Comment on ”Elastic constants from microscopic strain fluctuations”
Gwennou Coupier, Claudine Guthmann, Michel Saint Jean

To cite this version:


HAL Id: hal-00634266
https://hal.archives-ouvertes.fr/hal-00634266
Submitted on 20 Oct 2011

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L’archive ouverte pluridisciplinaire HAL, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d’enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.
Comment on “Elastic constants from microscopic strain fluctuations”

Gwennou Coupier,1,∗ Claudine Guthmann,2 and Michel Saint Jean2
1Laboratoire de Spectrométrie Physique, CNRS-UMR 5588, Université Grenoble I, BP 87, 38402 St. Martin d’Hères Cedex, France
2Laboratoire Matière et Systèmes Complexes, CNRS-UMR 7057, Université Paris 7, 10 rue Alice Domon et Léonie Duquet, 75205 Paris Cedex 13, France

(Received 11 May 2009; published 13 January 2010)

Sengupta et al. [Phys. Rev. E 61, 1072 (2000)] presented an elegant and simple finite-size scaling method for the calculation of elastic constants and their corresponding correlation lengths, which is suitable for many finite discrete systems considered through simulations or experiments. We take into account a mathematical finite-size effect that was neglected by the authors in order to propose a more accurate method. Consequences on the authors’ results are also discussed.

DOI: 10.1103/PhysRevE.81.013101 PACS number(s): 62.20.D−, 05.20.–y, 05.10.Cc

I. INTRODUCTION

Considering nonlocal elasticity effects is a central point in the study of disordered systems such as granular matter or foams, where small scales are easily observable, as pointed out in numerous recent papers [1–4]. But at small scale, even a well-ordered solid cannot be simply described in the standard continuous framework, where strain is simply proportional to stress at each point. Nonlocal effects must also be taken into account, that are due in particular to nonlocal interactions between the basic components of the solid, while derivation of standard continuous elasticity laws requires the hypothesis of surface contact forces between elementary volumes. Coherently, the associated length scale ξ is generally of the same order as the distance between these components [5–7]. However, quantitative methods allowing the determination of the correlation length ξ are seldom proposed in the literature.

In their paper entitled “Elastic Constants from microscopic fluctuations,” Sengupta et al. presented a versatile method to determine the elastic constants of a solid in the thermodynamic limit from the measurements of the fluctuations of the local strain tensor in a solid of finite size, when due to finiteness the strain can only be measured at small scale, where ξ is not negligible [8]. More precisely, they consider the fluctuations of the strain averaged over sub-boxes of varying sizes and compare it to a theoretical function in order to get the elastic constants and their associated correlation lengths. To calculate this function, they introduce a strain gradient in the elastic free energy in order to take into account non-local effects. In their derivation, they neglected some mathematical finite-size effects that slightly modify the determination of the elastic constants but greatly modify the estimation of correlation lengths.

II. MODIFICATION OF THE THEORETICAL CORRELATION FUNCTION

In chapter II, the authors consider a very general two-dimensional (2D) system of size \( L \times L \) described by a scalar order parameter \( \phi(r) \) and calculate the fluctuations of its averages over sub-blocks of size \( L_0 \times L_0 \). The function that is found is used to fit data obtained from simulations in order to find the susceptibility and the correlation length associated to this parameter. In case this parameter \( \phi \) is a component of the strain tensor, the susceptibility is a function of the elastic constants.

For simplicity, we consider in the following \( \beta=(k_B T)^{-1} \approx 1 \). For an infinite system, the correlation function \( G(r) = \langle \phi(r) \phi(0) \rangle \) is given by its Fourier transform (Eq. 2 of Ref. [8]),

\[
G(q) = \chi \frac{1}{1 + (q \xi)^2},
\]

where \( \chi \) is the susceptibility and \( \xi \) the correlation length. This implies

\[
G(r) = \frac{\chi}{(2\pi)^2} \int_{\mathbb{R}^2} \frac{e^{iq \cdot r}}{1 + (q \xi)^2} dq
\]

\[
= \frac{\chi}{(2\pi)^2 \xi^2} \int_0^{\infty} k dk \int_0^{2\pi} \frac{e^{ik \cos \theta}}{r^2 / \xi^2 + k^2} d\theta,
\]

which corresponds exactly to Eq. 6 of Ref. [8].

The latter integral can be calculated for instance by Mathematica software, and it is found that

\[
G(r) = \frac{1}{2\pi} \chi \xi^{-2} K_0(r/\xi),
\]

where \( K_0 \) is a Bessel function, which is Eq. 8 of Ref. [8] even if a factor 4 is missing because of a typo. Note that it is considered here that the correlation function \( G(r, r') = \langle \phi(r) \phi(r') \rangle = G(|r - r'|) \) is invariant by translation, which is true for simulations with periodic conditions, or far enough from walls in an experiment.

An error is made in Eq. 4 of Ref. [8] when switching from double to single integration using this invariance by translation. The fluctuations of the parameter \( \phi \) averaged over a sub-block of size \( L_0 \times L_0 \) (\( \bar{\phi} = \frac{1}{L_0^2} \int_{L_0} \phi(r) dr \)) are considered,
Then, probably by considering the new variable \( r = r' - r \),
the authors write that the latter expression is equal to
\( \int_{L_0} G(r) \, dr \) or \( \int_{L_0} G(r)^2 \, dr \).
It is obviously approximate: when \( r \) and \( r' \) are
varying in their 2D boxes of size \( L_0 \), the variable \( r - r' \)
clearly takes much more often small values than large ones
within the box of size \( 2L_0 \). More precisely, we can consider
each dimension separately, and in one dimension we would have

\[
\int_0^{L_0} \int_0^{L_0} G(x-x') \, dx \, dx' = \int_0^{L_0} dx' \int_0^{x'} \int_0^{L_0} G(x-x') \, dx \, dx' + \int_0^{L_0} dx' \int_0^{L_0} G(x-x') \, dx \, dx'.
\]

(6)

In the first integral we consider \( u = x' - x \) and in the second
one \( u = x - x' \). Using the parity of \( G \), we get

\[
\int_0^{L_0} \int_0^{L_0} G(x-x') \, dx \, dx' = \int_0^{L_0} dx' \int_0^{x'} G(u) + \int_0^{L_0} dx' \int_0^{L_0-u} G(u) \, du
\]

\[
= \int_0^{L_0} G(u) \, du \int_0^{L_0} dx' + \int_0^{L_0} G(u) \, du \int_0^{L_0-u} \, dx'
\]

\[
= \int_0^{L_0} 2(L_0-u)G(u) \, du.
\]

(7)

As expected, more weight is given to the low \( u \) values.

Finally, back to our 2D problem, we get for an infinite
system, instead of Eq. 4 of Ref. [8],

\[
L_0^2(\partial_r^2) = 4 \int_0^{L_0} \int_0^{L_0} w_L(r)G(r) \, dr,
\]

(8)

where \( w_L(r) = (1 - \frac{r}{L_0})(1 - \frac{r}{L_0}) \).

Similarly, the constant \( \Delta_L \) that is introduced by the
authors in their Eq. (7) in order to take into account the finite-
ness of the system becomes

\[
\Delta_L = \frac{4}{L^2} \int_0^{L_0} w_L(r)G(r) \, dr.
\]

(9)

This finally modifies the central result of the authors,
which is given in Ref. [8] by Eq. (11),

\[
L_0^2(\partial_r^2) = \chi \left[ \frac{L}{\xi} \psi(x, \frac{L}{\xi}) - x^2 \psi \left( \frac{L}{\xi} \right) \right] = f_L(\xi, \chi, x),
\]

(10)

where \( x = \frac{L_0}{L} \) and

\[
\psi(\alpha) = \frac{2}{\pi} \alpha^2 \int_0^1 w_1(z)K_0(\alpha z) \, dz,
\]

(11)

to be compared with the function proposed by the authors in
their equation (10),

\[
\psi_{\text{Sengupta}}(\alpha) = \frac{2}{\pi} \alpha^2 \int_0^1 K_0(\alpha z) \, dz.
\]

(12)

The consequences of these corrections by the \( w_1(z) \) term
need to be discussed. In the case of elastic systems, note that
the authors have introduced a quadratic correction to Eq.
(10) (see Eq. 20 in Ref. [8]), but they do not give any indication
about the values of the associated free parameter \( C \), so we
are not able to discuss it. Without this term, we have
\( f_L(\xi, \chi, 1) = 0 \). In most of their curves, this is rather well
verified, so we can deduce that this correction is small and will
not greatly modify the discrepancies presented in the next
paragraphs.

III. CONSEQUENCES ON THE ESTIMATION OF \( \chi \) AND \( \xi \)

We will now check that the modified function \( \psi \) still allows
description of the data presented in Ref. [8] and then
discuss how it influences the determination of the unknown
constants. Since we do not know these data, but since they
are well fitted by the function proposed by Sengupta et al., it
is equivalent to fit the curves obtained with the function
\( \psi_{\text{Sengupta}} \) using our modified function \( \psi \), and it should give
a good estimate of the errors made with their method. To do
this, we consider systems similar to the one considered in
Ref. [8]: Sengupta et al. ran simulations with up to 12 000
particles so that \( L \leq \sqrt{12000} \approx 110 \), where \( a_0 \)
is the lattice spacing. In the conclusion they indicate that \( \xi \approx 2
- 3 \), so \( L/\xi \leq 55 \). Finally, taking \( \xi = 1 \) as our length scale,
we consider the curves \( x f_L(\xi, \chi, x) \) as a function of \( x = L_0/L \)
(this choice of axes was made by the authors in most of their
figures) using the function \( \psi_{\text{Sengupta}} \) with \( \chi = 1 \) and \( 3 \leq L \)
\leq 55, and make a fit of them using our function \( \psi \). Results
are shown in Fig. 1.

The curve of their fitting function is well fitted by ours, so
we can deduce our new function would be able to describe
well defined and our correction should allow to determine much more precisely the elastic constants of the infinite solid.

The accuracy on the determination of the correlation length $\xi$ is greatly enhanced by our corrections: using $\psi_{\text{Sengupta}}$, overestimation is systematic, already of order 100% as soon as $L \approx 5$, and one order of magnitude is lost when $L = 50$. In particular, in Fig. 4 of Ref. [8], we can expect that these overestimations for $\xi$ would increase the discrepancy with theory. For the elastic systems considered by the authors, the correlation lengths would be finally lower than one lattice parameter (since they found $\xi \approx 2 - 3 \, a_0$). This is in qualitative agreement with the results of Maranganti and Sharma, who found that the length scale at which classical elasticity breaks down in simple solids is lower than the lattice spacing [6]. These errors in the determination of $\xi$ were probably not noticed by the authors because, unlike elastic constants, values for $\xi$ were not (and are still not) well documented in the literature. Moreover, it was not the main point of this paper. But it was important to propose a correction for $\psi$, since their method is also a simple method to determine $\xi$, with direct calculation in real space (no Fourier transform), even though calculation of the strain tensor is not that simple in such a discrete system, as noticed by the authors in their conclusion.

Finally, we have modified the method proposed by Sengupta et al. by taking into account mathematical finite-size effects that cannot be neglected. We found that this modification is necessary to determine accurately elastic constants in small systems and corresponding correlation lengths for systems of any size. We believe that their versatile method deserves to be more often tested on several ordered systems, but also on disordered ones, where discussions on nonlocal effects are central. In that latter case, a different free energy might be necessary to take into account the fact that the nonzero correlation length comes from inhomogeneities but not necessarily from nonzero interaction distance, as in granular systems.