Thermodynamic Theory of Weakly Excited Granular Systems

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We present a thermodynamic theory of weakly excited two-dimensional granular systems from the viewpoint of elementary excitations of spinless Fermions. We introduce a global temperature T that is associated with the acceleration amplitude Γ in a vibrating bed. We show that the configurational statistics of weakly excited granular materials in a vibrating bed obey the Fermi statistics. [S0031-9007(97)02860-3]

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Granular system is robust to thermal disturbances because its entity is a macroscopic object [1]. For this reason, the granular system is effectively in the ground state at any finite temperature and the excitation may be achieved by subjecting the system to vibration or shaking. Such an external stimulus will inject energy at a constant rate but the energy will be dissipated via collisions, leading the system to reach a steady state. Dynamics of such a steady state are quite complex, where convection [2], density waves [3], segregation [4], anomalous sound propagation [5], and even turbulent behaviors [6] have been observed.

There are some indications that fluctuations in physical quantities of granular systems persist over the size of the system [7] and intrinsically nonequilibrium clustering instabilities appear for particles with a large coefficient of restitution [8]. In such cases, we may eventually have to question the validity of the hydrodynamics [9] with the aid of kinetic theory [10], though some attempts have been made to capture some of the essential features of granular convections based on phenomenological hydrodynamics models [11].

In spite of the above negative signs, the validity of the thermodynamics concept has been suggested by several theoretical papers [12,13] and experimental papers [14–17]. In particular, Knight *et al*. [17] have observed a logarithmic relaxation in compaction processes in a three-dimensional vibrating bed, which can be understood as the consecutive transitions among the metastable (glassy) configurations. This suggests the validity of the free volume (or hole) theory [18] used for the dense liquid theory as will be shown later. In two dimensions, in particular, the situation is much simpler than in three dimensions, because the particles can form a lattice structure without glassy configurations. For example, the experiment by Clement and Rajchenbach [14] has suggested that nontrivial and distinctive *configurational* statistics appear to exist for excited granular systems in a vibrating bed. The experiment was conducted with steel balls that have small coefficient of restitution and was monitored carefully to suppress the convection with a suitable choice of the boundary condition. They then observed that the ensemble-averaged density profile obeys a universal function that is independent of the phase of oscillations. The experimental result in Ref. [14] has been recovered by a simulation based on the distinct element method [15] and has been generalized to the case of strong excitations [16]. The existence of such a distinctive configurational statistics, which resembles the problem of packing, appears to be a fairly convincing evidence that kinetic aspects of the vibrating bed might have been decoupled from the statistical configurations averaged over many ensembles and time sequences.

Such a simple observation in two-dimensional weak dissipation cases enables one to make some progress in characterizing the excitation of vibrating beds in two ways: first, if the kinetics is indeed separated out, then the configurational properties should be determined by the principle of maximum entropy or equivalently the minimization of free energy. Second, the validity of such variational methods should be carefully checked against experiments. The test may lead to further conceptual advances, establishing the fact that a weakly driven nonequilibrium dissipative vibrating bed with the vibration intensity Γ may be viewed as a thermodynamic equilibrium state at a finite temperature T in the near elastic limit, *if* one's focus is exclusively on the configurational properties. Here, $\Gamma = A\omega^2/g$ with g the gravitational acceleration, A and W the amplitude and the frequency of the oscillations. The precise relation between Γ and T, however, has yet to be determined. The purpose of this Letter is to advance such a simple observation into systematic investigations and to formulate a thermodynamic theory of powders, at least, in two-dimensional systems, from the viewpoint of elementary excitations such as the Fermi liquid theory [19] in condensed matter physics. Our formulation may open a way to visualize the invisible quantum behaviors of fermions or the microscopic behaviors of dense fluids through the manipulation of granular materials.

The starting point of our thermodynamic formulation [20] is the recognition that the granular state in a

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vibrating bed is an excited state and the degree of the excitation is controlled by the global parameter Γ. Since we are concerned here with the configurational property of such a system, it is natural to associate a similar *global* temperature T, but care must be taken here because the global temperature T must have a well defined thermodynamic meaning. One of the essential requirements is that T must satisfy the statistical definition of the thermodynamic temperature, namely, $T = \partial U/\partial S$, where U is the total energy and S is the entropy of the system. Notice that the conventional kinetic temperature, which is in general a local function, is not identical to the thermodynamic temperature. In fact, T can be nonzero without kinetic energy, because U contains the potential which is a function of the entropy. When the contribution from the kinetic energy is much smaller than the potential energy, the global temperature may be more appropriate than the local granular temperature to characterize the state of granules as the idea used in the free volume theory [18]. One can easily show that this parameter T is almost identical with the compactivity X defined through the free volume introduced by Edwards and his co-workers [12]. While the compactivity X has never been computed nor related in any manner with the experimental control parameters such as Γ, our formulation will enable us to determine the explicit relation between T and Γ. To be more specific, we first view the system of granular particles as the lattice gas, which can be regarded as the simplest version of the free volume (hole) theory [18]. We now assign virtual lattice points by dividing the vibrating bed of width L and the height μD into cells of $D \times D$ with the diameter of the grain D. Each row, i, is then associated with the potential energy $\epsilon_i = mgz_i$ with $z_i = (i - 1/2)D$ and m the mass of the grain. The degeneracy, Ω, of each row is $\Omega = L/D$. For a weakly excited system with $\Gamma \approx 1$, the kinetic energy may be neglected and the potential energy dominates, for which case the most probable configuration should be determined by the state that maximizes the entropy in the microcanonical ensemble approach.

The entropy, S, is defined as $S = \ln W$ with W the total number of ways of distributing N particles into a system. Excluded volume interactions do not allow two grains to occupy the same states and thus the statistics is given by the Fermi statistics. We find

$$W = \Pi_i[\Omega!/N_i!(\Omega - N_i)!], \tag{1}$$

where N_i is the number of particles in the ith row. We now maximize S with constraints that characterize the system, namely, the fixed number of particles N and the mean steady state system energy $\langle U(T(\Gamma))\rangle$, namely,

$$\sum_i N_i = N, \qquad \sum_i N_i \epsilon_i = U. \tag{2}$$

The maximization of S then yields that the density profile, $\phi(z)$, which is the average number of occupied cells at a given energy level, must be given by the Fermi distribution:

$$\phi(z) = N_i/\Omega = 1/\{1 + \exp[\beta(z - \mu)]\}, \tag{3}$$

where $\beta \to mgD/T$ in the low temperature limit, the height $z = z_i/D$, and the Fermi energy μ measured in units of D is the initial number of layers. Note that both z and μ are measured from the bottom layer. The Fermi analogy is valid when $\mu \gg n_l$ with n_l the number of fluidized layer. For a noninteracting electron gas, this ratio is of order 10 to 10^2. Now, since the injected energy per particle at the bottom layer, E_i, is of order $mA^2\omega^2/2$ and the potential energy, E_p, to fluidize a particle on the top n_l layers is of order mgn_lD, by equating the two, we find a necessary condition for the fluidization of the top n_l layers, namely, $n_l \sim \Gamma(A/2D)$. For $\Gamma \sim 1$, the Fermi statistics will be valid, if $\mu \gg A/D$.

Our only remaining task is then to relate the temperature T to the control parameter Γ. Here we do not calculate the entropy and the energy directly, because nonequilbrium and kinetic characteristics may appear in the relation between the temperature T and Γ. Since we have determined the density profile, we find from (2) the energy *per* particle:

$$\bar{u}(T) = \frac{U(T)}{N} = \frac{mgD\mu^2}{2}\left[1 + \frac{\pi^2}{3}\left(\frac{T}{mgD\mu}\right)^2\right] + \ldots, \tag{4}$$

where the first term is the ground state energy and the second term is the increase in energy due to *thermal* expansion, which results in the shift in the center of mass, $\bar{h}(T) = \bar{u}(T)/mg$.

$$\bar{h}(T) = h(0)\left[1 + \frac{\pi^2}{3}\left(\frac{T}{mgD\mu}\right)^2\right] + \ldots \tag{5}$$

with $h(0) = D\mu^2/2$. We now make a crucial observation that for a weakly excited granular system, most excitations occur near the Fermi surface, which may be effectively well represented by the motion of a *single* particle on the Fermi surface that is in contact with the vibrating plate. If the maximum height that a single ball bouncing in a vibrating plate with the intensity Γ is denoted by $H_0(\Gamma)$, then $H_0(\Gamma)$ is determined by the equation that describes the trajectory of a single ball on a vibrating plane with the intensity Γ [11,21]. The relative distance, $\Delta(t)$, between the ball and the vibrating plate is given by

$$\Delta(t) = \Gamma[\sin(t_0) - \sin(t)] + \Gamma\cos(t_0)(t - t_0) - \frac{1}{2}(t - t_0)^2 \tag{6}$$

in units of $g = \omega = 1$, where $t_0 = \sin^{-1}(1/\Gamma)$. The maximum, $H_0(\Gamma)$, can be obtained from (6) numerically and it is effectively equivalent to the expansion of the volume due to *kinetics*. Since the Fermi distribution near $T = 0$ can be approximated by a piecewise linear function and $H_0(\Gamma)$ is thought to be the edge of the function, we

expect $H_0(\Gamma)/2 \approx \Delta h = [\bar{h}(T) - h(0)]$. By equating the thermal expansion, (5), to the kinetic expansion, $H_0(\Gamma)g/\omega^2$ in physical units, we now complete our thermodynamic formulation by presenting the explicit relation between T and $\Gamma = A\omega^2/g$:

$$T = \frac{mg}{\pi\omega}[3DgH_0(\Gamma)]^{1/2}. \tag{7}$$

We point out that the energy is an extensive quantity along the horizontal direction, but is not in the vertical direction where strong anisotropy is present due to gravity. Further, T has a gap at $T = 0$ because the time between the launching and landing of the ball is always finite for $\Gamma > 1$. Figure 1 shows the fitting of the experimental density profile for $\Gamma = 4$ of Clement and Rajchenbach [14] by the scaled Fermi distribution, $\phi(z) \to \phi(z)\phi_c$, with $\phi_c \approx 0.92$ the closed packing density for the hexagonal packing. The fitting value of T/mg is 2.0 mm with $\mu D = 30.5$ mm, while Eq. (7) yields $T/mg \approx 2.6$ mm [22]. The agreement between the two is fairly good in spite of such a simple calculation. This expression also agrees with the simulation result [15]. Note that the detailed expression of $H_0(\Gamma)$ depends on the manner by which the grains are excited and we expect that our main scaling prediction of Eq. (7), namely, $T \propto g^{3/2}D^{1/2}/\omega$, will hold even for systems driven not by sinusoidal waves. Next, it is well known that the *specific heat* per particle, $C_v = d\bar{u}/dT$, can be written as the fluctuations in the energy, namely, $\langle(\Delta\bar{u})^2\rangle = \langle[\bar{u}(z) - \bar{u}]^2\rangle = T^2C_v$ and thus we predict the scaling relation for the fluctuations in potential energy, or in the center of mass,

$$\langle(\Delta\bar{u})^2\rangle = \frac{\pi^2}{3}\frac{T^3}{mgD} \propto g^{7/2}D^{1/2}\omega^{-3}. \tag{8}$$

Certainly, more experiments or simulations would be desirable to test our theory.

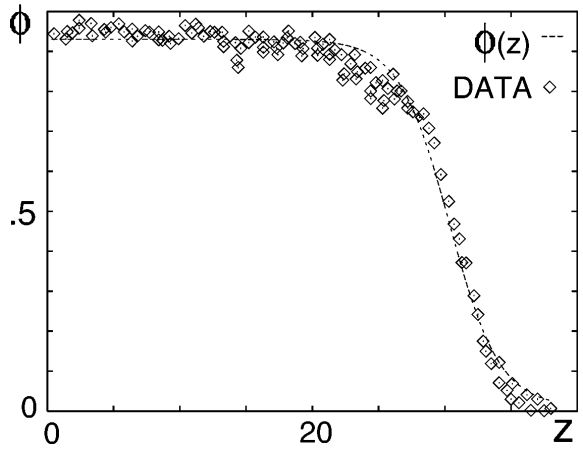

FIG. 1. Comparison between the experiment and the theoretical prediction. The diamonds are the data by Clement and Rajchenbach (Ref. [14]) and the dotted line is the Fermi distribution function $\phi(z)$ [Eq. (3)] multiplied by $\phi_c = 0.92$.

Three comments are in order: First, in three-dimensional systems the situations become far more complex and our ideal Fermi description based on a simple lattice gas picture certainly requires modification, primarily for two reasons: first, holes are not equivalent to particles and, second, many metastable configurations exist, which results in the hysteresis-dependent density profile as observed in the experiment of Knight *et al.* [17]. Even in this case, however, the lattice picture may be valid because the mean free path of the grains is of order of a few particle diameters and the basic granular state is not a gas but a crystal. Hence, the free energy approach adopted in this Letter is more appropriate than the kinetic theory in studying the granular state. Such an approach is consistent with the free volume theory of the liquid state [18], which assumes that the dominant process involving particle rearrangement is a hopping with the rate determined by the activation energy A. Within this picture, the probability of the hopping of a particle from a position $\mathbf{r}$ is proportional to $\exp[-A(\mathbf{r})/T]$ with $A(\mathbf{r}) \simeq a\phi(\mathbf{r})/[1 - \phi(\mathbf{r})]$. The relevant time scale τ that determines the time evolution of the compaction is then given by $\tau/\tau_0 \simeq \exp[b\phi/(1 - \phi)]$ with $b = a/T$, or $\phi(t) \simeq \ln(t/\tau_0)/[b + \ln(t/\tau_0)]$, where we have replaced τ by t. This is consistent with the experimental result reported by Knight *et al.* [17]. Notice that such an activation dominated process does not have a smooth increase of the density. Although this kind of slow relaxation may not be unexpected even in two-dimensional systems, the strong geometrical constraint may suppress such a slow process. We point out that attempts have been made to determine the thermodynamic temperature defined in this paper by measuring the effective viscosity for fluidized beds with a mixture of gas and particles. The results [23] seem to support the validity of the free volume theory. This is an indirect confirmation of the validity of our free fermion picture based on the free volume theory even in three dimensional systems.

Second, we comment on interactions among particles. It is known that even for hard core particles, an effective attractive interaction exists through the direct correlation function [24], which will induce the curvature term in the free energy. In the presence of such a curvature term, while it may be difficult to quantitatively compute the surface tension due to the spatial inhomogeneity, it is nevertheless obvious that we can define surface tension for excited granular materials in a vibrating bed. We may need more systematic experiments and careful theoretical argument to resolve the question of surface tension in excited granular materials [2].

Third, we comment on the effect of dissipation. For a simple one-dimensional system of $N(\gg 1)$ particles connected by springs, where the end particle at the bottom is driven by an external sinusoidal force, the equation of motion for nth bead is then given by $m\ddot{z}_n + m\zeta\dot{z}_n - k\partial_n^2 z_n = mA\omega^2\cos\omega t\,\delta_{n,0}$. For such a linear

system, it is easy to show that the effective amplitude A_{eff} felt by the particle at the top is expressed by $A_{\text{eff}} = A/\sqrt{1 + (\zeta/\omega)^2}$, where the dissipation constant $\zeta = -(\omega/\pi)\ln e$ with the restitution constant e [25]. Thus, the correction for A is very small.

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