“Stochastic Models for Granular Matter 1”

Kinetic theory for
granular gases (and liquids)

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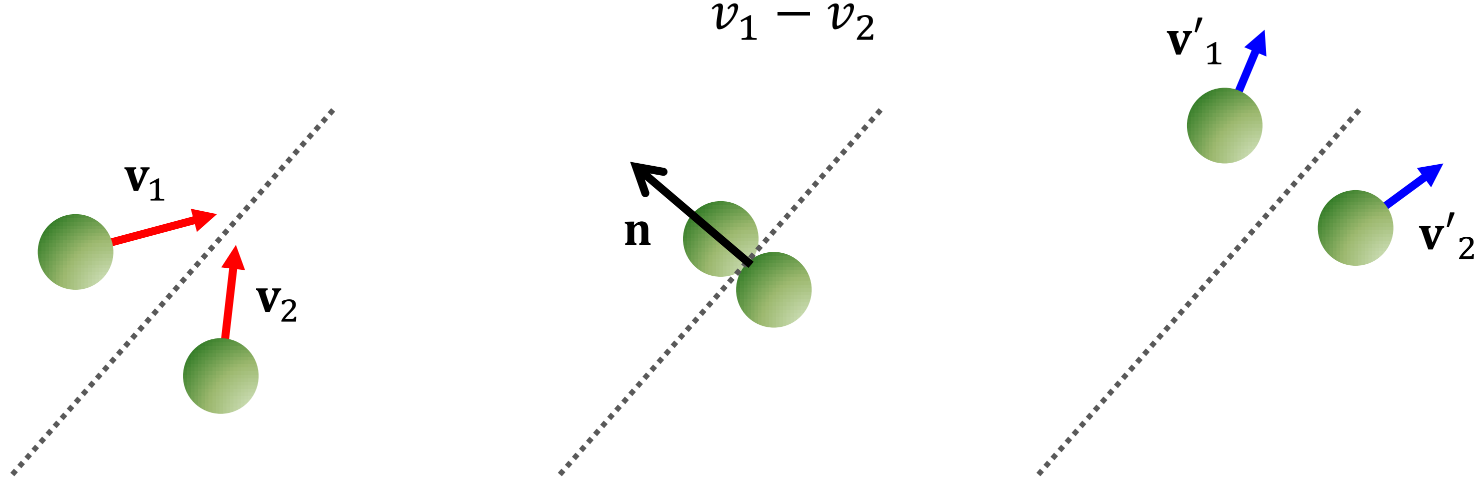
Inelastic binary collision

A model of granular materials:
Smooth (frictionless) spheres which dissipate their kinetic energy by **inelastic collisions**

Restitution coefficient

$$e \equiv -\frac{v'_1 - v'_2}{v_1 - v_2} < 1$$



Relative velocities

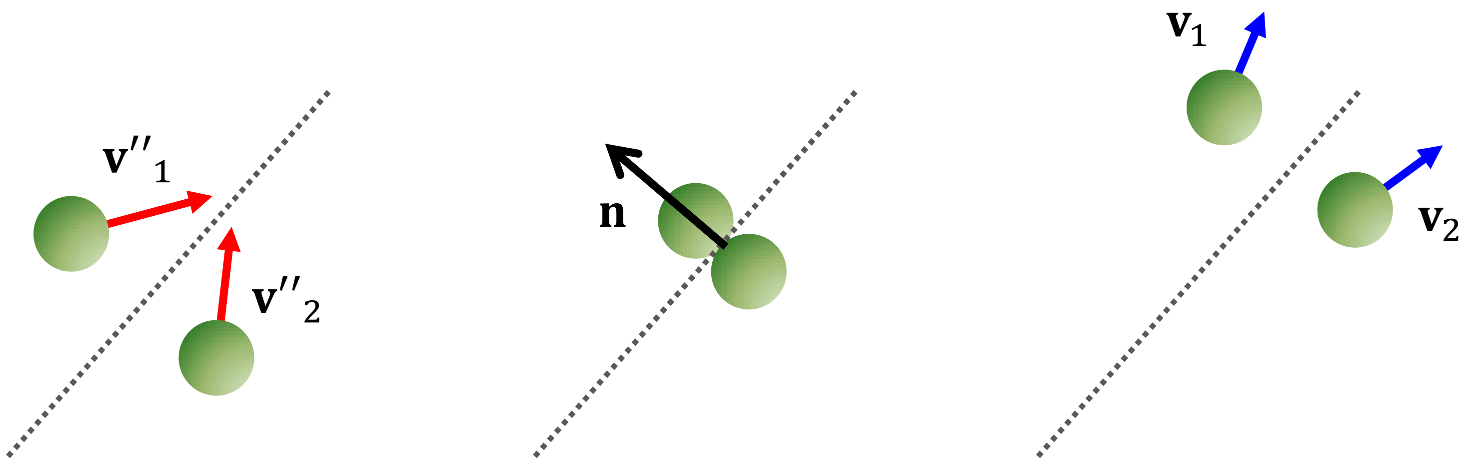
$$\mathbf{g} \equiv \mathbf{v}_1 - \mathbf{v}_2$$

$$\mathbf{g}' \equiv \mathbf{v}'_1 - \mathbf{v}'_2$$

$$\mathbf{g}' \cdot \mathbf{n} = -e(\mathbf{g} \cdot \mathbf{n})$$

Inelastic binary collision

Velocities, $\mathbf{v}''_1$ and $\mathbf{v}''_2$, which result in $\mathbf{v}_1$ and $\mathbf{v}_2$ after an inelastic collision:



$$\mathbf{g}'' \equiv \mathbf{v}''_1 - \mathbf{v}''_2$$

$$\mathbf{g}'' \cdot \mathbf{n} = -\frac{1}{e}(\mathbf{g} \cdot \mathbf{n})$$

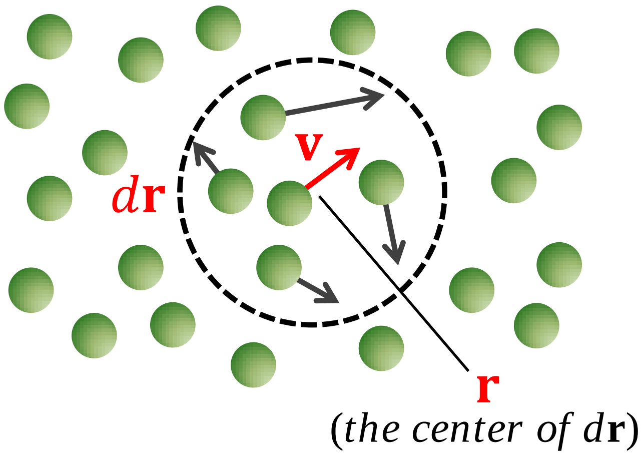
For *frictionless particles*, $\mathbf{g}'' = \mathbf{g} - \left(1 + \frac{1}{e}\right)(\mathbf{g} \cdot \mathbf{n})\mathbf{n}$

Exercise 1) Please derive the following relations.

$$d\mathbf{g}'' = \left|\frac{\partial \mathbf{g}''}{\partial \mathbf{g}}\right| d\mathbf{g} = \frac{1}{e} d\mathbf{g} \qquad d\mathbf{v}''_1 d\mathbf{v}''_2 = \frac{1}{e} d\mathbf{v}_1 d\mathbf{v}_2$$

Jacobian

Velocity distribution functions



"**The number of particles** in a volume $d\mathbf{r}$ with the velocities $\mathbf{v}$~$\mathbf{v}+d\mathbf{v}$ at time t" = $f(\mathbf{r}, \mathbf{v}, t)d\mathbf{r}d\mathbf{v}$

If there is no collision, we can trace the particles by

$$\mathbf{r} \rightarrow \mathbf{r} + \mathbf{v}dt$$

$$\mathbf{v} \rightarrow \mathbf{v} + (\mathbf{F}/m)dt$$

$$\mathbf{F} = m\frac{d\mathbf{v}}{dt}$$

External body force

The number of particles does not change:

$$\{f(\mathbf{r} + \mathbf{v}dt, \mathbf{v} + (\mathbf{F}/m)dt, t + dt) - f(\mathbf{r}, \mathbf{v}, t)\}d\mathbf{r}d\mathbf{v} = 0$$

Because of collisions, the number of particles change during dt:

$$\{f(\mathbf{r} + \mathbf{v}dt, \mathbf{v} + (\mathbf{F}/m)dt, t + dt) - f(\mathbf{r}, \mathbf{v}, t)\}d\mathbf{r}d\mathbf{v} \equiv \left(\frac{\partial f}{\partial t}\right)_{coll} d\mathbf{r}d\mathbf{v}dt$$

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \frac{\mathbf{F}}{m} \cdot \frac{\partial f}{\partial \mathbf{v}} \equiv \left(\frac{\partial f}{\partial t}\right)_{coll}$$

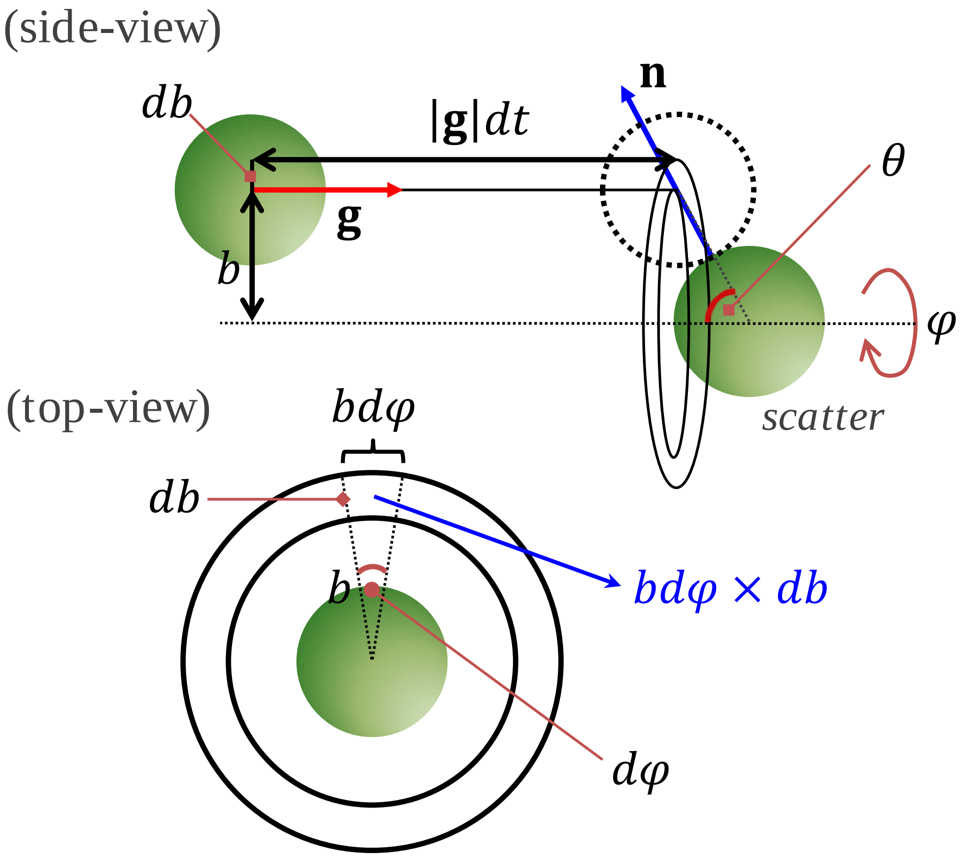
For simplicity, $\mathbf{F} = \mathbf{0}$

Boltzmann equation

The change of the number of particles after collisions: $\left(\frac{\partial f}{\partial t}\right)_{coll} d\mathbf{r}d\mathbf{v}dt$

- Case 1: *"Direct collision"*, $\mathbf{v} \rightarrow \mathbf{v}'(\neq \mathbf{v})$, ***lose*** the number of particles **with v**
- Case 2: *"Inverse collision"*, $\mathbf{v}''(\neq \mathbf{v}) \rightarrow \mathbf{v}$, ***gain*** the number of particles **with v**

Here, we assume that no particle goes out from the volume $d\mathbf{r}$.



The number of direct collisions:

The particles in a volume element
$dV \equiv bd\varphi \times db \times |\mathbf{g}|dt$
will collide with the scatter particle.

$$b = \sigma \sin\theta \,,\, db = \sigma \cos\theta \, d\theta$$

$$\therefore dV = \sigma^2 |\mathbf{g}\cdot\mathbf{n}| \sin\theta \, d\theta d\varphi dt$$
$$\equiv \sigma^2 |\mathbf{g}\cdot\mathbf{n}| d\Omega dt$$

"The number of particles in dV**"**
$$= f(\mathbf{r}, \mathbf{v}_1, t) dV d\mathbf{v}_1$$

"The number of scatters in $d\mathbf{r}$**"**
$$= f(\mathbf{r}, \mathbf{v}_2, t) d\mathbf{r} d\mathbf{v}_2$$

Boltzmann equation

The number of direct collisions:

(The number of particles in *dV*) × (The number of scatters in *d*r)

$$f(\mathbf{r},\mathbf{v}_1,t)f(\mathbf{r},\mathbf{v}_2,t)\sigma^2|\mathbf{g}\cdot\mathbf{n}|d\Omega d\mathbf{v}_1 d\mathbf{v}_2 d\mathbf{r}dt$$

The number of inverse collisions:

$$f(\mathbf{r},\mathbf{v}''_1,t)f(\mathbf{r},\mathbf{v}''_2,t)\sigma^2|\mathbf{g}''\cdot\mathbf{n}|d\Omega d\mathbf{v}''_1 d\mathbf{v}''_2 d\mathbf{r}dt$$

$$\mathbf{g}''\cdot\mathbf{n} = -\frac{1}{e}(\mathbf{g}\cdot\mathbf{n}) \qquad d\mathbf{v}''_1 d\mathbf{v}''_2 = \frac{1}{e}d\mathbf{v}_1 d\mathbf{v}_2$$ (Exercise 1)

$$\frac{1}{e^2}f(\mathbf{r},\mathbf{v}''_1,t)f(\mathbf{r},\mathbf{v}''_2,t)\sigma^2|\mathbf{g}\cdot\mathbf{n}|d\Omega d\mathbf{v}_1 d\mathbf{v}_2 d\mathbf{r}dt$$

The amount = (inverse collisions "*gain*") – (direct collisions "*loss*")

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = \sigma^2\int d\mathbf{v}_2\int_{\mathbf{g}\cdot\mathbf{n}<0} d\Omega\,|\mathbf{g}\cdot\mathbf{n}|\left[\frac{1}{e^2}f(\mathbf{r},\mathbf{v}''_1,t)f(\mathbf{r},\mathbf{v}''_2,t) - f(\mathbf{r},\mathbf{v}_1,t)f(\mathbf{r},\mathbf{v}_2,t)\right]$$

Boltzmann eq.

$$\left(\frac{\partial}{\partial t}+\mathbf{v}\cdot\nabla\right)f = \sigma^2\int d\mathbf{v}_2\int_{\mathbf{g}\cdot\mathbf{n}<0} d\Omega\,|\mathbf{g}\cdot\mathbf{n}|\left[\frac{1}{e^2}f''f''_2 - ff_2\right] \equiv I[f,f]$$

cf.) Note the similarity with the Master equation!

Boltzmann equation

$$\int \psi(\mathbf{v}) I[f,f] d\mathbf{v} = \frac{d^2}{2} \iint d\mathbf{v} d\mathbf{v}' \int_{\mathbf{g}\cdot\mathbf{n}<0} d\Omega \, |\mathbf{g}\cdot\mathbf{n}| \Delta[\psi(\mathbf{v}) + \psi(\mathbf{v}')] f f'$$

$$\Delta A(\mathbf{v}) \equiv A(\mathbf{v}') - A(\mathbf{v})$$

Collision invariants

Mass $\psi(\mathbf{v}) = m$ $\int m I[f,f] d\mathbf{v} = 0$

Momentum $\psi(\mathbf{v}) = m\mathbf{v}$ $\int m\mathbf{v} I[f,f] d\mathbf{v} = 0$

Kinetic energy $\psi(\mathbf{v}) = \frac{m\mathbf{v}^2}{2}$ $\int \frac{m\mathbf{v}^2}{2} I[f,f] d\mathbf{v} = -\frac{\pi m \sigma^2}{16}(1-e^2)\int |\mathbf{g}|^3 f f' d\mathbf{v} d\mathbf{v}'$

Exercise 2) Please derive above relations of collision invariants.

Hydrodynamics

Boltzmann eq. $$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla\right) f = I[f,f]$$

e.g.) Integrate over $\mathbf{v}$

- ✓ ∇ *and* $\mathbf{v}$ *is independent.*
- ✓ *Collision invariant*

$$\frac{\partial}{\partial t}\int f d\mathbf{v} + \nabla\cdot\int \mathbf{v} f d\mathbf{v} = \int I[f,f]d\mathbf{v} = 0$$

Continuity eq. $$\frac{\partial}{\partial t} n + \nabla\cdot(n\mathbf{u}) = 0$$

Number density $$n(\mathbf{r},t) = \int f(\mathbf{r},\mathbf{v},t)d\mathbf{v}$$

Velocity field $$\mathbf{u}(\mathbf{r},t) = \frac{1}{n(\mathbf{r},t)}\int \mathbf{v} f(\mathbf{r},\mathbf{v},t)d\mathbf{v}$$

Hydrodynamics

$\int d\mathbf{v}\, \mathbf{v} \times [\text{Boltzmann eq.}]$ ➡ **Equation of motion**

$$\frac{\partial}{\partial t}\mathbf{u} + \mathbf{u}\cdot\nabla\mathbf{u} = -\frac{1}{mn}\nabla\cdot\boldsymbol{\sigma}$$

$\int d\mathbf{v}\frac{mV^2}{2} \times [\text{Boltzmann eq.}]$ ➡ **Energy eq.**

$$\frac{\partial}{\partial t}T + \mathbf{u}\cdot\nabla T = -\frac{2}{3n}(\boldsymbol{\sigma}:\nabla\mathbf{u} + \nabla\cdot\mathbf{q}) - \zeta T$$

"Granular" temperature $\quad T(\mathbf{r},t) = \frac{2}{3n(\mathbf{r},t)}\int \frac{mV^2}{2} f(\mathbf{r},\mathbf{v},t)d\mathbf{v}$

Velocity fluctuation $\quad \mathbf{V} \equiv \mathbf{v} - \mathbf{u}(\mathbf{r},t)$

Exercise 3) Please derive the equation of motion from the Boltzmann eq.
(The derivation of the energy eq. is given in the lecture note.)

Hydrodynamics

Stress

$$\sigma_{ij} = nT\delta_{ij} + \int m\left(V_i V_j - \frac{1}{3}\delta_{ij}V^2\right) f d\mathbf{v} \equiv nT\delta_{ij} + \int D_{ij} f d\mathbf{v}$$

Heat flux

$$q_i = \int \left(\frac{mV^2}{2} - \frac{5}{2}T\right) V_i f d\mathbf{v} \equiv \int S_i f d\mathbf{v}$$

Cooling rate

$$\zeta = -\frac{m}{3nT}\int V^2 I[f,f] d\mathbf{v}$$

Chapman-Enskog method

"Slightly" inhomogeneous

$$\nabla \sim \mathbf{k} \qquad \epsilon \sim |\mathbf{k}| \ll 1$$

$$\nabla \to \epsilon \nabla$$

Dispersion relation

$$\begin{aligned}\omega(k) &= \omega_0 + k\omega_1 + k^2\omega_2 + \cdots \\ &\sim \omega_0 + \epsilon\omega_1 + \epsilon^2\omega_2 + \cdots\end{aligned}$$

Introduce different time scales

$$\omega \sim \frac{\partial}{\partial t} \qquad \omega_i \sim \frac{\partial}{\partial t_i}$$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t_0} + \epsilon\frac{\partial}{\partial t_1} + \epsilon^2\frac{\partial}{\partial t_2} \cdots$$

Perturbative expansion of $f(\mathbf{r}, \mathbf{v}, t)$

$$f = f_0 + \epsilon f_1 + \cdots$$

Chapman-Enskog method

Boltzmann eq. $$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla\right) f = I[f,f]$$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial t_0} + \epsilon\frac{\partial}{\partial t_1} + \cdots \qquad \nabla \to \epsilon\nabla \qquad f = f_0 + \epsilon f_1 + \cdots$$

$\boldsymbol{O}(\mathbf{1})$ $$\frac{\partial}{\partial t_0} f_0 = I[f_0, f_0]$$

Closed equation of f_0

$\boldsymbol{O}(\boldsymbol{\epsilon})$ $$\frac{\partial}{\partial t_0} f_1 - I[f_0, f_1] - I[f_1, f_0] = \left(\frac{\partial}{\partial t_1} + \mathbf{v}\cdot\nabla\right) f_0$$

Hydrodynamic eqs.

$\boldsymbol{O}(\mathbf{1})$
$$\frac{\partial n}{\partial t_0} = 0$$
$$\frac{\partial \mathbf{u}}{\partial t_0} = \mathbf{0}$$
$$\frac{\partial T}{\partial t_0} = -\zeta_0 T$$

$\boldsymbol{O}(\boldsymbol{\epsilon})$
$$\frac{\partial n}{\partial t_1} = -\nabla\cdot(n\mathbf{u})$$
$$\frac{\partial \mathbf{u}}{\partial t_1} = -\mathbf{u}\cdot\nabla\mathbf{u} - \frac{1}{mn}\nabla(nT)$$
$$\frac{\partial T}{\partial t_1} = -\mathbf{u}\cdot\nabla T - \frac{2}{3}T\nabla\cdot\mathbf{u}$$

Chapman-Enskog method

Assume that $f(\mathbf{r}, \mathbf{v}, t)$ depends on $\mathbf{r}$ and t through the hydrodynamic fields, $n(\mathbf{r}, t), u(\mathbf{r}, t)$, and $T(\mathbf{r}, t)$.

$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial n}\frac{\partial n}{\partial t} + \frac{\partial f}{\partial \mathbf{u}} \cdot \frac{\partial \mathbf{u}}{\partial t} + \frac{\partial f}{\partial T}\frac{\partial T}{\partial t}$$

$$\nabla f = \frac{\partial f}{\partial n}\nabla n + \frac{\partial f}{\partial \mathbf{u}} \cdot \nabla \mathbf{u} + \frac{\partial f}{\partial T}\nabla T$$

cf.) This idea, "*projection of phase-space functions on hydrodynamic fields*", is quite important in statistical mechanics, e.g. the mode-coupling theory (MCT).

Combined with the 1st-order hydrodynamics, the 1st-order Boltzmann eq. is now written as

$$\frac{\partial}{\partial t_0} f_1 - I[f_0, f_1] - I[f_1, f_0] = \mathbf{A} \cdot \nabla \log T + \mathbf{B} \cdot \nabla \log n + \mathbf{C} : \nabla \mathbf{u}$$

Exercise 4) Please show the explicit forms of A, B, and C.
Note that $A \propto V, B \propto V$, and C is a traceless tensor.

Chapman-Enskog method

$$\underbrace{\frac{\partial}{\partial t_0} f_1 - I[f_0, f_1] - I[f_1, f_0]}_{\textit{Linear in } f_1 \textit{ !!!}} = \mathbf{A} \cdot \nabla \log T + \mathbf{B} \cdot \nabla \log n + \mathbf{C} : \nabla \mathbf{u}$$

$$f_1 \equiv \boldsymbol{\alpha} \cdot \nabla \log T + \boldsymbol{\beta} \cdot \nabla \log n + \boldsymbol{\gamma} : \nabla \mathbf{u}$$

Substitute f_1 in the 1$^{\text{st}}$-order Boltzmann eq. and use the 0$^{\text{th}}$-order hydrodynamics

$$-\zeta_0 \left(T \frac{\partial}{\partial T} + \frac{1}{2} \right) \boldsymbol{\alpha} - J[f_0, \boldsymbol{\alpha}] = \mathbf{A}$$

$$-\zeta_0 \left(T \frac{\partial \boldsymbol{\beta}}{\partial T} + \boldsymbol{\alpha} \right) - J[f_0, \boldsymbol{\beta}] = \mathbf{B}$$

$$-\zeta_0 T \frac{\partial \boldsymbol{\gamma}}{\partial T} - J[f_0, \boldsymbol{\gamma}] = \mathbf{C}$$

$$J[a, b] \equiv I[a, b] + I[b, a]$$

$\boldsymbol{\alpha}$, $\boldsymbol{\beta}$, and $\boldsymbol{\gamma}$ are determined by solving the equations, i.e. f_1 is obtained.

Chapman-Enskog method

Stress $\sigma_{ij} = nT\delta_{ij} + \int D_{ij} f d\mathbf{v} \equiv p\delta_{ij} - \eta\left(\nabla_i u_j + \nabla_j u_i - \frac{2}{3}\delta_{ij}\nabla_k u_k\right)$

Kinetic theory **Phenomenological expression**

$\nabla \to \epsilon\nabla \qquad f = f_0 + \epsilon f_1 + \cdots$

$\boldsymbol{O(1)}$ $p = nT$ ***Hydrostatic pressure***

$\boldsymbol{O(\epsilon)}$ $\eta = -\frac{1}{10}\int (\mathbf{D}:\boldsymbol{\gamma}) d\mathbf{v}$ ***Shear viscosity***

Heat flux $q_i = \int S_i f d\mathbf{v} \equiv -\kappa\nabla_i T - \mu\nabla_i n$

$\boldsymbol{O(\epsilon)}$

$\kappa = -\frac{1}{3T}\int (\mathbf{S}\cdot\boldsymbol{\alpha}) d\mathbf{v}$ ***Thermal conductivity***

$\mu = -\frac{1}{3n}\int (\mathbf{S}\cdot\boldsymbol{\beta}) d\mathbf{v}$ ***"2nd-thermal conductivity"***

Chapman-Enskog method

e.g.) From the 0th-order Boltzmann eq.

$$f_0 \cong \frac{n}{(2T/m)^{3/2}} \exp\left[-\frac{\mathbf{v}^2}{2T/m}\right]\left\{1 + a_2(e) S_2\left(\frac{\mathbf{v}^2}{2T/m}\right)\right\}$$

Shear viscosity

$$\eta = \frac{15}{2(1+e)(13-e)d^2}\sqrt{\frac{mT}{\pi}}\left(1 + \frac{3(4-3e)}{8(13-e)} a_2(e)\right) \propto \sqrt{T}$$

Thermal conductivity

$$\kappa = \frac{75}{2(1+e)(9+7e)d^2}\sqrt{\frac{T}{\pi m}}\left(1 + \frac{797+211e}{32(9+7e)} a_2(e)\right) \propto \sqrt{T}$$

"2nd-thermal conductivity"

$$\mu = \frac{750(1-e)}{(1+e)(9+7e)(19-3e)nd^2}\sqrt{\frac{T^3}{\pi m}}\left(1 + h(e)a_2(e)\right) \propto (1-e)\frac{T^{3/2}}{n}$$

References

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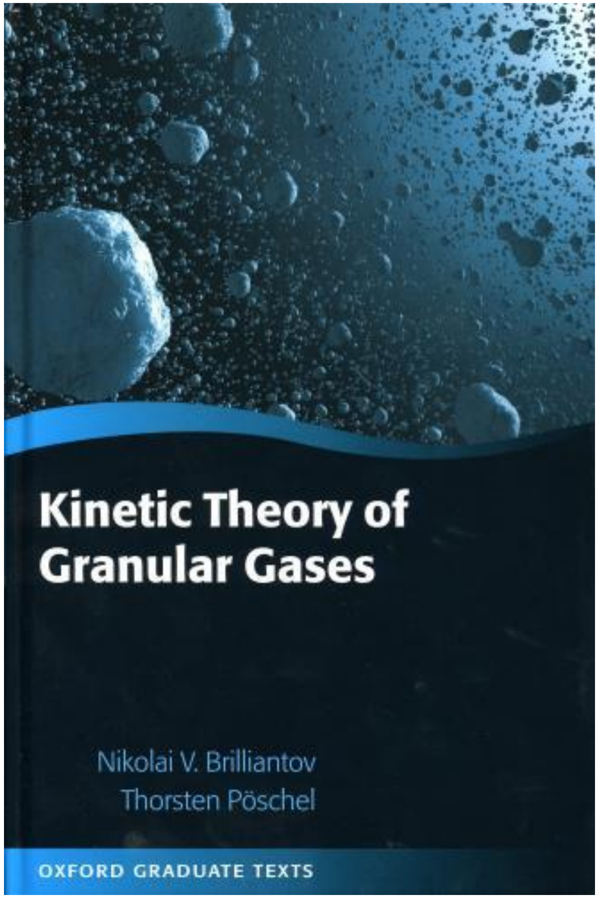
   "*Kinetic Theory of Granular Gases*"

2. S. Chapman and T.G. Cowling,
   "*The Mathematical Theory of Non-uniform Gases*"

3. Lecture note:
   http://www2.msm.ctw.utwente.nl/saitohk/pdf/kinetic.pdf



References

“**Negative normal restitution coefficient** found in simulations of nanocluster collisions”
K. Saitoh, A. Bodrova, H. Hayakawa, and N.V. Brilliantov

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Editors’ Suggestions

SUGGESTION

http://journals.aps.org/prl/abstract/10.1103/PhysRevLett.105.238001

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Negative Normal Restitution Coefficient Found in Simulation of Nanocluster Collisions

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The oblique impacts of nanoclusters are studied theoretically and by means of molecular dynamics. In simulations we explore two models—Lennard-Jones clusters and particles with covalently bonded atoms. In contrast with the case of macroscopic bodies, the standard definition of the normal restitution coefficient yields for this coefficient negative values for oblique collisions of nanoclusters. We explain this effect and propose a proper definition of the restitution coefficient which is always positive. We develop a theory of an oblique impact based on a continuum model of particles. A surprisingly good agreement between the macroscopic theory and simulations leads to the conclusion that macroscopic concepts of elasticity, bulk viscosity, and surface tension remain valid for nanoparticles of a few hundred atoms.

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Introduction.—Inelastic collisions, where part of the mechanical energy of colliding bodies transforms into heat, are common in nature and industry. Avalanches, rapid granular flows of sand, powders, or cereals may be mentioned as pertinent examples [1,2]. Moreover, inelastic collisions define basic properties of astrophysical objects, like planetary rings, dust clouds, etc. An important characteristic of such collisions is the so-called normal restitution coefficient e. According to a standard definition, it is equal to the ratio of the normal component of the rebound speed, $\mathbf{g}'$ (prime states for the postcollision value), and the impact speed, $\mathbf{g}$

$$e = -\frac{\mathbf{g}'\cdot\mathbf{n}}{\mathbf{g}\cdot\mathbf{n}}. \quad (1)$$

The unit intercenter vector $\mathbf{n} = \mathbf{r}_{12}/|\mathbf{r}_{12}|$ at the collision instant ($\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$) specifies the impact geometry. Since particles bounce in the direction opposite to that of the impact, e is positive, $e > 0$, and since the energy is lost in collisions, e is smaller than 1, that is, $0 \le e \le 1$. This is a common statement in the majority of mechanical textbooks, where it is also claimed that e is a material constant. Recent experimental and theoretical studies show, however, that the concept of a restitution coefficient is more complicated; first, it depends on an impact speed [3–5] and second, it can exceed unity for a special case of oblique collisions with an elastoplastic plate [6], where the energy of normal mo- numerically [7–10]. It was observed that the surface effects, due to the direct intercluster van der Waals interactions, play a crucial role: The majority of collisions of homogeneous clusters, built of the same atoms, lead to a fusion of particles [7]; they do not fuse for high impact speeds, but disintegrate into pieces [7]. This complicates the analysis of restitutive collisions, which may be more easily performed for particles with a reduced adhesion. Among possible examples of such particles are clusters of covalently bonded atoms, especially when their surface is coated by atoms of a different sort, such as for H-passivated Si nanospheres [8]. These particles can rebound from a substrate, keeping their form unaltered after an impact [8]. The bouncing nanoclusters demonstrate a surprising effect—the normal restitution coefficient can exceed unity even for strictly head-on collisions [9].

In this Letter we investigate the oblique impact of nanoclusters with the reduced adhesion by means of molecular dynamics (MD) and theoretically, using concepts of continuum mechanics. Unexpectedly, we have found that the normal restitution coefficient, as defined by Eq. (1), acquires for large incident angles negative values, $e < 0$. We explain this effect by the reorientation of the contact plane during an impact and quantify it. Moreover, we propose a modified definition of e, which preserves its initial physical meaning and always yields positive values.