Supplemental material for 'Exact non-equilibrium solutions of the Boltzmann equation under a time-dependent external force'

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In this supplemental material, we discuss the general case of non vanishing angular momentum solutions, providing more details on the derivation presented in the main text. We then establish that our solutions do possess a non-trivial scaling property and we generalize the analysis to the quantum case. Finally, the Monte Carlo numerical treatment is presented.

TIME-DEPENDENT SOLUTIONS WITH $J \neq 0$ FOR THE CLASSICAL BOLTZMANN EQUATION

We start by the set of equations

$$\boldsymbol{\nabla}_{\boldsymbol{r}}\,\beta \,=\, \mathbf{0}, \tag{S1}$$

$$v^2\partial_t\beta + \boldsymbol{v}\cdot\boldsymbol{\nabla}_{\boldsymbol{r}}(\boldsymbol{\gamma}\cdot\boldsymbol{v}) \,=\, 0, \quad \text{for all } \boldsymbol{v}, \tag{S2}$$

$$\partial_t\boldsymbol{\gamma} + \boldsymbol{\nabla}_{\boldsymbol{r}}\,\alpha + 2\beta\boldsymbol{F} \,=\, \mathbf{0}, \tag{S3}$$

$$\partial_t\alpha + \boldsymbol{F}\cdot\boldsymbol{\gamma} \,=\, 0. \tag{S4}$$

The inverse effective temperature β thus depends on time only, and the solution to Eq. (S2) is taken of the form $\boldsymbol{\gamma}(\boldsymbol{r},t) \,=\, \boldsymbol{J}\wedge\boldsymbol{r} \,-\, \dot\beta\,\boldsymbol{r}$ by a proper choice of velocity origin. It can be shown that $\boldsymbol{J}$ is proportional to the angular momentum $\langle \boldsymbol{r}\wedge\boldsymbol{v}\rangle$, where the angular brackets denote averaging over velocities at point $\boldsymbol{r}$. It has been noted in the main text that $\boldsymbol{J}$ is constant and uniform. Eq. (S3) then reads

$$-\ddot\beta\,\boldsymbol{r} + \boldsymbol{\nabla}_{\boldsymbol{r}}\,\alpha + 2\beta\boldsymbol{F} \,=\, \mathbf{0} \tag{S5}$$

which can be readily integrated with respect to position:

$$\alpha = \alpha_0(t) + 2\beta V + \ddot\beta\frac{r^2}{2}. \tag{S6}$$

The quantity $\alpha_0(t)$ can be absorbed in V without changing the resulting force, and will subsequently be set to 0. Inserting the above expression into (S4) yields

$$\begin{aligned} 2\dot\beta\,V \,+\, 2\beta\,\tfrac{\partial V}{\partial t} \,+\, \dddot\beta\,\tfrac{r^2}{2} \,&=\, \boldsymbol{\gamma}\cdot\boldsymbol{\nabla}_{\boldsymbol{r}}V \\ &= (\boldsymbol{J}\wedge\boldsymbol{r})\cdot\boldsymbol{\nabla}_{\boldsymbol{r}}V \,-\, \dot\beta\,\boldsymbol{r}\cdot\boldsymbol{\nabla}_{\boldsymbol{r}}V \end{aligned}$$

which can be recast

$$\dot\beta\,\left(2+\boldsymbol{r}\cdot\nabla_{\boldsymbol{r}}\right)V + 2\beta\,\frac{\partial V}{\partial t} + \dddot\beta\,\frac{r^2}{2} \,=\, (\boldsymbol{J}\wedge\boldsymbol{r})\cdot\boldsymbol{\nabla}_{\boldsymbol{r}}V. \tag{S7}$$

The case $\dot\beta \,=\, 0$ is uninteresting since it leads to the equilibrium distribution. The general solution to Eq. (S7) when $\dot\beta \neq 0$ is of the form

$$V(\boldsymbol{r}) = \frac{1}{2}\,\omega^2(t)r^2 + \frac{b}{r^2}, \tag{S8a}$$

$$\text{with} \quad \dddot\beta \,+\, 4\,\omega^2\dot\beta \,+\, 4\,\omega\,\dot\omega\,\beta \,=\, 0, \tag{S8b}$$

where the angular frequency ω can be time dependent, unlike b, which has to be t independent, but can depend on polar angle θ (defined from the $\boldsymbol{J}$ direction). In the simpler case where $\boldsymbol{J} \,=\, \mathbf{0}$, the function b can depend on both spherical angles, provided it does not depend on the radial distance $r \,=\, |\boldsymbol{r}|$. The solution uncovered should have $b \geq 0$ for normalizability. The mode under examination cannot be damped, since from momentum and energy conservation, it belongs to the kernel of the collision integral. We precise too that in practice, the $\boldsymbol{\gamma}$ coupling term in the definition of the distribution function, can be measured by time-of-flight experiments. In such setups, the confinement is removed at $t \,=\, 0$, meaning here that ω is set to 0, and the expanding size of the cloud is subsequently monitored as a function of time. From Eq. (S8b), we deduce that $\dddot\beta \,=\, 0$ which implies that $\langle r^2\rangle$ evolves as a quadratic function of time whose linear term is proportional to the position-velocity correlations.

The structure of Eq. (S7) explains why the anharmonic term in b/r^2 was hitherto missed [1, 2]. For solving Eq. (S7), one has to invert the operator $\mathcal{O} = 2+\boldsymbol{r}\cdot\boldsymbol{\nabla}_{\boldsymbol{r}}$. Power-laws in r^n are eigenfunctions of $\mathcal{O}$ with eigenvalue $n+2$, meaning that in addition to the particular solution in r^2, those with $n \,=\, -2$, belonging to the kernel of $\mathcal{O}$, should be considered. They have been omitted by previous authors. If V is not of the form (S8a), the only solution to Eq. (S7) is $\dot\beta \,=\, 0$, which implies $\alpha = 2\beta V$ and we retrieve the barometric equilibrium case.

SCALING PROPERTIES OF $f(\boldsymbol{r},\boldsymbol{v},t)$.

It is natural to rescale velocities by $\sqrt{T} \,\propto\, \beta^{-1/2}$, and to perform that operation in the center-of-mass frame. In addition, upon integrating $f(\boldsymbol{r},\boldsymbol{v},t)$ over $\boldsymbol{v}$ to get the particle density, it appears that $\beta^{1/2}$ sets the relevant length scale. We thus define

$$\widetilde{\boldsymbol{v}} = \sqrt{\beta}\boldsymbol{v} + \frac{\boldsymbol{\gamma}}{2\sqrt{\beta}} \quad \text{and} \quad \widetilde{\boldsymbol{r}} = \frac{\boldsymbol{r}}{\sqrt{\beta}}. \tag{S9}$$

Computing the (*a priori* time-dependent) joint distribution function of the couple $\widetilde{\boldsymbol{r}},\widetilde{\boldsymbol{v}}$, we have

$$\widetilde{f}(\widetilde{\boldsymbol{r}},\widetilde{\boldsymbol{v}},t) \,=\, \exp\left(-\alpha + \frac{\gamma^2}{4\beta} - \widetilde{v}^2\right). \tag{S10}$$

Remembering Eq. (S6) (with $\alpha_0 = 0$), this gives

$$\widetilde{f} \,=\, \exp\left(\frac{-\widetilde{r}^2}{4}\,[...] + \frac{(\boldsymbol{J}\wedge\widetilde{\boldsymbol{r}})^2}{4} - \frac{2b}{\widetilde{r}^2} - \widetilde{v}^2\right) \tag{S11}$$

where the term in square brackets is

$$[...] \,=\, 4\,\omega^2\beta^2 \,+\, 2\,\beta\ddot\beta \,-\, \dot\beta^2. \tag{S12}$$

An immediate consequence of the evolution equation (S8b) is that this term is constant ($d[...]/dt = 0$), so that $\widetilde{f}(\widetilde{\boldsymbol{r}}, \widetilde{\boldsymbol{v}})$ does not depend on time. Our solution corresponds to a rotating cloud at angular frequency $\boldsymbol{J}/2$ in the tilde position, which implies a time-dependent frequency $\boldsymbol{J}/(2\beta)$ in real space (faster rotation when β is small, and where thus the cloud is more compact). In terms of particle density and maintaining the same meaning as above for [...], we have

$$n(\widetilde{\boldsymbol{r}}) = \pi^{3/2} \exp\left(\frac{-\widetilde{r}^2}{4}[...] + \frac{(\boldsymbol{J}\wedge\widetilde{\boldsymbol{r}})^2}{4} - \frac{2b}{\widetilde{r}^2}\right), \quad \text{(S13)}$$

which is Gaussian whenever $b = 0$.

TIME-DEPENDENT SOLUTION FOR THE QUANTUM BOLTZMANN EQUATION

For the quantum Boltzmann equation [3, 4], the collision integral reads

$$I_{\rm coll}[\boldsymbol{v}|f,f] = \int \mathrm{d}^2\Omega\, \mathrm{d}\boldsymbol{v}_2\, \frac{\mathrm{d}\sigma}{\mathrm{d}^2\Omega}\, |\boldsymbol{v}_2 - \boldsymbol{v}| \times \Big[f(1')f(2')(1+\varepsilon f(1))(1+\varepsilon f(2)) - f(1)f(2)(1+\varepsilon f(1'))(1+\varepsilon f(2'))\Big],$$

where $\varepsilon = 1$ (resp. -1) describes a bosonic (resp. fermionic) gas, and $\mathrm{d}\sigma/\mathrm{d}^2\Omega$ is the differential cross section. In close analogy with our previous treatment, we shall search for a solution of the form

$$f_0(\boldsymbol{r},\boldsymbol{v},t) = \frac{1}{e^{-\mu+\Sigma(\boldsymbol{r},\boldsymbol{v},t)} - \varepsilon}, \quad \text{(S14)}$$

with Σ again a linear combination of collisional invariants

$$\Sigma(\boldsymbol{r},\boldsymbol{v},t) \;=\; -\alpha(\boldsymbol{r},t) - \beta(t)v^2 - \boldsymbol{\gamma}(\boldsymbol{r},t)\cdot\boldsymbol{v} \quad \text{(S15)}$$

The parameter μ is an effective chemical potential and is a priori time-dependent. The ansatz f_0 shall be included the kernel of the quantum collision integral $I_{\rm coll}[f_0] = 0$.This latter property can be readily demonstrated by noticing that:

$$\begin{aligned} &f_0(1')f_0(2')(1+\varepsilon f_0(1))(1+\varepsilon f_0(2)) \\ &= e^{-2\mu}e^{\Sigma(1)+\Sigma(2)} f_0(1)f_0(2)f_0(1')f_0(2'). \end{aligned} \quad \text{(S16)}$$

As shown hereafter, the chemical potential is a function of the quantity [...] which appears in Eq. (S12). To show this property we use a series expansion of the distribution function

$$\begin{aligned} 1 &= \int \mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{v}\frac{1}{e^{-\mu+\Sigma}-\varepsilon} = \int \mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{v}\frac{e^{\mu-\Sigma}}{1-\varepsilon e^{\mu-\Sigma}} \\ &= \int \mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{v} e^{\mu-\Sigma}\sum_{n=0}^{\infty}\varepsilon^n e^{n\mu-n\Sigma} \\ &= \sum_{n=1}^{\infty}\varepsilon^n (e^{\mu})^{n+1}\int \mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{v} e^{-(n+1)\Sigma}. \end{aligned} \quad \text{(S17)}$$

The integrals are of Gaussian kind, similar to those calculated in the classical case and depend only on the quantity [...]. The last step consists in injecting the ansatz (S14) in the l.h.s of the Boltzmann equation. We obtain a solution if the time-dependent parameters α, β and γ obey the same set of equations (S1,S2,S3,S4) as in the classical case. The time-dependent solution has therefore been generalized to the quantum Boltzmann equation.

COMPUTER SIMULATIONS

Our main goal here is to illustrate the reverse engineering viewpoint, and to put to the test the relevance of the shortcut to adiabaticity (STA) route in an interacting system. To this end, we have performed particle simulations of an open system of hard disks, by using the Direct Simulation Monte Carlo (DSMC) method [5]. This is a many body algorithm designed to generate the dynamics of a gas in the low density limit, where the Boltzmann equation description applies. The DSMC method is based on the discretization of both time and space. In the evolution of the system, the free flow of particles is considered to be uncoupled from collisions during a characteristic, small, time interval δt. Besides, space is discretized in cells of size smaller than the mean free path, and particles within the same cell collide with a probability proportional to their relative velocity. Large number of particles can be afforded, which improves the statistical accuracy of the results.

In the simulations presented here, a system with $N = 9{\cdot}10^5$ particles has been considered. No boundary conditions have to be imposed, as we are studying an open system confined by an external potential, taken harmonic of the form $\omega^2(t)\, r^2/2$. First of all, we successfully checked the validity and existence of the oscillating solutions predicted in the static confinement case ($\dot{\omega} = 0$). In a second step, we tested the STA protocol. The ultimate goal is to obtain an evolution of the (inverse) temperature given by Eq. (10), which sets the target. We thus wish to see if, by choosing $\omega(t)$ to be the solution of Eq. (9b) where β is given by Eq. (10), the system follows the predicted behavior with a temperature that is independent of space, and of the targeted form (10). We note in passing that the solution of Eq. (9b) can be obtained analytically, and reads

$$\omega^2(t) \;=\; \frac{1}{\beta^2}\left\{\omega_i^2\beta_i^2 + \frac{\dot{\beta}^2}{4} - \frac{\beta\ddot{\beta}}{2}\right\}. \quad \text{(S18)}$$

Hence, for any particular time dependent β, the associated ω is known.

The initial state was chosen so that the initial velocities of the particles obeyed a Gaussian distribution with zero mean and temperature $T(0) = T_i = (2k_B\beta_i)^{-1}$. The initial position of the particles, decoupled from their velocities, were generated from the barometric law, with a probability proportional to $\exp\left[-\omega_i^2 r^2/(2k_BT_i)\right]$. This provides the initial condition at $t = 0$. The system was then left to evolve during a time t_f, with a time dependent confinement given by Eq.

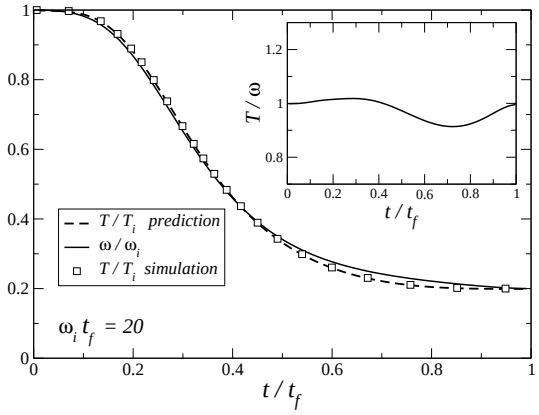

FIG. S1: Comparison of the predicted (dashed line) and measured temperatures T/T_i in the Monte Carlo simulations (open squares). The trap frequency $\omega(t)/\omega_i$ [as given by Eq. (S18) where $\beta(t)$ is the target, Eq. (10) of the main text], is shown by the continuous line. The inset provides a measure of 'non-adiabaticity', and shows $T(t)/\omega(t)$ normalized by T_i/ω_i, which equals 1 both at $t = 0$ and $t = t_f$. Here the protocol is slow ($t_f = 20/\omega_i$) and there are 54.9 collisions *per particle* in the time span t_f.

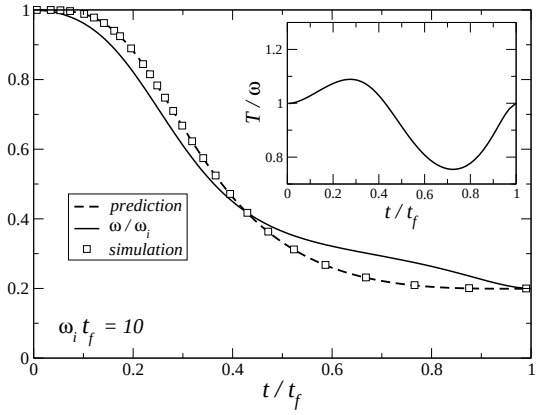

FIG. S2: Same as Fig. S1 for a faster protocol ($t_f = 10/\omega_i$). There are here 27.43 collisions per particle between $t = 0$ and $t = t_f$.

(S18). The temperature is measured locally at point $\boldsymbol{r}$ from the variance of the velocity distribution. It was always found to be $\boldsymbol{r}$ independent, in agreement with Eq. (S1).

When the transformation is slow (i.e. $t_f \gg \omega_i^{-1}$), the system evolves with $T(t)/T_i$ close to $\omega(t)/\omega_i$, as expected for an adiabatic transformation (see Fig. S1). Upon increasing the speed of the process (Figs. S2 and S3), we obtain significant non adiabatic effects (see the insets), but the measured T is always in remarkable agreement with the target: the squares (simulation data) and dashed line accurately superimpose, which proves the effectiveness of the STA route. We emphasize here that the collision rate has been modified, from small values to the collisional regime displayed, with a similar agreement in all cases.

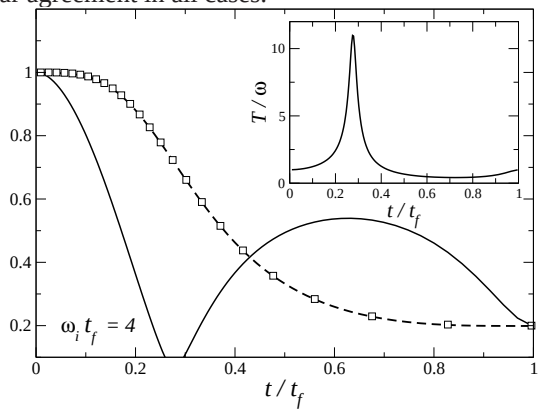

FIG. S3: Same as Figs. S1 and S2 for t_f close to τ_0 (see main text). Here, each particle undergoes on average 10.96 collisions between $t = 0$ and $t = t_f$.

[1] L. Boltzmann, in *Wissenschaftliche Abhandlungen*, edited by F. Hasenorl (J.A. Barth, Leipzig, 1909), Vol II, p. 83.

[2] C. Cercignani, *The Boltzmann equation and its applications* (Springer Verlag, New York, 1988).

[3] L. P. Kadanoff and G. Baym, *Quantum statistical mechanics* (W. A. Benjamin, New York, 1962).

[4] L. W. Nordheim, Proc. R. Soc. Lond. A **119** 689 (1928).

[5] G. Bird, *Molecular gas dynamics and the direct simulation of gas flows* (Clarendon Press, Oxford, 1994).