Rigorous solution for the elasticity of diluted Gaussian spring networks

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We present a rigorous solution of the elasticity of the diluted Gaussian spring networks (DGSNs) at zero temperature. We show that the deformation of a diluted DGSN is homogeneous provided that the displacements of the particles on the boundary are homogeneous. It follows that at zero temperature the nonvanishing elastic stiffness coefficients are proportional to the hydrostatic pressure in both two and three dimensions. Follows a rigorous proof of the equivalence of the elasticity of the DGSN and the conductance of the random resistor network at zero temperature.

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The elasticity of the diluted Gaussian spring networks (DGSNs), in which the particles interact with their nearest neighbors via the potential $\Phi(r)=\frac{1}{2}kr^2$, where r is the distance between particles, is a very important issue not only because it is the common limit of various systems under strong tension but also because it is equivalent to some other interesting systems, such as the random resistor network (RRN) [1]. It is believed that the elasticity of the DGSN has the same critical behavior as the conductance σ of the RRN and so can serve as a standard model system. However, a complete and rigorous solution of this equivalence is still elusive. In this note we show that at zero temperature (T) and with trivial boundary conditions, the nonvanishing elastic stiffness coefficients, which govern the elastic property of a stressed system [2–8], are proportional to the stress in both two and three dimensions at any concentration. As a consequence, we provide a complete and rigorous proof that the elasticity of the DGSN has exactly the same behavior as σ at any concentration. In contrast, the traditional elastic constants, which are the second derivatives of the free energy with respect to strain [2–8] and are also often confused with the elastic stiffness coefficients, are all identical to zero at $T=0$ and therefore play no role in the model system. Since the behavior of the conductance of the RRN is well known, our results provide a complete solution of the elasticity of the DGSN at $T=0$.

In a very influential letter in 1976 [9], de Gennes argued that the RRN and a diluted elastic network in which particles interact through isotropic forces are in the same universality class. More precisely, if σ vanishes at the geometric percolation concentration p_c as $\sigma \sim (p-p_c)^t$ and the elastic modulus of an elastic network $\sim (p-p_c)^f$ then the prediction is $f=t$. Since then, extensive work has been done to investigate whether the same conclusion can be drawn for other systems [10–13]. It has been shown, for instance, that at $T=0$ upon dilution, a tension-free network of particles interacting only through central two-body forces generically loses its ability to withstand shear at a concentration of particles p_r that is higher than the p_c. On the other hand, recent works suggest that at finite T the shear modulus of a diluted central force system has the same critical behavior as σ in the RRN [14–16]. Noting that in many cases a finite T plays a role similar to a finite stress, it is natural to think that an elastic network under tension may have a different critical behavior from the tension-free one. An intriguing question is then in what stressed elastic network is de Gennes' prediction valid exactly? It was in general believed that a simple analog between Kirchhoff's laws for a resistor network and the force balance conditions for the elastic network or the analog of energy functions between the two systems leads directly to a rigorous proof of de Gennes' prediction in the Gaussian spring network which is always stressed. However, a close examination of this argument shows ([1] and also in the following text) that such an analog in fact leads to the conclusion that the hydrostatic pressure P (positive for compression), but not the elastic stiffness coefficients, has the same behavior as σ. Since in general pressure does not even have the same critical point as the elastic stiffness coefficients such as in the tension-free state, to prove de Gennes' prediction in the DGSN it is necessary to study the relationship between the pressure and the elastic stiffness coefficients. In this paper we resolve this issue completely.

The proof for de Gennes' prediction in a tension-free isotropic force system is simple but instructive for the DGSN. Image a lattice with bonds of conductivity σ_{ij} connecting nearest neighbors sites i and j, Kirchhoff's law requires that

$$\sum_i \sigma_{ij}(U_i-U_j)=0 \text{ or } \sum_i I_{ij}=0, \tag{1}$$

where U_i is the voltage at the lattice site i and I_{ij} the current between sites i and j. But these equations are identical to the force balance equation

$$\sum_i \mathbf{f}_{ij}=\mathbf{0} \text{ or } \sum_i k_{ij}(\mathbf{R}_i-\mathbf{R}_j)=\mathbf{0}, \tag{2}$$

for an elastic network with energy $E=\frac{1}{2}\Sigma_{i<j}k_{ij}(\mathbf{R}_i-\mathbf{R}_j)^2$ (the isotropic Born model [9,10,17]) where k_{ij} corresponding to σ_{ij} now represents a set of spring constants and $\mathbf{R}_i$ is the displacement of the ith particle from its tension-free position.

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Explicitly, $\mathbf{R}_i = \mathbf{r}_i - \mathbf{R}_i^0$ where $\mathbf{r}_i$ is the coordinate of the ith particle and $\mathbf{R}_i^0$ the coordinate of particles in the tension-free state. It is clear that there is a one-to-one correspondence between the quantities in the two systems

$$I_{ij} \leftrightarrow f_x \text{ or } f_y \text{ or } f_z,$$

$$U_i - U_j \leftrightarrow X_i - X_j \text{ or } Y_i - Y_j \text{ or } Z_i - Z_j.$$

For the whole system, we have for the RRN: $I = GU$, where I is the macroscopic current, U is the macroscopic voltage drop, $G = \sigma L_0^{d-2}$ [1] is the macroscopic conductivity with d the dimension of the system and L_0 is the length of the undeformed system with the assumption that all directions have the same size for simplicity. Correspondingly for the elastic network

$$F = K' \delta L$$

and so

$$S = \frac{K' \delta L}{L_0^{d-1}} = \frac{K'}{L_0^{d-2}} \cdot \frac{\delta L}{L_0} = \frac{K'}{L_0^{d-2}} \epsilon = K\epsilon, \tag{3}$$

with $K = K'/L_0^{d-2}$, where F is a component of the total force on the boundary, δL is the corresponding deformation of the system, S is a component of the stress (negative for compression and $= -P$), and $\epsilon = \delta L/L_0$ is a macroscopic strain determined by the deformation. The uniqueness of the solution and the one-to-one correspondence between the two systems guarantee that K, the elastic constant, must have the same behavior as σ at all concentrations.

There is an important subtlety in this mapping associated with the boundary conditions [1]. In the RRN the net current flow can be in arbitrary directions so that G_α ($\alpha = x$, y, and z) can be obtained separately. However, in the spring problem, the frame acts equally in all Cartesian directions so that K'_α or K_α are strongly correlated. This is not a concern for high symmetry networks where $K'_x = K'_y = K'_z$. We shall follow Ref. [1] and refer to such networks as electrically isotropic. These are the only networks that we shall discuss in this work. This class of system includes square networks, triangular networks and cubic networks, either undiluted or randomly diluted. We should point out that there are in general three independent elastic constants in the square and cubic lattices so that their elastic properties are not in general isotropic. We also assume for convenience that the system has the shape of a hypercube. Note that the deformation δL is arbitrary, so we can conclude that all nonvanishing elastic constants should have the same critical behavior as σ.

It is clear that the above arguments can be applied only to a system with a tension-free reference (undeformed) state because $\mathbf{R}_i$ is measured from the tension-free state as is ϵ. Consequently, ϵ is finite and may be large for a state under tension. However, in this case in general Eq. (3) fails because the relationship between stress and δL (or ϵ) is no longer linear. For instance, a uniform dilation from the tension-free volume V_0 to V leads to $S = \int_{V_0}^{V} [B(V)/V] dV$, where B is the bulk modulus. In the simplest case of B being independent of V, we get $S = B \ln(V/V_0)$ but it can be reduced into Eq. (3) only if $(V - V_0)/V_0 \ll 1$. Therefore, the validation of de Gennes' prediction for a strongly stressed isotropic Born model is not self-evident. Equation (3) together with these explanations do not seem to be available in the literature.

It has been shown [1] that in DGSN P has the same behavior as σ. This can be understood by noting that the force balance equation in the system is

$$\sum_i k_{ij}(\mathbf{r}_i - \mathbf{r}_j) = \mathbf{0}, \tag{4}$$

and so the one-to-one correspondences between the two systems are

$$I_{ij} \leftrightarrow f_x \text{ or } f_y \text{ or } f_z$$

and

$$U_i - U_j \leftrightarrow x_i - x_j \text{ or } y_i - y_j \text{ or } z_i - z_j. \tag{5}$$

It follows that in the DGSN,

$$F = K'L = \frac{K'}{L^{d-2}} L^{d-1} = SL^{d-1}, \tag{6}$$

and S, the stress instead of any elastic constant, must have the same behavior as σ. More exactly, S must be proportional to σ at any concentration.

The elastic stiffness coefficients $c_{\alpha\beta\sigma\tau}$, which govern stress-strain relations are defined by

$$S_{\alpha\beta}(\eta) = S_{\alpha\beta}(0) + c_{\alpha\beta\sigma\tau}\eta_{\sigma\tau} \tag{7}$$

for a system without internal torques [2–5], where $S_{\alpha\beta}(0)$ is the stress of the reference state and $\eta_{\alpha\beta}$ the Lagrangian strain tensor [2,3,7].

For a central force system the stress tensor and the isothermal elastic stiffness coefficients can be calculated from [5]

$$S_{\alpha\beta} = \frac{1}{V}\left\langle \sum_{i<j} r_\alpha(ij) r_\beta(ij) \frac{\Phi'}{r_{ij}} \right\rangle - \frac{Nk_BT}{V}\delta_{\alpha\beta}, \tag{8}$$

$$\begin{aligned} c_{\alpha\beta\sigma\tau} = {} & \frac{1}{V}\left\langle \sum_{i<j} r_\alpha(ij) r_\beta(ij) r_\sigma(ij) r_\tau(ij) \frac{1}{r_{ij}^2}\left(\Phi'' - \frac{\Phi'}{r_{ij}}\right)\right\rangle \\ & - \frac{1}{k_BTV}\left\langle \Delta\left(\sum_{i<j} r_\alpha(ij) r_\beta(ij) \frac{\Phi'}{r_{ij}}\right) \right. \\ & \left. \times \Delta\left(\sum_{i<j} r_\sigma(ij) r_\tau(ij) \frac{\Phi'}{r_{ij}}\right)\right\rangle - \frac{1}{2}(2S_{\alpha\beta}\delta_{\sigma\tau} - S_{\alpha\sigma}\delta_{\beta\tau} \\ & - S_{\alpha\tau}\delta_{\beta\sigma} - S_{\beta\tau}\delta_{\alpha\sigma} - S_{\beta\sigma}\delta_{\alpha\tau}) \\ & + \frac{Nk_BT}{V}(\delta_{\alpha\sigma}\delta_{\beta\tau} + \delta_{\alpha\tau}\delta_{\beta\sigma}), \end{aligned} \tag{9}$$

where $\langle \cdots \rangle$ designates ensemble averages, $\Delta(A) = A - \langle A \rangle$, $r_\alpha(ij) = r_{i\alpha} - r_{j\alpha}$, and $r_{ij}^2 = (\mathbf{r}_i - \mathbf{r}_j)^2$.

Equations (8),(9) are valid in both $d = 2$ and $d = 3$, at any T and under arbitrary stress. At $T = 0$, for a homogeneously deformed system such as a perfect lattice with only one particle in the primitive cell, we can simply remove the ''fluctuation term,'' i.e., the second term in Eq. (9) and set $T=0$. However, for the lattice with more than one particle in the primitive cell or in our case the diluted lattice, at $T=0$ the ''fluctuation term'' tends to a limit called the ''relaxation'' term [18]. This ''relaxation'' term arises from the requirement of mechanical equilibrium that the total force on *each* particle be zero. As a consequence, there may be local rearrangements of the particles [18] and therefore the displacement is in general not homogeneous *everywhere*. The ''relaxation'' term is complex and is in general non-negligible. For instance, for a central force system, this term is non-vanishing and is comparable to the first term (''Born term'') in Eq. (9) at the critical point [19]. Therefore, to go further we have to check in a Gaussian system whether the homogeneous displacement guarantees the mechanical equilibrium of every particle.

Under a homogeneous deformation, the displacement of a point initially at $\mathbf{r}_i^0$ can be written as [2,3,6–8]

$$u_{i\alpha}(\mathbf{r}_i^0)=r_{i\alpha}(\mathbf{r}_i^0)-r_{i\alpha}^0=\sum_{\beta=1}^{d} u_{\alpha\beta}r_{i\beta}^0, \quad \alpha=1,2,\ldots,d, \tag{10}$$

where $u_{\alpha\beta}$ are constants everywhere. Requiring mechanical equilibrium in the reference state of the Gaussian system gives

$$F_{i\alpha}^0=\sum_j k_{ij}(r_{i\alpha}^0-r_{j\alpha}^0)=0. \tag{11}$$

After a homogeneous displacement, Eqs. (10),(11) lead to

$$F_{i\alpha}=\sum_j k_{ij}(r_{i\alpha}-r_{j\alpha})=F_{i\alpha}^0+\sum_{\beta=1}^{d} u_{\alpha\beta}F_{i\beta}^0=0. \tag{12}$$

Therefore in the DGSN, for an initially mechanically stable state, homogeneous displacement guarantees mechanical equilibrium after deformation. In other words, all particles in the system will be subjected to a homogeneous displacement provided that the displacements on the boundary are homogeneous. This boundary condition is trivial and is weaker than the one required for Eq. (3) since it allows the system to be anisotropic.

With the above result, it is easy to find the relation between elastic stiffness coefficients and stress tensor. Henceforth we focus on the system subjected to hydrostatic pressure since it is the most interesting case. First, from Eq. (8) the pressure is

$$P=-\frac{1}{dV}\sum_{i<j} k_{ij}r_{ij}^2=-\frac{1}{dV^{1-2/d}}\sum_{i<j} k_{ij}q_{ij}^2, \tag{13}$$

where the $\mathbf{q}_i=\mathbf{r}_i/L$ are scaled coordinates and must remain constant in a uniform dilation. It follows immediately that the pressure in $d=2$ for any lattice is independent of the size of the system, in agreement with Ref. [1]. As a consequence, B must be zero since a uniform dilation costs no (Gibbs') free energy. B can also be obtained from $B=-V(dP/dV)=(1-2/d)P\leqslant 0$. It gives again $B=0$ in $d=2$ at *any* concentration.

We can find every elastic stiffness coefficient in this way by applying to the system different kinds of homogeneous deformation. However, an equivalent but simple way is to use Eq. (9) by removing the ''fluctuation term'' and set $T=0$. The ''Born term'' in Eq. (9) vanishes so that all elastic stiffness coefficients are proportional to the pressure and therefore there is only one independent elastic stiffness coefficient. In the condensed Voigt notation [2,3,7], we have

$$c_{11}=c_{22}=c_{33}=\mu=c_{44}=c_{55}=c_{66}=-P, \tag{14}$$

$$c_{12}=c_{21}=c_{13}=c_{31}=c_{23}=c_{32}=P, \tag{15}$$

$$c_{\alpha\beta}=0 \text{ otherwise.} \tag{16}$$

where μ is the shear modulus. Equations (14),(15) give $B=(1-2/d)P$ again. Equations (14)–(16) complete the proof that the elasticity of the DGSN has exactly the same behavior at all concentrations as σ, or in other words, c_{ij} must be proportional to σ at any concentration. It is also interesting to note that for the high symmetry DGSN, which are electrically isotropic, $c_{11}-c_{12}=-2P=2\mu$. This means that the DGSN are elastically isotropic, and only two elastic constants are required. This is quite remarkable since Gaussian networks encompass diluted square and cubic lattices which in general are not isotropic, as mentioned earlier. For this reason this elastic isotropy has to be considered as ''accidental.'' We should emphasize again that these results are based on the homogeneity of the displacements in these networks.

It is interesting to note that at $T=0$ the traditional elastic constants consist of only the ''Born term'' [5] and therefore are equal to zero for the DGSN. It is another illustration of the fact that the traditional elastic constants are not the quantities which determine the elasticity of a system under tension [2–5]. We should also point out that the relationship between $c_{\alpha\beta}$ and the stress tensor can be easily derived in the same way for anisotropically stressed systems. For instance, $c_{11}=-c_{12}=-c_{13}=S_{11}$, $c_{44}=\frac{1}{2}(S_{22}+S_{33})$, etc.

Since the DGSN is a limiting case of the isotropic Born model, it is reasonable to think that at arbitrary tension, the μ of the Born model has the same critical behavior as σ. Meanwhile, because the DGSN is also the infinite tension limit of the central force system, it is clear that the critical behavior of the $c_{\alpha\beta}$'s of the central force network must depend on the tension. A previous work focusing on the displacement gradient moduli [20] made this point, though a convincing conclusion should be drawn from the investigation of the behavior of $c_{\alpha\beta}$ which describes the elasticity more precisely.

At finite T, the P of the DGSN still has the same behavior as σ. To show this we need only to replace the quantities appearing in Eqs. (4)–(6) by their ensemble averages. It is also easy to show, since the interparticle interactions are completely separable, that Eqs. (15) and (16) are still satisfied for DGSN. A direct consequence is that for an isotropic system $B=\mu+P$ in $d=2$ and $B=(3\mu+2P)/3$ in $d=3$. We can also expect that the critical points at finite T remain the same as at $T=0$ since entropy favors rigidity [14–16]. However, it is not easy to find a rigorous relationship between the $c_{\alpha\beta}$ and P at finite T even for a perfect lattice.

In summary, we completely solve the problem of the elasticity of the DGSN at $T=0$. We show that at $T=0$ the displacement of the particles in the diluted DGSN is homogeneous provided a trivial boundary condition is imposed, i.e., the displacements of the particles on the boundary are homogeneous. As a consequence, the bulk modulus is zero at any concentration for a two-dimensional system and those nonvanishing elastic stiffness coefficients are proportional to the stress in both two and three dimensions. This proves *completely* and rigorously that the elasticity of the DGSN has exactly the same behavior as σ at *any concentration*. In contrast, the traditional elastic constants are all identically equal to zero. Moreover, the elasticity of all electrically isotropic DGSN (i.e., all high symmetry networks) under hydrostatic pressure are ''by accident'' isotropic. Our results may also shed light on the tight-binding Hamiltonian and spin waves in a Heisenberg ferromagnet at low T since it has been shown that these three systems are equivalent [1]. Finally, our conclusions hold for either the bond or site percolation problem.

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