

Reply to comment on “Failure of the Volume Function in Granular Statistical Mechanics and an Alternative Formulation”

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(Dated: May 11, 2017)

We recently argued [1] that the volume function (VF), being insensitive to most of the degrees of freedom (DFs), is unsuitable as the granular ‘Hamiltonian’ and proposed an alternative. The previous comment [2] contests with the following arguments:

(1) Changes in positions of bulk particles in granular systems (GSs) may lead to rearrangements that change the boundary position, making the latter implicitly sensitive to many configurational changes.

(2) The Hamiltonian does not determine the number of microstates and the entropy.

(3) The ideal gas Hamiltonian, H_{ig} , for example, is also independent of some DFs, yet it is a good model in thermal statistical mechanics.

(4) The VF insensitivity to the bulk particle positions agrees with Edward’s hypothesis of equiprobable microstates, supporting the VF.

As detailed next, we agree with argument (2), refute (1), (3) and (4), and clarify why the VF is not a useful Hamiltonian analogue for GSs.

Argument (1): That the microscopic VF changes when particle displacement reaches the boundary is correct, but structural perturbations well inside a GS affect the boundary negligibly if at all, except near the jamming point, as the authors concede. Away from this point, where most realistic GSs exist, the range of the response to internal perturbations is much shorter than the system size and is hardly likely to affect the boundary particle positions and, therefore, the VF. This is independent of the existence of rattlers, whose change of positions does not affect the boundary either.

Argument (2): Indeed, the statement in our paper, that the VF fails to account correctly for the entire entropy, was incorrect. Nevertheless, this is not the main reason for the failure of the VF, as we explain next.

Argument (3): This is the comment’s main argument. The main aim of our paper was to construct a statistical mechanical formalism to describe usefully *all* GSs. The objective of statistical mechanics in general is to make possible derivation of measurable macroscopic properties as expectation values over a partition function, which can apply to *all* systems. A thermal system’s energy

need not depend on all the DFs, but if it does, the Hamiltonian will also depend on all of them. This makes it applicable to *all* thermal systems. E.g., put the ideal gas in a gravitational field and H_{ig} would also depend on the position DFs, otherwise one could not calculate the macroscopic pressure or gas density as functions of position (height). In contrast, the VF cannot depend on the internal structural DFs for all GSs. Consequently, we cannot use it to derive expectation values of quantities that depend on internal DFs. For example, a GS permeability to fluid flow through it depends on the distribution of its inter-pore passageways. The VF provides no way to calculate this distribution.

Argument (4): Edwards’s hypothesis of equiprobable microstates was shown to fail for a range of GSs [3–5] away from the jamming point, further undermining the applicability of the VF and the basis for this argument.

Thus, the Hamiltonian applies to all thermal systems, involving all relevant DFs when necessary. The VF lacks this feature, depending only on few DFs. Therefore, it is unusable for calculating all possible structure-based expectation values. The argument that changes in the internal structure would affect the boundary particle positions is wrong – such changes affect only a small region in most systems. The argument that equiprobability of microstates obviates dependence on internal DFs is misconceived because the microstates of GSs are not always equiprobable.

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