Strength of disordered solids

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The response of a bond-diluted elastic network, when it is subjected to an external stress, is discussed. For low-bond-dilution concentration, the statistics of lattice animals can provide a measure of the strength (fracture stress) of such a system and lead to the conventional Weibull form for the flaw distribution function $g(\sigma)$. Near the percolation threshold p_c of the system, we use the "node-link-blob" model of the percolation cluster to study the critical behavior of the strength of such a bond-diluted elastic network. As $p \to p_c$, strength goes to zero with the critical exponent T'. A scaling relation for T' is obtained, which is exact for dimension $d \geq 6$ and gives a lower bound for $d < 6$. Agreement of the scaling relation with experimental results are discussed. Finally we present a Monte Carlo renormalization-group (MCRG) study in a very simplistic elastic model in $d = 2$ dimensions, along with a straightforward Monte Carlo simulation (MCS) for the elastic response and strength of the same model system of size 50×50. The elastic exponent T and the fracture exponent T', obtained for the model either from MCRG or from MCS, are in perfect conformity (within the limit of statistical errors) with our scaling relation.

I. INTRODUCTION

It has been known for quite a long time that defects play a very crucial role in determining the mechanical properties of a system. Griffith, as early as 1920, pointed out (see p. 5 of Ref. 1) that defects, in the form of very narrow atomically sharp (micro) flaws, act like stress concentrators (concentrating stresses at the sharp notches of the flaw) and are the chief cause for the characteristic low load-bearing capacity of brittle materials like ceramics, glass, etc. He also gave a formula for the variation of the strength of a system with the variation of the dimension (length) of such a sharp flaw. According to Griffith, the equilibrium extension of a flaw is governed by a balance between the mechanical energy released and surface energy gained, as the flaw propagates. This energetics of flaw propagation gives the Griffith's instability condition (see Ref. 1)

$$\sigma_c = \left[\frac{2\gamma Y}{\pi c} \right]^{1/2} \equiv \left[\frac{k}{c} \right]^{1/2} , \tag{1}$$

where σ_c is the maximal stress that can be sustained by a sharp hairlike flaw of length $2c$ placed perpendicularly to σ_c within a system having an elasticity Y and a free-surface energy per unit area γ.

In real engineering samples, the presence of a large number of flaws with various sizes, shapes, and orientations (with respect to the applied load) makes the situation far more complex. In fact, due to these random flaws, brittle materials generally exhibit a wide scatter of fracture strengths, when nominally identical specimens are tested under nominally identical loading conditions and one generally talks of average strengths for such materials. In the case of such random flaws, the only parameter that seems to be relevant is the density (volume fraction) of flaws within the system.

Much physical insight into the strength of disordered systems comes from the microscopic consideration as in McClintock's discrete lattice model,[2] where one considers a lattice with the atoms or grains at the lattice sites and the bonds which link them via a potential energy is diluted with a finite probability q $(=1-p)$. Thus there is a chance p, that each material grain is bonded to its neighbor and a chance q, that it is not, thereby forming a flaw. This gives a finite probability (in terms of q) of occurrence (due to fluctuation of average dilution) of flaws with various shapes and sizes, and one can have the size distribution of flaws in terms of q. In this paper we discuss how the strength of an elastic network changes with the concentration q of randomly diluted bonds in the network.

At low q, the flaws are well separated and do not interact with each other in the sense that the (elastic) energy-released region of one flaw does not overlap with that of the other. When q is very low, the statistics of flaws is given by that of lattice animals (see Ref. 3 for lattice animals). In Sec. II, we very briefly discuss how the lattice-animal statistics provides a microscopic explanation of the strength of disordered systems in the limit of very weak disorder $(q \to 0)$.

However, as the system is diluted more and more, the average flaw size can no longer be represented definitely in terms of the cut bonds and flaw condensation and their interaction becomes common. The elastic and fracture behaviors (variation of elastic modulus and strength with flaw density) cross over to the power-law regime, and the modulus and strength vanish, at the percolation threshold[3] of the system, with some singularity essentially because of the critical divergence of the correlation length at this point. The singular behavior exhibited by elastic modulus and fracture stress are characterized in terms of the critical exponents, and in Sec. III we discuss the fracture exponent of a system near p_c. Using the "node-link-blob" picture[3] of the percolation cluster near p_c, we obtain a scaling relation for the fracture ex-

ponent T'

$$T' \geq [T+(d-d_B)\nu]/2 \ . \tag{2}$$

Here, T and ν are, respectively, the elasticity and correlation length exponents and d_B is the fractal dimensionality of the percolating backbone (see Ref. 3). This provides us with a rigorous lower-bound estimate of T' for any dimension d less than the upper-critical dimension d_c $(=6)$, at which the equality becomes exact. In fact, to check the validity of the scaling relation as well as to gain insight of how the strength scales near p_c, we artifice a very simple elastic model. In this model, the bond angles are considered to be perfectly rigid and all the neighboring sites in the backbone are assumed to be elastically connected, irrespective of their actual connection through bonds. This model, in spite of its oversimplification, is useful as the essential dynamic nature of the elasticity problem gets reduced in this model to a static one (like the electrical conductivity problem) and this helps in very precise determination of the elasticity and strength of the system and the critical exponents associated with them near the percolation transition point. Our MCRG study of this model gives $T=0.38\pm0.05$ and $T'=0.84\pm0.03$ which satisfy our scaling relation. Lastly, our MCS study of elasticity and strength of such a model gives the phase diagram for this quantities over the entire dilution range in addition to the exponents T and T' near p_c of the system.

II. WEAK-DISORDER LIMIT ($p \lesssim 1$)

In the weak-disorder limit, the flaws are almost noninteracting. For a system having N such noninteracting randomly distributed flaws, each with a probability $f(\sigma)$ to fail at or above the tensile stress σ, the survival probability of the entire sample under stress σ can be written as (see Ref. 2)

$$P(\sigma)=\prod_{i=1}^{N}[1-f_i(\sigma)] \simeq \exp\left[-\sum_{i=1}^{N} f_i(\sigma)\right] \equiv \exp\left[-\int g(\sigma)d\nu\right] , \tag{3}$$

where $g(\sigma)$ is the density of flaws which propagate under a minimum stress σ and the integration is over the entire volume of the sample.

When q is very low and close to zero, different configurations of the vacancy clusters are given by the statistics of "lattice animals."[3] Thus, typically, the number n_s of s clusters (formed by s adjoining vacant bonds) for large s is given by $n_s \sim \exp[-|\ln(\lambda q)|\, s]$ apart from some less-important contributing factor. Here λ is a lattice-dependent constant (e.g., $\lambda \simeq 4.06$ for a square lattice). The clusters would be of different shapes and sizes, but the average radius R_s of the s-clusters behaves as s^{ϕ} for large s, where ϕ is a critical exponent (for example, $\simeq 0.64$ in two dimensions). The density distribution $g(\sigma)$ of flaws is readily obtained as

$$g(\sigma)=\int_{\sigma^{-2/\phi}}^{\infty} n_s ds \simeq \frac{(\lambda q)^{1/\sigma^{2/\phi}}}{|\ln(\lambda q)|} , \tag{4}$$

if we assume the validity of Griffith's law [Eq. (1)] even for the clusters of arbitrary shapes. However, again, this assumption is questionable for finite q.

Perhaps a more straightforward approach is to visualize a flaw as was done[4] by McClintock, by considering vacant bonds in successive columns between any two adjacent rows. The number of vacant bonds defines the length of the flaw and Griffith's law is more applicable in this case. However, for small q, $g(\sigma)$ turns out[5] to be of Weibullian form, $(\sigma/\sigma_0)^m$, with some intricate q dependence of σ_0 and m as

$$\sigma_0=\sqrt{k}\,[\,|\ln q\,|/q(1-q)^2]^{1/m} , \qquad m=2\,|\ln(2q)|/|\ln(|\ln q\,|/\ln 2) . \tag{5}$$

Figure 1 shows $g(\sigma)$ versus σ curves for $q=0.01$ and 0.001 in both the cases [Eq. (4) and Eq. (2) in Ref. 5]. The curves for the two cases are almost identical for small q. The average strength thus obtained for small q very well satisfies the results (see Ref. 5) obtained from the molecular-dynamic study of the strength of a randomly bond-diluted (for low dilution concentration) square lattice with Lennard-Jones interaction between neighboring sites and is also apparent in the experimental result[6] of strength of a porous sheet of aluminum. Nevertheless, the complicated phenomenon of crack nucleation and its interactions with various external and internal agents render the actual situation, one faces in day to day engineering applications, very complicated and almost intractable.

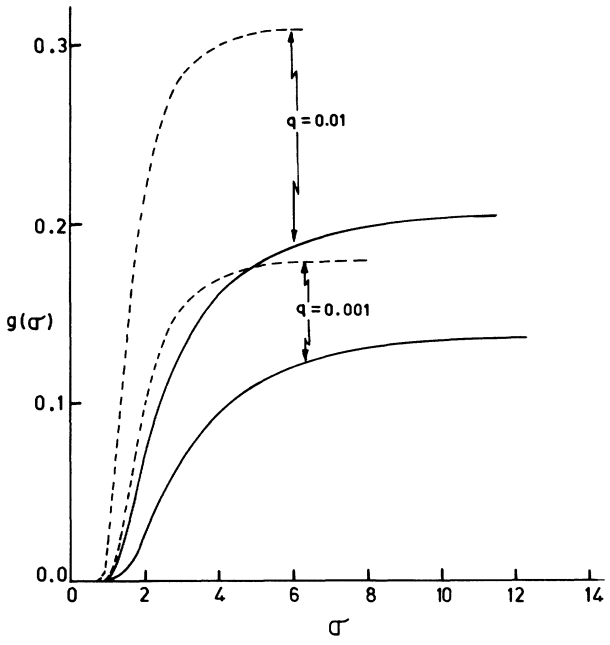

FIG. 1. $g(\sigma)$ vs σ curves for $q=0.01$ and 0.001. The dashed curves are obtained using Eq. (4) with $\lambda=4.06$ and $\phi=0.641$. The solid curves are obtained using Eq. (2) in Ref. 5 with $k=1$.

III. STRONG DISORDER OR PERCOLATION REGIME ($p \simeq p_c$)

As the concentration of the bond dilution increases, the elasticity as well as strength of a system gets lowered. This is schematically shown by the curve $AB'C'$ in Fig. 2. The elasticity as given by the slope AB' is much less than the elasticity obtained from the slope AB before dilution. Similarly the strength given by the breaking stress σ_c' is much less than its previous value σ_c. It is to be noticed that the curve $AB'C'$ is drawn much straighter than ABC to imply that, along with the elasticity and strength, the plastic region, where the stress-strain relation is nonlinear, is also affected by dilution and shrinks (see Ref. 7). When the bond-dilution concentration q is very large, so that the bond occupation concentration $p=(1-q)$ is less than the percolation threshold p_c of the system, the system is no longer connected. For $p>p_c$, the system would have finite elasticity and strength and, as $p \to p_c$ from above, the curve $AB'C'$ (in Fig. 2) merges with the strain axis and each of the above quantities goes to zero with a criticality. For example, the dependence of the effective elastic constant Y on p, near p_c, is given[8] by $Y \sim |p-p_c|^T$, where T is the elasticity exponent. Similarly, breaking stress also exhibits[9] criticality at p_c and is characterized by the exponent T'. These singular behaviors are essentially caused due to the divergence of the correlation length $\xi \sim |p-p_c|^{-\nu}$ and depend on the percolation geometry of the network. The elasticity exponent T also depends on the elastic Hamiltonian concerned; it differs[8] from a central-force system to a bond-bending-force system. The disappearance of elasticity at p_c actually corresponds to the tortuosity and stringiness of the connecting paths in the backbone of the infinite cluster. Such paths certainly would have[10] vanishing force constants.

On the other hand, the stress concentration on the stringy percolating structure and how that scales and

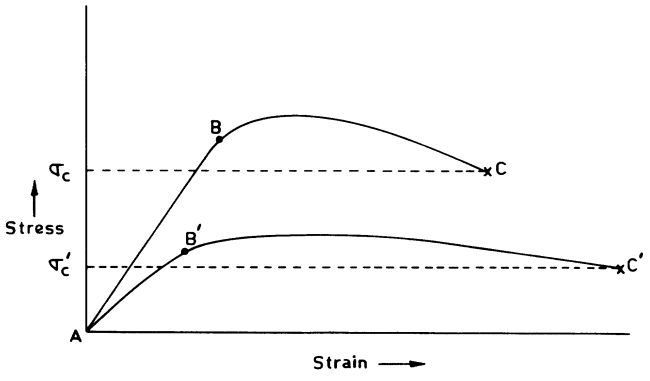

FIG. 2. Schematic diagram of the stress-strain curve commonly observed for solids. ABC represents the stress-strain curve when the solid is not disordered, whereas $AB'C'$ represents the stress-strain curve after the solid has been disordered. AB and AB' represent the Hooke's region, whereas σ_c and σ_c' represent the fracture stresses for the two cases, respectively.

makes the strength vanish at p_c with some criticality is not that apparent. One may argue,[5,9,11] very naively, that the most vulnerable flaw, at least in two dimensions, can be considered to be of the order of correlation length ξ and the effect of other flaws can be ignored. It is then just the Griffith system with a single crack of length $c=\xi \sim |p-p_c|^{-\nu}$ in a medium whose effective elasticity is $Y \sim |p-p_c|^T$. These values, in conjunction with Eq. (1), can provide[5,9] a measure for the fracture exponent T' $[=(T+\nu)/2]$. However, the argument has some drawbacks and moreover, it is not applicable to higher dimensions.

To see what crucial aspects of the percolation geometry govern the strength of a dilute network at $p \approx p_c$, we consider the node-link-blobs (NLB) model[12] of the percolating backbone, which describes the backbone on length scale $L \gg \xi$, as a network of "elements" of mean size $\xi \sim |p-p_c|^{-\nu}$. Each such element consists of regions of multiply connected bonds linked by chains of singly connected bonds. The force constant K_ξ of such a typical element is related[10] to ξ by $K_\xi \sim \xi^{(d-2)-T/\nu}$. If σ denotes the macroscopic stress applied on the system, then the stress on each element becomes $\sigma_\xi \sim \sigma \xi^{d-1}$, and the corresponding strain is $S_\xi \sim \sigma_\xi / K_\xi \sim \sigma \xi^{(T+\nu)/\nu}$. It is, in fact, the total strain $\sigma \xi^{T/\nu}$ shared by $1/\xi$ number of strings or "elements." Since, typically, there are ξ^{d_B} (d_B being the fractal dimensionality of the backbone) bonds in an "element" of length ξ, the average strain of a bond, constituting the superlattice element, comes out to be $S_B \sim S_\xi \xi^{-d_B}$ and the average strain energy of such bonds becomes

$$E_B = \sigma_\xi S_B \sim \sigma^2 \xi^{(d-d_B)+T/\nu} . \tag{6}$$

To determine the fracture stress, we assume each bond to remain elastic up to the point of its breaking, and equate E_B to its limiting value E_F, beyond which the bond ruptures. It may be mentioned that one could have calculated[7] the average strain of a bond and equated it to a limiting strain at rupture. However, near p_c, as the connecting paths become extremely tortuous, there would be enormous apparent strain without any real cost of elastic energy and the later calculation would lead to a gross underestimation of strength σ_c, except when the bond-bending force is fairly high. Thus, for equilibrium propagation of fracture $E_B = E_F$ and using Eq. (6) we get

$$E_F = \sigma_c^2 \xi^{(d-d_B)+T/\nu} . \tag{7}$$

This gives

$$\sigma_c \sim E_F^{1/2} |p-p_c|^{[T+(d-d_B)\nu]/2} \sim |p-p_c|^{T'} ,$$

where

$$T' = [T+(d-d_B)\nu]/2 .$$

Since in an actual case the strain would be higher for singly connected bonds than for multiply connected

ones, the average strain per bond that we calculate is less than the actual strain for a singly connected bond. Thus the fracture stress of the network that we estimate is always higher than the actual one, and the expression (2) we obtained for T' is a lower bound on T'. It is only for $d \geq 6$, when the elements of the superlattice network would be made up[12] totally of singly connected bonds, that the equality relation (2) becomes exact. For a bond-bending-force system,[10] $\nu = \frac{1}{2}$, $d_B = 2$, and $T = 4$ for $d \geq 6$; we obtain $T' = 3$ at and above the upper critical dimension (see also Ref. 7). For such systems in two dimensions, $T \simeq 3.96$ (see Zabolitzky *et al.* in Ref. 8). Together with the estimate[13] $d_B \simeq 1.60$, our scaling relation leads to $T' \geq 2.26$. This result is consistent with the experimental results[14] $T' \simeq 2.5$ for a porous sheet of aluminum and copper. For the central-force system, however, the situation is not very clear. The problem appears to belong to a different universality class altogether with the elasticity exponent $T \sim 1.4$ and correlation length exponent $\nu \sim 1.05$ (see Ref. 15). The value of d_B, fractal dimension of the backbone, is not known. The value of the fracture exponent T' obtained[16] from the molecular-dynamic simulation study of fracture in a two-dimensional Lennard-Jones system is nearly equal to unity, and this indicates that d_B for central-force system might be less than that for ordinary percolation backbone.

An idea of how the fracture stress σ_c scales down to zero at p_c is obtained from the Monte Carlo renormalization determination of T'. To simplify the problem we consider a rigid bond-angle system and assume that all the neighboring sites in the backbone are elastically connected, irrespective of the presence of bonds between them. Strain can then only take place along the lattice edges so that the lattice symmetries are preserved, except for the elongation of the cells. We use the H-type cell[17] for the square lattice and for a certain scale factor b, the bonds are first filled up with probability $p = p_c = 0.50$ by means of a random-number generator. The cluster that connects the top to the bottom end of the cell is determined, and the backbone is extracted by removing the dangling ends. For each such realization, the fracture stress σ_c as well as the elasticity modulus Y are evaluated. In this model the layers of bonds normal to the applied force always remain so, and the bonds along the force are only stressed. The response of the system to a tensile stress is thus identical to that of a series of springs of different force constants between the neighboring layers normal to the force; the number of (parallel) bonds between any two layers determine the force constant of the corresponding spring between those layers. Elasticity is given by the series combination of such springs and the fracture stress is given by the weakest of them. The probability distributions $P_b(\sigma_c)$ and $P_b(Y)$ are obtained by repeated sampling (20 000–30 000 realizations). The entire process is repeated for different b ($b = 2$–13). At p_c, $P_b(\sigma_c)$ is expected to approach a scale-invariant form

$$P_b(\sigma_c) \sim b^{T'/\nu} \tilde{P}(\sigma_c / b^{-T'/\nu}) \tag{8}$$

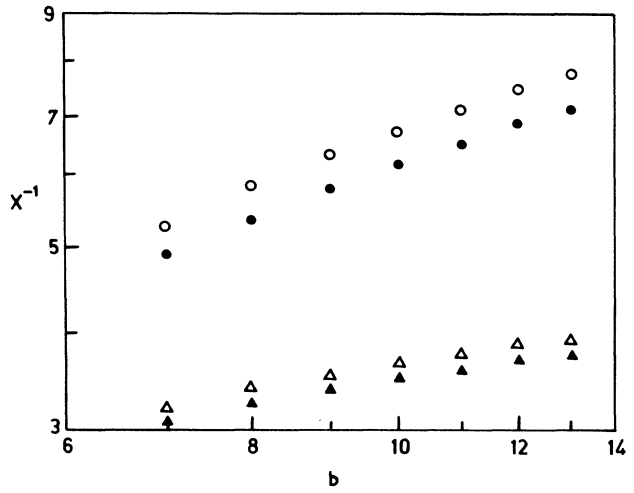

FIG. 3. X^{-1} vs b (in logarithmic scale) for Monte Carlo RSRG in our model system, where $X = \langle \sigma_c \rangle_b$, $(\langle \sigma_c^2 \rangle_b)^{1/2}$, $\langle Y \rangle_b$, and $(\langle Y^2 \rangle_b)^{1/2}$. The corresponding points are marked by ○, ●, △, and ▲, respectively. The limiting slopes give $T = 0.38 \pm 0.05$ and $T' = 0.84 \pm 0.03$.

for large b [the same is true for $P_b(Y)$, with T' replaced by T]. Similar scaled probability distribution for other quantities have been studied before.[18] The mean and root-mean-square fracture stress are

$$\langle \sigma_c \rangle_b \approx c_1 b^{-T'/\nu}, \qquad (\langle \sigma_c^2 \rangle_b)^{1/2} \approx c_2 b^{-T'/\nu}, \tag{9}$$

where $c_1 = \int x \tilde{P}(x) dx$ and $c_2^2 = \int x^2 \tilde{P}(x) dx$. Figure 3 shows the plots (in logarithmic scale) of $\langle \sigma_c \rangle_b$ [and also

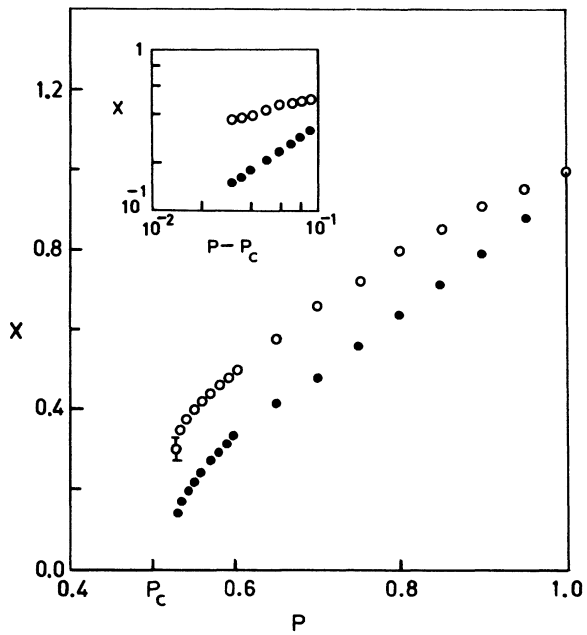

FIG. 4. X vs p (●, $X = \langle \sigma_c \rangle$; ○, $X = \langle Y \rangle$) for the Monte Carlo simulation in our model system of size 50×50. The inset shows a $\log X$ vs $\log(p - p_c)$ plot, giving $T = 0.42 \pm 0.07$ and $T' = 0.85 \pm 0.05$.

of $(\langle \sigma_c^2 \rangle_b)^{1/2}$] against b. Similar curves for the elasticity Y are also shown in the figure. From the limiting slope (for $b \to \infty$) of the curves we find $T' = 0.84 \pm 0.03$ and $T = 0.38 \pm 0.05$ in two dimensions (with $\nu = \frac{4}{3}$).

Since only the bonds of the backbone, which are along the applied force, are only stressed, the chemical length l_c of the stressed bonds for $b \ll \xi$ (in the fractal regime) satisfies $l_c \sim b$: the fractal dimension d_B of the stressed bonds of the backbone turns out to be unity in this model. We find that the T and T' we obtain for our model satisfy the scaling relation very well.

Finally, in the same model and in a 50×50-site lattice, we find fracture stress and elasticity for various values of p above p_c. The bonds are occupied randomly at some concentration p by means of a random-number generator and the backbone is sorted out as before. The average fracture stress $\langle \sigma_c \rangle$ and elasticity $\langle Y \rangle$ are determined for 15–20 realizations at each p and the entire process is repeated for different values of p. The variations of $\langle \sigma_c \rangle$ and $\langle Y \rangle$ with p are shown in Fig. 4. Both are found to approach zero at $p = p_c = 0.5$ with exponents $T' = 0.85 \pm 0.05$ and $T = 0.42 \pm 0.07$, respectively.

IV. SUMMARY

We consider a bond- (or site) diluted lattice model for disordered solids containing random voids or flaws. The variation of the strength of such solids with lattice dilution concentration $(1-p)$ is studied. In the low-concentration limit ($p \lesssim 1$), the average strength of the specimen is justified using animal statistics for the flaws or the vacancy clusters (Sec. II). Near the percolation point ($p \gtrsim p_c$; with fixed specimen volume V), the node-link-blob model of the percolation cluster is used to derive the relation

$$T' \geq [T + (d - d_B)\nu]/2$$

for the average fracture stress exponent T' (Sec. III). Reported agreement of the experimental results[14(b)] [see also Ref. 14(a)] with the above scaling relation (from an unpublished version of this paper) is discussed. It is also checked in a very simple elastic network, for which T and T' are obtained straightforwardly using Monte Carlo and Monte Carlo RSRG.

Note added in proof. In Eq. (2), an upper bound of T' can also be obtained easily by considering only the singly-connected bonds in the links constituting the superlattice network. For the singly-connected bonds $d_B = 1/\nu$ (see Ref. 12) and the fracture exponent, T' is then given by $(T + d\nu - 1)/2 \geq T' \geq [T + (d - d_B)\nu]/2$. For $d \geq 6$, the two bounds coincide and give $T' = 3$ exactly for bond-bending force systems. For such systems in two dimensions the above relation predicts $2.81 \geq T' \geq 2.26$ which agrees with the experimental result $T' = 2.5 \pm 0.4$.[14] For the central-force system the relation gives (with[15] $\nu \simeq 1.05$ and $T \simeq 1.4$) $T' \leq 1.3$ which again agrees with $T' \simeq 1.0$, obtained[16] from molecular dynamic simulation.

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