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The numerical analysis of the rotational theory for the formation of lunar globules

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Lunar globules are smooth glassy objects which were discovered by the astronauts on the moon. These objects are small - most are less than a tenth of a millimeter in diameter - though some are a good deal larger. The shapes of the globules vary on a continuum from spheres to prolate spheroids to dumbbells. Figure 1 contains two photographs, one of a prolate globule and one of a dumbbell shaped globule.

Several theories have been proposed for their creation. All these theories assume that molten rock is shot from the surface of the moon, solidifies in space above the moon and then falls back to the surface.

The rotational theory which we study in this paper makes the following assumptions: The volume of the molten rock does not change during cooling. The angular momentum is conserved. There are no internal motions because of the high viscosity of the molten rock, i.e., in equilibrium the globule is rotating as a rigid body. Finally, we assume that the kinetic reaction of the globule to the forces is fast relative to the rate of cooling, i.e., we assume that the globule reaches equilibrium at constant energy. For more discussion of this theory see [1].

Most thermodynamists would agree that with these assumptions equilibrium will be achieved at a local minimum of the internal energy and that the relevant part of the internal energy is

$$E = \frac{1}{2} I(\Omega)\omega^2 + T \cdot A(\partial\Omega)$$

Here Ω is the region occupied by the globule in a coordinate system fixed in the body. $I(\Omega)$ is the moment of inertia of the globule with respect to its axis of rotation. $A(\partial\Omega)$ is the surface area of the globule. T is a positive constant which describes the surface tension properties of the molten rock (this number is effectively constant over wide variations of temperature), and ω is the angular velocity.

We remark that from the standpoint of rational thermokinetics there is a need to justify these claims theoretically. However, we will assume here that equilibrium will be achieved at a local minimum of this internal energy expression.

We therefore consider the mathematical problem:

Minimize: $$E = \frac{1}{2} I\omega^2 + T \cdot A(\partial\Omega) \tag{1}$$

Subject to: $\text{Volume}(\Omega) = V(\Omega) = k_1$ = given constant

$I\omega = k_2$ = given constant.

It is sometimes more convenient to consider the problem in the following equivalent form.

Minimize: $$\bar{E} = \frac{ck_2^2}{I} + A(\partial\Omega) \tag{2}$$

Subject to: $V(\Omega) = k_1$ = given constant

The class of globules over which we minimize will always be some subset of the smoothly bounded axisymmetric (with respect to the axis of rotation) configurations. Here axisymmetric with respect to the z-axis means that if (x,y,z) is a point in the globule then so is $(-x,-y,z)$.

We would first like to point out that for this variational problem there is no configuration for which E (or $\bar{E}$) attains its absolute minimum, so that we can only expect to find a local minimum. To see this, consider problem (2). Let $\varepsilon > 0$ be given. By detaching two small identical pieces from the sphere at volume k_1 and placing them symmetrically on either side of the remainder of the sphere on an axis which is perpendicular to the axis of rotation, it is possible by pushing the two small pieces far away from the sphere to obtain a configuration, Ω, such that $\bar{F}(\Omega) = a_1 + \varepsilon$ where a_1 is the surface area of the sphere of volume k_1. Thus the absolute minimum for $\bar{E}$ is a_1 if it exists. But clearly no configuration has this value for $\bar{E}$ provided that $k_2 \neq 0$, since the sphere of volume k_1 is the only possibility.

Applying the classical methods of the calculus of variations we obtain as the Euler-Lagrange equation for this problem the equation:

$$C(p) = -(Ar^2 + B), \tag{3}$$

where $C(p)$ is the mean curvature of the surface $\partial\Omega$ at the point $p \in \partial\Omega$, $r^2 = x^2 + y^2$ where we have taken the z-axis is the axis of rotation, and A and B are constants which involve Lagrange multipliers and must be chosen to satisfy the constraints. It is reassuring to note that this equation can be obtained directly by balancing the forces at each point on $\partial\Omega$ without considering the variational problem at all. Since the pressure inside the globules must be greater than the outside pressure, we may conclude that the constants A and B are positive. Here we have adopted the convention that inward curvature is negative.

It is possible to write this equation as a free boundary value problem for a nonlinear partial differential equation. But this problem seems difficult to treat even numerically. We will introduce additional symmetries into the problem so that we are led to consider an approximate problem involving ordinary differential equations.

The oblate solutions

There exist exact solutions to (3) which are surfaces of resolution with respect to the z-axis (the axis of rotation). By taking advantage of the assumed symmetries, we see that these solutions will be solutions to the free boundary value problem.

$$f f'' = (1 + (f')^2)(1 - 2f(1 + (f')^2)^{\frac{1}{2}} (Af^2 + B)) \tag{4}$$

$$f'(0) = 0 : f(b) = 0,\ f'(b) = -\infty.$$

Here, f and b are unknown and A and B are positive constants which must be chosen to satisfy the constraints. The function $x = f(z)$ generates the surface of the globule when rotated about the z-axis. Remarkably, this equation can be integrated exactly in terms of elliptic integrals. (See Chandrasehkar [2].) However, it is easier to do numerically. These solutions while they are exact solutions to the Euler-Lagrange equation (3), they almost surely are not local minima for our variational problem except possibly near the sphere i.e., for small values of the angular momentum. Nevertheless, there is a smooth one parameter family of these solutions for a given volume starting with the sphere ($k_2 = 0$) and becoming more and more oblate. A convenient parameter to index these solutions is, I, their moment of inertia. Table 1 contains some important numbers for a few members of this family.

The approximate prolate and dumbbell solutions

Motivated by the fact that the actually occurring shapes are close to being surfaces of revolution with respect to an axis (which we call the x-axis) which is perpendicular to the axis of rotation, we consider the variational problem modified so as to include in the class of possible globules only those which are surfaces of revolution with respect to the x-axis. Now the appropriate functional to minimize is

$$\int_0^b \frac{\rho\Pi}{8} f^4\omega^2 + \frac{\rho\Pi}{2} f^2x^2\omega^2 + 2\Pi\ T\ f\ \sqrt{1 + (f')^2}$$

$$+ \lambda_1\ \Pi f^2 + \lambda_2\ [\frac{\rho\Pi}{4} f^4 + \rho\Pi\ f^2x^2]\omega\ dx$$

where the function $y = f(x)$ generates the surface of the globule by rotation about the x-axis, ρ is the density, and λ_1 and λ_2 are Lagrange Multipliers. Here ω is treated as a parameter. As before, both f and b are unknown. This leads to the free boundary value problem,

$$f f'' = (1 + (f'^2))(1 - 2f(1 + (f'^2))^{\frac{1}{2}} (Ax^2 + \frac{A}{2} f^2 + B)) \tag{5}$$

$$f'(0) = 0 : f(b) = 0, \quad f'(b) = -\infty.$$

As before, the positive constants A and B must be chosen to satisfy the constraints. As in the oblate case, if we fix the volume, we can generate, numerically, a continuous one parameter family of solutions starting at this sphere and proceeding through prolate shapes to dumbbell shapes with narrower and narrower necks. Again, I, the moment of inertia is an increasing parameter along this family of deformations of the sphere. Figure 2 contains graphs of some of the members of this family. The volumes of all the globules in this graph are equal. The reader is asked to compare the shapes in this figure with the photographs in Figure 1. Mathematically, this equation is more difficult to handle than (4). It cannot be integrated in terms of elliptic integrals and no existence theorem is known for this free boundary value problem. Table 2 contains extensive information about this family. The number e is defined as the thickness at the axis of rotation divided by the length of the globule. The number, D, is defined by $D = \frac{A}{B^3}$. We note that both of these numbers are invariant under similarity transformations and that if a globule is a solution to our free boundary value problem then so is any similar globule. Both Tables 1 and 2 were computed assuming that the volume is one and that the density is one.

We have, therefore, two families of deformations of the sphere each parameterized by, I, the moment of inertia of the globule with respect to its axis of rotation. We denote the oblate family by $\Omega_0(I)$ and the prolate family by $\Omega_p(I)$. For given I, the two corresponding members are local minimum for the variational problem modified in two ways. First, we add the constraint that I = const. Second, we restrict the variations allowed to be such that they produce in the case of the oblate family surfaces which are surfaces of revolution with respect to the axis of rotation (the x-axis) and in the prolate family surfaces which are surfaces of revolution with respect to the x-axis. We caution that if more general variations are allowed the prolate family globule cannot be a local minimum since they do not satisfy (3). While the oblate family globule is also not a local minimum, at least sufficiently far from the sphere, even though it does satisfy (3).

The first constraint, I = constant, is eliminated by considering $\bar{E}$ as a function of I along either of the families. We have

$$\bar{E}(I) = \frac{ck_2^2}{I} + A(I) .$$

At a minimum for the problem where the constraint, I = constant, is dropped but the restrictions on the variations are retained we must have $\frac{d\bar{E}}{dI} = 0$. That is $I^2\frac{dA}{dI} = c\, K_2^2$.

Also we must have $\frac{d^2\bar{E}}{dI^2} > 0$. Some simple calculations show that this condition is equivalent to the condition $\frac{d}{dI}\left(I^2\frac{dA}{dI}\right) > 0$ assuming that $\frac{d\bar{E}}{dI} = 0$ at the point considered. An examination of Table 2 leads to the conclusion that these globules are no longer a minimum beyond globule #25. That is beyond this point the globules are clearly unstable. If this theory is correct, the dumbbell shaped globule in Figure 1 is near the limit of stability. If it were much narrower at the neck it would break apart.

Comparison of the energies

We assume now that this volume of all globules is fixed at one. If k_2 is sufficiently small, there is exactly one local minimum for the modified variational problems along each of the families $\Omega_0(I)$ and $\Omega_p(I)$. The value of $\bar{E}$ at a point where $\frac{d\bar{E}}{dI} = 0$ is given by the expression $I\frac{dA}{dI} + A$ which forms the last column in the tables. By inspecting Tables 1 and 2 we see that for a given k_2 the energy, $\bar{E}_p(k_2)$ of the minimizing globule from the $\Omega p(I)$ family is smaller than the energy $\bar{E}_0(k_2)$ at the minimizing globule from the $\Omega_0(I)$ family from globules #16 or #17 on to the end of the table, while up to that point $\bar{E}_0(k_2)$ is smaller than $\bar{E}_p(k_2)$. However, since there exist purturbations of any of the prolate family globules which produce an even smaller energy there are globules near the prolate family which produce smaller values of $\bar{E}$ nearer to the sphere than globule #16.

We conjecture that there is a one parameter family of globules which start from the sphere and develops essentially like the prolate family but which contains true local minimum for the variational problem (1). (Chandrasehkar [2] expects that the oblate spheroids are stable near the sphere and that a bifurcation occurs along this family which contains ellipsoids with different lengths for all three axes.)

Conclusion

The good agreement between the actual shapes of the Lunar globules and the numerical results in Figure 2 certainly lend some support to the rotational theory. However, since the existence of true local minima has not been established and since the theoretical understanding of the thermokenetics is still to be attained, there is certainly room for doubt.

The numerical computation

The simplification of the variational problem yields a second order ordinary differential equation (ODE) for f(x)

$$\frac{d^2f}{dx^2} = \frac{1}{f(x)} \left(1 + \left(\frac{df}{dx}\right)^2\right) \left[1 - 2f(x) \sqrt{1 + \left(\frac{df}{dx}\right)^2} \quad (Ax^2 + B + C\,(f(x))^2)\right] \tag{6}$$

and one must find a positive value of the independent variable, say x_f, so that the following boundary conditions hold

$$\left.\frac{df}{dx}\right|_{x=0} = 0; \qquad f(x_f) = 0; \qquad \left.\frac{df}{dx}\right|_{x=x_f} = -\infty \tag{7}$$

i.e., the function should start off flat from the f-axis and should cross the x-axis going straight down.

The numerical solutions present in this paper were computed using 14 digit precision BASIC on a Z-80 based microcomputer employing two routines from the small machine oriented library of mathematical software, SCRUNCH [4] to solve this variant of a two-point boundary value problem by simple shooting. ZEROIN, a robust root finder developed by L. F. Shampine and R. C. Allen, Jr. which uses a careful combination of bisection and the secant rule, was used to find the missing end point, x_f. RKF45, a fourth/fifth order Runge-Kutta-Fehlberg method originally coded by H. A. Watts and L. F. Shampine for solving the initial value problem for systems of first order differential equations with automatic step selection and reliable error control, integrated the ODEs for each trial value of x_f.

The differential equations and boundary conditions were reformulated in terms of arc length and integrated from $x=x_f$ to $s=0$ using a suggestion of C. W. Gear to avoid the singularities present at the boundaries and the instability due to a large, positive eigenvalue of the ODE system (6) at $x=x_f$. Changing the direction of integration caused the system to be initially stiff due to the large, negative eigenvalue present, but this causes no problem due to the small step sizes typically necessary to start the integration. Letting $x = x(s)$; $y = y(s) = f(x(s))$, the problem actually computed was

$$\begin{aligned} \frac{d^2x}{ds^2} &= -2\frac{dy}{ds}\,(Ax^2 + B + Cy^2) - \frac{dy}{ds}\left(\frac{dx}{ds}\,\frac{1}{y(s)}\right) \\ \frac{d^2y}{ds^2} &= 2\frac{dx}{ds}\,(Ax^2 + B + Cy^2) + \frac{dx}{ds}\left(\frac{dx}{ds}\,\frac{1}{y(s)}\right) \end{aligned} \tag{8}$$

with boundary conditions at $x_f = x(0)$:

$$x(0) = x_f; \quad \left.\frac{dx}{ds}\right|_{s=0} = 0; \quad y(0) = 0; \quad \left.\frac{dy}{ds}\right|_{s=0} = 1 \tag{9}$$

and defining the total length of the arc, s_T, by the condition $x(s_T) = 0$

$$x(s_T) = 0; \quad \left.\frac{dx}{ds}\right|_{x=s_T} = -1; \quad y(s_T) = \text{positive}; \quad \left.\frac{dy}{ds}\right|_{s=s_T} = 0. \tag{10}$$

The singularity still present at the starting point x_f due to the term $\frac{dx}{ds}\frac{1}{y(s)}$ in (8) is avoided by using the approximation

$$\left.\left(\frac{dx}{ds}\frac{1}{y(s)}\right)\right|_{s=0} \doteq -\left.(Ax^2 + B + Cy^2)\right|_{\substack{x=x_f\\y=0}} = -(Ax_f^2 + B)$$

which comes from using the first two terms of a Taylor series for $\frac{dx}{ds}$ and $y(s)$ near $s=0$ and the known properties of the problem.

The final BASIC program takes as input the values of the parameters A and B (using the relation that $C = A/8$) and an interval (x_1,x_2) in which to search for the unknown x_f, the root of the function

$$G(x) \equiv \left.\frac{dy}{ds}\right|_{s=s_T}$$

obtained by integrating (8) backwards from the trial starting point x using initial conditions (9) until the function crosses the y-axis. The differential equations were integrated using a mixed relative and absolute error tolerance of 10^{-6} and the root was found to a similar mixed tolerance of 10^{-5}. These tolerances were easily met using the 14 digit BASIC now that the problem is formulated in a numerically stable manner. Once the missing value x_f was obtained, the initial value problem (8 and 9) was solved and the values (x,y) obtained at each step of the integration were plotted using a simple line-printer/plotter routine.

Table 1

C V=1	20	25	50	75	150
I	.12768	1.9094	.19978	.20477	.21300
A	4.8833	4.9297	4.9742	5.0022	5.0523
$\frac{dA}{dI}$	3.499	5.034	5.611	6.087	7.107
$I^2\frac{dA}{dI}$	.1105	.1835	.2239	.2553	.3235
$I\frac{dA}{dI} + A$	5.505	5.891	6.065	6.249	6.566

Table 2

#	e	D	I	A	$\frac{dA}{dI}$	$I^2 \frac{dA}{dI}$	$I \frac{dA}{dI} + A$
1	1	0	.15401	4.8363	.26		
2	1.05	.125	.15554	4.8367	1.09		
3	1.07	.25	.15691	4.8382	1.98		
4	1.10	.5	15934	4.8430	2.59		
5	1.14	.75	.16181	4.8494	3.22		
6	1.21	1.25	.16694	4.8659	4.14		
7	1.43	2.5	.18516	4.9413	4.52		
8	1.45	2.625	.18815	4.9548	4.55		
9	1.47	2.6375	.18848	4.9563	4.57		
10	1.48	2.6875	.18986	4.9626	4.46	.161	5.81
11	1.49	2.71875	.19078	4.9667	4.54	.165	5.83
12	1.50	2.75	.19175	4.9711	4.50	.166	5.83
13	1.55	3.05	.20779	5.0433	4.38	.189	5.95
14	1.92	3.0	.23741	5.1729	4.13	.233	6.15
15	2.02	2.875	.25021	5.2257	3.99	.250	6.22
16	2.15	2.6875	.26628	5.2898	3.87	.275	6.32
17	2.15	2.6375	.26770	5.2953	3.88	.278	6.33
Dumbell 18	2.18	2.625	.27139	5.3096	3.78	.278	6.34
19	2.26	2.5	2.8150	5.3478	3.62	.287	6.37
20	2.41	2.25	.30217	5.4227	3 42	.312	6.46
21	2.58	2.0	.32432	5.4984	3.20	.336	6.54
22	2.67	1.75	3.4908	5.5775	2.98	.363	6.62
23	2.95	1.5	.37758	5.6623	2.75	.392	6.70
24	3.21	1.25	.41136	5.7552	2.34	.396	6.72
25	3.98	.75	.50533	5.9755	1.98	.506	6.98
26	4.66	.5	.57291	6.1059	1.52	.500	6.98
27	6.30	.25	.65168	6.2258	1.02	.431	6.88
28	9.15	.125	.68487	6.2595			

Figure 1

Photographs supplied courtesy of Dr. Gertrude Hinsch, Department of Biology, University of South Florida and Dr. H. Fertig, Max Plank Institute für Kerm Physik, Heidelberg, Germany.

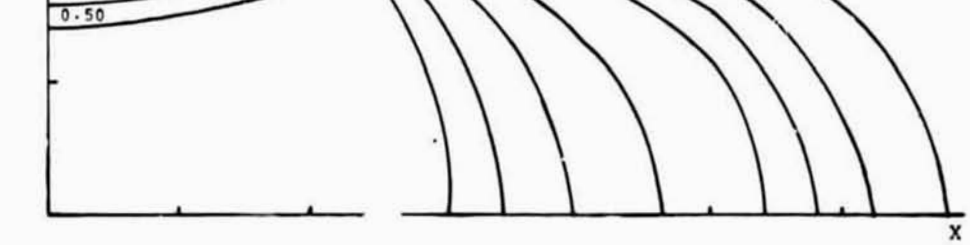

Figure 2

The numbers appearing on the graph are values of D.

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