Fate of Boltzmann's breathers: Stokes hypothesis and anomalous thermalization

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Boltzmann showed that in spite of momentum and energy redistribution through collisions, a rarefied gas confined in a isotropic harmonic trapping potential does not reach equilibrium; it evolves instead into a breathing mode where density, velocity and temperature oscillate. This counterintuitive prediction is upheld by cold atoms experiments. Yet, are the breathers eternal solutions of the dynamics even in an idealized and isolated system? We show by a combination of hydrodynamic arguments and Molecular Dynamics simulations that an original dissipative mechanism is at work, where the minute and often neglected bulk viscosity eventually thermalizes the system, that thus reaches equilibrium.

Ludwig Boltzmann was among the very "first creative thinkers in any field to look at the world in a fully twentieth-century manner" [1]. Together with J.C. Maxwell, he was the founding father of kinetic theory unifying Newtonian mechanics with thermodynamics, two approaches that had been impervious to each until then. This accomplishment is epitomized in the so-called Boltzmann equation of which we celebrated the 150th anniversary in 2022. It remains an important branch in basic sciences, be it in mathematics [2], physics [3] and engineering [4, 5]. Lesser known is the fact that a few years after having laid the foundations, Boltzmann found outlandish solutions to the eponymous equation, where a confined dilute gas never reaches equilibrium but rather organizes into a perpetual oscillating "breathing mode" [6, 7]. For lack of an experimental realization in a three dimensional system, Boltzmann's prediction long remained peripheral, garnering limited interest. The situation changed recently when a large collection of Rb cold atoms confined in a harmonic trap was shown to clearly vindicate the breather mode, in full agreement with the theory [8, 9].

Since the Boltzmann equation features irreversibility [7], the possibility of breathing modes is surprising in two respects. First, they do emerge under the action of viscous forces, but are themselves shear-less and undamped [10, 11]. Second, they provide eternal solutions, a priori trustworthy in the limit where the framework applies, ie a dilute system with short range interactions. Under such conditions, far from a critical point or from the crowding environment that are found in kinetically arrested states of matter or glasses [12], the system should eventually thermalize and reach equilibrium [13]. Yet, the kinetic theory framework of the Boltzmann equation fails

to identify any damping mechanism for the breathers. It is our main purpose to study their fate, from the formation to their possible disappearance, under a dissipative mechanism that necessarily requires a description beyond the Boltzmann equation. While kinetic theory itself is a possible venue for such an analysis [14], we will see that hydrodynamics provides a direct answer: not only does it allow to recover the breathing modes in a economical fashion, but more importantly, it sheds lights on their damping, beyond the Boltzmann equation level. In essence, the damping is associated to the non locality of collisions [15]. Hence, it vanishes in the low density limit, while it is related to the bulk viscosity for finite densities. Our analytical results will be confronted against Molecular Dynamics (MD) simulations.

The setting. We consider a dilute system of interacting atoms (or molecules), trapped in a harmonic potential. Each atom at position r is subjected to an external force $-m\omega^2 r$; all masses m are identical. A sketch of the system is shown in Fig. 1. We adopt a classical description, stressing that quantum effects are negligible in the experiment of Ref. [8], and also that the breathers survive to quantum effects [16]. While pure isotropic harmonic potentials do not exist in reality, they provide an excellent approximation in the context of the experiments carried out in Ref. [8]. We restrict to monoatomic gases; the analysis relies on energy and momentum conservation during collisions: it is not necessary to specify the type of interatomic potential studied, provided that interactions are short range and the system dilute. Under this proviso, the Boltzmann equation framework applies [14], and, unexpectedly, does not lead at long times to Maxwell-Boltzmann distribution n_e for the particle den-



FIG. 1. (Color online) Sketch of the system. The particles, shown with the disks, are confined in the (red) parabolic potential. Under generic initial conditions, the system evolves towards a breathing state, oscillating between a dense configuration with high temperature (left) and a more dilute configuration with a smaller temperature and a higher potential energy (right).

sity n:

$$n(\mathbf{r},t) \neq n_e(\mathbf{r}) = n_0 \exp\left[-\frac{m\omega^2 r^2}{2kT}\right],$$
 (1)

where k is Boltzmann constant, T the temperature, n_0 is a normalization factor and $r = |\mathbf{r}|$. While one may have expected long-time thermalization starting from arbitrary initial conditions, solutions indeed exist with avoided equilibration, where the density, velocity and temperature oscillate with time t at 2ω , twice the natural trapping frequency [6–8]. These solutions are readily characterized as follows.

Due to density, momentum, and energy conservation in collisional events, the density, velocity and temperature fields, resp n, u, T, obey the generic hydrodynamic equations [17]

$$\partial_t n + \boldsymbol{\nabla} \cdot (n\boldsymbol{u}) = 0, \qquad (2)$$

$$\partial_t u_i + (\boldsymbol{u} \cdot \boldsymbol{\nabla}) u_i + \frac{1}{mn} \partial_j \mathcal{P}_{ij} + \omega^2 x_i = 0, \qquad (3)$$

$$\frac{d}{2}n\partial_t T + \frac{d}{2}n\boldsymbol{u}\cdot\boldsymbol{\nabla}T + \mathcal{P}_{ij}\partial_j u_i + \nabla\cdot\boldsymbol{q} = 0, \qquad (4)$$

where d denotes space dimension, the summation over repeated indices is assumed and the x_i denote the Cartesian coordinates of position \boldsymbol{r} . The total number of atoms is $N = \int n(\boldsymbol{r}, t) d\boldsymbol{r}$, a conserved quantity. To first order in the gradients of the fields, the heat flux is $\boldsymbol{q} = -\kappa \nabla T$ and the pressure tensor $\boldsymbol{\mathcal{P}}$ reads [17]

$$\mathcal{P}_{ij} = p\delta_{ij} - \eta \left[\partial_i u_j + \partial_j u_i - \frac{2\delta_{ij}}{d} \nabla \cdot \boldsymbol{u}\right] - \nu \nabla \cdot \boldsymbol{u} \,\delta_{ij}, \quad (5)$$

where p is the pressure, η the shear viscosity, ν the bulk viscosity (also called the volume viscosity, and sometimes the "second" or "expansive" viscosity), κ the heat conductivity; the expressions of these quantities in terms of n and T depend on the system. By substituting the expression of the fluxes into the balance equations, Eqs. (2)-(4), the Navier-Stokes equations are obtained. On general grounds, the system's total entropy S increases under the action of the various dissipative mechanisms at work, thermal conduction and internal friction due to viscous forces. This results in [17]

$$\frac{dS}{dt} = \int d\boldsymbol{r} \left\{ \frac{\kappa}{T^2} (\nabla T)^2 + \frac{\eta}{2T} \left(\partial_k u_i + \partial_i u_k - \frac{2}{d} \delta_{ik} \nabla \cdot \boldsymbol{u} \right)^2 + \frac{\nu}{T} (\nabla \cdot \boldsymbol{u})^2 \right\}.$$
(6)

Recovering the breathing modes. More often than not, the bulk viscosity ν is neglected [7, 18]. This "tradition" dates back to the early days of hydrodynamics, and bears the name of Stokes' hypothesis [19–21]. Since the term in brackets in Eq. (5) is traceless, Stokes' hypothesis implies that the mechanical and thermodynamic pressures coincide. In a polyatomic system where energy can be transferred from translational to other degrees of freedom (rotational, vibrational), such an assumption would fail, but it holds in a dilute monoatomic gas [22, 23] and is often considered to be correct without the diluteness restriction for such gases, see eg [21, 24–27]. Being interested in monoatomic species, we momentarily endorse Stokes' hypothesis, setting $\nu = 0$. For consistency with the dilute assumption we also have $\mathcal{P}_{ij} = p\delta_{ij}$, where p = nkT. By taking moments in Eqs. (2) and (3), it is easily seen that the quantities $\langle r^2 \rangle = \int r^2 n d\mathbf{r} / N$ and $\langle \boldsymbol{r} \cdot \boldsymbol{v} \rangle = \int \boldsymbol{r} \cdot \boldsymbol{u} n d\boldsymbol{r} / N$ fulfill a closed set of first order differential equations, that can be transformed into a closed second order differential equation for $\langle r^2 \rangle$ [16, 28, 29]

$$\frac{d^2\langle r^2\rangle}{dt^2} = \frac{4e}{m} - 4\omega^2 \langle r^2\rangle,\tag{7}$$

where the total energy per particle, that is a constant of the motion, has been introduced, $e = \frac{1}{2N} \int d\mathbf{r} n(\mathbf{r},t) \left[mu^2(\mathbf{r},t) + dT(\mathbf{r},t) + m\omega^2 r^2 \right]$. The solution of Eq. (7) is simply

$$\langle r^2 \rangle = \rho^2 + \Delta \cos(2\omega t - \varphi),$$
 (8)

where $\rho^2 \equiv e/m\omega^2$ is the equilibrium value of $\langle r^2 \rangle$, φ is an irrelevant phase factor, and Δ is a parameter quantifying the amplitude of the oscillations that can be written in terms of the initial condition as $\Delta = \sqrt{\frac{\langle r \cdot v \rangle_0^2}{\omega^2} + (\langle r^2 \rangle_0 - \rho^2)^2}$, where the index 0 refers to averages over all atoms in the initial condition. Let us stress that Eq. (8) is exact in the low density limit. It holds for *all times*, independently of the initial condition, and it clearly shows that, in general, the system will perpetually oscillates at twice the trap natural frequency (the exception being $\Delta = 0$ that will be analyzed latter).

The maximum entropy solution, corresponding to the long-time evolution of our interacting system (that in the following will be denoted by the subscript *B*), is such that the first two terms in parenthesis in Eq. (6) vanish. Thus, the temperature should be spatially homogeneous $(\nabla T_B = \mathbf{0})$, and $\partial_k u_{B,i} + \partial_i u_{B,k} - \frac{2}{d} \delta_{ik} \nabla \cdot \mathbf{u}_B = 0$ ($\forall i, k =$

 $1, \ldots, d$) that, in turn, imply that $u_B(\mathbf{r}, t) = a(t)\mathbf{r} + \mathbf{j}(t) \times \mathbf{r} + \mathbf{u}_0(t)$. By a proper choice of the rest frame, and discarding globally rotating system, we set \mathbf{u}_0 and \mathbf{j} to $\mathbf{0}$, so that $u_B(\mathbf{r}, t) = a(t)\mathbf{r}$. By substituting the specific form of the velocity and temperature field into Eq. (3), it is obtained that the density is gaussian with the above identified variance

$$n_{\scriptscriptstyle B}(\boldsymbol{r},t) = N \left[\frac{d}{2\pi \langle r^2 \rangle} \right]^{d/2} \exp\left(-\frac{d}{2 \langle r^2 \rangle} r^2 \right).$$
(9)

Performing the same in Eq. (2) by taking into account the gaussian density profile, the time-dependent coefficient, a(t), is identified, $a(t) = (1/2)\partial_t \log \langle r^2 \rangle$ and, if Eq. (4) is used, it is obtained that $T_B(t)\langle r^2 \rangle$ is a constant. This is a signature of the kinetic to potential energy conversion at work in the present swing mechanism: when the cloud is extended, with a large value of $\langle r^2 \rangle$ (*ie* a large potential energy), the temperature is small, and the temperature is conversely maximal when $\langle r^2 \rangle$ is minimal, and the peak density (at the origin) maximal. To summarize, starting from arbitrary initial conditions, in the long time limit the system reaches a state that is characterized by the parameters describing the dynamics of $\langle r^2 \rangle$ (N, e, Δ and φ): the density is gaussian given by Eq. (9) and

$$\boldsymbol{u}_B(\boldsymbol{r},t) = rac{\boldsymbol{r}}{2} \partial_t \log \langle r^2 \rangle, \quad T_B(t) = rac{C}{\langle r^2 \rangle}, \quad (10)$$

where C is a constant that depend on the same parameters [14]. The velocity field is shear-less, and thus immune to shear-viscosity effects. In fact, this is exactly the breathing mode solution obtained by Boltzmann. The equilibrium solution (n_e in Eq. (1)) corresponds to $\Delta = 0$, which requires highly specific initial conditions [30]. Note that the interatomic interaction specifics are immaterial here.

Damping mechanism for the breathing modes. It is appropriate at this point to revisit Stokes hypothesis [31]. Physically, the bulk viscosity arises because collisions involve particles that are not exactly located at the same point in space; in other words, there is a transfer of momentum through a given surface due to the interaction of a pair of particles located at different sides of the surface. The rationale for setting $\nu = 0$ is that dilatational dissipation is often small compared to its shear counterpart. In the context of the Boltzmann equation, the pressure tensor is purely kinetic and the bulk viscosity vanishes. The Boltzmann equation is derived in the low density limit, whereas the bulk viscosity makes an appearance at higher densities. For the breathers, shear dissipation vanishes and attention should be paid that the bulk viscosity, no matter how small, may cause dissipation. As it has been discussed, for a monoatomic gas, what can be shown rigorously is that $\nu/\eta \to 0$ when $n \to 0$, but taking $\nu = 0$ does not yield a valid description at all times. Interestingly, the hydrodynamics framework above is convenient for the analysis where $\nu \neq 0$,

that aims at going beyond the low density approximation. In particular, the maximum entropy argument now demands that the three terms in parenthesis in Eq. (6) do vanish, so that $a = 0 = \nabla \cdot \boldsymbol{u}$: the long-time maximum entropy solution thus has $\boldsymbol{u} = \boldsymbol{0}$ (in the rest frame, assuming again no global rotation), a uniform temperature, and a profile set by Eq. (3), *ie* the hydrostatic balance $\nabla p + mn\omega^2 \boldsymbol{r} = 0$, which is the equilibrium solution. Beyond the dilute limit, the explicit form of the pressure *p* depends on the specific interactions at work, which modifies the Gaussian profile on the rhs of Eq. (1). We have just shown that the bulk viscosity dissipation drives equilibrium: ultimately, the breathers have to decay to thermal equilibrium This takes place at constant energy per particle *e* in our conservative system [32].

The damping time. What is the lifetime of a Boltzmann breather? From Eqs. (2)-(4), we obtain on general grounds

$$\frac{d^2 \langle r^2 \rangle}{dt^2} = \frac{4e}{m} - 4\omega^2 \langle r^2 \rangle + \frac{2d}{mN} \int d\boldsymbol{r} [\Delta p - \nu \boldsymbol{\nabla} \cdot \boldsymbol{u}], \quad (11)$$

where $\Delta p \equiv p - nkT$ is the excess pressure that depends on density n and temperature T, themselves time and position dependent. This opens the way to a multiple time scale analysis. Indeed, plugging the breather expressions into Eq. (11) and linearizing around the equilibrium value, $\langle r^2 \rangle_e$, a differential equation for $x \equiv \langle r^2 \rangle - \langle r^2 \rangle_e$ is obtained

$$\ddot{x} + \frac{2}{\tau}\dot{x} + \Omega^2 x = 0, \qquad (12)$$

where a new time scale τ appears, which measures the life time of the breathers. We have $\tau = \frac{2mN\rho^2}{d^2\int dn\nu_e}$, that is a functional of the equilibrium bulk viscosity ν_e , itself position dependent. The frequency of the oscillations, $\Omega = \left[4\omega^2 + \frac{2d}{mN}\int d\mathbf{r}\frac{\delta\Delta p}{\delta\langle \tau^2\rangle}\right]^{1/2}$, differs from the Boltzmann value, 2ω , due to the excess pressure contribution and its explicit expression depends on the particular equation of state. Here, the excess pressure contribution does not affect the relaxation time because, to linear order, is \dot{x} -independent. As expected, in the low-density limit $\tau \to \infty$ and $\Omega \to 2\omega$. In contrast with Eq. (7), Eq. (12) does not hold for all times, but it describes the *universal* long time behavior in which the initial condition is forgotten and the fields are close to their breather counterparts.

Comparison to numerical simulations. To proceed, we specify the analysis to the simplest non-trivial monoatomic case possible: the hard-sphere system, for which all quantities of interest are known [33]. For this model, the explicit expressions for τ and Ω^2 are $\tau = \frac{d2^{(d-1)/2}\Gamma(d/2)N^{1/d}}{\pi^{d/2}\phi^{(d+1)/2}\omega}$ and

$$\Omega^2 = 4\omega^2 \left[1 + \frac{(d+2)\pi^{d/2}}{2^{(d+4)/2}d\Gamma(d/2)}\phi \right],$$
(13)



FIG. 2. $\langle r^2 \rangle / \rho^2$ as a function of the dimensionless time, ωt , for $\phi = 9 \times 10^{-3}$. The circles are the simulation results and the solid line the Boltzmann theoretical prediction (8). In the inset, the envelope of the oscillations (dashed line) is plotted on a much longer time scale (the dotted line at unity is plotted for reference).

where the maximum (dimensionless) density at equilibrium at Boltzmann level, $\phi \equiv N \left(\frac{d}{2\pi\rho^2}\right)^{d/2} \sigma^d$, has been introduced. We have also neglected position correlations at contact.

We have put our predictions to the test with MD simulations of a system with N = 1000 hard disks (twodimensional system), where the particle trajectories are followed with time, under the action of the harmonic onebody confinement potential, and of instantaneous interparticle collisions [34]. Figure 2 shows that the cloud spread, $\langle r^2 \rangle$, for a system with $\phi = 9 \times 10^{-3}$, oscillates in time as predicted for the breather state around the (equilibrium) value, ρ^2 . The circles are the simulation results and the solid line the Boltzmann theoretical prediction. The agreement between both in the shown time window is excellent taking into account that there are no adjustable parameters. Nevertheless, a tiny discrepancy with the theoretical frequency, 2ω , can be appreciated (specially for times $\omega t \sim 50$ as it is a cumulative effect). In the inset, the envelope of the oscillations is plotted on a much longer time scale (dashed line), where the damping becomes visible. Both effects, shifting of the frequency and damping, are precisely those predicted by our hydrodynamical theory. In addition, the breather state characterized by the hydrodynamic fields (9) and (10) is only reached for times $\omega t > 40$. This can be appreciated by checking the constancy of $T_{\scriptscriptstyle B} \langle r^2 \rangle$ with time.

For different small densities and starting with an initial condition close to equilibrium, $\Delta/\rho^2 = 0.2$, (the density has to be "close to Boltzmann" and the amplitude of $\langle r^2 \rangle$ small for the theory to be valid), MD simulations have been performed. The frequency and the relaxation time of the oscillations have been measured by counting the number of maxima (minima) per unit time and by fitting



FIG. 3. $\left(\frac{\Omega}{\omega}\right)^2$ as a function of the dimensionless density, ϕ . The dots are the simulation results and the solid line is the theoretical prediction (13).



FIG. 4. $\omega\tau$ as a function of the dimensionless density, ϕ , in logarithmic scale. The points are the simulation results, the solid line is the theoretical prediction for τ as defined above (13) and the dashed line is the linear fitting of the simulation results.

the envelope to an exponential, respectively. In Fig. 3, the frequency is plotted. The points are the simulation results (the error bars are not plotted because they can not be seen in the figure) and the solid line the theoretical prediction. The agreement between the theoretical prediction and the simulation results is excellent in the whole range of densities. Note that the corrections to the Boltzmann prediction are of the order of ϕ , $\sim 10^{-2}$. In Fig. 4, $\omega \tau$ is plotted as a function of ϕ in logarithmic scale. The points are the simulation results (as above, the error bars are not plotted), the solid line is the theoretical prediction and the dashed line is the linear fitting of the simulation results with slope -1.53 ± 0.02 , in perfect agreement with the theoretical prediction for d = 2, $\tau \sim \phi^{-3/2}$. The quotient between the theoretical and measured relaxation times is of the order of 1.5, indicating that, although the density dependence is perfectly captured by the theory, there are other not considered ingredients that "renormalize" the amplitude of $\phi^{-3/2}$.

The only approximation made in the theory has been to take for the hydrodynamic fields the corresponding ones of the breather state. It seems that it is perfectly valid to first order in ϕ (the frequency Ω fits the theoretical prediction), but it fails beyond first order. Yet, the agreement is satisfactory taking into account the simplicity of the theory.

In conclusion, treading in Boltzmann's footsteps, we have recovered that an isolated low-density system confined in a harmonic trap generically evolves towards a time-dependent breathing mode. Such a solution however cannot be eternal: it holds in a finite time-window, all the larger as the system is more dilute, and we could characterize the ultimate fate of a breather. Under an original dissipation mechanism that is insensitive to usual shear viscous forces, but involves dilatational dissipation, the system reaches asymptotically thermal equilibrium, as expected. The key player is the bulk viscosity, that is minute compared to the shear viscosity for dilute systems: neglecting it allows to recover Boltzmann's results in a convenient fashion; yet, it rules the long-time dynamics. This dissipation mechanism, which operates as consequence of the breathing mode spherical symmetry, is unique and provides a platform for measuring the elusive bulk viscosity.

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