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Microscopic and macroscopic stress with gravitational and rotational forces

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Many recent papers have questioned Irving and Kirkwood's atomistic expression for stress. In Irving and Kirkwood's approach both interatomic forces and atomic velocities contribute to stress. It is the velocity-dependent part that has been disputed. To help clarify this situation we investigate (i) a fluid in a gravitational field and (ii) a steadily rotating solid. For both problems we choose conditions where the two stress contributions, potential and kinetic, are significant. The analytic force-balance solutions of both these problems agree very well with a smooth-particle interpretation of the atomistic Irving-Kirkwood stress tensor.

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I. INTRODUCTION

In 2003 Zhou [1] published his lengthy and detailed paper "New Look at the Atomic Level Virial Stress" in the *Proceedings of the Royal Society of London.* He criticized the usual Irving-Kirkwood virial expression [2] for the pressure tensor P as a sum of potential and kinetic terms. The pressure tensor is the same thing as the comoving corotating momentum flux, and is also minus the stress tensor, $\sigma \equiv -P$. The detailed microscopic Irving-Kirkwood approach has been used for more than 50 years in the interpretation of atomistic molecular-dynamics simulations [3–6]. Averaged over a homogeneous periodic volume V, the Irving-Kirkwood expression for the pressure tensor gives

$$-\sigma V \equiv PV = P^{\Phi}V + P^{K}V = \sum_{i<j} (Fr)_{ij} + \sum_{i} (pp/m)_i .$$

Here F_{ij} is the force (for simplicity we assume a pairwise-additive potential) exerted on particle i by particle j, where the vector from j to i is r_{ij}. Particle i, at location r_i with mass m_i and momentum p_i, obeys Newton's equation of motion,

$$m_i \ddot{r}_i \equiv F_i^{\text{ext}} + \sum_{j \neq i} F_{ij}, \quad F_{ij} = -\nabla_i \phi(|r_{ij}|), \quad \Phi \equiv \sum_{i<j} \phi_{ij} .$$

Zhou [1] stated that only the tensor force sum, $\Sigma(Fr)_{ij} \equiv \Sigma F_{ij} r_{ij}$, contributes to the stress, while the tensor momentum sum, $\Sigma(pp/m)_i \equiv \Sigma(p_i p_i/m_i)$, does not.

This idea—including the forces but not the momenta–is not quite so outlandish as it seems. In solids, where the longtime average of the particle location is a sensible quantity, the virial theorem *can* be written in a similar tensor form omitting the momenta:

$$\langle PV \rangle = \sum_{i<j} \langle (FR)_{ij} \rangle, \quad R_i \equiv \langle r_i \rangle .$$

This form is derived in Sec. IIC of Ref. [4]. We use angular brackets here to indicate longtime averages. In situations including external forces the tensor force sum must also include either $(F^{\text{ext}} r)_i$ or $(F^{\text{ext}} R)_i$.

Subramaniyan and Sun [7] tested Zhou's ideas [1] with molecular dynamics, heating a model atomistic solid subject to a variety of external boundary conditions on the particle coordinates. Their simulations showed that only the full Irving-Kirkwood pressure tensor, potential plus kinetic, was consistent with macroscopic thermodynamics. Liu and Qiu [8] recently provided a useful list of references supporting both sides of the question. In addition they suggested that the Zhou prescription is correct provided that external fields and rotation are not involved. Here we explore those latter two conditions separately and explicitly, showing that both (i) an external field (gravity) and (ii) a condensed-phase rotation can be analyzed properly with the Irving-Kirkwood pressure tensor, in a way compatible with macroscopic continuum mechanics. This suggests that the original Irving-Kirkwood approach is more generally useful than is the suggested modification of it by Zhou [1].

In order to compute continuous differentiable field variables (density, velocity, energy, stress, heat flux, etc.) from atomistic molecular-dynamics simulations, for comparison to corresponding fields generated by continuum mechanics solutions, we recommend the use of "smooth-particle" averages. These correspond to smearing individual particle properties over a spatial region of size h, the range of the smooth-particle weighting function, as described in a recent text [9], summarized in Sec. II, and applied in Sec. III.

Because the derivation of the pressure tensor is familiar and applies both at and away from equilibrium [4,5], we do not repeat that here. Instead, in Secs. III and IV, we describe and study two especially instructive problems involving gravitational and rotational forces. We reserve our conclusions and closing remarks for Sec. V.

II. SMOOTH-PARTICLE AVERAGES OF ATOMISTIC PROPERTIES

Irving and Kirkwood [2] chose to localize *particle* properties *at* the particle locations using delta functions. Though this is convenient for formal analyses, and even natural for mass and momentum, a smoothed or smeared-out particle contribution to potential energy and to fluxes often simplifies comparisons with continuum mechanics. The smeared approach can provide field variables with two continuous spatial derivatives, as we show below.

Because "action at a distance" makes the exact location of momentum and energy fluxes ambiguous, we choose to smear out particle contributions within a spatial region somewhat larger in extent than the spacing between particles. We use a local weight function with a range h, $w(r,h)$, to convert particle properties to continuum field properties. Consider, for example, the density ρ and the velocity v in a fluid or solid composed of particles with individual masses and velocities $\{m_i, v_i\}$. In the smooth-particle approach [9,10] field variables, such as the density and velocity at the point r, are *defined* as h-dependent (range-dependent) sums of nearby particle contributions:

$$\rho(r) \equiv \sum_j m_j w(|r - r_j|),$$

$$\rho(r)v(r) \equiv \sum_j m_j v_j w(|r - r_j|).$$

The sums include all particles within a distance h of point r. A good feature of this approach is that these definitions of density and velocity satisfy the continuity equation $\dot{\rho}/\rho \equiv -\nabla \cdot v$ exactly. Here, as usual, the dot indicates a comoving time derivative following the motion.

Lucy [10] was one of the inventors of the smooth-particle approach. For convenience we use his form for the weighting function in all of our smooth-particle sums,

$$w^D_{\text{Lucy}}(|r| < h) = C_D(1 - 6x^2 + 8x^3 - 3x^4), \quad x = |r|/h.$$

This form has two continuous derivatives everywhere. The normalizing prefactor C_D depends on the dimensionality D,

$$C_1 = (5/4h), \quad C_2 = (5/\pi h^2), \quad C_3 = (105/16\pi h^3).$$

C is chosen so that the spatial integral of the weight function is unity:

$$\int_0^h w^1(r)2dr = \int_0^h w^2(r)2\pi r dr = \int_0^h w^3(r)4\pi r^2 dr \equiv 1.$$

Lucy's polynomial form [10] is the simplest normalized weight function with a maximum value at the origin and two continuous derivatives everywhere. In Sec. III, where we consider the mechanical equilibrium of a two-dimensional fluid in a one-dimensional gravitational field, we compute average values of the pressure tensor using the one-dimensional form of Lucy's weight function [10].

III. GRAVITATIONAL EQUILIBRATION

Gravitational equilibration is a problem in which both the potential and kinetic contributions to stress can play a role. Where a constant gravitational acceleration acts downward in y, the simple force-balance equation for mechanical equilibrium is

$$dP/dy = (dP/d\rho)(d\rho/dy) = -\rho g.$$

The stationary density profile $\rho(y)$ can be found provided that the dependence of pressure P on the density ρ is known. As a simple example problem, chosen to highlight the kinetic and potential contributions to the virial, we choose to study the molecular dynamics of an atomistic system which closely approximates the isothermal fluid equation of state

$$P(\rho,T) = (\rho^2/2) + \rho T, \quad T \equiv 1.$$

This equation of state closely corresponds to the virial equation of state for two-dimensional particles of unit mass at unit temperature interacting with a "cusp" potential chosen to have a spatial integral of unity:

$$\phi_{\text{cusp}}(r < h) = (10/\pi h^2)(1 - x)^3, \quad x = |r|/h$$

$$\rightarrow \int_0^h 2\pi r \phi_{\text{cusp}}(r) dr \equiv 1.$$

$$\langle p_x^2/m \rangle = \langle p_y^2/m \rangle = kT \equiv 1.$$

We use this cusp interaction for the interparticle forces because the model closely corresponds to the simple and useful thermodynamic equation of state given above. We choose the range of the cusp pair potential $h=3$, so that the deviation of the potential part of the pressure tensor from that macroscopic equation of state is on the order of 1%.

For periodic two-dimensional systems the virial-theorem expression for the potential part of the pressure tensor can be expressed in terms of sums over all $N(N-1)/2$ pairs of interacting particles [4,5]. For a hydrostatic fluid, where P^Φ_{xx} and P^Φ_{yy} are each equal to the potential part P^Φ of the hydrostatic pressure P, we have

$$\begin{aligned} P^\Phi_{xx}V &= \sum (xF_x)_{i<j} \\ &= P^\Phi_{yy}V = \sum (yF_y)_{i<j} = (1/2)\sum (F \cdot r)_{i<j} = P^\Phi V. \end{aligned}$$

For a completely random distribution of particles in the volume V, the potential part of the pressure is then given by a force integral. The integral can be related to the integral of the pair potential using integration by parts. With our particular choice of pair potential ϕ, with an integral of unity, and particle mass, unity, the resulting hydrostatic pressure is simply half the square of the density:

$$\begin{aligned} P^\Phi V &= (1/2)\sum (F \cdot r)_{i<j} \\ &\simeq -[N(N-1)/(4V)]\int_0^h 2\pi r^2 \phi' dr \\ &\equiv +[N(N-1)/(2V)]\int_0^h 2\pi r \phi dr \\ &\equiv N(N-1)/(2V) \simeq N\rho/2 \rightarrow P^\Phi \simeq (1/2)\rho^2. \end{aligned}$$

A snapshot from an isokinetic (constant-kinetic-temperature) simulation appears in Fig. 1.

For convenience we have chosen a situation in which the potential and kinetic parts of the pressure are equally

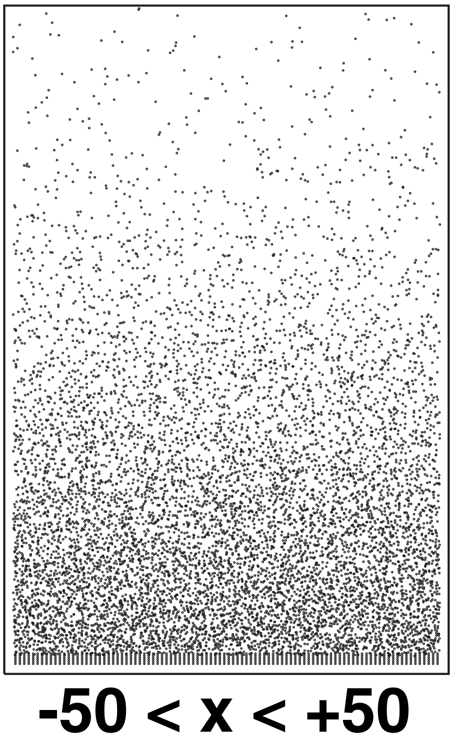

FIG. 1. Gravitational isothermal equilibrium at unit temperature for $n_x n_y = 96\times 96 = 9216$ moving particles above $6\times 96 = 576$ boundary particles fixed at the bottom of the system. The width of the system is $n_x = 96$. The height is unbounded. The field strength $g = 4/n_y$ is chosen so that the maximum density matches that of the fixed particles at the bottom: $\rho = N/V = 2$ at $y = 0$. This snapshot is typical of a long simulation used to calculate the smooth-particle pressure profiles shown in Fig. 2. In all of the figures dimensionless (or "reduced") units are used. These follow from the definitions of unity for the particle mass, Boltzmann's constant, and the length and energy scales in the interparticle forces derived from the cusp potential in Sec. II and the Hooke's-law potential in Sec. IV.

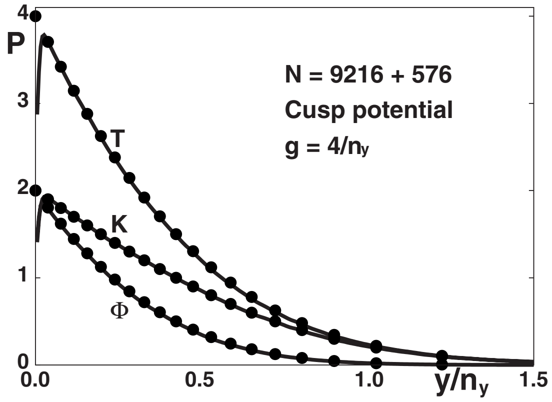

FIG. 2. Comparison of the observed and analytic pressure profiles for the gravitational problem shown in Fig. 1. From top to bottom the three curves are the total (T or Irving-Kirkwood), kinetic (K), and potential (Φ or Zhou) contributions to the pressure profile. These observed pressure contributions are calculated as smooth-particle averages. The points correspond to the analytic expressions from the isothermal equation of state $P_T = P_\Phi + P_K = (\rho^2/2) + \rho$.

important. At unit temperature ($kT = 1$) and a density of $2(\rho = Nm/V = N/V = 2)$, we have

$$P^\Phi \simeq (N^2/2V^2) = \rho^2/2 = 2, \quad P^K = \rho kT = 2.$$

We choose the gravitational acceleration g so that the "weight" of a column of unit width and containing n_y particles is equal to the maximum pressure, 4, at the maximum density, $\rho(y = 0) = 2$. In this case the mechanical equilibrium force-balance density and pressure profiles are

$$(\rho + 1)(d\rho/dy) = -\rho g \rightarrow \rho - 2 + \ln(\rho/2) = -gy,$$

$$P(y) = P^\Phi(y) + P^K(y) = g\int_y^\infty \rho(y)dy.$$

We test these analytic results against a molecular-dynamics simulation carried out *isothermally* [4–6] at a constant temperature of unity. At and below the bottom $y = 0$ of the column, we place $6n_x$ boundary particles in an area of $3n_x$ (corresponding to the maximum density, 2). See Fig. 1. We also include a short-ranged repulsive force,

$$F^{\mathrm{rep}}(y < 0) \equiv -100y^3,$$

which is applied to those few moving particles which occasionally penetrate the boundary at $y = 0$.

With periodic boundaries in x and a repulsive boundary at $y = 0$, a 9216-particle simulation gives the typical configuration we showed in Fig. 1. The corresponding kinetic and potential pressure profiles, averaged vertically with Lucy's one-dimensional weight function [10], are compared to the analytic force-balance profile in Fig. 2. Evidently the agreement is quite good, and would be qualitatively in error were the kinetic contribution to the pressure tensor omitted.

IV. ROTATIONAL EQUILIBRATION

Next we consider the influence of the kinetic pressure on the mechanical equilibrium of a rotating *solid*. We can use molecular dynamics to determine the thermal (velocity-dependent) properties of an isolated *rotationless* crystal. For this study we have chosen a nearest-neighbor Hooke's-law interaction,

$$\phi_{\mathrm{Hooke}} = \frac{\kappa}{2}(|r| - d)^2,$$

with the force constant κ, characteristic length d, and particle mass m all set equal to unity. To make contact with continuum mechanics we write the stress tensor in terms of the displacement vector u and elastic constants λ and η:

$$\sigma = \lambda \nabla \cdot uI + \eta[(\nabla u) + (\nabla u)^t],$$

where I is the unit tensor, with $I_{xx} = I_{yy} \equiv 1$ and $I_{xy} = I_{yx} = 0$. For the nearest-neighbor Hooke's-law crystal the Lamé constants are known,

$$\lambda = \eta = \sqrt{3/16}\kappa,$$

as is also the complete vibrational frequency distribution along with the bulk and surface entropies. See Chap. 4 of Ref. [5] for details.

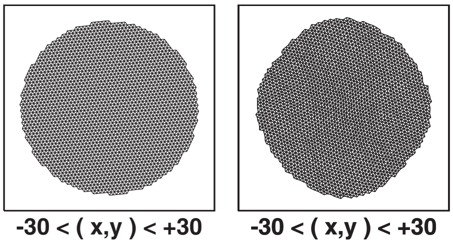

FIG. 3. Stationary rotation snapshots of two 2335-particle Hooke's-law crystals. In the rotationless stress-free case all 6828 nearest-neighbor distances are unity. In the steady rotational situations shown here, both with an angular frequency $\omega = 0.01$, the tensile strain offsetting the centrifugal forces is maximized at the center of the rotating solid. The left view is a cold solid. The right view has a temperature $kT = 0.01$.

The radial displacement in a rotating disk of radius R, $u(r)$, as well as the corresponding stress tensor σ, is well-known result of linear-elastic theory [11]. A derivation for our two-dimensional situation is sketched in the Appendix. The results are

$$u(r) = (\omega^2 r/18)[5R^2 - 2r^2],$$

$$\sigma_{rr} = (\rho\omega^2/12)[5R^2 - 5r^2], \quad \sigma_{\theta\theta} = (\rho\omega^2/12)[5R^2 - 3r^2].$$

The stress components satisfy the radial force-balance equation for a plane-polar-coordinate volume element $r dr d\theta$ rotating at the angular frequency ω:

$$+\rho\ddot{r} = -\rho r\omega^2 = (d\sigma_{rr}/dr) + (\sigma_{rr} - \sigma_{\theta\theta})/r.$$

In the comoving and corotating frame, where stress is the negative of the momentum flux, rotation provides a centrifugal force per unit mass varying as ω^2.

To compare these results from linear elasticity to molecular-dynamics simulations, consider the stationary rotation of a Hooke's-law lattice. Figure 3 shows two nominally stationary states of a 2335-particle solid with an angular velocity of $\omega = 0.01$. The cold crystal is shown at the left. The kinetic temperature of the warm crystal shown on the right is $kT = 0.01$. The 2335-particle crystal is nearly circular. It is the smallest with 36 particles equidistant from the origin (at $\sqrt{637} \simeq 25.239$). Both these rotational problems were initialized by thermostating the radial momenta [4,5] while rescaling the angular momenta to generate thermally equilibrated, steadily rotating solid disks. During the first half of each run two separate rescaling, or "Gaussian," thermostats were applied, so as to keep the radial temperature and the angular velocity constant.

Figure 4 illustrates the approximately quadratic dependence of the maximum tensile stress on the rate of rotation for small angular velocities. For comparison with the simulation results the linear-elastic stress at the center of a disk with the same mass, $Nm = 2335$, and a series of rotation rates ω is also shown. The agreement is correct to four figures as $\omega \to 0$.

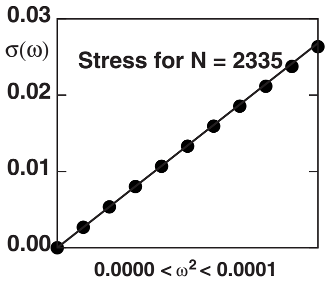

FIG. 4. Angular velocity dependence of the cold-crystal maximum tensile stress on rotation rate. The molecular-dynamics data, shown here as points, for nearly circular solids of the type shown in Fig. 3, agree with the linear-elastic result (shown as a straight line in the figure) for disks to four figures as the rotation rate goes to zero. The linear-elastic result is $\sigma_{\max} V/N = (5N\sqrt{3/4}/12\pi)\omega^2$.

Let us next consider the stresses in a thermally excited rotating crystal, computed according to the virial theorem using the formulation of the atomistic stresses by Irving and Kirkwood [2]. The Hooke's-law nature of the particle interactions guarantees that our model crystals will not melt. But as temperature rises the deformation can become quite large, so that linear-elastic theory no longer applies. Figure 5 is a typical view of a rotating specimen at a rotation rate of $\omega = 0.01$ and a kinetic temperature (relative to rigid-body rotation) $kT = 0.02$.

The simplest route to the polar-coordinate stress tensor is, first, to calculate the kinetic and potential parts of each particle's pressure tensor in Cartesian coordinates:

$$(P^K_{xx}V)_i = (p_x^2/m)_i, \quad (P^K_{xy}V)_i = (p_x p_y/m)_i, \quad (P^K_{yy}V)_i = (p_y^2/m)_i,$$

$$(P^\Phi_{xx}V)_i = \frac{1}{2}\sum_j (xxF/r)_{ij}, \quad (P^\Phi_{xy}V)_i = \frac{1}{2}\sum_j (xyF/r)_{ij},$$

$$(P^\Phi_{yy}V)_i = \frac{1}{2}\sum_j (yyF/r)_{ij}.$$

In keeping with the Irving-Kirkwood picture, the potential contributions to the pressure tensor are divided evenly between pairs $\{i,j\}$ of interacting particles. The polar-coordinate representation for each particle's pressure tensor follows from the Cartesian representation by a simple rotation, which can be written as a pair of matrix multiplications:

$$(PV)_{\text{polar}} = R \cdot (PV)_{\text{Cartesian}} \cdot R^t,$$

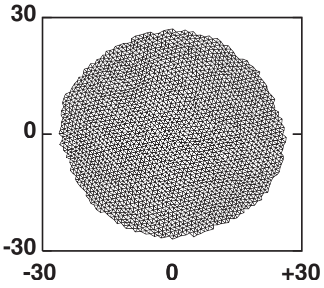

FIG. 5. View of a rotating 2335-particle Hooke's-law crystal at an angular velocity of 0.01 and a temperature $kT = 0.02$.

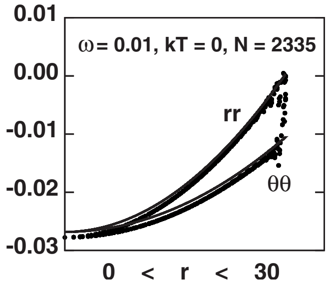

FIG. 6. *PV* in the rotating cold crystal in Fig. 3 with ω=0.01. The theoretical radial and circumferential components are shown as lines based on the expressions derived in the Appendix.

$$R_i = \begin{bmatrix} +\cos(\theta_i) & +\sin(\theta_i) \\ -\sin(\theta_i) & +\cos(\theta_i) \end{bmatrix}, \qquad \theta_i = \arctan(y/x)_i .$$

Figure 5 illustrates a thermally excited rotating Hooke's-law crystal. For the figure we have chosen the temperature so that the thermal stresses make a significant contribution to the pressure tensor. The radial stress vanishes at the disk boundary, while the circumferential "hoop" stress remains tensile there in conformity to the predictions of linear elasticity.

The stresses in two rotating crystals, one cold and one hot, are compared with the theoretical results from elastic theory in Figs. 6 and 7. The agreement is nearly perfect, and would be spoiled if the kinetic contributions were not included. In particular, omitting the kinetic contribution to the radial stress would be quite inconsistent with the vanishing of that stress component at the boundary of the disk.

V. CONCLUSION

Both the gravitational and the rotational problems show excellent correspondence between conventional continuum mechanics and atomistic mechanics *provided that both the kinetic and potential parts of the pressure tensor are included* in the analysis. Although for stationary solids the solely potential form for the virial theorem is correct, the number and type of problems which can be studied numerically are greatly enhanced by including the ideas of Irving and Kirkwood [2] coupled with the smooth-particle averaging introduced by Lucy and Monaghan in 1977. For well-defined local properties, both at and especially away from equilibrium, it is essential that these properties be measured in a coordinate frame that moves with the material. It is no accident that the fundamental equations of continuum mechanics take their simplest form in the comoving frame. In particular, the pressure (or stress) and temperature tensors, as well as the heat flux, only make sense in this frame. Stress and pressure cannot depend upon the chosen coordinate system. Hence we must choose the "comoving" "corotating" "Lagrangian" frame. In that frame the pressure tensor is simply the momentum flux, and has both potential and kinetic contributions, as shown clearly in the two problems solved here.

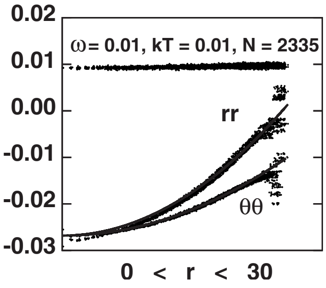

FIG. 7. Time-averaged stresses in the warm rotating thermally excited crystal in Fig. 3 with ω=0.01 and kT=0.01. The thermal contributions to $(PV)_{rr}$ and $(PV)_{\theta\theta}$ are the points at the top. The theoretical expressions for the stress (based on the cold-crystal elastic constant) shown as lines in the figure agree well with the points representing results from molecular dynamics. The molecular-dynamics results include both the potential and kinetic contributions to the comoving corotating stresses.

APPENDIX

The stationary rotation, at angular velocity ω, of an elastic disk of radius R with equal Lamé constants $\lambda = \eta = \sqrt{3/16}$ obeys the force-balance equation in the comoving frame,

$$0 = +\rho\omega^2 r + (\partial\sigma_{rr}/\partial r) + (\sigma_{rr} - \sigma_{\theta\theta})/r .$$

This macroscopic problem corresponds to a microscopic model composed of unit-mass particles linked by nearest-neighbor Hooke's-law springs. Both the spring constant and the rest length of the springs are taken equal to unity. The displacement responsible for the radial strain $\epsilon_{rr} = (du_{rr}/dr)$ causes a corresponding strain in the circumferential direction, $\epsilon_{\theta\theta} = (u/r)$. The stresses

$$\sigma_{rr} = \eta[3(du/dr) + (u/r)], \qquad \sigma_{\theta\theta} = \eta[(du/dr) + 3(u/r)]$$

convert the force balance to an ordinary differential equation,

$$r^2(d^2u/dr^2) + r(du/dr) - u = -\omega^2 r^3 \rho/(3\eta),$$

with a unique solution such that the radial stress vanishes at R:

$$u(r) = (\rho\omega^2 r/48\eta)[5R^2 - 2r^2] = (\omega^2 r/18)[5R^2 - 2r^2].$$

This solution can be used to generate the maximum tensile stress in the disk as well as the stress and strain profiles,

$$\sigma_{rr} = (\rho\omega^2/12)[5R^2 - 5r^2], \qquad \sigma_{\theta\theta} = (\rho\omega^2/12)[5R^2 - 3r^2].$$

[1] M. Zhou, Proc. R. Soc. London, Ser. A **459A**, 2347 (2003).

[2] J. H. Irving and J. G. Kirkwood, J. Chem. Phys. **18**, 817 (1950).

[3] B. J. Alder and T. E. Wainwright, J. Chem. Phys. **31**, 459 (1959).

[4] Wm. G. Hoover, *Molecular Dynamics*, Lecture Notes in Physics Vol. 258 (Springer, Berlin, 1986), available at the homepage http://williamhoover.info/MD.pdf

[5] Wm. G. Hoover, *Computational Statistical Mechanics* (Elsevier, Amsterdam, 1991), available at the homepage http://williamhoover.info/book.pdf

[6] D. J. Evans and G. P. Morriss, *Statistical Mechanics of Nonequilibrium Liquids* (Academic, London, 1990), available at the authors' websites.

[7] A. K. Subramaniyan and C. T. Sun, Int. J. Solids Struct. **45**, 4340 (2008).

[8] B. Liu and X. Qiu, e-print arXiv:0810.0803.

[9] Wm. G. Hoover, *Smooth Particle Applied Mechanics—The State of the Art* (World Scientific, Singapore, 2006), available from the publisher at the publisher's site, http://www.worldscibooks.com/mathematics/6218.html

[10] L. B. Lucy, Astron. J. **82**, 1013 (1977).

[11] T. B. Bahder, e-print arXiv:physics/0211004.