

Effective temperatures in nonequilibrium statistical physicsJ. S. Langer *Kavli Institute for Theoretical Physics, Kohn Hall, University of California, Santa Barbara, California 93106-9530, USA*

(Received 4 December 2023; accepted 3 June 2024; published 18 June 2024)

This paper summarizes two related effective-temperature analyses of nonequilibrium phenomena: first, dislocations in deforming crystals and, second, chaotic behaviors of defects in thermally driven Rayleigh-Bénard hydrodynamic systems. The results are encouraging for broader applications of this statistical concept.

DOI: [10.1103/PhysRevE.109.064139](https://doi.org/10.1103/PhysRevE.109.064139)**I. INTRODUCTION**

My purpose here is to describe the roles played by effective temperatures in two special nonequilibrium situations. I hope that this theoretical strategy will prove useful in developing predictive physics-based understandings of a wider range of complex phenomena.

The basic idea is that complex systems, when driven persistently by external forces, often can be described by distinctly different sets of degrees of freedom that fall out of thermodynamic equilibrium with each other. My favorite example is a crystal deforming under shear stress that develops a population of line defects, i.e., dislocations. These defects carry the strain and have a well-defined temperature that, in accord with the second law of thermodynamics, is distinctly different from the conventional temperature of the system as a whole [1].

As far as I know, the idea of an effective temperature dates back to a 1989 paper by Mehta and Edwards [2]. Those authors considered an athermal powder consisting of differently sized hard spheres, and introduced a temperaturelike quantity—the derivative of the volume with respect to the entropy—that they called the “compactivity.” They used this quantity to describe both fluidlike states at low densities and jammed states at higher densities.

My own experience with effective temperatures started with my attempts [3,4] to use them to describe the populations of shear-transformation zones (STZs), ephemeral localized regions in which rearrangements occur in glass-forming, multicomponent materials. At present, this example of the effective-temperature concept does not seem to me to be as well defined as other examples to be discussed below. Realistic glass transitions do not seem to fit neatly into the theory [5]. I do not know how to specify sizes or other properties of STZs near a glass transition, nor do I know in what sense glass transitions really exist in the limit of infinitely large systems. But a molecular simulation of a two-dimensional binary glass-forming system by Haxton and Liu [6] produces reasonable and internally consistent values of an effective temperature over a wide range of strain rates. Thus, this topic deserves more attention.

In the present paper, I focus on two related examples of systems in which the effective temperature seems more sharply defined than it is for STZs in glasses. First, I present a slightly modified version of my thermodynamic dislocation

theory [1], emphasizing aspects that are especially relevant to the effective-temperature concept. Then I turn to the case of defect turbulence in Rayleigh-Bénard systems [7] where there remain some interesting complications and uncertainties.

II. DISLOCATIONS

Dislocations are line defects in crystals whose motions determine irreversible shear deformations. The effective-temperature theory of dislocations is discussed in detail in my recent review article [1] and in earlier papers (for example, see Refs. [8–11]). Here, I want to emphasize a few basic features of that theory and reformulate it in a way that is more systematic and relates more closely to the defect turbulence to be discussed in the following section.

The central idea is that, in steadily deforming solids, the dislocations and the rest of the system, i.e. the fast, atomic-scale, kinetic-vibrational modes, constitute two distinct, weakly coupled subsets of dynamic degrees of freedom. I assume that each of these subsystems is ergodic. We can think of them almost as if they were two different objects, at different temperatures, connected by weak thermal contacts that conduct heat slowly from one to the other.

To explore the subsystem of dislocations, and to construct a plausibly realistic caricature of it, start by considering a slab of material lying in the x, y plane, undergoing irreversible shear deformation in that plane in response to an applied shear stress. Assume cubic symmetry. Let the area of this slab be A_0 and, for simplicity, let its thickness in the z direction be a characteristic dislocation length, say L_0 . Let ρ denote the areal density of dislocations or, equivalently, the total length of dislocation lines per unit volume.

The relevant dislocations are lines running perpendicular to this plane, i.e., in the z direction, marking the edges of partial planes of atoms. If these partial planes extend in the $+y$ direction, and if they move in the $+x$ direction, then we say that the resulting shear is positive and that these dislocations have “+” signs. Conversely, if the partial planes extend in the $-y$ direction, then these dislocations have “−” signs and the associated shear is negative. It was this duality of the dislocation population that I ignored in my previous dislocation-theory caricatures, but an analogous duality will be needed for describing defect chaos in the next section.

Note also that I am considering only edge dislocations and can ignore screw dislocations for present purposes.

Denote the configurational energy and entropy of the dislocations in this slab by $U_0(\rho)$ and $S_0(\rho)$, respectively. Here, $U_0(\rho) = A_0 e_D \rho$, where e_D is a characteristic energy of a dislocation of length L_0 . In this approximation, I do not include the energy of long-range interactions between the dislocations. These elastic interactions produce cellular dislocation patterns at small driving rates and may be quantitatively important in other respects, but they can be neglected for present purposes.

To compute the configurational entropy, start by dividing the area A_0 into N squares of side a , where a is the minimum spacing between noninteracting dislocations—an atomic-scale length—i.e., $N = A_0/a^2$. Then $S_0(\rho) = \ln W$, where W is the number of ways in which we can distribute the $N_+ + N_-$ dislocations among the N sites. In accord with the neglect of elastic interactions between the dislocations, assume that $N_+ = N_-$.

The statistical weight W is approximately

$$W \approx \frac{N!}{(N - N_+ - N_-)! N_+! N_-!}, \quad (1)$$

where $N!/(N - N_+ - N_-)!$ is the number of ways to distribute $N_+ + N_-$ dislocations among N sites, and $1/(N_+! N_-!)$ corrects for the fact that the N_+ and N_- dislocations are statistically identical to each other; it does not matter in what order they are placed in the system. Let $n \equiv N_+ + N_- = \rho a^2 N$. Then the entropy S_0 is

$$S_0 \approx \ln W \approx n \ln(2N/n) + n = A_0[\rho - \rho \ln(\rho a^2/2)], \quad (2)$$

where I have used Stirling's approximation and have dropped small terms of relative order n/N . This result differs from the previous one (in Ref. [1]) only by the factor 2 in the argument of the logarithm.

As before, compute the density of dislocations by minimizing the free energy

$$F_0(\rho) = U_0(\rho) - \chi S_0(\rho), \quad (3)$$

where χ is the effective temperature which enters here as the inverse of a Lagrange multiplier in an optimization problem. That is, we maximize the entropy S_0 for a fixed value of the energy U_0 . Minimization of F_0 with respect to ρ produces the familiar result

$$\rho_{ss} = \frac{2}{a^2} e^{-e_D/\chi_{ss}}, \quad (4)$$

where the subscript “ss” reminds us that this is a steady-state formula, and the prefactor 2 is the only reminder of the dislocation-duality hypothesis.

The big question now is how do we evaluate the effective temperature χ ? In my opinion, χ is just as fundamental a quantity as the ordinary temperature T . The problem is that we generally do not have a thermometer for measuring χ , even in principle. But consider the following.

I argued in Ref. [1] that, when the shear rate is slow enough that the fast kinetic-vibrational subsystem has time to relax between dislocation-rearrangement events, then the steady-state dislocation-rearrangement time is effectively the only timescale in the system, and therefore the density of dislocations must be a constant independent of the shear rate.

It cannot depend on how we set our clocks. I further argued that the transition between the two kinds of behaviors ought to occur (as in a Lindemann melting transition) when the spacing between the dislocations is roughly ten interaction lengths a . This led me to estimate from Eq. (4) that $\chi_{ss}/e_D \approx 0.25$, which is remarkably close to the observed value in a wide range of experiments. Thus, in this case, we do have an approximate first-principles argument for evaluating the effective temperature.

This argument breaks down at larger strain rates (of order $10^6/s$ for real crystals) where the kinetic-vibrational and dislocation-rearrangement timescales do become comparable to each other. Here, as shown in Eq. (15) of Ref. [1], I introduced an approximate formula to fit the Livermore computer-simulation data [12]. This formula correctly predicts that the underlying crystalline structure melts at high strain rates, but it is not strictly a first-principles result.

The effective-temperature analysis is only one of the two most unconventional ingredients of the dislocation theory presented in Ref. [1] and in earlier papers. The second major heresy is that I have taken Cottrell's “bird's-nest” analogy quite literally. Instead of trying to define a “Peierls stress” that drives the average motion of dislocations across a variety of obstacles, as has been done in the conventional literature since about 1940, I have assumed that the fundamental timescale is set by the thermally activated rate at which entangled dislocations come apart from each other at the bird's-nest-like pinning points. With this assumption, I recover Taylor's formula for stress proportional to $\sqrt{\rho}$, and I predict yield stresses, Hall-Petch (grain-size) effects, adiabatic shear banding, fracture toughness, etc. These results are strongly supported by a scaling test [11] originally devised by Le. See Ref. [1] for details of these analyses.

III. DEFECT CHAOS

I turn now to the question of how the statistical methods developed for the thermodynamic dislocation theory [1] may be extended to deal with defect turbulence as observed by Daniels and Bodenschatz (DB) [7] in Rayleigh-Bénard systems.

The DB experiments were performed with an array of parallel Rayleigh-Bénard (RB) rolls driven by a negative temperature difference between the bottom and the top of a tilted slab of compressed CO_2 . The RB rolls form when the situation is such that uniform heat flow from bottom to top becomes hydrodynamically unstable. The result is the formation of a spatially periodic pattern of fluid flow, i.e., an array of parallel rolls. The orientation of this pattern is stabilized in the direction of the tilt of the slab. I arbitrarily assume for counting purposes that the pairs of rolls are those in which the warmed fluid is flowing upward between them and cooled fluid back down on their opposite sides.

The defects in this system are points where pairs of rolls are created or destroyed, producing either one extra pair or one missing pair in the uphill direction. These will be denoted “+” or “-” defects. They are analogous to dislocations, except that they are not extended lines perpendicular to the plane and there is no analog of entanglement. On the other hand, the analogy is close in that the +/− signs tell us whether the

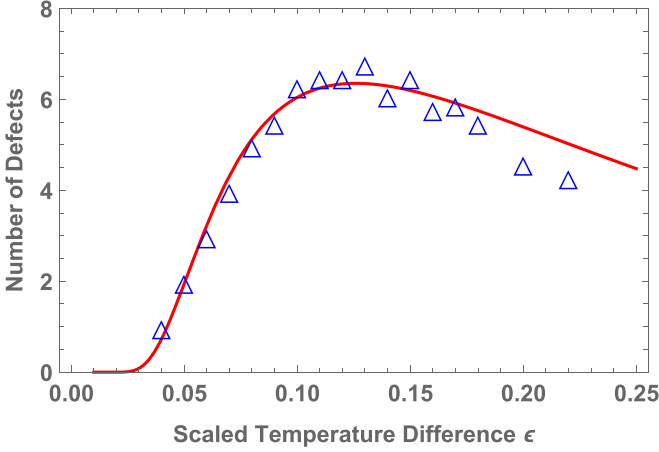


FIG. 1. Daniels-Bodenschatz data for the number of positive defects $\langle N_+ \rangle$ in their sample area as a function of ϵ . The red curve is the theoretical approximation given by Eqs. (7) and (8), with a linear approximation for the energy $e_D(\epsilon)$.

extra pair of rolls, such as an extra half plane of atoms, lies uphill or downhill from the defect.

Now we can adapt our earlier statistical analysis to the DB experiments. Consider an array of parallel Rayleigh-Bénard rolls driven by a dimensionless temperature difference $\epsilon = (T_{\text{hot}} - T_{\text{cold}})/T_{\text{cold}}$. Suppose that there are N_+ positive defects and an equal number N_- of negative ones, and again let $N_+ + N_- \equiv n$ be the total number of defects. Let the area of the system be Na^2 , where a is the characteristic size of a defect in the sense that defects separated by distances greater than a do not interact with each other. Unlike DB, assume periodic boundary conditions for the system of area Na^2 .

The statistical weight W of this system is the same as that given by Eq. (1), and the entropy $S(n)$ is the same as $S_0(n)$ given by Eq. (2), i.e.,

$$S(n) \approx \ln W \approx n \ln(2N/n) + n. \quad (5)$$

Let the energy of a defect be $e_D(\epsilon)$. Then the free energy is

$$F(\epsilon, n) = e_D(\epsilon)n - \chi(\epsilon)S(n), \quad (6)$$

where the effective temperature χ must now be a function of ϵ . Minimizing with respect to n , we find

$$n(\epsilon, \chi) = 2N \exp[-e_D(\epsilon)/\chi(\epsilon)]. \quad (7)$$

This formula presumably describes the data shown in DB Fig. 4, where the number of positive defects inside some subarea of the Rayleigh-Bénard system is plotted as a function of the dimensionless temperature difference ϵ . I show these data by the blue triangles in Fig. 1.

Also shown in Fig. 1, in red, is a theoretical curve based on Eq. (7), with a linear approximation $e_D(\epsilon) \approx e_0 \epsilon$, and $\chi(\epsilon) \equiv e_0 \tilde{\chi}(\epsilon)$. I find that I can fit the DB data by assuming that

$$\tilde{\chi}(\epsilon) = \frac{\tilde{\chi}_0 \epsilon^3}{\epsilon_0^3 + \epsilon^3}. \quad (8)$$

That is, the effective temperature is assumed to vanish cubically at small driving force ϵ and to go to a constant as

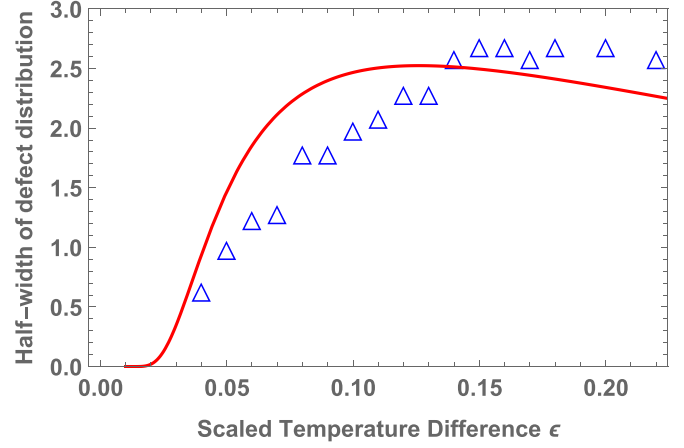


FIG. 2. Daniels-Bodenschatz data for the half widths of the distributions of the numbers of + defects as a function of ϵ . The red curve is the theoretical approximation.

ϵ becomes large. In evaluating Eq. (7) with this assumption, I used $N = 7$, $\epsilon_0 = 0.1$, and $\tilde{\chi}_0 = 0.24$, the latter being approximately the same as its predicted value for low to moderate strain rates in the thermodynamic dislocation theory. The agreement between theory and experiment shown here appears to be quite good except for the two points at large ϵ . That discrepancy might easily be fixed by adding a realistic nonlinear term to the formula for $e_D(\epsilon)$.

In their Fig. 4, Daniels and Bodenschatz also show vertical bars indicating the widths of the defect distributions at the chosen values of ϵ . My representation of that data is shown here by the blue triangles in Fig. 2. To make rough theoretical estimates of these widths, I have assumed that the probability distribution over n is proportional to a Gaussian approximation for $\exp[-F(\epsilon, n)/\chi(\epsilon)]$ and then computed the curvature at the peak of this distribution for fixed ϵ . That is, from Eqs. (5) and (6), I find that $\partial^2 F/\partial n^2 \approx \chi/n$, and thus the half width is approximately $\sqrt{n(\epsilon, \chi)}$ with $n(\epsilon, \chi)$ given by Eq. (7) with $2N = 14$.

This theoretical result is shown by the red curve in Fig. 2. Agreement between theory and experiment is modest at best, but given the uncertainties in my Gaussian approximation and in my interpretation of the half widths shown in BD Fig. 4, this may be the best that could have been expected. I have introduced no new fitting parameters, but the general trend and the orders of magnitude look roughly correct.

IV. CONCLUDING REMARKS

As the problems we are facing in physics—especially those with applications in chemistry, biology, artificial intelligence, etc.—become more and more complex, we increasingly need new ideas. We cannot afford to repeat the mistakes of those of us who denied the relevance of the second law of thermodynamics to dislocation theory and delayed progress in that field for over half a century. The effective temperature plays a central role in what I believe is a correct, predictive dislocation theory, and the idea seems to be confirmed by the Daniels-Bodenschatz [7] measurements of defect chaos. It should be interesting to see where we can go from here.

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