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TOPICAL REVIEW — Statistical physics and complex systems

Effective temperature and fluctuation-dissipation theorem in athermal granular systems: A review*

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The definition and the previous measurements of a dynamics-relevant temperature-like quantity in granular media are reviewed for slow and fast particle systems. Especially, the validity of the fluctuation-dissipation theorem in such an athermal system is explored. Experimental evidences for the fluctuation-dissipation theorem relevant effect temperature support the athermal statistical mechanics, which has been widely explored in recent years by physicists. Difficulties encountered in defining temperature or establishing thermodynamics or statistical mechanics in non-equilibrium situations are discussed.

Keywords: granular systems, fluctuation-dissipation relation, non-equilibrium thermodynamics

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1. Introduction

It has been an active research area in granular physics to find whether comparable statistical thermodynamics at the atomic level exists for the dissipative grain-level fluctuations. In this paper, we start with a review of temperature in equilibrium thermodynamical systems in Section 2, followed by the introduction of different proposals and experimental evidences on temperatures in non-equilibrium granular systems of dense slow moving particles in Section 3, and that of fast moving particles in Section 4. In the last section, we discuss the challenges in establishing the athermal statistical mechanics.

2. Temperature in equilibrium thermodynamic systems

Temperature is one of the fundamental physical quantities in equilibrium thermodynamics and statistical mechanics.[1] In equilibrium thermodynamics, the definition of temperature is supported by two fundamental laws: the zeroth law of thermodynamics, which defines the empirical temperature related to the transitivity of mutual thermal equilibrium; the second law of thermodynamics, which relates temperature to heat transfer. The second law states the continuity and ordering properties, i.e., the direction of the flow of heat from a high-temperature object to a low-temperature object, and defines an absolute thermodynamic temperature independent of the material properties of the reference used to evaluate it. The standard definition of the absolute temperature in equilibrium thermodynamics is given by $T_{\mathrm{eq}} = (\partial U/\partial S)_{V,\{N\}}$, where U is the internal energy, S is the entropy, V the volume, and $\{N\}$ denotes all numbers of moles.

Statistical mechanics describes the connection between microscopic properties and collective many-body properties for systems in thermal equilibrium. In equilibrium statistical mechanics, the kinetic theory is used to define an absolute temperature as the average translational kinetic energy of the random motions of all the particles, where it is often assumed that it remains valid even in the absence of thermal equilibrium. The simplest case is non-interacting particles of the ideal gas, we have $\frac{3}{2}k_{\mathrm{B}}T_{\mathrm{eq}} = \left\langle \frac{1}{2}m\boldsymbol{v}^2 \right\rangle$, where k_{B} is the Boltzmann constant, m is the mass of the particle, $\boldsymbol{v}$ is the velocity of the particles, and the angular brackets denote the average over the velocity of all the particles.

In a gas at equilibrium, the distribution of the particle velocities must satisfy a statistical distribution function in Gaussian form

$$f_{\mathrm{eq}}(\boldsymbol{v}) \propto \exp\left(-\frac{1}{2}\frac{m\boldsymbol{v}^2}{k_{\mathrm{B}}T_{\mathrm{eq}}}\right).$$

Here, we can see that T_{eq} is connected not only to the average value of the energy, but also to the form of the distribution function.

In classical equilibrium statistical mechanics, temperature usually appears as a parameter in equilibrium ensembles, a measure of fluctuations, or a dynamical quantity. In equilibrium ensembles, Boltzmann showed that the energy distribution function in any system at thermal equilibrium at temperature T_{eq} has a canonical form $f_{\mathrm{eq}}(E) \propto \exp\left(-E/k_{\mathrm{B}}T_{\mathrm{eq}}\right)$, where E is the energy of the system. In the canonical ensemble, the

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internal energy of the system fluctuates, and the second moments of the energy fluctuations are related to temperature. To be able to go from a dynamical description to a thermodynamical one for a classical Hamiltonian system, the system must exhibit ergodicity, i.e., the dynamical time averages may be replaced with ensemble averages. The fundamental aspects of temperature in equilibrium states are related to the atomic level particle fluctuation and are well defined. Defining the concept of temperature related to the granular level fluctuations in non-equilibrium steady or quasi-steady states, however, remains challenging.

3. Temperature in non-equilibrium dense granular systems with slowly moving particles

Granular matters,[2–7] foams,[8] and colloids[9–11] are examples of non-equilibrium model systems. They are considered as athermal systems because the usual atomic level thermal temperature does not play a role compared with that defined by the granular level fluctuations.[12,13] For example, the ‘kinetic temperature’ corresponding to translation velocities of 1 cm$\cdot$s^{-1} of small beads in typical silicate glass is 11 orders of magnitude higher than room temperature.[1–7] The thermal kinetic energy of each particle, $k_{\rm B}T_{\rm eq}$, is therefore considered irrelevant compared to the kinetic energy of the grain level. In such systems, the assembly of particles possesses a large number of degrees of freedom with energy dissipation through inelastic collisions or internal friction, which are, in steady state, balanced by some non-thermal sources (vibrations, tapping, shearing, ...).[14–21] The validity of the concept temperature is not guaranteed in such non-equilibrium systems.[22–28] The thermal energy $k_{\rm B}T_{\rm eq}$ at room temperature is too small to induce any macroscopic grain fluctuations, and the fluctuation-dissipation theorem is therefore in general not expected to be valid.

To define temperature of such an athermal system when one considers only the grain level fluctuations, one must first compute the system’s entropy. Edwards and collaborators[29–31] have proposed analogies between dense granular systems and classical statistical systems. They introduced a method to calculate the entropy (the number of all possible configurations) for dense, slowly moving (gently sheared, tapped or vibrated) granular systems. This entropy is a function of the number of blocked configurations $\Omega_{\rm Edw}$ (in which every grain is unable to move) of given system volume V and total energy E, as $S_{\rm Edw} = k_{\rm B}\ln\Omega_{\rm Edw}(E,V)$. Edwards’ entropy is considered strictly in Boltzmann–Gibbs statistics. All blocked configurations are assigned the same statistical weight, in analogy to the microcanonical ensemble of classical systems. Edwards then explored the physical meaning of the derivatives of the entropy, namely, $T_{\rm Edw}^{-1} = \partial S_{\rm Edw}/\partial E$, $X_{\rm Edw}^{-1} = \partial S_{\rm Edw}/\partial V$, where an Edwards temperature and a quantity $X_{\rm Edw}$, called the compactivity, are defined. Although it is not an easy task to test Edwards’ theory, because experimentally, the rate of energy input and the density are normally non-uniform, in recent years some efforts in both simulations and experiments have been made.[24,32–40]

Attempts to test the validity of Edwards’ theory are worth reviewing here. In 2000 Barrat *et al.*[32] carried out a numerical study in some microscopic models, and obtained a dynamical temperature from the diffusion constant and the particle mobility, following the Einstein relation. The dynamical temperature is found to match well the Edwards temperature obtained from the blocked configurations as shown in Fig. 1.

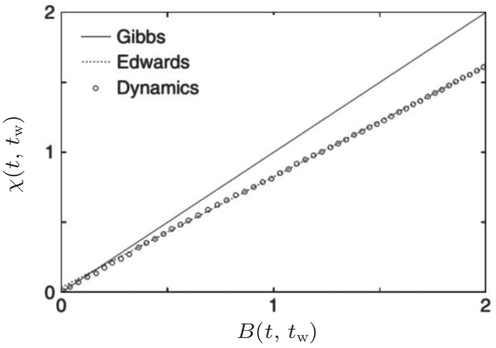

Fig. 1. Einstein relation in the Kob–Andersen model: plot of the mobility $\chi(t,t_{\rm w})$ vs. the mean square displacement $B(t,t_{\rm w})$. The slope of the full straight line corresponds to the equilibrium temperature, and the dashed one to Edwards’ prescription.[32]

In 2002, Makse and Kurchan[33,34] carried out a numerical model of a dense, slowly sheared granular system. An effective temperature is obtained from measuring the diffusivity and mobility of some trace particles. The temperature is found to be independent of the shear rate and the tracer particle characteristic features. Its value is found to be consistent with the Edwards temperature,[35] although the agreement between dynamical and Edwards temperatures is not as good when the rate of energy input through tapping or shearing increases.

Later, Makse *et al.*[36,37] verified the effective temperature with experimental measurements of near jamming granular materials in a slowly sheared three-dimensional Couette cell with refractive index and density matching fluid (see Fig. 2(a)). Effective temperatures can be obtained from the slope of the mean square displacements versus the average displacement of the trace particles shown in Fig. 2(b). The well overlapped data points provide an evidence that the obtained temperatures are independent of the slow-shear rate and the tracer-particle features.

To describe the behavior of diffusivity and mobility, Geng and Behringer[38] experimented on a dense two-dimensional (2D) granular system, as seen in Fig. 3. They introduced random motion by stirring, and characterized diffusivity by particle tracking. To obtain the mobility, they measured the force needed to push a particle through the medium at a fixed veloc-

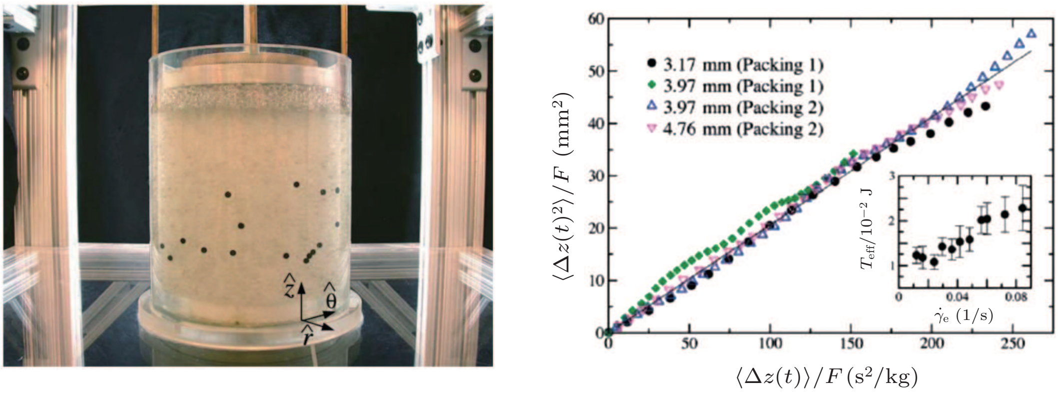

Fig. 2. (a) Picture of slowly sheared Couette cell. (b) Effective temperatures for various tracers and different packings. Inset shows the dependence of $T_{\rm eff}$ on the shear rate in packing 2.[36]

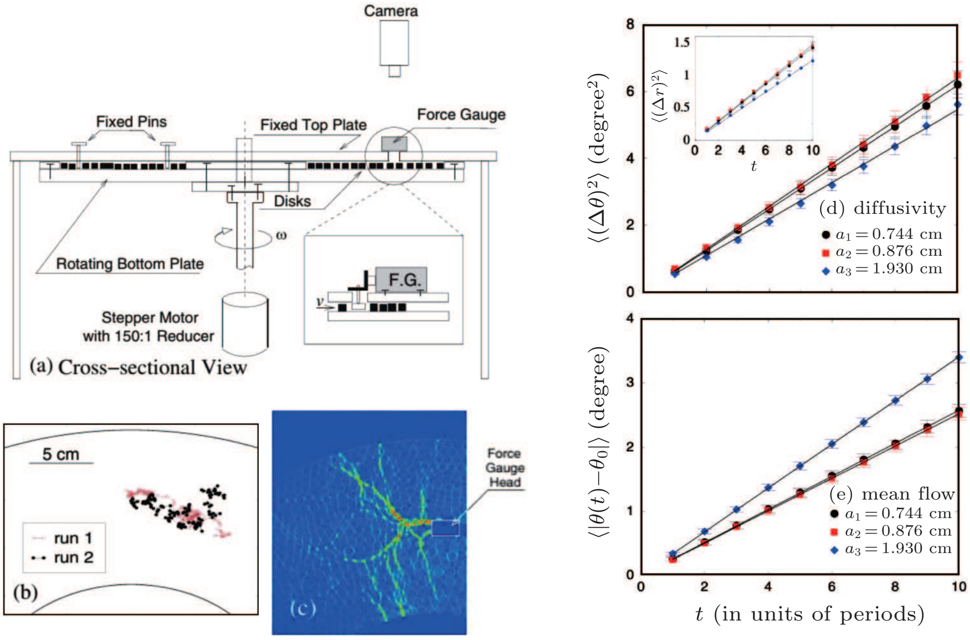

Fig. 3. (a) Cross-sectional view of the schematic of the apparatus. (b) Typical trajectories of the tracer. (c) Stress image showing force chain structures. (d) Variance of $\Delta\theta$ vs. time. Inset shows diffusivities in the radial direction. (e) Mean angular displacement as a function of observation time.[38]

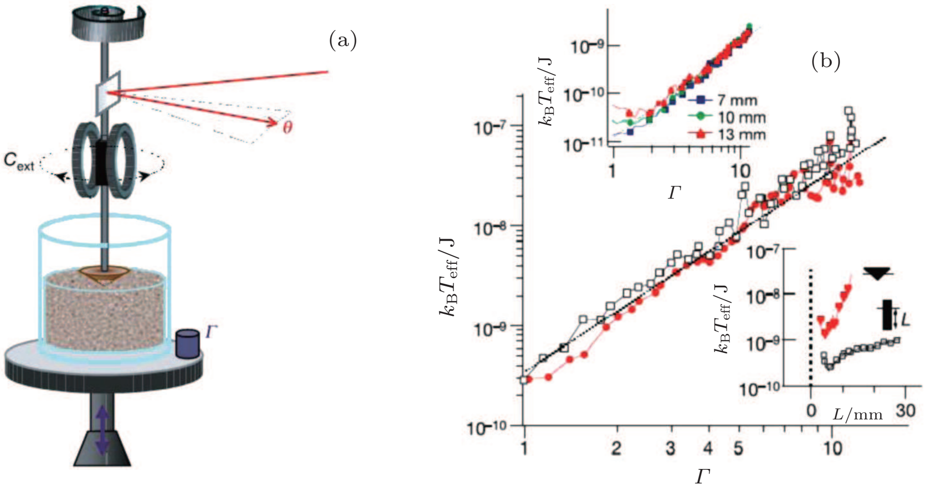

Fig. 4. (a) Sketch of the torsion setup in a granular bath. (b) Effective temperature versus vibration intensity Γ. Upper inset: the effective temperature $T_{\rm eff}$ versus Γ, obtained using cylindrical probes of different diameters with the same immersion depth. Lower inset: the effective temperature $T_{\rm eff}$ at fixed Γ versus the immersion depth of the oscillator, L, for conical (red) and cylindrical (black) probes.[39]

ity. They found that diffusions in the radial direction and the tangential direction are identical. Both the mean square displacement and the average displacement change linearly with time.

Other experimental efforts by Mayor *et al.*[39,40] measured the motion of a torsion oscillator, which was immersed in an externally vibrated granular medium of glass spheres. They observed Brownian-like motions. They found that an approximate fluctuation-dissipation relation holds, and a temperature-like quantity, i.e., the effective temperature T_{eff}, can be defined. The temperature T_{eff} is found to be independent of the probe properties, but depends on the area of the oscillator's interaction with the granular medium: the more the oscillator interacts with the granular medium, the higher the T_{eff}, as is seen in Fig. 4.

4. Temperature in non-equilibrium granular systems with fast moving particles

Edwards' theory is for slow moving particles. For fast moving particles in granular systems that are vigorously shaken,[41–43] the erratic motion of the particles is similar to the thermal motion of molecules in a normal gas and therefore it is possible to introduce the concept of granular temperature as

$$\frac{3}{2}k_{\text{B}}T_{\text{gr}} = \frac{1}{2}m\left(\langle v^2\rangle - \langle v\rangle^2\right).$$

When the system receives a high-energy input, it approaches the behavior of gases,[44] and thus some generalizations of the Boltzmann equation can be applied to such situations.[45–47] With a two-layer, vertically vibrated granular system, shown in Fig. 5(a), in which an oscillating plate drives a horizontal layer of heavy grains, which in turn drives an overlying horizontal layer of lighter grains, Baxter and Olafsen[48] observed that, driven by collisions with the first-layer heavy particles, the velocity distribution of the top layer particles can be Gaussian (Fig. 5(b)). Their system may therefore be ideally suited to developing a kinetic theory of granular gases.

Inspired by some non-zero temperature gradient thermo-osmotic trap experiments,[9] we built a non-zero "viscosity" gradient on the surface of a plate.[49] A granular chain shaken by vertical vibration bounces on the plate. Directional drift of the chain from a low viscosity region towards a high viscosity region is observed. In the system, the motion of this bouncing chain on the unevenly grooved plate is recorded by a high speed camera. Line-grooves carved on the supporting plate are denser at the middle and gradually decreasing towards both ends of the plate. Figure 6 is a sketch of our experimental setup. This uneven roughness along the chain direction causes the shaken chain to collide with the supporting plate more frequently at the rough side than that at the smooth end, inducing a net drift towards the rough center.[49]

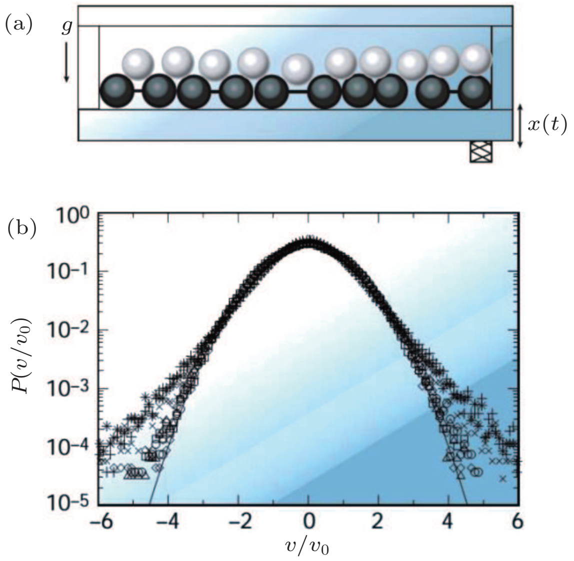

Fig. 5. (a) The two-layered experimental setup. (b) Velocity statistics for the first- and the second-layer grains. First layer: crosses, plus symbols, and asterisks. Second layer: diamonds, squares, circles, and triangles.[48]

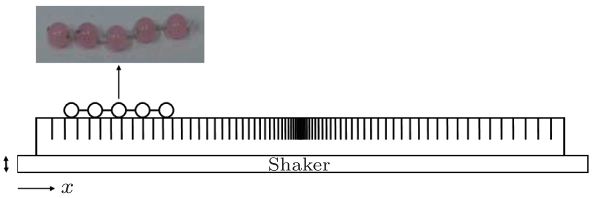

Fig. 6. Schematic illustration of the setup. Inset is a photo of the granular chain.

Classical irreversible thermodynamics, based on the local-equilibrium hypothesis, assumes that the basic thermodynamic concepts do not require a reformulation for non-equilibrium systems, but that usual equilibrium quantities shall be locally applied to systems in non-equilibrium states. In our system, a viscosity gradient exists. We needed to check if the local-equilibrium hypothesis is valid. We divided the length of the plate into bins. The width of each bin was chosen to be small enough so that within each bin the "friction" coefficient and the instantaneous driving force induced by the viscosity gradient can be assumed as constants, and at the same time large enough so that there are sufficient statistical data. The distribution functions of the displacement, the local instantaneous velocities, and the instantaneous accelerations were analyzed and found to be Gaussian. This tells us that the local-equilibrium hypothesis is valid.

The chain's motion is similar to a stochastic process that a viscous friction force and a random force act on the object. The Langevin equation[50] for a stochastic process driven by a constant viscous friction force $-\gamma v$, proportional to the velocity, and a constant random force f, i.e., a Gaussian white noise, can be written as $\dot{x} = v$, and $m\dot{v} = -\gamma v + f$, where f satisfies $\langle f(t)\rangle = 0$ and $\langle f(t)f(t')\rangle = C\delta(t-t')$. Solving for $v(t)$, we obtain $\langle v(t)v(t)\rangle = C/2\gamma$. Since $\frac{1}{2}m\langle v^2\rangle = \frac{1}{2}k_{\text{B}}T$, we obtain $C = 2\gamma k_{\mathrm{B}}T$. The mean square displacement can be calculated once we know $x(t)$. Then, from the Einstein relation $\langle (x(t+t_0)-x(t_0))^2\rangle = 2Dt$, where D is the diffusivity, the fluctuation-dissipation relation can be easily reached $\gamma D = k_{\mathrm{B}}T$. In our situation, since the chain particle moves along a plate with a viscosity gradient, the friction coefficient γ and the random force f are not independent of position x. In this case, we can only examine locally the values of γ and D in each bin.

Since we are only interested in the translational motion of the chain induced by the "field" gradient, we record only the position of the center-of-mass of the chain. Both quantities of the MSD and fluctuation-induced displacement $\langle x(t+t_0) - x(t_0)\rangle$ show good linear dependence on time. From the slopes of $\langle [x(t+t_0)-x(t_0)]^2\rangle = 2Dt$ versus $\langle x(t+t_0)-x(t_0)\rangle = v_{\mathrm{d}}t$, we are able to obtain the local $D(x)$ and $v_{\mathrm{d}}(x)$ the drift velocity, respectively.

Figure 7 plots MSD versus $\langle x(t+t_0)-x(t_0)\rangle/F$, where F is the driving force obtained from the average of the instantaneous acceleration, which is assumed to be constant in each bin. The width of each bin is chosen to be 5 mm so that it is small enough such that variables driving force F, diffusion coefficient D, and etc. can be assumed as constants, and the average of the random force f be zero, meanwhile large enough to contain sufficient statistical data. The local effective temperature can then be obtained from the slope $\langle [x(t+t_0)-x(t_0)]^2\rangle = 2T_{\mathrm{eff}}\langle x(t+t_0)-x(t_0)\rangle/F$.

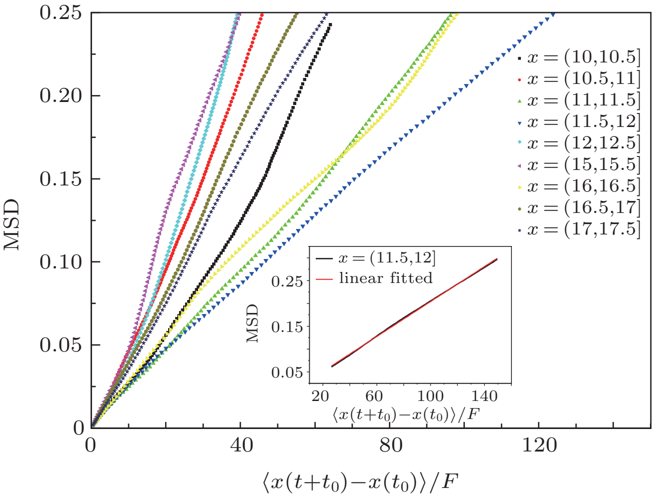

Fig. 7. Effective temperatures for various positions obtained from a parametric plot of their diffusion versus mobility. The inset shows the linear fit.

We compare this effective temperature with the so called granular temperature defined by the average instantaneous fluctuation kinetic energy of the chain, i.e., $T_{\mathrm{g}} = \langle |v - \langle v\rangle|^2\rangle \approx \langle v^2\rangle$. Figure 8 plots all the measured T_{g} and T_{eff} under different experimental conditions. It is found that $T_{\mathrm{eff}} = T_{\mathrm{g}}$, i.e., they are in good agreement within experimental accuracies.

This fast moving particle experiment provides a one-variable model system that reflects granular stochasticity with two temperature-like quantities: one is given by the average kinetic energy of the grain, the other by the width of the distribution profile around the average kinetic energy. The fact that the two temperatures are found to have the same values within experimental accuracies provides an additional support to the athermal statistical mechanics.

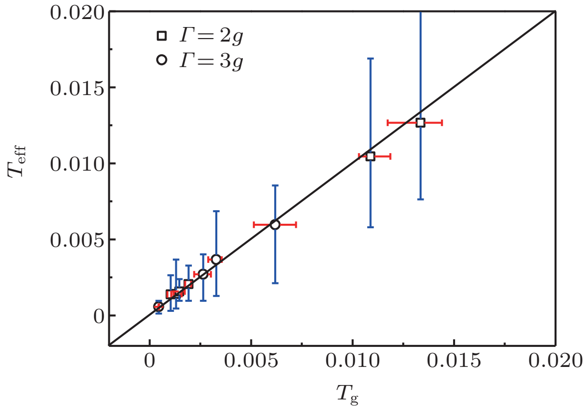

Fig. 8. Effective temperature versus granular temperature for chains of different materials (resin, glass, aluminum, iron, and steel).

5. Conclusion and perspectives

Temperatures in non-equilibrium systems are being examined in recent years in a very active way in systems such as glasses,[26,51,52] sheared fluids,[53–55] amorphous semiconductors,[56,57]and turbulent fluids,[58,59] other than granular materials. It is a great challenge to compare proposals in these different systems and to appraise their mutual consistency. A good review of temperature in non-equilibrium situations in different systems, given by Casas-Vázquez and Jou,[1] provides a good summary with the intention to stimulate the connection of different proposals. Despite the success in recent experimental and simulation works on the consistency of non-equilibrium temperatures, a general overview of the definitions and problems of non-equilibrium effective temperatures is given in their review.[1] The main difficulty in non-equilibrium systems is that in equilibrium, all the temperature definitions lead to the same result, but for non-equilibrium situations, different definitions, implying different methods of measurements, may yield different results. In non-equilibrium systems, the zeroth and the second laws of thermodynamics are not satisfied, since the definition of temperature from the former depends on interaction, and the definition from the latter assumes thermal equilibrium. From the statistical mechanics point of view, distribution functions out of equilibrium are usually non-Gaussian, and the implications for a non-equilibrium temperature are unknown.

In this paper, starting from the definitions of temperature in equilibrium thermodynamics and in equilibrium statistical mechanics, we reviewed Edwards' entropy, which defines temperature and compactivity of non-equilibrium dense granular systems with slow moving particles. Several simulation and experimental studies have found agreement between effective temperatures and the Edwards temperature. For fast moving particles, the concept of granular temperature is often defined by the average fluctuation of the kinetic energy of particles. The distribution function of such systems is found to be reproducible, but often not Gaussian. The forms of the distribution function depend strongly on the driving methods. Baxter and Olafsen[48] showed for the first time a Gaussian velocity distribution of a fast moving granular system with bulk excitation. Our recent experiment, using a single granular chain to mimic a stochastic process driven by a viscous friction force and a random force by bouncing on a vertically vibrated unevenly grooved plate, showed good agreement between temperatures obtained from the average kinetic energy of the grain and from the fluctuation of the average value. The finding provides a useful experimental support to the athermal statistical mechanics.

Finally, as pointed out in granular solid hydrodynamics proposed by Jiang and Liu,[60] we would like to remind ourselves that the basic laws, such as thermal fluctuations at the microscopic atomic level (involving the zeroth, the first, or the second law of thermodynamics, the fluctuation-dissipation relation, the Boltzmann statistical laws, etc.), must be obeyed by any material including granular systems. There is only one temperature these laws are related to — the thermal temperature T_{eq}. When we say a granular system is athermal and try establishing non-equilibrium thermodynamics by defining a temperature-like quantity, we actually consider only the mechanical energy of the grain level, and treat the heat loss (in phonon level) due to inelastic collision or friction as dissipation. It is convenient, phenomenological, and challenging to build a non-equilibrium thermodynamic and statistical mechanic theory at the grain level in the framework of classical thermodynamics and/or statistical mechanics. However, we are not sure if a natural law similar to the classical thermodynamics exists for such athermal systems, although under specific conditions, experimental and simulation results as mentioned in Sections 3 and 4 support agreements of athermal dynamic temperatures of thermodynamics and/or statistical mechanics.

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