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Heat conduction in a rotating disk via nonequilibrium molecular dynamics

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Nonequilibrium molecular dynamics is used to study the conduction of heat due to a radial temperature gradient in a rotating two-dimensional disk of dense fluid. These calculations show that Coriolis's force contributes to the heat flux.

I. INTRODUCTION

Transport simulations of linear phenomena, such as Fick's-law diffusion, Newtonian viscosity, and Fourier heat conduction, are in good agreement with theoretical predictions based on the Boltzmann equation and the Green-Kubo theory. Less is known of the richer class of nonlinear problems. Recent work has shown that some nonlinear problems, such as the propagation of strong shock waves in dense fluids, can be treated successfully using the linear transport theory. Because the nonlinear theory is still in the process of development, microscopic computer simulations are particularly valuable for testing theoretical models and suggesting new approaches. See, for instance, the shock wave and shear flow simulations described in Refs. 1 and 2.

Up to now rotating molecular systems have not been simulated. But the attention of theorists has already been attracted to the coupling of diffusive processes with rotational accelerations in rotating systems. For example, the Coriolis accelerations, linear in the rotational frequency, and the centrifugal accelerations, quadratic in frequency, can couple with gradients of momentum and temperature. Here we explore the simplest problem involving this coupling, the flow of heat in a rotating system. The microscopic equations of motion, solved in the "comoving" coordinate frame rotating with the material, reveal the dependence of the heat-flux vector and the density profile on the rotational motion.

Several authors[3] have considered heat conduction in rotating disks from the two different theoretical standpoints, microscopic and macroscopic. Those favoring microscopic kinetic theory find that Coriolis's force should lead to an angular heat-flux vector component in the presence of a purely radial temperature gradient. Those favoring the macroscopic continuum concept of "frame indifference" believe instead that the heat-flux vector (in a comoving frame) must be purely radial, as Fourier's linear law $q=-\lambda\nabla T$ predicts. These conflicting views have stimulated the present work.

An experimental test of the conflicting predictions is made difficult by the extreme angular frequencies required. Perhaps real tour de force experiments could be carried out by using electric and magnetic fields to suspend and spin conducting microspheres.

Lacking experimental evidence, we sought to satisfy the curiosity piqued by this apparent theoretical disagreement by applying a much more direct approach, solving the N-body problem numerically. In this work we simulate a dense-fluid system with a wholly radial temperature gradient to find out which of the two theoretical views agrees with that derived from Newton's equations of motion.

We study a spinning disk, hot at the center and cold on the outer boundary. Despite the large fluctuations that characterize two-dimensional systems, the results indicate that angular accelerations *do* influence the flow of heat so that the qualitative predictions of low-density kinetic theory are justified in dense media. In the present paper we describe first our understanding of the conflicting theoretical predictions, next the numerical example chosen to test the relative merits of the predictions, and last the numerical results.

II. THEORETICAL PREDICTIONS

The Boltzmann equation correctly describes the transport of mass, momentum, and energy at low density provided that the gradients are sufficiently small and that the system under consideration is sufficiently large relative to the mean free path. Not only does Boltzmann's derivation of his equation appear very plausible, but also the comparison of its predictions with experimental data provides strong independent evidence for the equations's validity.[4] Outside the regime of linear transport theory, Boltzmann's equation is not to be trusted. Kinetic theorists have recently shown that the Burnett coefficients describing flux contributions quadratic in the gradients are divergent, at least in principle.[5] For this reason we must view with suspicion the application of Boltzmann's equation to the nonlinear coupling of two different linear effects, a temperature gradient, and Coriolis's force.

The theoretical treatment of this coupling can be based on the relaxation-time approximation to Boltzmann's equation, as described in McQuarrie's recent textbook.[6] For a motionless (nonrotating) but conducting disk composed of mass m particles at a temperature T with a radial temperature gradient dT/dr, the relaxation-time Boltzmann equation

$$\left[\frac{df}{dt}\right]=\frac{(f^o-f)}{\tau} \tag{1}$$

gives

$$\frac{f}{f^o}=1-\tfrac{1}{2}v_r\tau\left[\left[\frac{mv^2}{kT}\right]-4\right]\left[\frac{d\ln T}{dr}\right]. \tag{2}$$

This result is obtained by combining f^o functions corresponding to particles at local equilibrium a time of order τ in the past. f^o is the equilibrium one-particle distribution function and τ is the collisional relaxation time. For simplicity we ignore any dependence of τ on velocity. In a frame rotating counterclockwise at angular velocity ω, a particle moving in the θ direction has a radial Coriolis acceleration $\dot{v}_r=2\omega v_\theta$. Thus, a particle now with v_r had, a time τ previously, radial velocity component $v_r-2\omega\tau v_\theta$. To first order in ω, v^2 is unchanged by Coriolis's forces so that the combined effects of temperature gradient and rotation give

$$\frac{f}{f^o}=1-\tfrac{1}{2}(v_r-2\omega\tau v_\theta)\left[\left[\frac{mv^2}{kT}\right]-4\right]\left[\frac{d\ln T}{dr}\right]. \tag{3}$$

The resulting θ heat-flux component varies linearly with ω:

$$\frac{q_\theta}{q_r}=-2\omega\tau\,. \tag{4}$$

Thus, the microscopic kinetic theory predicts a heat flux lagging behind the disk's rotation.

The continuum view can lead to a different conclusion. Continuum mechanics appears to be based upon a judicious mixture of mechanics, macroscopic thermodynamics, and intuition. The principles of the subject are that no material can violate known thermodynamic laws and that, under reasonable conditions, the results of experiments should not depend upon the time of the experiment or upon the coordinate frame from which that experiment is observed. If a macroscopic body obeying Fourier's law $q=-\lambda\nabla T$ is viewed in a comoving coordinate system, rotating with the body, the "principle of frame indifference" suggests that Fourier's law is still obeyed, so that a radial temperature gradient can excite only radial heat flow. On the other hand, microscopic Newtonian mechanics implies that Coriolis's force causes field-free particles to follow curved trajectories. From the macroscopic standpoint of continuum mechanics the microscopic motion is simply a part of the internal energy. There is no macroscopic motion in a comoving frame so that no Coriolis's phenomena can occur.

III. MICROSCOPIC FORMULATION OF ROTATION AND HEAT FLOW

The mechanics of rotation was described by G. G. Coriolis[7] (1792–1843, a French mathematician and professor of mechanical engineering). He was the first to consider the effect of relative accelerated motions, such as rotations, on dynamical observations. If a system obeying Hamilton's equations of motion in an inertial laboratory frame is viewed from a Cartesian xy frame rotating at angular frequency ω, a transformation of the coordinates to the rotating frame gives the result[8]

$$H = H_{eq} - \sum \omega(xp_y - yp_x)$$
$$= \sum \sum \phi_{ij} + \sum \frac{m}{2}(\dot{x}_i^2 + \dot{y}_i^2 - \omega^2 x^2 - \omega^2 y^2) , \tag{5}$$

where the single sum ranges over all N particles and the double sum ranges over all $N(N-1)/2$ pairs of particles. The equations of motion in the moving frame follow by differentiation:

$$\dot{x} = (p_x/m) + \omega y, \quad \dot{p}_x = F_x + \omega p_y ,$$
$$\dot{y} = (p_y/m) - \omega x, \quad \dot{p}_y = F_y - \omega p_x , \tag{6}$$

and are well suited to numerical integration. Positive angular velocity corresponds to the counterclockwise motion of the xy frame relative to the laboratory frame. It should be noted that the momenta in the (fixed) laboratory frame are identical with the (comoving) rotating-frame momenta.

There is an apparent similarity between the Hamiltonian (5) and the Doll's tensor Hamiltonian[9] used to describe adiabatic deformation. The latter formulation would describe the equations of motion in an inertial frame, viewed from a rotating laboratory frame, and therefore is not useful for the present problem. In the Doll's tensor formulation the momenta are products of moving-frame velocities and particle masses, while in the present description of a rotating system the momenta are products of laboratory-frame velocities and particle masses.

Special boundary conditions must be added in order to maintain a temperature gradient in the rotating-frame heat-flow simulation based on the microscopic Hamilton's equations (6). It is necessary to provide a heat source and a heat sink. One way to accomplish this[10] is to partition the system into separate "reservoir" and "bulk" regions with mathematical walls. The reservoir regions can then be maintained at steady temperatures by rescaling the moving-frame velocities at each time step. We tried this method, using reservoirs of different sizes, but the reservoirs proved ineffective. The centrifugal forces $m\omega^2 r$ inhibited thermal contact between the two reservoirs and the bulk region. We therefore adopted a different method for introducing and extracting heat, rescaling the radial velocities of a fixed number of particles nearest the inner boundary of the system to maintain a nearly-constant hot temperature, and rescaling the radial velocities of the same number of particles nearest the outer boundary to maintain a nearly-constant cold temperature. This rescaling process was carried out at time intervals of $0.1(m\sigma^2/\epsilon)^{1/2}$. Except at the times of these heat transfers (which affect no angular velocities) the ordinary equations of motion were solved. The negative temperature gradient $dT/dr < 0$ inhibits convection by reinforcing the positive density gradient due to centrifugal forces.

In order to describe the heat transfer process in terms of thermal conductivity, it is necessary that the radial extent of the system be more than a few mean free paths. The number of particles required can be greatly reduced by using periodic boundary conditions in plane polar coordinates as shown in Fig. 1. The boundaries at $r/\sigma = 12$ and 28 were implemented with a wall potential of the form $\phi_{wall} = \epsilon(\sigma/10\delta r)^{12}$. With this geometry the periodic images required to compute the forces on particles near the periodic "boundary" are rotated

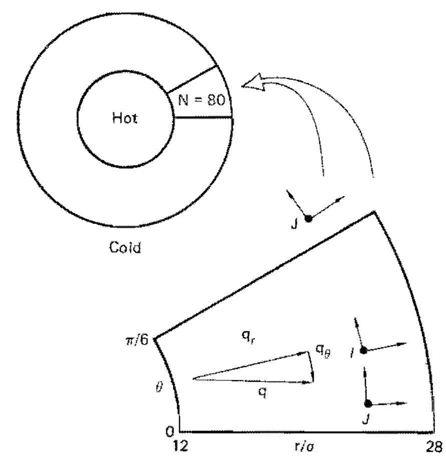

FIG. 1. Geometrical configuration of the system under study. The 30° slice between the inner and outer radii contains 80 particles, all interacting with the soft-disk potential, modified by adding a very small Hooke's law attraction to make the force and energy vanish at $r = 3\sigma$. The radial temperature in the inner region (defined by the 20 particles closest to the center) is constrained to be $10\epsilon/k$ and the temperature in the outer region (defined by the 20 particles closest to the outer boundary) is $2\epsilon/k$. The two particles i and j shown in the figure lie at different angles θ_i and θ_j. When the potential contribution of this pair to the heat-flux vector is computed, basis vectors lying at the point $(r_i + r_j)/2$ are used. This ambiguity in the radial and theta components of the potential contribution to q is negligible for the short-range forces used here, but could not be ignored with long-range interactions.

relative to the particles "inside" the system, so that the sum of the forces on particle i due to j and particle j due to i is not necessarily zero. These forces must be properly taken into account in computing the potential contribution to the heat flux. Conservation of energy (in any frame) and angular momentum (in the inertial laboratory frame only) serve as powerful checks of the numerical work. To suppress fluctuations in angular velocity in the comoving frame, the theta velocities were adjusted ($\delta\dot{\theta}_i = A + Br_i + Cr_i^2$) at the rescaling intervals of $0.1(m\sigma^2/\epsilon)^{1/2}$ to constrain the three sums $\sum\dot{\theta}, \sum\dot{\theta}r, \sum\dot{\theta}r^2$ to vanish in the comoving frame.

To interpret the microscopic solution of the equations of motion in terms of macroscopic quantities, a heat-flux vector must be defined. The accepted definition results in a natural way if the microscopic flow of heat is treated in parallel with the flow of momentum, as described by the virial theorem.[11] It is not usually emphasized that these momentum and heat theorems can be applied not only to equilibrium fluids or solids, but also to fluids or solids in steady nonhydrostatic heat-conducting nonequilibrium states. Both the momentum-flux (pressure tensor) and the heat-flux vector are always defined relative to the comoving (rotating) frame.

The virial theorem derivation proceeds by computing the time average of the tensor product of the particle coordinates and the time rate of change of particle momenta. By equating the external-force contributions to the time rate of change, the virial theorem is obtained. For the particular case in which the interaction is pairwise additive, the theorem has the form

$$PV = \sum \frac{pp}{m} + \sum\sum rr\frac{F}{r} , \tag{7}$$

where the double sum includes all distinct pairs of particles.

Heat flow can be described in a similar way. We follow Kirkwood and Irving[12] in associating half the energy of each pair interaction with each of the interacting particles. If we indicate the external contribution to the time rate of change of particle i's energy with a superscript e then

$$\dot{E}_i = \dot{E}_i^e + \left[2p_iF_i - \sum(F_{ij}p_i + F_{ji}p_j)\right]\frac{1}{2m} ,$$
$$\dot{E}_i = \dot{E}_i^e + \sum F_{ij}\frac{(p_i+p_j)}{2m} , \tag{8}$$

where the sum in (8) includes all particles j with which i interacts. Notice that the time rate of change of particle i's energy depends explicitly on particle j's momentum. If we next construct the sum, over all particles in the volume V, of particle i's position multiplied by $\dot{E}_i$ from (8), and average over time, replacing the external heat flow with the product of the volume and the heat-flux vector q, we get

$$qV = \sum \dot{r}_i E_i + \sum\sum (r_i - r_j)(F_{ij})\cdot(\dot{r}_i + \dot{r}_j)/2 . \tag{9}$$

This form is well suited to numerical calculation. The force terms linking particles i and j have been combined, so that the heat flux, like the momentum flux, has both an individual-particle convective part and a two-particle potential part.

Because we are interested in finding both the angular and radial components of the heat flux, it is essential to write the macroscopic vector qV in (9) as a sum of microscopic short range, nearly local vectors. In (9) this has been done; the contribution to the heat flux of the force exerted by particle j on particle i depends on the relative separation vector $r_i - r_j$. Unless the ij terms are combined in this way, the division of the microscopic vectors into radial and angular parts loses physical significance.

IV. NUMERICAL RESULTS

We decided to study a simple soft-disk fluid, rather than a solid, in order to avoid long phonon free paths and to enhance the expected contribution of the Coriolis force to the heat-flux vector. The soft-disk system, with particles interacting with an inverse 12th-power potential $\phi = \epsilon(\sigma/r)^{12}$, has been carefully investigated by Cape.[13] His numerical work located the freezing transition and showed that a truncated virial expression provides a useful analytic expression for the fluid-phase equation of state:

$$PV/NkT = 1 + 1.773x + 2.362x^2 + 1.484x^3 + 9.477x^4 - 11.544x^5 + 11.038x^6 ,$$

with

$$x \equiv (N\sigma^2/V)(\epsilon/kT)^{1/6} . \tag{10}$$

This equation of state allows us to estimate the thermal conductivity for the soft disks from Gass's two-dimensional Enskog theory.[14] Gass's expression for the ratio of the dense-fluid thermal conductivity to the low-density conductivity is

$$\lambda/\lambda_0 = b\rho[(1/b\rho\mathcal{X}) + 1.5 + 0.872 b\rho\mathcal{X}]\,, \quad (11)$$

where $b\rho$ and $\mathcal{X}$ follow from Cape's equation of state, (10), for the soft disks:

$$b\rho = 1.478(N\sigma^2/V)(\epsilon/kT)^{1/6} \equiv 1.478x\,,$$
$$b\rho\mathcal{X} = 1.478x + 1.575x^2 + 0.742x^3 + 3.159x^4 - 1.924x^5\,. \quad (12)$$

Gass quotes the low-density hard-disk conductivity, $\lambda_o(s) = (1.16/s)(k^3T/m)^{1/2}$, in terms of the hard-disk diameter s. We estimate the soft-disk conductivity at low density by matching the second virial coefficient contributions to the thermal pressures:

$$1.571s^2 = 1.478\sigma^2(\epsilon/kT)^{1/6}\,. \quad (13)$$

The resulting soft-disk thermal conductivity at $T = 6\epsilon/k$ and

$$N\sigma^2/V = 80/[(\pi/12)(28^2 - 12^2)] = 0.477$$

is

$$6.1k(\epsilon/m\sigma^2)^{1/2}\,,$$

in fairly good agreement with the value deduced from our numerical radial-heat-flux data $4.4k(\epsilon/m\sigma^2)^{1/2}$ discussed below.

Mechanical equilibrium requires that the centrifugal force on an element of mass at r and θ, $(r\,dr\,d\theta)m\rho\omega^2 r$, must balance the pressure-gradient force $-(r\,dr\,d\theta)dP/dr$. An exact solution of the corresponding mechanical equilibrium equation, including heat flow, is tedious, and the resulting density profile differs only slightly from the simpler isothermal profile, as shown in Fig. 2. Cape's equation of state indicates that rotational frequencies, up to the maximum we used, all correspond to wholly fluid-phase states.

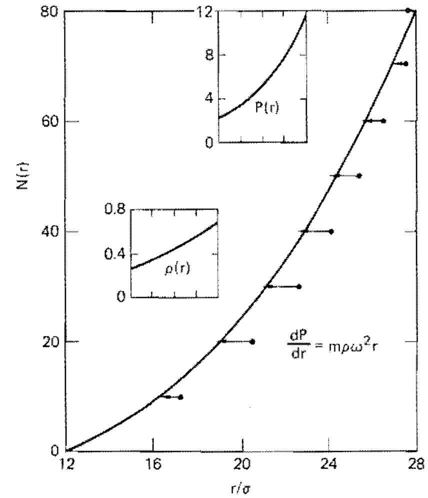

FIG. 2. Density profile for a rotating two-dimensional disk with $\omega = 0.25(\epsilon/m\sigma^2)^{1/2}$. Cape's equation of state for the soft-disk fluid, at a temperature of $6\epsilon/k$, was used to solve the mechanical-equilibrium equation for a system rotating at the highest angular frequency shown in Table I, and with the same number of particles. The profile has been integrated to display the average number of particles $N(r)$ lying within a circle of radius r. The points shown along the curve correspond to average locations of the 10th, 20th, 30th, . . . , particle, counting outward from the center, from the corresponding molecular dynamics simulation. In the drawing, the figure ϵ, m, σ, and k have all been set equal to one. The arrows indicate the shifts required at zero frequency to match the isothermal mechanical-equilibrium calculation with the corresponding microscopic heat-conducting simulation.

The numerical results given in Table I and illus-

TABLE I. Numerical results for six rotational frequencies ω. The time, radial, and angular heat fluxes in the volume V are tabulated. In the table the units correspond to setting ϵ, m, σ, and k all equal to one.

		Radial[a]		Angular	
Frequency	Time	qV (potential)	qV (kinetic)	qV (potential)	qV (kinetic)
0.00	400	322	241	4	9
0.05	200	328	215	−23	1
0.10	200	308	214	−25	−4
0.15	1400	350	233	−33	−35
0.20	400	379	250	−22	−24
0.25	400	389	237	−57	−36

[a]Most of the increase in the radial heat flux with frequency corresponds to the decrease of effective system width with frequency. The centrifugal forces increase the effective temperature gradient. We have not made a precise estimate because the accuracy of the results does not warrant it. Energy was conserved to at least one part in 10^5 in integrating over the time intervals between momentum rescalings.

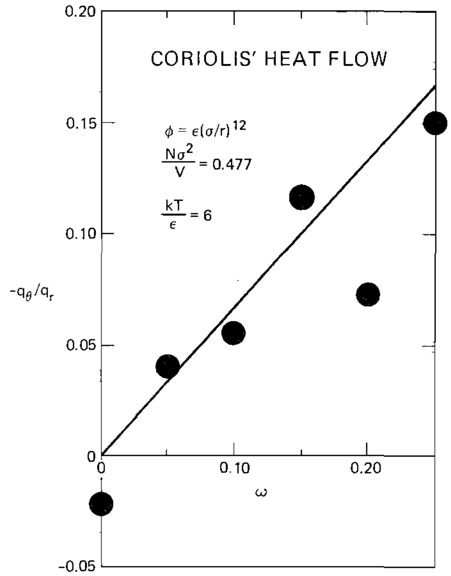

FIG. 3. Ratio of the angular to the radial heat flux as a function of rotational frequency. Despite considerable fluctuations the data establish that the qualitative predictions of kinetic theory are correct. The slope of the line drawn through the data agrees well with the collisional relaxation time estimated in the text.

trated in Fig. 3 all refer to the geometrical situation indicated in Fig. 1. A periodic 30° portion of an annulus, containing 80 particles, was followed for a sufficiently long time to estimate the radial and angular parts of the heat flux. The radial part corresponds to a thermal conductivity which is not significantly affected by rotation and which agrees fairly well with the Enskog theory. This indicates that ordinary Fourier heat conduction is an adequate description of the radial heat flow in this small two-dimensional system.

The angular part of the heat flux found here contains nearly equal potential and kinetic parts. It fluctuates wildly with time and is considerably smaller than the radial part. The angular flux is equal to twice the product of minus the radial flux, the angular frequency, and the relaxation time, according to the approximate Boltzmann treatment given in Sec. II. Our observed angular heat flux confirms this order-of-magnitude estimate. The data correspond to a relaxation time $\tau = 0.30(m\sigma^2/\epsilon)^{1/2}$. An independent estimate for τ can be obtained from the exponential relaxation theory (ERT). That theory predicts a thermal conductivity $\lambda_{\mathrm{ERT}} = 2\rho k^2 T\tau/m$. Setting this equal to the kinetic part of the conductivity estimated from Table I and Fig. 2, $1.9k(\epsilon/m\sigma^2)^{1/2}$ gives $\tau = 0.33(m\sigma^2/\epsilon)^{1/2}$.

We conclude that the approximate kinetic theory and Enskog's dense-fluid modification of Boltzmann's equation correctly predict a violation of Fourier's heat conduction law. In dense media a radial temperature gradient induces an angular heat flux in a comoving frame.

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