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Free thermal convection driven by nonlocal effects

Jorge Ibsen, Rodrigo Soto, and Patricio Cordero*
Departamento de Física, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile, Casilla 487, Santiago 3, Chile
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We quantify a convective phenomenon (thermal slip) that cannot be classified either as a hydrodynamics instability nor as a macroscopically forced convection. Two complementary arguments show that the velocity field by a nonuniform thermalizing wall is proportional to the ratio between the heat flux and the pressure. This prediction is quantitatively corroborated by our molecular dynamics simulations.

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Free thermal convection—driven by buoyancy or by surface tension—is a perfectly well understood and familiar phenomenon derivable from Navier-Stokes (NS) equations [1,2]. Simulations of free thermal convection by means of molecular dynamics (MD) techniques can be achieved with systems with as few as 10^3 particles and already these small systems exhibit hydrodynamic behavior as seen, for example, in [3–7]. Moreover MD is useful in studying fluid phenomena at the microscopic level without having to make assumptions concealed behind the NS equations such as the Fourier law, Newton's law of viscosity, and local thermodynamic equilibrium.

Rarefied gases present a variety of phenomena near the walls of the container [8,9]. When they are correctly described in terms of hydrodynamic fields they can be used as boundary conditions (BC) to solve Navier Stokes equations.

For a nonuniform thermalizing wall there exists a phenomenon known as *thermal slip*: the gas is forced to move tangential to the wall. As we shall see this phenomenon is related to the variation of the temperature field in one mean free path ℓ through the Knudsen number $\ell\nabla T/T$. This number can be interpreted as a measure of how far from local thermal equilibrium the system is at a given point. The mechanism can be sketched as follows: the particles that approach a point P of the wall come from an anisotropic distribution while the particles that hit the wall at P come back to the system with a distribution that is isotropic or at least less anisotropic than the incoming flux. A careful assessment of the difference between the incoming and outgoing fluxes at P yields the conclusion that there is a net mass flux parallel to the wall. This phenomenon implies a particular type of macroscopic BC.

We have observed this phenomenon in MD simulations. In the following we are going to derive the explicit form for this velocity field by the wall which, as we will see, coincides with what we observe in our simulations.

We have made MD simulations of a two dimensional gas of hard disks in a square box using our own efficient algorithm [10] and the carefully devised measurement routines described in [11]. Each numerical experience consisted of two runs: (1) The system with periodic vertical walls was subjected to a vertical temperature difference, relaxed for 200 thermal diffusion times t_T, and then the temperature profile $T(z)$ was carefully measured for another $200t_T$. (2) A second simulation was run under the same conditions as in (1) except that the periodic (vertical) walls were replaced by new walls: each particle hitting them returns to the system with a velocity taken from a heat bath at the local temperature $T(z)$. The sign of the vertical component of this velocity was random and therefore microscopically it is a *nonslip* BC in the sense that the emerging particles do not remember the velocity with which they came. In our main simulations the particles hitting anyone of the thermalizing walls emerged on the opposite one (cylindrical topology) to reduce boundary effects even though this feature does not affect the appearence of the phenomenon we are reporting. Again the system was relaxed for $200t_T$ and then measurements were averaged in time during the next $600t_T$. The measurements were done dividing the system in square cells. Densities and the velocity field were measured in every cell and fluxes were measured across the cell walls.

Units are chosen such that particle's mass and diameter, the Boltzmann constant, and the temperature at the bottom m, D, k_B, and T_b, respectively, are fixed to unity. With this particular choice of units the lengths are in diameter units, the temperature in energy units, and the time in units of $\sqrt{mD^2/k_BT_b}$. The control parameters of each simulation are the number of particles N, the bulk number density n_B, and the temperature at the top T_t where $T_t < T_b$.

Our main simulation considered a system of $N = 1444$ hard disks, bulk number density $n_B = 0.05$, implying a box side of 170 and a mean free path of about 7 and at the top the temperature was fixed to be $T_t = 0.1$.

The main observation is the following: a convective current stabilizes in the neighborhood of the vertical walls moving towards the warmer zone. In Figs. 1 and 2 it is possible to see the velocity field $\vec{v}$ and the mass flux $mn\vec{v}$. At the bottom the convective current necessarily bends towards the center to come up along the central part of the box. Since the gas is highly compressible the eye of the convective rolls are far from the expanded hotter zone. The velocity component v_z in the cells by the vertical walls is almost constant (even though the den-

*Electronic address: pcordero@tamarugo.cec.uchile.cl

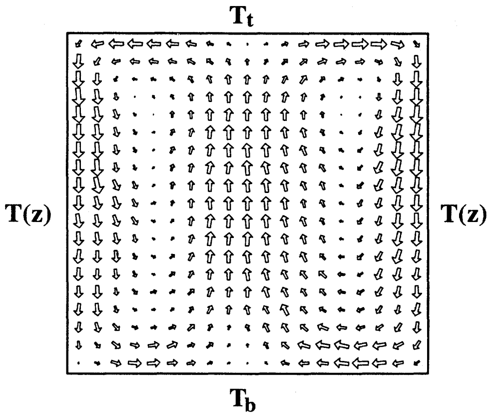

FIG. 1. Velocity field measured using MD simulations. The horizontal walls are kept at a uniform temperature, the warmer wall is at the bottom, and the vertical walls have a different temperature at each point. The number of particles, the bulk number density, and the top temperature were $N = 1444$, $n_B = 0.05$, and $T_t = 0.1$, respectively.

sity varies by a factor of 10 from top to bottom) and its average was

$$v_z = -0.015 \pm 0.002 \qquad \text{(observed)} \tag{1}$$

after excluding ten cells in the upper and lower extremes and with 76×76 the total number of cells.

Thermal slip was observed in all the other situations we simulated: (i) $n_B = 0.01$, $N = 8100$, $T_b = 1.0$, and $T_t = 0.01$; (ii) $n_B = 0.25$, $N = 1444$, $T_b = 1.0$, and $T_t = 0.1$. The velocity component v_z measured near the vertical walls in (i) was $v_z = 0.014 \pm 0.003$ and it shows the same behavior as the preceding simulation. The vertical component of the velocity in (ii), however, is no longer constant, it increases with height. The theoretical derivations that we make below are not applicable to this denser case but it is interesting to observe that the phenomenon still exists.

Finally we made another simulation in which the temperature profile of the thermalizing wall was not the one obtained from a first run but rather $T(z)$ was chosen arbitrarily to be a smooth monotonic profile. In this case we used $n_B = 0.05$, $N = 1444$, and $T_t = 0.1$. Again a convective current was created with similar characteristics to the previous ones. This result and the theoretical calculations below illustrate that in order to obtain this convective motion it is enough to have a temperature gradient parallel to a thermalizing wall so that each particle emerging from the wall comes from a (at least partially) thermalized distribution.

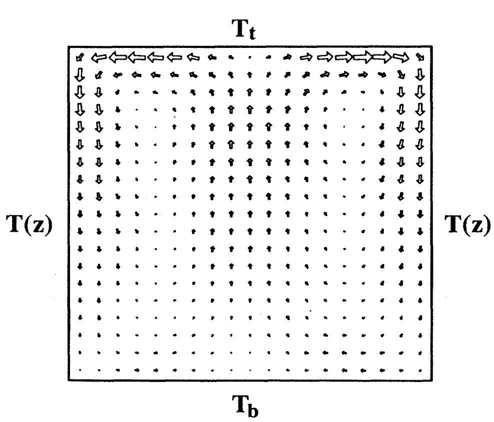

FIG. 2. Mass flux measured in the same simulation shown in the previous figure.

To derive the correct macroscopic BC one should solve the corresponding Boltzmann equation. Instead, in what follows we give two heuristic and complementary derivations for a rarefied two dimensional hard disk gas one based on local nonequilibrium distribution functions and the other one based on the mean free path theory of transport. Both derivations yield essentially the same prediction for the velocity field near the vertical thermalizing wall. What the calculations below imply is that the vertical wall exerts an effective tangential force on the gas such that a velocity field — proportional to the ratio between the heat flux and the pressure — pointing against the heat flux is established.

The basic idea behind the following two derivations is that particles hitting the thermalizing wall at a point P (see Fig. 3) come from an anisotropic nonequilibrium environment while the particles emerging from P come from an equilibrium isotropic distribution. It is understandable then that some fluxes do not necessarily cancel and, in particular, we are able to quantify the net velocity field at the thermalizing walls.

Nonequilibrium interpretation. The velocity distribution function near a point P of the thermalizing wall (Fig. 3) has two contributions: (a) one from the particles that come towards P from a nonequilibrium velocity distribution and (b) the other one from the outgoing particles that come from the thermal bath at P. The nonequilibrium distribution function for a system under a heat flux adapted from [12] to the case of a two dimensional system is

$$f_{\text{neq}} = \left(1 + \frac{m}{2pT}\left[\frac{mv^2}{2T} - 2\right] \vec{v} \cdot \vec{q}\right) f_{\text{eq}} \ , \tag{2}$$

where f_{eq} is the usual Maxwellian distribution. Then the

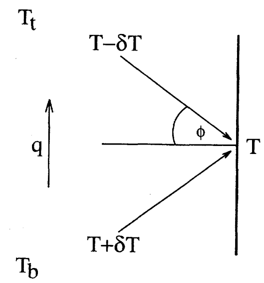

FIG. 3. Contributions to the mass flux from different directions. Particles come from regions at different temperatures and emerge with velocities from an isotropic distribution at temperature T.

velocity distribution near the right wall is

$$f = \begin{cases} f_{\rm neq}(\vec{v}), & v_x > 0 \\ f_{\rm eq}(\vec{v}), & v_x < 0 \,. \end{cases} \tag{3}$$

Using this distribution the x-z component of the stress exerted by the fluid against the wall ($\sigma_{xz} = mn\langle v_x v_z\rangle_f$) is

$$\sigma_{xz} = \frac{q}{8}\sqrt{\frac{2m}{\pi T}} \,. \tag{4}$$

Then the force per unit length exerted by the wall on the fluid is, by the action-reaction principle, the negative of the previous expression and hence it points *antiparallel to the heat flux.* The velocity near the wall can be estimated using Newton's law ($\sigma_{xz} = \eta\partial v_z/\partial x$ where η is the shear viscosity) and the assumption that this velocity decays at distances comparable with the mean free path ℓ and it is

$$v_z = -\frac{\ell\sigma_{xz}}{\eta} \,. \tag{5}$$

Replacing the expressions for the shear viscosity $\eta = \frac{1}{2}\sqrt{T/\pi}$, the mean free path $\ell = \frac{1}{2\sqrt{2}n}$ and using the equation of state for an ideal gas yields

$$v_z = -\frac{1}{8}\frac{q}{p} \,. \tag{6}$$

Kinetic interpretation. Let us consider the mass flux balance at an arbitrary point P of the wall as shown in Fig. 3. The mass flux coming from an angle between ϕ and $\phi + d\phi$ with respect to the normal to the wall and reaching P is

$$d\vec{\jmath} = m\,n\sqrt{\frac{T}{m}}\,a(\phi)(\cos\phi, -\sin\phi)\,d\phi \,, \tag{7}$$

where n and T are the number density and temperature at the points where the particles come from, whereas $a(\phi)$ is a geometrical factor depending on the incident angle. We do not give a value for $a(\phi)$ since it is well known that the mean free path theory of transport is too simple to produce the correct numerical factor [13]. Since the number density is small then $p = nT$.

The combined inward mass flux from the directions ϕ and $-\phi$ to P is then

$$d\vec{\jmath}_{\rm in}(\phi) = \sqrt{m}\,p\,a(\phi)\left[\cos(\phi)\left(\frac{1}{\sqrt{T(\phi)}} + \frac{1}{\sqrt{T(-\phi)}}\right)\hat{\vec{x}} - \sin(\phi)\left(\frac{1}{\sqrt{T(\phi)}} - \frac{1}{\sqrt{T(-\phi)}}\right)\hat{\vec{z}}\right] d\phi \,.$$

The combined outward mass flux from directions ϕ and $-\phi$ can only be in the $\hat{\vec{x}}$ direction since the flux comes from the local equilibrium distribution at the wall and it is $d\vec{\jmath}_{\rm out}(\phi) = -m\,n\sqrt{\frac{T}{2\pi m}}\cos(\phi)\,\vec{x}\,d\phi$. The density n in $d\vec{\jmath}_{\rm out}$ cannot be replaced by p/T because the equation of state is not valid at wall points. This number density is unknown and can be determined imposing null net mass flux in the $\hat{\vec{x}}$ direction.

The total flux in the $\hat{\vec{z}}$ direction is

$$\vec{J}\cdot\hat{\vec{z}} = \int_0^{\pi/2}(d\vec{\jmath}_{\rm in} + d\vec{\jmath}_{\rm out})\cdot\hat{\vec{z}} = A\sqrt{m}\,\frac{p\,\ell}{T^{3/2}}\,\frac{dT}{dz} \tag{8}$$

with

$$A = \int_0^{\pi/2} a(\phi)\sin^2\phi d\phi$$

and where we have set $T(\phi) = T + \ell\sin(\phi)\,dT/dz$ with ℓ the mean free path. It must be remarked that from the previous expression the velocity field near the wall can be estimated dividing this flux by the mass density and it reduces to

$$v_z = {\rm const}\times\left(\frac{\ell}{T}\frac{dT}{dz}\right)\,v_{\rm th} \,, \tag{9}$$

where $v_{\rm th}$ is the thermal velocity. The previous result implies that a mass flux parallel to the temperature gradient is induced near the wall and it is proportional to the adimensional Knudsen number $\frac{\ell}{T}\frac{dT}{dz}$ which is a measure of how far from local thermal equilibrium the system is at a given point.

Using the Fourier law, the expressions for the mean free path, the thermal conductivity $k = 2\sqrt{T/\pi}$, and the equation of state for an ideal gas v_z becomes

$$v_z = -\frac{A}{4}\sqrt{\frac{\pi}{2}}\frac{q}{p} \,. \tag{10}$$

This result predicts the same behavior as (6). The velocity is independent of the point P—due to the absence of external forces and energy sources, p and q are uniform—as it can be appreciated in Fig. 1. Our predicted value for v_z from our observations of q and p is

$$v_z = -0.016 \pm 0.003 \quad \text{(predicted)} \,, \tag{11}$$

which should be compared with (1) and $v_z = -0.020 \pm 0.001$ for the simulation with $n_B = 0.01$, $N = 8100$, $T_b = 1.0$, and $T_t = 0.01$.

The extension to three dimensions is straightforward giving essentially the same result indicating that this convective motion could be observed in gases. For example, using gaseous helium at atmospheric pressure with a temperature gradient of $\nabla T = 100$ K/cm the velocity near the wall that we are predicting is $v_z = 3.8$ mm/s. It may be somewhat smaller because in a real experiment the average flux coming out from every point at the thermalizing wall is not totally isotropic.

Regarding the heat flux $\vec{q}$ there has been an interesting recent proposal applicable to the case of systems under a heat flux saying that one should observe a departure from the standard Fourier law [14] (which actually motivated our series of simulations). What we observe (see Fig. 4) is that the energy flux is consistent with the Fourier law plus the kinetic flux $\frac{1}{2}\langle m\, n\, v^2\, \vec{v}\rangle$ of an ideal gas. The effect predicted in [14] for our system is about an order of magnitude smaller than the total flux and since fluxes are noisier than densities we cannot yet see if such an effect exists.

In summary, we have observed and quantified the macroscopic BC for a case of thermal slip and have seen how it arises from nonlocal effects due to the presence of nonequilibrium distributions, which implies free thermal convection. The velocity by the wall (proportional to $\ell\nabla T/T$) coincides with that observed in our MD simulations.

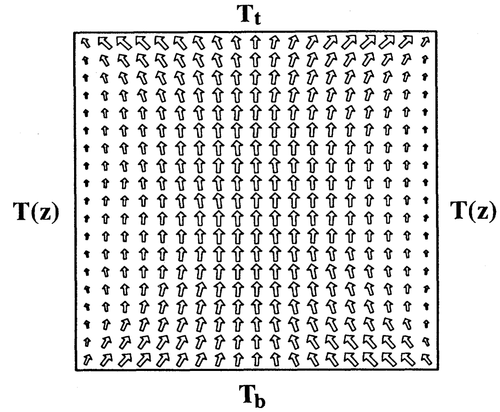

FIG. 4. Energy flux measured in the same simulation as in previous figures. The x component has been amplified four times to show how it is distorted by the convective current.

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[1] S. Chandrasekar, *Hydrodynamics and Hydrodynamic Stability* (Clarendon Press, Oxford, 1961).
[2] C. Normand, Y. Pomeau, and M. Velarde, Rev. Mod. Phys. **49**, 581 (1977).
[3] M. Mareschal and E. Kestemont, J. Stat. Phys. **48**, 1187 (1987).
[4] D. C. Rapaport, Phys. Rev. Lett. **60**, 2480 (1988).
[5] A. Puhl, M. Malek-Mansour, and M. Mareschal, Phys. Rev. A **40**, 1999 (1989).
[6] D. C. Rapaport, Phys. Rev. Lett. **43**, 7046 (1991).
[7] D. Risso and P. Cordero, in *Proceedings of the IV Instabilities and Nonequilibrium Structures*, edited by E. Tirapegui and W. Zeller (Kluwer Academic, Dordrecht, 1993).
[8] H. Ferziger and H. G. Kaper, *Mathematical Theory of Transport Processes in Gases* (North-Holland, Amsterdam, 1972).
[9] E.M. Lifshitz and L.P. Pitaevskii, *Physical Kinetics* (Pergamon Press, New York, 1993).
[10] M. Marín, D. Risso, and P. Cordero, J. Comput. Phys. **109**, 306 (1993).
[11] D. Risso, Ph.D. thesis, Universidad de Chile, 1994.
[12] H. Grad, *Principles of the Kinetic Theory of Gases*, Handbuch der Physik Vol. XII, edited by S. Flunge (Springer, Berlin, 1958).
[13] D. McQuarrie, *Statistical Mechanics* (Harper Collins Publishers, New York, 1976).
[14] J. Casas-Vázquez and D. Jou, Phys. Rev. E **49**, 1040 (1994).