Comment on "Elastic constants from microscopic strain fluctuations"

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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.

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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 subboxes 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 $\phi(\mathbf{r})$ and calculate the fluctuations of its averages over sub-blocks of size $L_b\times L_b$. 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 ϕ is a component of the strain tensor, the susceptibility is a function of the elastic constants.

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

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

where χ is the susceptibility and ξ the correlation length. This implies

$$G(r)=\frac{\chi}{(2\pi)^2}\int_{\mathbb{R}^2}\frac{e^{i\mathbf{q}\cdot\mathbf{r}}}{1+(q\xi)^2}d\mathbf{q} \tag{2}$$

$$=\frac{\chi}{(2\pi)^2\xi^2}\int_0^\infty kdk\int_0^{2\pi}\frac{e^{ik\cos\theta}}{r^2/\xi^2+k^2}d\theta, \tag{3}$$

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

$$G(r)=\frac{1}{2\pi}\chi\xi^{-2}K_0(r/\xi), \tag{4}$$

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 $G(\mathbf{r},\mathbf{r}')=\langle\phi(\mathbf{r})\phi(\mathbf{r}')\rangle=G(\mathbf{r}-\mathbf{r}')$ 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 ϕ averaged over a sub-block of size $L_b\times L_b$ ($\bar{\phi}=L_b^{-2}\int_{L_b}\phi(\mathbf{r})d\mathbf{r}$) are considered,

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$$L_b^2\langle\bar{\phi}^2\rangle = L_b^{-2}\int_{L_b}\int_{L_b} G(\mathbf{r}-\mathbf{r}')d\mathbf{r}d\mathbf{r}'. \tag{5}$$

Then, probably by considering the new variable $\mathbf{r}=\mathbf{r}-\mathbf{r}'$ the authors write that the latter expression is equal to $\int_{L_b} G(\mathbf{r})d\mathbf{r}$. It is obviously approximate: when $\mathbf{r}$ and $\mathbf{r}'$ are varying in their 2D boxes of size L_b, the variable $\mathbf{r}-\mathbf{r}'$ clearly takes much more often small values than large ones within the box of size $2L_b$. More precisely, we can consider each dimension separately, and in one dimension we would have

$$\int_0^{L_b}\int_0^{L_b} G(x-x')dxdx' = \int_0^{L_b} dx' \int_0^{x'} G(x-x')dx + \int_0^{L_b} dx' \int_{x'}^{L_b} G(x-x')dx. \tag{6}$$

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

$$\begin{aligned}
&\int_0^{L_b}\int_0^{L_b} G(x-x')dxdx' \\
&= \int_0^{L_b} dx' \int_0^{x'} G(u)du + \int_0^{L_b} dx' \int_0^{L_b-x'} G(u)du \\
&= \int_0^{L_b} G(u)du \int_u^{L_b} dx' + \int_0^{L_b} G(u)du \int_0^{L_b-u} dx' \\
&= \int_0^{L_b} 2(L_b-u)G(u)du.
\end{aligned} \tag{7}$$

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],

$$L_b^2\langle\bar{\phi}^2\rangle = 4\int_0^{L_b}\int_0^{L_b} w_{L_b}(\mathbf{r})G(\mathbf{r})d\mathbf{r}, \tag{8}$$

where $w_{L_b}(\mathbf{r})=(1-\frac{x}{L_b})(1-\frac{y}{L_b})$.

Similarly, the constant Δ_L that is introduced by the authors in their Eq. (7) in order to take into account the finiteness of the system becomes

$$\Delta_L = \frac{4}{L^2}\int_L w_L(\mathbf{r})G(\mathbf{r})d\mathbf{r} \tag{9}$$

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

$$L_b^2\langle\bar{\phi}^2\rangle = \chi\left[\psi\left(x\frac{L}{\xi}\right) - x^2\psi\left(\frac{L}{\xi}\right)\right] \equiv f_L(\xi,\chi,x), \tag{10}$$

where $x=\frac{L_b}{L}$ and

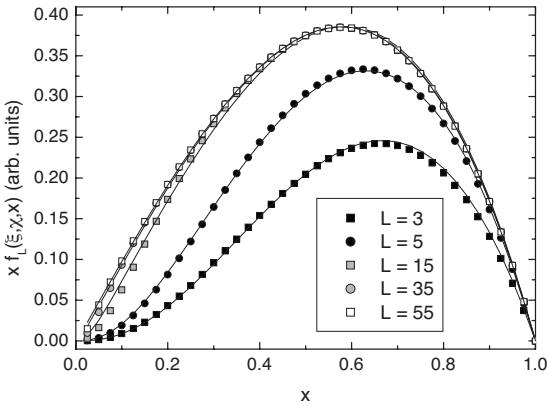

FIG. 1. Theoretical curves for $xf_L(\xi,\chi,x)$ as a function of $x=L_b/L$ for different L. Symbols: using ψ_{Sengupta} (Eq. (12)) with $\chi=1$ and $\xi=1$. Full lines: fits with the proposed ψ (Eq. (11)).

$$\psi(\alpha) = \frac{2}{\pi}\alpha^2\int_1 w_1(\mathbf{z})K_0(\alpha z)d\mathbf{z}, \tag{11}$$

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

$$\psi_{\text{Sengupta}}(\alpha) = \frac{2}{\pi}\alpha^2\int_1 K_0(\alpha z)d\mathbf{z}. \tag{12}$$

The consequences of these corrections by the $w_1(\mathbf{z})$ 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 χ AND ξ

We will now check that the modified function ψ 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 ψ_{Sengupta} using our modified function ψ, 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 $L\lesssim\sqrt{12\,000}\ a_0\simeq 110\ a_0$, where a_0 is the lattice spacing. In the conclusion they indicate that $\xi\simeq 2-3\ a_0$, so $L/\xi\lesssim 55$. Finally, taking $\xi=1$ as our length scale, we consider the curves $xf_L(\xi,\chi,x)$ as a function of $x=L_b/L$ (this choice of axes was made by the authors in most of their figures) using the function ψ_{Sengupta}, with $\chi=1$ and $3\leq L\leq 55$, and make a fit of them using our function ψ. Results are shown on 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

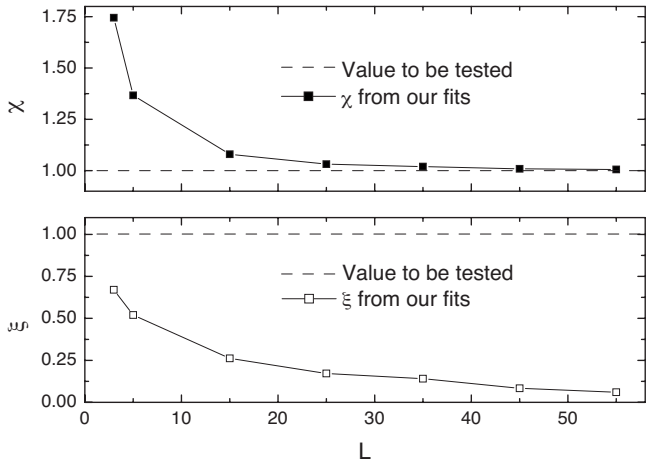

FIG. 2. Values for χ and ξ found with our function ψ, to be compared with the values $\chi=1$ and $\xi=1$ that would be found with function ψ_{Sengupta}, for different system sizes L.

the data considered by the authors. However, our procedure does not yield the same parameters, as shown on Fig. 2.

It appears that in Ref. [8], χ was systematically underestimated, therefore the elastic constants overestimated, since χ scales as their inverse. However, this underestimation of χ drops below 10% for a large enough (but still rather small) system ($L \gtrsim 15$). This is probably why the authors have not noticed their errors, since in addition their fits were good and yield good agreement with values calculated with other methods. In other papers based on Sengupta *et al.*'s method [9–13], the results will even not be modified at all, since they focus only on elastic constants and use the property $\lim_{x\to 0} x f_L(\xi,\chi,x)=\chi$, which does not require any knowledge on ξ, and remains true after our modifications $[\lim_{\alpha\to 0} \psi(\alpha)=\lim_{\alpha\to 0} \psi_{\text{Sengupta}}(\alpha)=1]$. However, in some experiments or simulations, the number of particles can be rather low, thus L small, and in such case the latter limit less 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 ξ is greatly enhanced by our corrections: using ψ_{Sengupta}, overestimation is systematic, already of order 100% as soon as $L \gtrsim 5$, and one order of magnitude is lost when $L \simeq 50$. In particular, in Fig. 4 of Ref. [8], we can expect that these overestimations for ξ 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 $\xi \simeq 2-3\ a_0$). 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 ξ were probably not noticed by the authors because, unlike elastic constants, values for ξ were not (and are still not) well documented is the literature. Moreover, it was not the main point of this paper. But it was important to propose a correction for ψ, since their method is also a simple method to determine ξ, 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.

[1] C. Goldenberg, A. P. F. Atman, P. Claudin, G. Combe, and I. Goldhirsch, Phys. Rev. Lett. **96**, 168001 (2006).
[2] C. E. Maloney, Phys. Rev. Lett. **97**, 035503 (2006).
[3] C. Goldenberg, A. Tanguy, and J.-L. Barrat, EPL **80**, 16003 (2007).
[4] F. Léonforte, A. Tanguy, J. P. Wittmer, and J.-L. Barrat, Phys. Rev. Lett. **97**, 055501 (2006).
[5] X. Zhang and P. Sharma, Phys. Rev. B **72**, 195345 (2005).
[6] R. Maranganti and P. Sharma, Phys. Rev. Lett. **98**, 195504 (2007).
[7] K. Franzrahe, P. Keim, G. Maret, P. Nielaba, and S. Sengupta, Phys. Rev. E **78**, 026106 (2008).
[8] S. Sengupta, P. Nielaba, M. Rao, and K. Binder, Phys. Rev. E **61**, 1072 (2000).
[9] S. Sengupta, P. Nielaba, and K. Binder, Phys. Rev. E **61**, 6294 (2000).
[10] K. Zahn, A. Wille, G. Maret, S. Sengupta, and P. Nielaba, Phys. Rev. Lett. **90**, 155506 (2003).
[11] K. Franzrahe *et al.*, Comput. Phys. Commun. **169**, 197 (2005).
[12] A. Ricci, P. Nielaba, S. Sengupta, and K. Binder, Phys. Rev. E **74**, 010404(R) (2006).
[13] K.-Q. Zhang and X. Y. Liu, Langmuir **25**, 5432 (2009).