at the leading order in a gradient expansion. This corresponds to an energy functional of the form

\[ H_c = \int d^2x \mathcal{H}_c(\mathbf{x}) \]

with an energy density \( \mathcal{H}_c(\mathbf{x}) \) depending only on \( \mathbf{r}_1(\mathbf{x}) \) and \( \mathbf{r}_2(\mathbf{x}) \) and their leading-order gradients at \( \mathbf{x} \). After introduction of sum and difference coordinates \( \mathbf{r} = \frac{1}{2}(\mathbf{r}_1 + \mathbf{r}_2) \), \( \mathbf{s} = \mathbf{r}_1 - \mathbf{r}_2 \), invariance under translations in the three-dimensional ambient space implies that \( \mathcal{H}_c \) cannot depend on \( \mathbf{r} \), but only on its derivatives. In the leading order of a gradient expansion, we will thus assume that \( \mathcal{H}_c(\mathbf{x}) \) depends only on the local separation vector \( \mathbf{s} \) and on the tangent vectors \( \partial_\alpha \mathbf{r} \), neglecting dependence on higher derivatives such as \( \partial_\alpha \mathbf{s} \) or \( \partial^2 \mathbf{r} \). As it will be seen below, this level of approximation is analogous to the approach in Ref.\textsuperscript{39}, where the coupling energy is derived by discretization of a continuum three-dimensional elasticity theory. As a remark, we notice that the assumption of locality is broken by the presence of infinite-range van der Waals interactions\textsuperscript{52} (see Ref.\textsuperscript{53} for a study in presence of dipole-dipole interactions) and coupling with gapless electrons\textsuperscript{54,55}. Effects of non-local interactions are beyond the scope of this work, and will be neglected.

The most general form of \( \mathcal{H}_c \), consistent with rotational and inversion symmetries of the three-dimensional ambient space is a generic function of the scalar products\textsuperscript{56}

\[ \partial_\alpha \mathbf{r} \cdot \partial_\beta \mathbf{r}, \quad \mathbf{s} \cdot \partial_\alpha \mathbf{r}, \quad s^2. \]

In the configuration of mechanical equilibrium, neglecting a small uniform strain induced by interlayer coupling, \( \mathbf{r}(\mathbf{x}) = x_\alpha \mathbf{v}_\alpha \). The relative displacement between layers in this minimum-energy state is \( \mathbf{s}(\mathbf{x}) = l \mathbf{n} \), where \( l \) is the interlayer distance and \( \mathbf{n} = \mathbf{v}_1 \times \mathbf{v}_2 \) is an unit vector directed along the normal to the plane. For small fluctuations, the coupling energy can thus be expanded in powers of the strain tensor \( U_{\alpha\beta} = \frac{1}{2} (\partial_\alpha \mathbf{r} \cdot \partial_\beta \mathbf{r} - \delta_{\alpha\beta}) \), the field \( \mathbf{s} \cdot \partial_\alpha \mathbf{r} \), which measures interlayer shear, and \( s^2 - l^2 \), which describes local dilations of the layer-to-layer distance.

Consistency with the dihedral \( D_{3d} \) symmetry of the AB-stacked bilayer graphene\textsuperscript{57} (see Figs. 1a and 1b) selects, among general combinations of these terms, a subset of allowed invariant functions. Symmetry-consistent terms can be directly constructed by group theory arguments, or, equivalently, by adapting invariants from theory of three-dimensional elastic media. Identification of \( \mathbf{s}/l = (\mathbf{r}_1 - \mathbf{r}_2)/l \) with a discrete version of \( \partial_\mathbf{r} \) in a corresponding three-dimensional theory, indicates that \( \mathbf{s} \cdot \partial_\alpha \mathbf{r}/l \) and \( (s^2 - l^2)/l^2 \) have the same transformation properties of strain tensor components \( U_{\alpha\alpha} = \partial_\alpha \mathbf{r} \cdot \partial_\alpha \mathbf{r} \) and \( U_{\alpha\beta} = \partial_\alpha \mathbf{r} \cdot \partial_\beta \mathbf{r} - 1 \), respectively. The general elastic free-energy of uniaxial media with \( D_{3d} \) point group subject to uniform deformation reads\textsuperscript{14,58}

\[ F = \frac{1}{2} C_1 U_{\alpha\alpha}^2 + C_2 U_{\alpha\beta} U_{\alpha\beta} + \frac{1}{2} C_3 U_{\alpha\alpha}^2 U_{\alpha\beta}^2 + \frac{1}{2} C_4 U_{\alpha\beta}^2 + C_9 U_{\alpha\alpha} U_{\alpha\beta} + \frac{1}{2} C_4 \left[ (U_{xx} + U_{yy}) U_{xz} - 2 U_{xy} U_{yz} \right], \]  

where Greek indices run over \( x \) and \( y \) components, and \( C_i \) and \( C_i \) are constants. In Eq. (6) and in the following, reference-space coordinates are interchangeably denoted

\[ \mathbf{r}(\mathbf{x}) = x_\alpha \mathbf{v}_\alpha. \]
as \((x_1, x_2)\) or \((x, y)\). Returning to the bilayer case, by drawing from analogous invariants in Eq. (6), we can write the functional \(H_c\) as

\[
H_c = \int d^2x \left[ \frac{g_1}{8l^4} (s^2 - l^2)^2 + \frac{g_2}{2l^2} (\mathbf{s} \cdot \partial_r \mathbf{r})^2 \right. \\
+ \frac{g_3}{4l^2} (s^2 - l^2) U_{\alpha\alpha} + \frac{g_4}{2l} \left( (\mathbf{s} \cdot \partial_r \mathbf{r})(U_{xx} - U_{yy}) \right) \\
\left. - 2(\mathbf{s} \cdot \partial_r \mathbf{U}_{xy}) \right],
\]

up to terms of quadratic order in the strains. Additional terms, manifestly consistent with symmetries, could be added to Eq. (7). One is an isotropic tension, \(\sigma \int d^2x U_{\alpha\alpha}\), reflecting uniform strain due to a small difference in lattice constants between monolayer and bilayer graphene. This tension can be eliminated by modifying the reference state about which strain is defined (see Refs. 7, 15, 59 for a discussion on thermally-induced uniform stretching). Such redefinition of the point of expansion implies a small shift in the elastic moduli. In addition, symmetry does not rule out a coupling of the form

\[
\frac{\lambda}{2}(U_{\alpha\alpha})^2 + \mu' U_{\alpha\beta} U_{\alpha\beta},
\]

which contributes to the stretching elasticity of the bilayer as a whole. Due to the large difference in scale between covalent carbon-carbon interactions and interlayer van der Waals interactions, it is expected that \(\lambda'\) and \(\mu'\) are much smaller than the monolayer Lamé moduli \(\lambda\) and \(\mu\). Similarly, it is expected that corrections to \(\lambda, \mu, \kappa\) due to uniform strain are small. These effects are thus neglected in Eq. (7).

Collecting terms in Eq. (2), the model Hamiltonian for graphene bilayer thus reduces to:

\[
H = H_1 + H_2 + \int d^2x \left[ \frac{g_1}{8l^4} (s^2 - l^2)^2 \right. \\
+ \frac{g_2}{2l^2} (\mathbf{s} \cdot \partial_r \mathbf{r})^2 + \frac{g_3}{4l^2} (s^2 - l^2) U_{\alpha\alpha} \\
\left. + \frac{g_4}{2l} \left( (\mathbf{s} \cdot \partial_r \mathbf{r})(U_{xx} - U_{yy}) - 2(\mathbf{s} \cdot \partial_r \mathbf{U}_{xy}) \right) \right].
\]

Within the harmonic approximation, after neglect of the anisotropic term in the last line, Eq. (9) reduces to the functional derived in Ref. 39.

In this work, similarly to the approach of Ref. 39, interlayer fluctuations will be treated within a harmonic approximation. However, nonlinearities in the soft flexural mode fluctuations will be taken into account, which is crucial in the long-wavelength scaling regime. For further analysis, it is convenient to parametrize the coordinate vectors \(\mathbf{r}(x)\) and \(\mathbf{s}(x)\) by separating in-plane and out-of-plane displacement fields: \(\mathbf{r}(x) = (x_\alpha + u_\alpha) \mathbf{v}_\alpha + h \mathbf{n}\) and \(\mathbf{s}(x) = \bar{u}_\alpha \mathbf{v}_\alpha + (l + \bar{h}) \mathbf{n}\), where \(\mathbf{u}, \mathbf{u}, \mathbf{n} \in \mathbb{R}^2, h, \bar{h} \in \mathbb{R}\), and \(\mathbf{n} = v_1 \times v_2\) denotes the normal to the plane. Fluctuations of relative coordinate \(\bar{h}\) and the shear mode \(\bar{u}_\alpha + l \delta_{\alpha\beta} h\) are bounded by the couplings \(g_1\) and \(g_2\). For simplicity, a harmonic approximation in \(\bar{u}\) and \(\bar{h}\) will be considered.

In the theory of a single crystalline membrane, it is generally assumed that nonlinearities in the free energy of in-plane fluctuation modes and the contribution of in-plane phonons to the curvature energy are irrelevant for the calculation of universal properties in the scaling regime. The neglect of such terms can be rigorously justified by power counting within a perturbative \(\epsilon\)-expansion method.

In the case of bilayer graphene, similarly, we neglect nonlinearities in the field \(u_\alpha\), which describes collective in-plane displacement of the bilayer as a whole. The exact strain tensor

\[
U_{\alpha\beta} = \frac{1}{2} (\partial_\alpha \mathbf{r} \cdot \partial_\beta \mathbf{r} - \delta_{\alpha\beta})
\]

is thus replaced with the approximate form

\[
\bar{u}_\alpha + l \delta_{\alpha\beta} h \partial_\beta h + \partial_\alpha u_\alpha \partial_\beta u_\beta.
\]

These simplifications do not affect the universal properties of the long-wavelength scaling behavior, although they can affect the amplitudes of power-law behavior and correlation functions at finite wavevector \(q\). In the following, the reduced theory is assumed as a starting point for the description of finite-wavelength phenomena.

After expansion of Eq. (9), neglecting in-plane nonlinearities, anharmonicity in \(\bar{h}\), and in-plane curvature energies leads to the effective Hamiltonian

\[
\bar{H} = \int d^2x \left[ \kappa (\partial_\alpha \bar{h})^2 + \lambda (u_{\alpha\alpha})^2 + 2\mu u_{\alpha\beta} u_{\alpha\beta} \right.
\]

\[
+ \frac{\kappa}{4} (\partial_\alpha \bar{h})^2 + \frac{\lambda}{4} (\partial_\alpha \bar{u}_\alpha)^2 + \frac{\mu}{8} (\partial_\beta \bar{u}_\alpha + \partial_\alpha \bar{u}_\beta)^2
\]

\[
+ \frac{g_1}{2l^2} \bar{h}^2 + \frac{g_2}{2l^2} (\bar{u}_\alpha + l \delta_{\alpha\beta} h)(U_{xx} - U_{yy}) - 2(\bar{u}_\alpha + l \delta_{\alpha\beta} h) U_{xy}) \right].
\]

In the transition from Eq. (9) to Eq. (11), neglected nonlinearities lead to an explicit breaking of rotational symmetry. However, as it is well known in the theory of crystalline membranes, the underlying invariance is preserved in a deformed form. A simple analysis shows that \(\bar{H}\) is invariant under the transformations

\[
\bar{h}(x) \rightarrow \bar{h}(x) + A_\alpha x_\alpha + B, \]

\[
u_\alpha(x) \rightarrow u_\alpha(x) - A_\alpha \bar{h}(x) - \frac{1}{2} A_\alpha A_\beta x_\beta + B'_\alpha, \]

\[
u_\alpha(x) \rightarrow \bar{u}_\alpha(x) - A_\alpha l, \]

\[
\bar{h}(x) \rightarrow \bar{h}(x).
\]

for arbitrary coordinate-independent \(A_\alpha, B, B'_\alpha\). The fields \(h\) and \(u_\alpha\), which describe collective displacement of the bilayer as a whole, transform as in the conventional effective theory of crystalline membranes.
This deformed symmetry and the subsequent Ward identities are crucial in the renormalization of the theory of membranes, and, most importantly, in the protection of the masslessness of flexural modes, which ensures the criticality of the theory without fine-tuning of parameters\textsuperscript{2,6,8–10}.

### A. Effective theory for flexural fluctuations

By systematically integrating out fields, we can construct an effective theory describing the statistics of flexural fluctuations $h(x)$: this approach, which emphasizes the most strongly fluctuating degrees of freedom, has been adopted in several theoretical approaches to single crystalline membranes\textsuperscript{4,7,9,10,13,15,17,18,51}.

In the case of double-layer membranes, we consider Eq. (11) as a starting point. Since the Hamiltonian is quadratic in $\bar{h}$, $\bar{u}_\alpha$, and $\bar{u}_\alpha$, the effective theory can be explicitly constructed by Gaussian integration.

After integration over relative fluctuations $\bar{h}$ and $\bar{u}_\alpha$, the theory reduces to an effective Hamiltonian controlling coupled fluctuations of $u_\alpha$ and $h$ fields. An explicit calculation leads to

$$
\hat{H}'_\text{eff} = \int \frac{1}{2} \kappa_0(q) q^4 |h(q)|^2 + \frac{1}{2} \lambda_0(q) |u_{\alpha\alpha}(q)|^2 + \mu_0(q) |u_{\alpha\beta}(q)|^2 + \frac{g_2^2}{16 g_2} (\lambda + \mu) d_L(q) d_T(q) |A(q)|^2 - \frac{g_2^4}{4g_2} (\lambda + 2\mu) d_L(q) q^2 h(q) A^*(q),
$$

(13)

where $h(q)$ and $u_{\alpha\beta}(q)$ are Fourier components of $h(x)$ and $u_{\alpha\beta}(x)$, and $A(q)$ is the Fourier transform of the anisotropic $D_{3h}$-invariant field

$$
A(x) = \partial_x u_{xx} - \partial_y u_{yy} - 2\partial_y u_{xy}.
$$

(14)

In Eq. (13), we introduced the dimensionless functions

$$
d_L(q) = \left[1 + \frac{(\lambda + 2\mu) q^2}{2g_2}\right]^{-1},
$$

$$
d_T(q) = \left[1 + \frac{\mu q^2}{2g_2}\right]^{-1},
$$

$$
d(q) = \left[1 + \frac{\kappa q^2}{2g_1}\right]^{-1},
$$

(15)

and defined

$$
\kappa_0(q) = 2\kappa + \frac{(\lambda + 2\mu) q^2}{2} d_L(q),
$$

$$
\lambda_0(q) = 2\lambda - \frac{g_2^2}{4g_1} d(q) + \frac{g_2^2}{4g_2} d_T(q),
$$

$$
\mu_0(q) = 2\mu - \frac{g_2^2}{4g_2} d_T(q).
$$

(16)

The notation $\int d^2q/(2\pi)^2$ denotes momentum integration.

The interactions $\int q^4 |\bar{A}(q)|^2$ and $\int q^2 h(q) A^*(q)$ are damped at small wavelengths by powers of the wavevectors $q$. A power counting analysis shows that they are irrelevant in a renormalization-group sense at least in the framework of a field-theoretic $\varepsilon=(4-D)$-expansion. In the following, the role of these interactions at intermediate wavelength and their effect on the amplitude of the scaling functions will be neglected for simplicity.

The effective Hamiltonian $\hat{H}'_\text{eff}$ thus reduces to

$$
\hat{H}'_\text{eff} = \frac{1}{2} \int q \left[ \kappa_0(q) q^4 |h(q)|^2 + \lambda_0(q) |u_{\alpha\alpha}(q)|^2 + 2\mu_0(q) |u_{\alpha\beta}(q)|^2 \right],
$$

(17)

which is identical in form to the standard effective theory of crystalline membranes\textsuperscript{4,6,8,12}.

$$
\hat{H}_0 = \frac{1}{2} \int d^2x \left[ \kappa (\bar{\partial}^2 h)^2 + \lambda (u_{\alpha\alpha})^2 + 2\mu u_{\alpha\beta} u_{\alpha\beta} \right],
$$

(18)

although elastic moduli $\kappa$, $\lambda$, and $\mu$ are replaced by $q$-dependent quantities. The remaining integration over in-plane fields, therefore, proceeds in an usual way\textsuperscript{4,7,10,12} (see also Chap. 6 of Ref.\textsuperscript{1}). The resulting effective Hamiltonian for the flexural field $h(x)$ reads:

$$
\hat{H}_\text{eff} = \frac{1}{2} \int q \left[ \kappa_0(q) q^4 |h(q)|^2 + Y_0(q) \left| \frac{K(q)}{q^2} \right|^2 \right],
$$

(19)

where

$$
Y_0(q) = \frac{4\mu_0(q)(\lambda_0(q) + \mu_0(q))}{\lambda_0(q) + 2\mu_0(q)}
$$

(20)

is a $q$-dependent Young modulus and $K(q)$ is the Fourier transform of the composite field

$$
K(x) = -\frac{1}{2} (\bar{\delta}_{\alpha\beta} \bar{\partial}^2 - \bar{\partial}_{\alpha} \bar{\partial}_{\beta})(\bar{\partial}_{\alpha} h \bar{\partial}_{\beta} h)
$$

$$
= \frac{1}{2} \left[(\bar{\partial}^2 h)^2 - (\bar{\partial}_{\alpha} h \bar{\partial}_{\beta} h)(\bar{\partial}_{\alpha} \bar{\partial}_{\beta} h)\right].
$$

(21)

At leading order for small deformations, $K(x)$ coincides with the Gaussian curvature\textsuperscript{4}.

### III. Model Parameters for AB-Stacked Bilayer Graphene

As discussed above, the bending rigidity $\kappa$ and the Lamé coefficients $\lambda$ and $\mu$ are approximated by their values for monolayer graphene, which is justified by the weakness of van der Waals interactions in comparison with in-plane bonding. In the case of the in-plane Young modulus $Y$ this approximation is consistent with experimental values illustrated in Ref.\textsuperscript{37}, which indicate for bilayer graphene a value of $Y$ approximately equal to twice the corresponding monolayer modulus.
The elastic moduli and the bending stiffness of a monolayer graphene have been investigated extensively (see e.g.\textsuperscript{37}). Theoretical predictions and estimates of $\kappa$ lead to values between 0.69 eV and approximately 2.4 eV\textsuperscript{61,62}.

By comparing results of atomistic Monte Carlo simulations and continuum membrane theory, the bare bending rigidity $\kappa$ was predicted to present a significant temperature-dependence\textsuperscript{19}. This was attributed to anharmonic interactions between acoustic modes and other phonon branches, or, more generally, with degrees of freedom not captured by the membrane model. In Ref.\textsuperscript{34}, a similar result was obtained for bilayer graphene. In addition, by a similar fitting method Ref.\textsuperscript{34} determined temperature-dependences of the interlayer compression modulus, analogue to $g_1$ in Eq. (11).

In the following, we neglect these temperature dependences and, similarly, effects of thermal expansion on the lattice constant $a$ and the interlayer distance $d$. In further calculations, we adopt the values $\lambda \simeq 3.8$ eVÅ$^{-2}$ and $\mu \simeq 9.3$ eVÅ$^{-2}$, which we deduced from the first-principle results of Ref.\textsuperscript{63}, and assume $\kappa = 1$ eV\textsuperscript{21,22}.

An estimate of $g_3$ from the identification $g_3 = 2c_{13}$ and the value experimental value $c_{13} = (0 \pm 3)$GPa for graphite\textsuperscript{64,65} gives $|g_3| \lesssim 0.1$ eVÅ$^{-2}$. As it will be shown by \textit{ab-initio} calculations $g_1 \simeq 0.8$ eVÅ$^{-2}$ (see below). The correction $-\frac{g_3^2}{4g_1}d(\varphi)$ in Eq. (16) is thus much smaller than the Lamé coefficients $2\lambda$ and $2\mu$. Similarly, it is expected that the terms $\frac{g_3^2}{4g_2}d(\varphi)$ play a minor role. As a result, for any wavevector the effective Young modulus $Y_0(q)$ is well approximated by $2Y$, where $Y$ is the Young modulus of monolayer graphene. This approximation is consistent with the derivation of Eq. (9), where additional terms of the form (8) have been neglected\textsuperscript{66}.

To determine interlayer coupling parameters $g_1$ and $g_2$, we have performed density functional theory (DFT) calculations on AB-stacked bilayer graphene (see Figs. 1a and 1b). We use the plane-wave based code PWscf as implemented in the Quantum-Espresso \textit{ab-initio} package\textsuperscript{67}. A vacuum layer of more than 15 Å has been added in order to avoid perpendicular interaction between neighbouring cells. The quasi-Newton algorithm for ion relaxation is applied until the components of all forces are smaller than 10$^{-5}$ Ry/bohr. The interlayer distance $l$ and the lattice parameter $a$ obtained after relaxation are shown in Table I. For the self consistent calculations, we use a 36 $\times$ 36 $\times$ 1 grid. The kinetic energy cutoff is set to 100 Ry. Projector augmented wave (PAW) pseudopotentials within the Perdew-Burke-Ernzerhoff (PBE) approximation\textsuperscript{68} for the exchange-correlation functional are used for the C atoms. Van der Waals dipolar corrections are introduced during relaxation through the Grimme-D2 model\textsuperscript{69}.

To calculate the interlayer shear modulus $g_2$ and the out-of-plane compression modulus $g_1$, we apply deformations as shown in Fig. 2(a) and 2(b) respectively to the bilayer graphene unit cell. For simplicity, a frozen-ion approximation is assumed: during deformation, all atoms are displaced rigidly without allowing for a relaxation of the internal structure of the unit cell. After application of a sequence of relative shifts $\delta x$ between carbon layers and variations $\delta l$ of the layer-to-layer distance, the total energy per unit area $E/A$ is fitted as:

$$ \frac{E}{A} = \frac{E_0}{A} + \frac{g_1}{2} \frac{\delta l^2}{l^2}, \quad (22) $$

$$ \frac{E}{A} = \frac{E_0}{A} + \frac{g_2}{2} \frac{\delta x^2}{l^2}. \quad (23) $$

The resulting values for $g_1$ and $g_2$ are illustrated in Table I.

It is natural to compare the values of $g_1$ and $g_2$ with corresponding three-dimensional elastic moduli in graphite. A stack of membranes with interactions of the form (11) between nearest-neighbouring layers and vanishing interactions between non-neighbouring layers exhibits three-dimensional elastic moduli $c_{33} = g_1/l$ and $c_{44} = g_2/l$, where $c_{33}$ and $c_{44}$ are defined according to the Voigt notation:

$$ \frac{E}{V} = \frac{1}{2} \sum_{i,j} c_{ij} \epsilon_i \epsilon_j , \quad (24) $$

where $E/V$ is the energy density of the three-dimensional solid under uniform strain. In Table I, our results for bilayer graphene are compared with \textit{ab-initio} calculations for ideal AB-stacking graphite reported in Ref.\textsuperscript{64}. The comparison indicates that values of $g_1$ and $g_2$ calculated in this work are of the same order of the corresponding graphite stiffnesses. We note, however, that the exact value of the shear modulus in multilayer graphene is still far from being understood. Reported values for the interlayer shear modulus exhibit a large dispersion (see e.g.\textsuperscript{37,46}). Raman measurements give values of the order of 4-5 GPa, while direct measurements using mechanical approaches give values of 0.36-0.49 GPa, increasing with the number of layers. This big discrepancy calls for a better understanding of interlayer dipolar or van der Waals interactions in layered materials, which is beyond the scope of this work. Experimental values of the interlayer shear modulus in graphite also exhibit a large scatter\textsuperscript{47}.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig2.png}
\caption{Scheme of the shear and out-of-plane strains.}
\end{figure}
TABLE I. Parameters for bilayer graphene obtained from first-principle calculations, compared with the elastic constants of AB-stacking graphite reported in Ref. 1.4. In the elastic moduli of graphite, results in brackets were calculated considering van der Waals corrections.64. The lattice constant a and interlayer distance l are expressed in Å, the couplings g₁ and g₂ in eV Å⁻², and the elastic moduli c₃₃, c₄₄ in GPa. In the case of graphite, the values of g₁ and g₂ in the table are defined by the identifications g₁ ≡ c₁₁l, g₂ ≡ c₄₄l, where l is the graphite interlayer distance.

|       | a    | l     | g₁    | g₂    | c₃₃   | c₄₄   |
|-------|------|-------|-------|-------|-------|-------|
| Bilayer | 2.46 | 3.2515| 0.80  | 0.11  | -     | -     |
| Graphite | 2.45 | 3.42±0.01| 0.62(0.90) | 0.096(0.10) | 29(42) | 4.5(4.8) |

IV. SELF-CONSISTENT SCREENING APPROXIMATION

Equilibrium correlation functions of the flexural field \( h(x) \) at a temperature \( T \) can be calculated by functional integration from the effective Hamiltonian \( H_{\text{eff}} \), Eq. (19). In this work, the two-point correlation function \( G(q) = \langle |h(q)|^2 \rangle \) is calculated within the self-consistent screening approximation \(^9,10,51\).

In the considered model for bilayer graphene, the problem differs from conventional membrane theory only by the \( q \)-dependence of \( \kappa_0(q) \) and \( Y_0(q) \). Therefore, SCSA equations can be written in a standard way \(^10\), by adapting the conventional equations with the replacements \( \kappa \rightarrow \kappa_0(q) \), \( Y \rightarrow Y_0(q) \).

a) \[ \frac{\tilde{b}(q)}{q^4} = b_0(q)/q^4 + G(q-k) \]

b) \[ G(q) = G_0(q) + \frac{\tilde{b}(q)}{q^4} G(q-k) \]

FIG. 3. Graphical representation of the self-consistent screening approximation.

The SCSA is defined diagrammatically in Fig. 3: by neglect of vertex corrections, Dyson equations are truncated to a closed set of integral equations for \( G(q) \) and a screened-interaction propagator \( D(q) \). For physical two-dimensional membranes in three-dimensional space, SCSA equations read \(^10\):

\[
G^{-1}(q) = G_0^{-1}(q) + \Sigma(q) ,
\]

\[
\tilde{b}^{-1}(q) = b_0^{-1}(q) + 3I(q) ,
\]

where the self-energy \( \Sigma(q) \) and the polarization bubble \( I(q) \) are, respectively,

\[
\Sigma(q) = 2 \int_k [\eta^2 k^2 - (q \cdot k)^2] \frac{2b(k)}{k^4} G(q-k)
\]

and

\[
I(q) = \frac{1}{3q^4} \int_k [\eta^2 k^2 - (q \cdot k)^2]^2 G(q-k)G(k)
\]

For membranes described by Eq. (17), the zero-order propagators are

\[
G_0^{-1}(q) = \frac{\kappa q^4}{T} , \quad b_0(q) = \frac{Y}{2T} .
\]

For bilayer graphene, after the approximation \( Y_0(q) \approx Y_0 = 2Y \), the zero-order flexural-field and interaction propagators for bilayer graphene read

\[
G_0^{-1}(q) = \frac{\kappa_0(q)q^4}{T} , \quad b_0(q) = \frac{Y_0}{2T} ,
\]

where, as in Eq. (16),

\[
\kappa_0(q) = 2\kappa + \frac{(\lambda + 2\mu)l^2}{2} \left( 1 + \frac{(\lambda + 2\mu)l^2q^2}{2g_2} \right)^{-1} .
\]

In the long-wavelength limit, identification of power-law solutions of SCSA equations within the strong-coupling assumption \( \Sigma(q) \gg G_0^{-1}(q) \), \( I(q) \gg b_0^{-1}(q) \) yields analytical equations for the universal exponent \( \eta \). After generalization to a theory of \( D \)-dimensional membranes embedded in a \( (D + d_c) \)-dimensional ambient space, the SCSA exponent \( \eta(D,d_c) \) is exact to first order in \( \varepsilon = 4 - D \), to leading order in a \( 1/d_c \)-expansion and for \( d_c = 0 ^{9,10} \). For the physical case \( D = 2, d_c = 1 \), the SCSA exponent \( \eta = 4/(1 + \sqrt{15}) \approx 0.821 \), shows a good agreement with complementary approaches such as numerical simulations and the nonperturbative renormalization group \(^11\). As compared with the SCSA, a second-order generalization which includes dressed diagrams with the topology of \( O(1/d_c^2) \) graphs in a large-\( d_c \) expansion, leads to quantitatively small corrections to universal quantities for \( D = 2, d_c = 1 ^{51} \), which supports the accuracy of the method. Recently, SCSA predictions have been compared with exact analytical calculations of \( \eta \) in second-order large-\( d_c \) and \( \varepsilon \)-expansions \(^17,18\). In Ref. \(^{17}\), it was shown that the SCSA equations are exact at \( O(\varepsilon^2) \) within a non-standard dimensional continuation of the theory to arbitrary \( D \). A more general two-loop theory was developed in Ref. \(^{18}\), where a larger space of theories was considered. For models equivalent to the conventional dimensionally-continued membrane theory, the \( O(\varepsilon^2) \) was shown to deviate from the SCSA prediction.

In order to determine correlation functions at an arbitrary wavevector \( q \), we solve SCSA equations numerically by an iterative algorithm. Starting from non-interacting
propagators $G(\mathbf{q}) = G_0(\mathbf{q})$, $\tilde{b}(\mathbf{q}) = b_0(\mathbf{q})$, Eqs. (27) and (25) are used to determine the zero-order polarization bubble $I(\mathbf{q})$ and the first approximation to the screened interaction $\tilde{b}_0(\mathbf{q})$. The self-energy diagram in Fig. 3b is then calculated as a loop integral of $\tilde{b}_1(\mathbf{q})$ and $G_0(\mathbf{q})$, leading to a dressed Green’s function $G_1(\mathbf{q})$. Iteration of the process generates a sequence of screened interactions and dressed propagators

$$G_{n+1}(\mathbf{q}) = G_0(\mathbf{q}) + \Sigma_n(\mathbf{q}),$$

$$\tilde{b}_{n+1}(\mathbf{q}) = b_0(\mathbf{q}) + 3I_n(\mathbf{q}),$$

$$\Sigma_n(\mathbf{q}) = 2 \int_{\mathbf{k}} [q^2 k^2 - (\mathbf{q} \cdot \mathbf{k})^2] \frac{2 \tilde{b}_{n+1}(\mathbf{k})}{k^4} G_n(\mathbf{q} - \mathbf{k}),$$

$$I_n(\mathbf{q}) = \frac{1}{3q^4} \int_{\mathbf{k}} [q^2 k^2 - (\mathbf{q} \cdot \mathbf{k})^2] G_n(\mathbf{q} - \mathbf{k}) G_n(\mathbf{k}),$$

(31)

which, after convergence, approach solutions to the SCSA equations. At each step in the iteration process, correlation functions are calculated on a grid of 50 wavevector points, evenly spaced in logarithmic scale and ranging between $10^{-7} \text{Å}^{-1}$ and $110 \text{Å}^{-1}$. Calculations with grids of 26 and 29 points are also performed to estimate the numerical accuracy.$^{71}$

![FIG. 4. Sequence of correlation functions (red solid lines) and screened interactions (blue dashed lines) obtained by 25 iterations of the convergence algorithm. Data in the graph refer to a bilayer membrane with the parameters $\lambda = 3.8$ eV Å$^{-2}$, $\mu = 9.3$ eV Å$^{-2}$, $\kappa = 1$ eV, $l = 3.2515$ Å, $g_2 = 0.11$ eV Å$^{-2}$ and $T = 300$ K. Correlation functions evaluated at the last iteration on the 50-point grid are shown by dots.]

Twenty-five steps of the iteration algorithm are illustrated in Fig. 4. In order to calculate loop integrals, at each iteration $G(\mathbf{q})$ and $\tilde{b}(\mathbf{q})$ are interpolated by cubic splines$^{72}$ in logarithmic scale: $G(\mathbf{q})$ and $\tilde{b}(\mathbf{q})$ are interpolated as $G_n(\mathbf{q}) = A_1 \exp[f_1(\ln(q/B))]$, $\tilde{b}_n(\mathbf{q}) = A_2 \exp[f_2(\ln(q/B))]$, where $f_1$ and $f_2$ are cubic splines and $A_1$, $A_2$, $B$ are constants. In the region $q < 10^{-7} \text{Å}^{-1}$, which is not covered by the wavevector grid, functions are extrapolated as pure power laws, $G_n \propto q^{-\eta(n)}$ and $\tilde{b}_n \propto q^{\eta(n)}$ with exponents and amplitudes matching the first two points in the grid.

In the calculation of integrals, we split two-dimensional wavevector integration into a sequence of one-dimensional integrals over $k_y$ and $k_x$, the components of $\mathbf{k}$ respectively transverse and longitudinal to the external wavevector $\mathbf{q}$. In the computation, we use an adaptive algorithm for single-variable integration$^{74}$, and include $k_y$-integration in the function called by the outer $k_x$ integral. Inner and outer integrals are evaluated within a relative accuracy $1.49 \times 10^{-8}$ and $10^{-7}$ respectively.

Although the self-energy and polarization bubble are convergent, a hard ultraviolet cutoff $\Lambda = 100 \text{Å}^{-1}$ is imposed in explicit calculations. To estimate the numerical error due to the finite UV cutoff, we compared data sets calculated with $\Lambda = 100 \text{Å}^{-1}$ and $\Lambda = 1000 \text{Å}^{-1}$, which were obtained by calculating numerical solutions on wavevector grids consisting of 26 and 29 points respectively. Upon this change in UV cutoff, data sets for $G(\mathbf{q})$ and $\tilde{b}(\mathbf{q})$ deviate by less than $10^{-5}$.71

In the numerical calculations, difficulties stem from the rapid variation of functions in regions of much smaller size than the integration domain and from the slow decay of integration tails at large $k$. To address these problems, integrals are performed piecewise. Specifically, the $k_y$ integration domain is split into contiguous intervals with extrema $\{0, 10^{-1} q_1, q_1, 10 q_1, q_2, 10 q_2, 10^2 q_2, 10^3 q_2\}$, where $q_1 = \sqrt{|q|/|\mathbf{k}|}$ and $q_2 = \max [|q|, |\mathbf{k}|]$. For any $q$ and $k_x$ and at any steps in the iteration process, characteristic scales $q_1$ and $q_2$ define roughly the width in $k_y$ integration which contributes mostly to the integral value. The piecewise calculation defined above is then able to capture a small-scale peak in the integrand function and a long tail for $k_y \gg q_2$. In the subsequent $k_x$ integrations, similarly, subintervals are chosen as $\{\ldots, -10 q, 0, q, 10 q, 100 q, \ldots\}$.

After 25 iteration of the algorithm, the values of $G_n(\mathbf{q})$ and $\tilde{b}_n(\mathbf{q})$ at the grid of sampled wavevector points converge within a relative deviation smaller than $10^{-10}$. The final results (see Sec. V) reproduce the analytically-known SCSA exponent and amplitude ratio$^{9,10,51}$ closely: an estimate of the exponents $\eta$, $\eta_n$ and the amplitudes $z_1$, $z_2$ of the scaling behavior

$$G^{-1}(\mathbf{q}) = z_1 q^{4-\eta}, \quad \tilde{b}(\mathbf{q}) = z_2 q^{\eta_n},$$

(32)

from the first two points of the wavevector grid gives values in the range $\eta = 0.8208515 \div 0.8208524$, $\eta_n = 0.35829478 \div 0.35829524$, and $z_1/z_2 = 0.1781321 \div 0.1781381$ for considered data sets for monolayer graphene at $T = 300$ K and bilayer graphene at different temperatures between 10 and 1500 K. These results are in close agreement with the analytical predictions $\eta = 4/(1+\sqrt{15}) \approx 0.8208525$, $\eta_n = 2 - 2\eta \approx 0.35829523$, and...
\[
\frac{z_1^2}{z_2} = \frac{3}{16\pi} \Gamma^2(1+\eta/2)\Gamma(1-\eta) \approx 0.17813212 \ldots
\] (33)

The individual amplitudes \(z_1\) and \(z_2\) and the crossover behaviors at finite \(q\) are more sensitive to numerical error. A limitation to numerical accuracy derives from the need to interpolate \(G(q)\) and \(\hat{b}(q)\) from a discrete set of data points. To estimate the order of the corresponding error, the numerical solution of SCSA equations was repeated after reduction to a broader grid, consisting of 26 wavevector points. Compared to data evaluated with the 50 \(q\)-point grid, interpolating functions exhibit a maximum relative deviation of the order of 2% in all considered sets of data (see71 for a more detailed analysis). The amplitudes \(z_1\) and \(z_2\) of the long-wavelength scaling regime exhibit a smaller discrepancy, of the order of \(10^{-3}\), upon change from the finer to the broader wavevector grid.

Numerical results indicate that the numerical values of the exponent and the amplitude ratio \(z_1^2/z_2\) are much more accurate than the numerical precision in calculations of non-universal properties such as the amplitude and finite-wavelength dependences of \(G(q)\) and \(\hat{b}(q)\). Qualitatively, universal properties are only sensitive to the region of small momenta, where \(G(q)\) and \(\hat{b}(q)\) approach pure powers and the precision of numerical interpolation improves significantly.

V. RESULTS

The numerical algorithm described in Sec. IV was used to determine solutions to the SCSA equations for a graphene monolayer and for graphene bilayers at temperatures \(T = 10, 300,\) and 1500 K. Results are illustrated in Figs. 5, 6, 7, and 8. Numerical data are reported in Ref. 71.

The correlation function \(G(q)\) and the renormalized elastic modulus \(\hat{b}(q)\)9,10 for single-layer graphene at room temperature are illustrated by blue dashed lines in Fig. 5. As it is completely general within the framework of the elasticity model, Eq. (18), interaction effects are weak for \(q \gtrsim q_*\), where \(q_* = \sqrt{3TY/(16\pi\kappa^2)}\)9,19. In the limit \(q \gg q_*\), \(\tilde{\kappa}(q)\) and \(\hat{b}(q)\) approach their bare values \(\kappa\) and \(Y/(2T)\), with negligible renormalizations. In contrast, for \(q \lesssim q_*\) a strong coupling regime sets in. For \(q \ll q_*\) the self-energy \(\Sigma(q)\) and the polarization function \(P(q)\) are much larger than the harmonic propagators \(G^{-1}(q)\) and \(b_0^{-1}(q)\); correlation functions scale as power laws9,10,51:

\[
G^{-1}(q) = z_1 q^{4-\eta}, \quad \hat{b}(q) = z_2 q^{\eta_0}.
\] (34)

As mentioned above, numerical results are in close agreement with the scaling relation \(\eta_0 = 2 - 2\eta\), and the predictions, exact within SCSA, \(\eta = 4/(1 + \sqrt{15})\) and \(z_1^2/z_2 \approx 0.17813212^9,10,51\).

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig5.png}
\caption{Effective bending rigidity \(\tilde{\kappa}(q) = TG^{-1}(q)/q^4\) and renormalized elastic coefficient \(\hat{b}(q)\) for monolayer (blue dashed lines) and bilayer graphene (red solid lines) at \(T = 300\) K. For \(q \to 0\), \(\tilde{\kappa}(q)\) diverges for both curves as \(q^{-\eta}\) and \(\hat{b}(q)\) approaches 0 as \(q^{2-2\eta}\).
}
\end{figure}

By a simple rescaling, the numerical solution obtained for monolayer graphene can be adapted to any membrane described by the elasticity model, Eq. (18). For any such membrane, the statistics of out-of-plane fluctuations is governed by a Hamiltonian of the form (19) with a wavevector-independent rigidity \(\kappa_0(q) = \kappa\) and Young modulus \(Y_0(q) = Y\). A scaling analysis then shows that

\[
G(q) = \frac{T}{\kappa q^2} g \left( \frac{q}{q_*} \right)
\] (35)

and

\[
\hat{b}(q) = b_0 f \left( \frac{q}{q_*} \right) = \frac{Y}{2T} f \left( \frac{q}{q_*} \right),
\] (36)

where \(g(x)\) and \(f(x)\) are independent of temperature and elastic parameters. In particular, the coefficient \(z_1\) governing the amplitude of the scaling behavior has the form73

\[
z_1 = \tilde{z}_1 \frac{\kappa q_*^2}{T},
\] (37)

where \(\tilde{z}_1\) is independent of \(T, \kappa,\) and \(Y\). An estimate from the amplitude of \(G\) in monolayer graphene gives \(\tilde{z}_1 \approx 1.177\). In the following, the scaling-analysis relations (35) and (36) are used to convert numerical data collected for monolayer graphene at \(T = 300\) K to single membranes with arbitrary elastic parameters and temperature.

As Figs. 5, 6 and 7 show, correlation functions in bilayer graphene exhibit a more intricate crossover behavior which extends from microscopic to mesoscopic scales. In contrast with the monolayer elasticity theory, the behavior of a bilayer is controlled by several length scales.
The effective bare bending rigidity $\kappa_0(q)$, Eq. (30), approaches limiting values $2\kappa$ and $\bar{\kappa}_0 = 2\kappa + (\lambda + 2\mu) l^2 / 2$ for $q \gtrsim q_{1c}$ and for $q \lesssim q_{2c}$ respectively, where

$$q_{1c} = \sqrt{\frac{2g_2}{2\kappa}} \approx 0.2 \text{Å}^{-1}$$

and

$$q_{2c} = \frac{1}{l} \sqrt{\frac{2g_2}{\lambda + 2\mu}} \approx 3 \times 10^{-2} \text{Å}^{-1}.$$  

A crossover in the mechanical behavior\(^{39}\) takes place between these two scales: $q_{2c} < q < q_{1c}$. The strong $q$-dependence of $\kappa_0(q)$ has a crucial impact on the harmonic correlation functions. The effective rigidity $\tilde{\kappa}(q)$ and elastic coefficient $\tilde{b}(q)$ in the harmonic approximation, which coincide with their bare value $\kappa_0(q)$ and $b_0(q)$, are illustrated by dashed lines in Fig. 6 and by grey dotted lines in Fig. 7. The effective elastic coefficient $b_0(q)$, conversely, displays a weak wavevector dependence and it is approximated as a constant in this work (see Sec. III).

At finite temperatures, for a single membrane, crossover from weak to strong coupling is marked by the Ginzburg scale $q_* = \sqrt{3TY/(16\pi\kappa^2)}$. In the case of bilayer graphene, two scales analogue to $q_*$ can be anticipated:

$$q_{1*} = \sqrt{\frac{3T}{16\pi} \frac{(2Y)}{(2\kappa)^2}} = \frac{q_*}{\sqrt{2}}$$

and

$$q_{2*} = \sqrt{\frac{3T}{16\pi} \frac{(2Y)}{\kappa_0}}.$$  

While $q_{1*}$ is close to the Ginzburg scale for a monolayer graphene, $q_{2*}$ is smaller by two orders of magnitude due to the strong enhancement of $\kappa_0 \gg 2\kappa$.

In order to study the interplay and overlap between these crossover effects, we analyzed fluctuations in bilayer graphene at temperatures $T = 10, 300,$ and 1500 K. For small temperatures, the mechanical and the weak-strong coupling crossovers are disentangled. At $T = 10$ K both $q_{2*} \approx 4 \times 10^{-4} \text{Å}^{-1}$ and $q_{1*} \approx 2 \times 10^{-2} \text{Å}^{-1}$ are smaller than $q_{1c}$, and furthermore $q_{2*} \ll q_{2c}$. As it is confirmed by the numerical results, throughout the region $q_{2c} < q < q_{1c}$ thermal effects are negligible. Strong coupling behavior sets in only at $q < q_{2*} < q_{2c}$, a region where $\kappa_0(q)$ has already converged to its limiting value $\bar{\kappa}_0$. A more detailed analysis of the collected numerical data shows that for $q > 4 \times 10^{-4} \text{Å}^{-1}$, $\tilde{\kappa}(q)$ and $\tilde{b}(q)$ differ from their harmonic approximations $\kappa_0(q)$ and $b_0(q)$ by less than 3%. For $q < 4 \times 10^{-3} \text{Å}^{-1}$, instead, numerical data agree within 3% with correlation functions of a single membrane with Young modulus $2Y$ and rigidity $\bar{\kappa}_0$, which was obtained by rescaling monolayer graphene results via Eqs. (35) and (36). In particular, in the scaling region $q \ll q_{2*}$, the amplitude $z_1$ of the power-law behavior $G^{-1}(q) = z_1 q^\eta$ differs from the corresponding single-membrane value

$$z_1 = \frac{z_1}{2} \frac{\tilde{\kappa}_0 g_2^2}{T} \approx 1.17 \frac{\kappa_0 g_2^2}{T}$$

only by a deviation of the order of $10^{-3}$.

Fig. 7 illustrates an explicit comparison between full correlation functions for bilayer graphene at $T = 10$ K, their harmonic approximation, and the corresponding functions for single membranes having Young modulus $2Y$ and bending rigidity $2\kappa$ and $\bar{\kappa}_0$. Ratios between corresponding functions are presented in Fig. 8.

At room temperature, the mechanical and the weak-strong coupling crossovers have a more sizeable overlap: the characteristic scale $q_{1*} \approx 0.13 \text{Å}^{-1}$ is of the same order of $q_{1c}$. As it can be seen in Fig. 8(b), the renormalized bending rigidity $\tilde{\kappa}(q)$ exhibits a larger deviation from the harmonic approximation at scales of the order of $10^{-1} \text{Å}^{-1}$. However, the effect is relatively small. For $q \gtrsim 10^{-2} \text{Å}^{-1}$, $\tilde{\kappa}(q)$ and $\tilde{b}(q)$ differ from the corresponding functions in the harmonic approximation by less than 10%. In the long wavelength region $q \lesssim 10^{-2} \text{Å}^{-1}$, instead, $\tilde{\kappa}(q)$ and $\tilde{b}(q)$ agree within 9% with the renormalized rigidity $\tilde{\kappa}_1(q)$ and elastic modulus $\tilde{b}_1(q)$ of a single membrane with bare bending stiffness $\kappa_0$ and Young
FIG. 7. Effective bending rigidity and renormalized elastic modulus for bilayer graphene at $T = 10$ K (top panel) and $T = 300$ K (bottom panel). Solid red lines represent $\tilde{\kappa}(q)/T$ and $\tilde{b}(q)$ obtained by numerical solution of SCSA equations for bilayer graphene. The corresponding functions in the harmonic approximation are illustrated as grey dotted lines. The blue dashed curves show the SCSA correlation functions for a single membrane with rigidity Young modulus $2Y$ and bending rigidity $2\kappa$, i.e., twice as large than in monolayer graphene. The correlation functions of a single membrane with Young modulus $2Y$ and the much larger bending rigidity $2\kappa + (\lambda + 2\mu)l^2/2$ is illustrated by green dash-dotted lines.

modulus $2Y$. An explicit comparison is illustrated graphically in Fig. 7.

The effects of thermal renormalizations are more pronounced at $T = 1500$ K, as Fig. 8(c) shows. Within the considered model, the amplitude of the long-wavelength power-law behavior $\tilde{\kappa}(q) = Tz'' q^{-n}$ differs from the scaling limit of $\tilde{\kappa}_1(q)$, $\tilde{\kappa}_1(q) = z_1 \tilde{\kappa}_0(q_{2c}q)^n$, by approximately 10%.

In correspondence with crossover regions for $\tilde{\kappa}(q)$,

FIG. 8. Ratio between the renormalized bending rigidity $\tilde{\kappa}(q)$ and the bare effective rigidity $\tilde{\kappa}_0(q)$ (grey dotted lines), the renormalized rigidity $\tilde{\kappa}_1(q)$ of a single-layer membrane with parameters $2Y$ and $2\kappa$ (blue dashed line), and the analogue function $\tilde{\kappa}_2(q)$ for parameters $2Y'$ and $2\kappa_0$ (red solid line). Panels (a), (b), and (c) refer to data at $T = 10$, 300, and 1500 K respectively. A horizontal line at 1 is drawn as guide to the eye.
the renormalized elastic coefficient $\tilde{h}(q)$ exhibits a flexion (see Fig. 7). Since $h_{0}(q)$ is assumed to be wavevector-independent, this behavior reflects corresponding crossovers in the polarization function $\Pi(q)$.

VI. INCLUSION OF INTERLAYER FLEXURAL NONLINEARITIES

In the model considered in this work, nonlinearities in $\tilde{h} = h_{1} - h_{2}$ and $\tilde{u}_{\alpha}$ have been neglected. As a result of the harmonic approximation, however, Eq. (11) fails to recover the theory of two independent nonlinearly-fluctuating layers in the complementary limit $g_{1}, g_{2}, g_{3}, g_{4} \to 0$. A minimal extension of the theory necessary to connect this limiting regime can be constructed by including nonlinearities in the interlayer flexural field $\tilde{h}$, while neglecting anharmonicity in the in-plane displacement fields. With this extension, an analogue of Eq. (11) reads:

$$\tilde{H} = \frac{1}{2} \int d^{2}x \left[ \kappa (\partial^{2} h_{1})^{2} + \lambda (u_{1\alpha\alpha})^{2} + 2\mu (u_{1\alpha\beta})^{2} \ight. \\
+ \kappa (\partial^{2} h_{2})^{2} + \lambda (u_{2\alpha\alpha})^{2} + 2\mu (u_{2\alpha\beta})^{2} \
+ \frac{g_{1}}{2} \tilde{h}^{2} + \frac{g_{2}}{2} (\tilde{u}_{\alpha} + (l + \tilde{h}) \partial_{\alpha} h_{1})^{2} + \frac{g_{3}}{2} (u_{1\alpha\alpha} + u_{2\alpha\alpha}) \\
+ \frac{g_{4}}{2} ((\tilde{u}_{\alpha} + (l + \tilde{h}) \partial_{\alpha} h_{1}) (u_{xx} - u_{yy}) \\
- 2(\tilde{u}_{y} + (l + \tilde{h}) \partial_{y} h_{1}) u_{xy}) \right],$$

(43)

where $u_{i\alpha\beta} = \frac{1}{2} (\partial_{\alpha} u_{i\beta} + \partial_{\beta} u_{i\alpha} + \partial_{\alpha} h_{i} \partial_{\beta} h_{1})$ are approximate strain tensors of the $i$-th layer. For $g_{1}, g_{2}, g_{3}, g_{4} = 0$, Eq. (43) reduces to two copies of the well-known nonlinear effective theory for monolayer membranes.\textsuperscript{4,6,8,12}

Developing a general theory for weakly coupled membranes with large interlayer-distance fluctuations is a complex problem. If the field $\tilde{h}$ is regarded as critical, with a propagator scaling as $q^{-4}$, power counting indicates an infinite number of relevant and marginal perturbations (see e.g.\textsuperscript{74} for a related analysis). Eq. (43), therefore, is not a general Hamiltonian but rather, a minimal extension which connects the harmonic theory to a nonlinear decoupled regime of the two membranes.

The theory defined by Eq. (18) is invariant under the transformations (see\textsuperscript{2,8})

$$h_{1}(x) \rightarrow h_{1}(x) + A_{\alpha} x_{\alpha} + B$$
$$h_{2}(x) \rightarrow h_{2}(x) + A_{\alpha} x_{\alpha} + B$$
$$u_{1\alpha}(x) \rightarrow u_{1\alpha}(x) - A_{\alpha} \left( \frac{l}{2} + h_{1}(x) \right) - \frac{1}{2} A_{\alpha} A_{\beta} x_{\beta} + B'_{\alpha}$$
$$u_{2\alpha}(x) \rightarrow u_{2\alpha}(x) + A_{\alpha} \left( \frac{l}{2} - h_{2}(x) \right) - \frac{1}{2} A_{\alpha} A_{\beta} x_{\beta} + B'_{\alpha},$$

(44)

which represent deformed versions of rotations in the embedding space, adapted to match the neglection of in-plane nonlinearities.

Qualitatively, in the case of bilayer graphene, anharmonic terms in $\tilde{h}$ are expected to play a minor role.

VII. SUMMARY AND CONCLUSIONS

In summary, this work analyzed the statistical mechanics of equilibrium thermal ripples in a tensionless sheet of suspended bilayer graphene. The individual graphene membranes forming the bilayer were described as continuum two-dimensional media with finite bending rigidity and elastic moduli. For the description of interlayer interactions a phenomenological model in the spirit of elasticity theory was constructed. Although the fluctuation energy is expanded to leading order for small deformations, anharmonicities emerge as a necessary consequence of rotational invariance, which forces the energy to be expressed in terms of nonlinear scalar strains.

For explicit calculations, the model was simplified by neglecting nonlinearities in the interlayer shear and compression modes, and by dropping anharmonic interactions of collective in-plane displacements. An effective theory describing the statistics of soft flexural fluctuations was then derived by Gaussian integration. The resulting model is controlled by bending rigidity and a long-range interactions between local Gaussian curvatures and it is identical in form to the analogue theory for a monolayer membrane. However, the bare bending rigidity $\kappa_{0}(q)$ exhibits a strong wavevector dependence at mesoscopic scales. Relevant phenomenological parameters governing the strength of interlayer interactions were derived in the case of AB-stacked bilayer graphene through ab-initio density functional theory calculations, by combining an exchange-correlation functional within the Perdew-Burke-Ernzerhoff approximation and van der Waals corrections in the Grimme-D2 model.

Due to the formal equivalence to a corresponding single-membrane theory, the statistical mechanics of fluctuations can be addressed by well-developed approaches. In this work, the field theory integral equations of motion were solved within the self-consistent screening approximation. In order to access correlation functions at arbitrary wavevector $q$, SCSA equations were solved numerically by an iterative algorithm.

The numerical solutions recover with good accuracy analytical SCSA predictions for universal properties in the long-wavelength scaling behavior. At mesoscopic lengths, the calculated correlation functions exhibit a rich crossover behavior, driven by the harmonic coupling between bending and interlayer shear and by renormalizations due to nonlinear interactions.

In the final part of the paper, a minimal extension of the theory, including nonlinearities in the flexural fields of both layers was briefly discussed.
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FIG. 9. Top and bottom panels illustrate, respectively, the ratios \( \Delta G/G = |G_1 - G_2|/|G_1| \) and \( \Delta \tilde{b}/\tilde{b} = |\tilde{b}_1 - \tilde{b}_2|/|\tilde{b}_1| \), where \( G_1 \) and \( \tilde{b}_1 \) are calculated with a 50-point wavevector grid, while \( G_2 \) and \( \tilde{b}_2 \) are obtained with a broader 26-point grid. Data illustrated in the figure refer to monolayer graphene at \( T = 300 \) K, with the choice of parameters discussed in the main text (\( \lambda = 3.8 \text{ eVÅ}^{-2}, \mu = 9.3 \text{ eVÅ}^{-2}, \kappa = 1 \text{ eV} \)). Dots illustrate the values of \( \Delta G/G \) and \( \Delta \tilde{b}/\tilde{b} \) at the points of the broader wavevector grid, which, by construction, coincide with a subset of \( q \)-points of the finer grid. The deviation between interpolating functions in the two data sets is illustrated by continuous lines. Overall, the maximum relative deviations between interpolating functions is \( 4 \times 10^{-3} \), while for points in the discrete grid, the maximum relative discrepancy is approximately \( 4 \times 10^{-4} \). In the long-wavelength limit, the deviation becomes approximately constant. Extracting the scaling exponents \( \eta \) and \( \eta_u \) from the first two points in the wavevector grids gives, for the 50-point and the 26-point data sets, the same exponent within an absolute deviation \( 3 \times 10^{-11} \). The amplitude ratio \( z_1^0/z_2 \simeq 0.1781321 \) (see the main text), extracted from the first two points in the grid, deviates by approximately \( 10^{-10} \) between 50- and 26-points sets. The amplitude \( z_1 \) of the scaling behavior deviates by less than \( 2 \times 10^{-4} \) in the two data sets. It should be noted, however, that the precision of calculations is limited by other sources of error. For example the tolerance of wavevector integrals is set to \( 1.49 \times 10^{-8} \) for \( k_y \)-integrals and to \( 10^{-7} \) for \( k_x \)-integrals.

SUPPLEMENTAL MATERIALS

Data sets illustrated in the main text are reported in the text files `data_set_1.txt` and `data_set_2.txt` (see Ancillary files). In particular, `data_set_1.txt` reports \( G_0(q), b_0(q), G(q), \) and \( b(q) \) for monolayer graphene at \( T = 300 \) K. As discussed in the main text, a logarithmic wavevector grid consisting of 50 wavevector points ranging between \( 10^{-7} \) and \( 110 \text{Å}^{-1} \) is used and integrations are performed by introducing a hard UV cutoff \( \Lambda = 100 \text{Å}^{-1} \). Data for bilayer graphene are calculated with an identical set of wavevector points, and by imposing the same cutoff \( \Lambda = 100 \text{Å}^{-1} \) on momentum integrations. Data obtained at \( T = 10K, T = 300K \) and \( T = 1500 \) K are collected in the text file `data_set_2.txt`.

In order to estimate the numerical inaccuracy due to discretization of the wavevector grid and the subsequent interpolation, correlation functions were recalculated using a broader wavevector grid consisting of 26 points. To facilitate comparison, the \( q \) grid was chosen in such way that the first 25 points coincide with a subset of wavevector points used in the finer grid. Results for monolayer and bilayer graphene are reported in `data_set_3.txt` and `data_set_4.txt`, respectively. A graphical comparison between data obtained with denser and broader grids is illustrated in Figs. 9 and 10.

Finally, Figs. 11 and 12 analyze the effect of a modified ultraviolet cutoff \( \Lambda \) on numerical results. Corresponding data are reported in files `data_set_5.txt` and `data_set_6.txt`. 
FIG. 10. Comparison between data sets calculated with 50-point and 26-point wavevector grids for bilayer graphene at (a) $T=10\text{K}$, (b) $T = 300 \text{ K}$, and (c) $T=1500\text{K}$. As in Fig. 9, the top and bottom panels in each figure illustrate the relative deviations $\Delta G/G$ and $\Delta \tilde{b}/\tilde{b}$ respectively, where $G_1$ and $\tilde{b}_1$ are calculated with a 50-point wavevector grid, while $G_2$ and $\tilde{b}_2$ are obtained with a broader 26-point grid. The maximum relative deviation of interpolating functions reaches 2%. However, the maximum error at the discrete sampling points is of the order of $10^{-3}$. For each of the three considered temperatures, taken separately, the estimated scaling exponents $\eta$ and $\eta_u$ deviate by an absolute discrepancy smaller than $5 \times 10^{-7}$ between 26-point and 50-point data sets. The discrepancy in amplitude ratios $z_1^2/z_2$ are instead smaller than $10^{-7}$. In the long-wavelength limit, the amplitude $z_1$ exhibit deviations of the order of $2 \times 10^{-4}, 6 \times 10^{-4}$, and $10^{-3}$ for the data sets at $T = 10, 300, $ and $1500 \text{K}$ respectively.

FIG. 11. Comparison between results for monolayer graphene using different UV cutoffs: $\Lambda = 100$ and $1000\text{Å}^{-1}$. Top and bottom panels illustrate, respectively $\Delta G/G = |G_1 - G_2|/G_1$ and $\Delta \tilde{b}/\tilde{b} = |\tilde{b}_1 - \tilde{b}_2|/\tilde{b}_1$ where $G_1$ and $\tilde{b}_1$ are calculated with $\Lambda = 100\text{Å}^{-1}$ while $G_2$ and $\tilde{b}_2$ are evaluated with a larger cutoff $\Lambda = 10^3\text{Å}^{-1}$. Calculations for $G_1$ and $\tilde{b}_1$ were performed using the 26-point data reported in data_set_3.txt. $G_2$ and $\tilde{b}_2$ were determined instead by using a grid of 29 wavevector points, extending between $10^{-7}$ and approximately $2.15 \times 10^3 \text{Å}^{-1}$. By construction, $q$ points in the two grids are identical in the common range. Evaluations at the discrete set of data points are illustrated by dots, whereas ratios of the corresponding interpolant functions are shown as continuous lines. Overall, the maximum relative deviations between between interpolant functions is smaller than $10^{-5}$. Extracting the scaling exponents and amplitudes from the first two wavevector points leads to the same values of $\eta$ and $\eta_u$ within less than $10^{-14}$ in the two data sets. For the amplitude ratio $z_1^2/z_2$, the discrepancy between values extracted from the two data sets is of the order of $2 \times 10^{-13}$. The numerical precision, however, is limited by other sources of error, such as the tolerance of integrations, which was set to a relative error of $1.49 \times 10^{-8}$ and $10^{-7}$ for inner and outer integrals.
FIG. 12. Comparison between results for bilayer graphene using different UV cutoffs: $\Lambda = 100$ and $1000\,\text{Å}^{-1}$. Panels (a), (b), and (c) correspond to $T = 10$, 300, and 1500 K respectively. As in Fig. 11, top and bottom panels illustrate $\Delta G/G = |G_1 - G_2|/G_1$ and $\Delta \tilde{b}/\tilde{b} = |\tilde{b}_1 - \tilde{b}_2|/\tilde{b}_1$ respectively, where $G_1$ and $\tilde{b}_1$ are calculated with $\Lambda = 100\,\text{Å}^{-1}$ while $G_2$ and $\tilde{b}_2$ are evaluated with $\Lambda = 10^3\,\text{Å}^{-1}$. Calculations for $G_1$ and $\tilde{b}_1$ were performed using the 26-point data reported in data set 4.txt. $G_2$ and $\tilde{b}_2$ were determined instead by using an extended grid of 29 wavevector points, ranging between $10^{-7}$ and approximately $2.15 \times 10^3\,\text{Å}^{-1}$. The wavevector grids are constructed in such way that $q$ points in the two data sets are identical in the common range. Evaluations at the discrete set of data points are illustrated by dots, whereas ratios of the corresponding interpolant functions are shown as continuous lines. Overall, the maximum relative deviations between between interpolant functions is smaller than $10^{-5}$. Exponents and the amplitude ratio $z_1^2/z_2$ were extracted as explained above (see captions of Figs. 9, 10, 11). For each of the three considered temperatures, deviations of $\eta$ and $\eta_u$ between data with $\Lambda = 100\,\text{Å}^{-1}$ and $\Lambda = 1000\,\text{Å}^{-1}$ are less than $10^{-10}$. The discrepancy of the corresponding amplitude ratios $z_1^2/z_2$ is within $2 \times 10^{-12}$. The numerical precision, however, is limited by other sources of error, such as the tolerance of integrations, which was set to a relative error of $1.49 \times 10^{-8}$ and $10^{-7}$ for inner and outer integrals.