Thermodynamic Theory of Weakly Excited Granular Systems

Hisao Hayakawa and Daniel C. Hong

1. Graduate School of Human and Environmental Studies, Kyoto University, Yoshida, Sakyo, Kyoto 606-01, Japan
2. Department of Physics, Lewis Laboratory, Lehigh University, Bethlehem, Pennsylvania 18015

Abstract

We present a thermodynamic theory of weakly excited two-dimensional granular systems from the viewpoint of elementary excitations of spinless Fermion systems. We introduce a global temperature \( T \) that is associated with the acceleration amplitude \( \Gamma \) in a vibrating bed. We show that the configurational statistics of weakly excited granular materials in a vibrating bed obey the Fermi statistics.

P.A.C.S. numbers 81.35.+k, 46.10.+z, 05.70.-a, 05.20.Dd

Granular system is robust to thermal disturbances because its entity is a macroscopic object. 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, density waves, segregation, anomalous sound propagation and even turbulent behaviors have been observed.

There are some indications that fluctuations in physical quantities of granular systems persist over the size of the system and intrinsically nonequilibrium clustering instabilities

*E-mail address: hisao@phys.h.kyoto-u.ac.jp
†E-mail address: dh09@lehigh.edu
appear for particles with 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 $\Gamma$ 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. The precise relation between $\Gamma$ 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 granular state in a vibrating bed is an excited state and the degree of the excitation is controlled by the global parameter $\Gamma$. Since we are concerned here with the configurational property of such a system, it is natural to associate a similar global temperature $T$, but a care must be taken here because the global temperature $T$ must have a well defined thermodynamic meaning. One of the essential requirement 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 coworkers. \[12\] While the compactivity $X$ has never been computed nor related in any manner with the experimental
control parameters such as $\Gamma$, our formulation will enable us to determine the explicit relation between $T$ and $\Gamma$. 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 $\mu D$ 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, $\Omega$, 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:

$$W = \Pi_i[\Omega!/N_i!(\Omega - N_i)!].$$ (1)

We now maximize $S$ with constraints that characterize the system, namely the fixed number of particles $N$ and the mean steady state system energy $<U(T(\Gamma))>$, namely

$$\sum_i N_i = N, \quad \sum_i N_i \epsilon_i = U.$$(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:

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

where $\beta \rightarrow mgD/T$ in the low temperature limit, the height $z = z_i/D$ and the Fermi energy $\mu$ measured in units of $D$ is the initial number of layers. Note that both $z$ and $\mu$ are measured from the bottom layer. The Fermi analogy is valid when $\mu \gg n_l$ with $n_l$ is the number of fluidized layer. For a non-interacting electron gas, this ratio is of order $10$ to $10^2$. Now, since the injected energy, $E_i$, to the system is of order $mA^2\omega^2/2$ and the potential energy,
\(E_p\), to fluidize particles on the top \(n_t\) layers is of order \(mgn_tD\), by equating the two, we find a necessary condition for the fluidization of the top \(n_t\) layers, namely: \(n_t \sim \Gamma(A/2D)\). 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 \(\Gamma\). Here we do not calculate the entropy and the energy directly, because nonequilibrium and kinetic characteristics may appear in the relation between the temperature \(T\) and \(\Gamma\). Since we have determined the density profile, we find from (2) the energy per particle:

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

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, \(\bar{h}(T) = \bar{u}(T)/mg\).

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

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 \(\Gamma\) 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 \(\Gamma\). \(^{[11,21]}\)

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 \(H_0(\Gamma) \approx \Delta h/2 = (\bar{h}(T) - h(0))/2\). 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 \(\Gamma = A\omega^2/g\):
\[ T = \frac{mg}{\pi \omega} (3DgH_0(\Gamma))^{1/2}. \] (7)

We point out that the energy is an extensive quantity along the horizontal direction, but is not in 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, \( \phi(y) = \rho(y)/\rho_c \), with \( \rho_c \approx 0.92 \) 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 \( <(\Delta \bar{u})^2> = <(\bar{u}(z) - \bar{u})^2> = T^2C_v \) and thus we predict the scaling relation for the fluctuations in potential energy, or in the center of mass,

\[
< (\Delta \bar{u})^2 > = \frac{\pi^2}{3} \frac{T^3}{mgD} \propto g^{7/2}D^{1/2}\omega^{-3}.
\] (8)

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

Three comments are in order: First, in three dimensional systems the situations become far more complex and our ideal Fermi description based on 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, 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 paper is more appropriate than the kinetic theory in studying the granular state. Such an approach is consistent with the free volume theory of
liquid state \cite{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 $\tau$ 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 $\tau$ by $t$. This is consistent with the experimental result reported by Knight et al. \cite{17}. Notice that such an activation dominated process does not have 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 \cite{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, interactions among particles. It is known that even for hard core particles, an effective attractive interaction exists through the direct correlation function \cite{24}, which will induce the curvature term. 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 \cite{2}.

Third, 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 $n-$th bead is then given by: $m\ddot{z}_n + m\zeta\dot{z}_n - k\partial_n^2 z_n = mA_0^2 \cos \omega t \delta_{n,0}$. For such a linear system, the effective amplitude $A_{eff}$ felt by the particle at the top is expressed by $A_{eff} = A/\sqrt{1 + (\zeta/\omega)^2}$, where the dissipation constant $\zeta = -(\omega/\pi) \ln e$ with the restitution constant $e$ \cite{25}. Thus, the correction for $A$ is very small.
After we have submitted this Letter, we became aware of two recent papers in which thermodynamic concepts such as one developed in this paper are useful in highly excited vertical vibration of granular materials [26] and in horizontal vibration of granular materials [27]. In these papers, the authors have demonstrated that stationary nonequilibrium state of the vibrating bed exhibits similarities with the thermally equilibrated fluid, consistent with the assumption of this paper, and the spatial correlation function (two-point correlation) can be an index of solid-fluid transition of granular materials and can be approximated by the equilibrium distribution function in the fluid phase.

We would like to express our sincere gratitude to N.Goldenfeld for his encouragement of this study during HH’s stay at U. of Illinois and his collaboration in the early stage of this study, Y. Oono, G. Baym, and H.J.Herrmann for helpful discussions concerning the Fermi liquid theory, Ryan Mitchell for graphical assistance, and J. A. McLennan on various aspects of the kinetic theory of dense gases. HH is, in part, supported by Grant-in-Aid for Scientific Research from Japanese Ministry of Education, Science and Culture (No. 08226206 and 08740308).
REFERENCES

[1] For recent reviews, see: H.M. Jaeger, S.R. Nagel and R.P. Behringer, Physics Today, 49, 32 (1996), Rev. Mod. Phys. 68, 1259 (1996); H. Hayakawa, H. Nishimori, S. Sasa and Y-h. Taguchi, Jpn. J. Appl. Phys. Part 1, 34, 397 (1995) and references therein.

[2] P. Evesque and J. Rajchenbach, Phys. Rev. Lett. 62, 44 (1989); E. Clement, J. Duran and J. Rajchenbach, Phys. Rev. Lett. 69, 1189 (1992); F. Melo, P. Umbanhowar and H. Swinney, Phys. Rev. Lett. 72, 172 (1994), Phys. Rev. Lett. 75, 3838 (1995); P. Umbanhowar, F. Melo and H.L. Swinney, Nature 382, 793 (1996).

[3] G.W. Baxter, R.P. Behringer, T. Fagert and G.A. Johnson, Phys. Rev. Lett. 62, 2825 (1989); T. Poschen. J. Phys. (Paris) 3, 24 (1993).

[4] J.C. Williams. Powder Tech. 15, 245 (1976); J. Knight, H. Jaeger, and S. Nagel. Phys. Rev. Lett. 70, 3728 (1993) and reference therein.

[5] C-h Liu and S.R. Nagel, Phys. Rev. Lett. 62, 40 (1989).

[6] Y-h Taguchi. Europhys. Lett. 24, 203 (1993); K. Ichiki and H. Hayakawa, Phys. Rev. E 51, 658 (1995).

[7] R.P. Behringer, Bull. Amer. Phys. Soc. 41, No.1, 684 (1996).

[8] S. McNamara and W. R. Young, Phys. Fluids A 4, 496 (1992), Phys. Rev. E 53, 5089 (1996); I. Goldhirsch and G. Zanetti, Phys. Rev. Lett. 70, 1619 (1993).

[9] Y. Du, H. Li and L.P. Kadanoff, Phys. Rev. Lett. 74, 1268 (1995).

[10] J.T. Jenkins and S.B. Savage, J. Fluid Mech. 130, 187 (1983); B. Bernu, F. Deylon, and R. Dazighi, Phys. Rev. E. 50, 4551 (1994); J.J. Brey, F. Moreno and J.W. Dufty, Phys. Rev. E 54, 445 (1996).

[11] M. Bourzutschky and J. Miller, Phys. Rev. Lett. 74, 2216 (1995); H. Hayakawa, S. Yue and D.C. Hong, Phys. Rev. Lett. 75, 2328 (1995).
[12] S.F.Edwards and R.B.S. Oakeshott, Physica A 157, 1080 (1989); A.Mehta and S.F.Edwards, Physica A 168, 714 (1990).

[13] H.J.Herrmann, J.de Physique (Paris) II 3, 427 (1993).

[14] E. Clement and J. Rajchenbach. Europhys. Lett. 16, 133 (1991)

[15] J.A.C.Gallas, H.Herrmann, and S.Sokolowski, Physica A 189, 437 (1992).

[16] S.Warr, J.M. Huntley and G.H. Jacques, Phys.Rev. E 52, 5583 (1995).

[17] J.B.Knight, C.G.Fandrich, C.N.Lai, H.M.Jaeger and S.R.Nagel, Phys.Rev. E 51, 3957 (1995).

[18] see e.g. T.L.Hill, Statistical Mechanics (Dover, New York,1987) Chap.8; See also, H. Caram and D. C. Hong, Phys. Rev. Lett. 67, 828 (1991)

[19] L.D.Landau, J. Phys. USSR. 10, 25 (1946).

[20] Preliminary argument of the Fermi analogy was first presented at the International Conference on Nonlinear Dynamics and Chaos, July, 1995, Pohang, Korea, by H. Hayakawa and D.C. Hong, Proceedings to be published in Int. J. Bifurcations and Chaos.

[21] J.M. Luck and A.Mehta, Phys. Rev. E 48, 3988 (1993) and references therein.

[22] This good agreement may be a little surprising for strong excitation. For $\Gamma = 4$, $t_0 = 0.25268$, and the solution of $d\Delta(t)/dt = 0$ is given by $t_{max} = 4.59483$, for which case $H_0(4) = 12.3623$. In ref. [14] $D = 3[mm]$ and $\omega/(2\pi) = 20[Hz]$. For $\Gamma = 4$, the bouncing solution becomes chaotic.

[23] K.Ichiki and H.Hayakawa(unpublished). For earlier experiment, see; J. Furukawa and T. Ohmae, Ind. Emg. Chem. 50, 821 (1958).

[24] J.-P. Hansen and McDonald, Theory of Simple Liquids, 2nd Edition (Academic, London, 1986).
[25] Y-h. Taguchi, Phys. Rev. Lett. 69, 1367 (1992).

[26] S. Warr and J-P. Hansen, preprint.

[27] G.H. Ristow, G. Strassburger and I. Rehberger, preprint.
Figure Caption

Fig. 1. Comparison between the experiment and the theoretical prediction. The circles are the data by Clement and Rajchenbach (ref.14) and the dotted line is the Fermi distribution function \( \phi(z) \) (eq.(3)).
DATA

\[ \phi(z) \]

\[ \phi \]

\[ Z \]

\[ .5 \]

\[ 0 \]