VIRUSES, VESICLES AND MULTI-ELECTRON BUBBLES: THE THOMSON PROBLEM REVISITED

- DEFECTS AND THE GROUND STATES OF PARTICLES PACKED IN TWO DIMENSIONS geometrical frustration

- PARTICLE PACKINGS ON A SPHERE

  1. J. J. Thomson's theory of the periodic table.

  2. Icosahedral Packings in Viral Shells D. Caspar & A. Klug
     disclination buckling

  3. Multi-electron bubbles -- an experimental realization of the Thomson problem

- CONTINUUM ELASTIC TREATMENT OF DEFECTS AND *ICOSADELTAHEDRAL* GROUND STATES
  Euler's Theorem $\Longrightarrow N_5 - N_7 = 12$

- NEED FOR ***GRAIN BOUNDARIES*** IN THE GROUND STATE WITH SPHERICAL GEOMETRIES grain boundaries can terminate inside curved media!!

- EXPERIMENTAL TESTS: Colloids absorbed onto Spherical and Toroidal Vesicles; Hyperbolic phases of lipid bilayers

Collaborators

Michael Rubinstein
Subir Sachdev

Alex Travessett & Mark Bowick
Phys. Rev. B62, 8738 (2000)
Jack Lidmar

Related Work

* Alar Toomre (unpublished)

M. Dodgson, M. Moore, A. Pérez-Garrido
Phys. Rev. B56, 3640 (1997)
Phys. Rev. B60, 15628 (1999)

Motivation:

VIRUSES

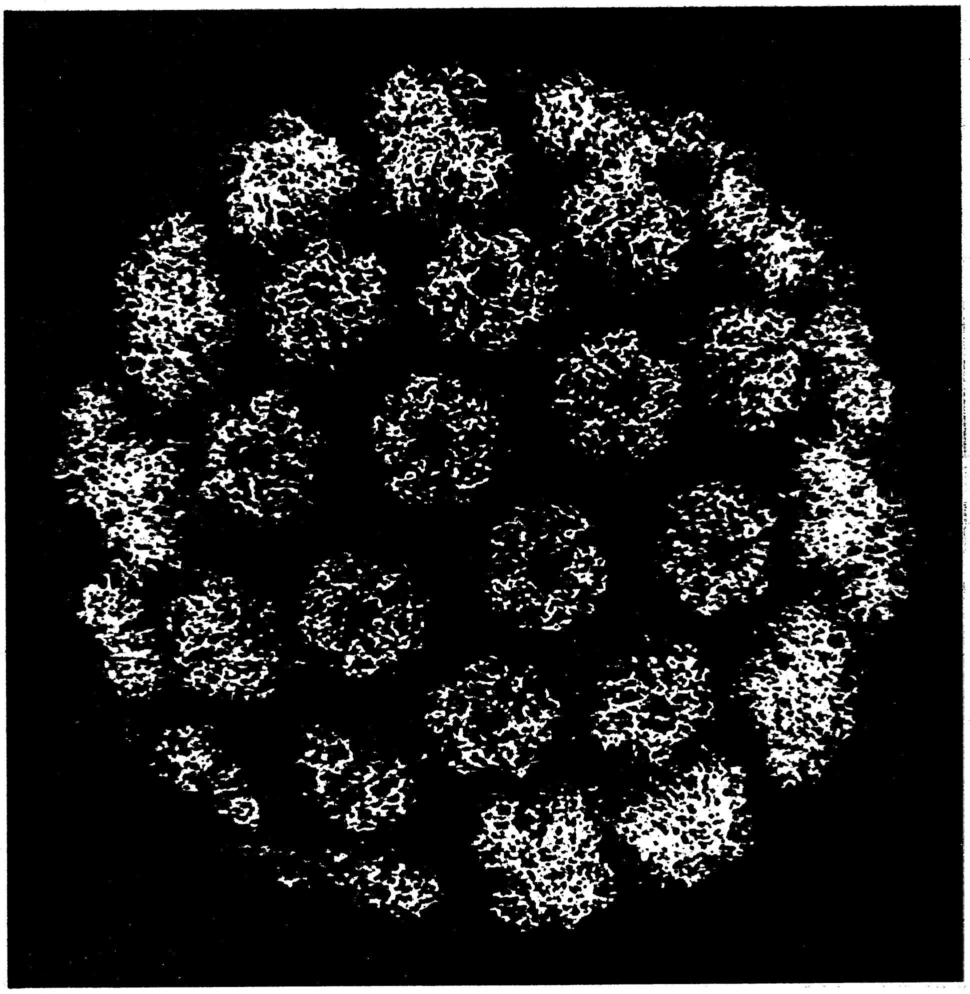
SV40, POLYOMAVIRUS (Steve Harrison)

* 12 pentamers in a 5-fold environment

* 60 pentamers in a 6-fold environment

* overall icosahedral symmetry

* it's chiral!



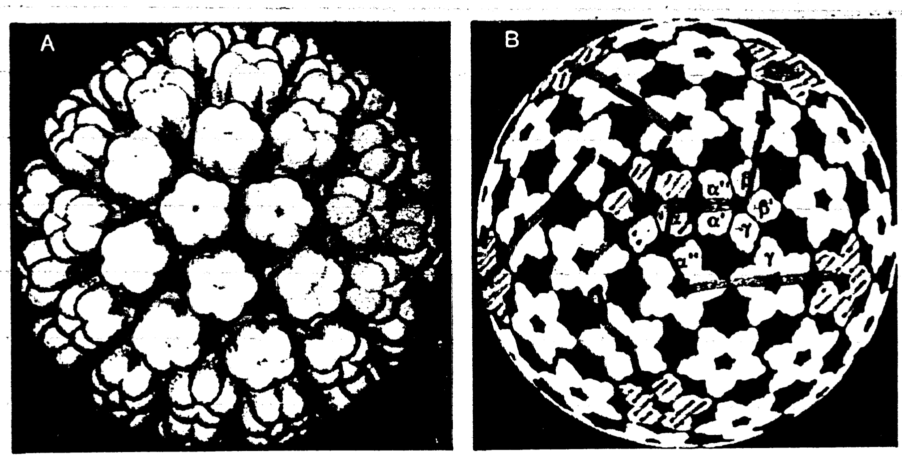


FIGURE 7.3 Overall view of the polyomavirus virion. The shell is composed of 360 copies of VP1 organized into 72 pentamers. The pentamers are situated at the points of a $T = 7d$ icosahedral surface lattice. There are 12 five-coordinated pentamers and 60 six-coordinated pentamers. The three kinds of interpentamer clustering are indicated. Three subunits (α, α', α'') form a threefold interaction, the subunits labeled β and β' form one sort of twofold interaction, and the γ subunits form another kind of twofold interaction across an icosahedral twofold axis. (Adapted from Salunke et al., 1986.)

Crystallography on the sphere:

D. Caspar & A. Klug, Cold Spring Harbor Sym on Quant. Biology 27, 1-24 (1962)

DENSE - PACKED ARRAYS

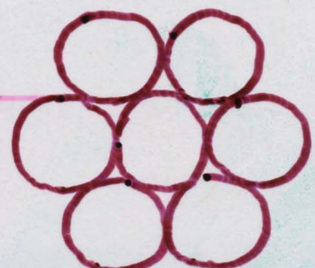
ground state
of a 2d crystal ...

Two Dimensions:

maximize density via
equilateral triangles

six triangles

HEXAGON



TRIANGULAR LATTICE

NUCLEATION AND GROWTH ON A SPHERE

a = particle diameter

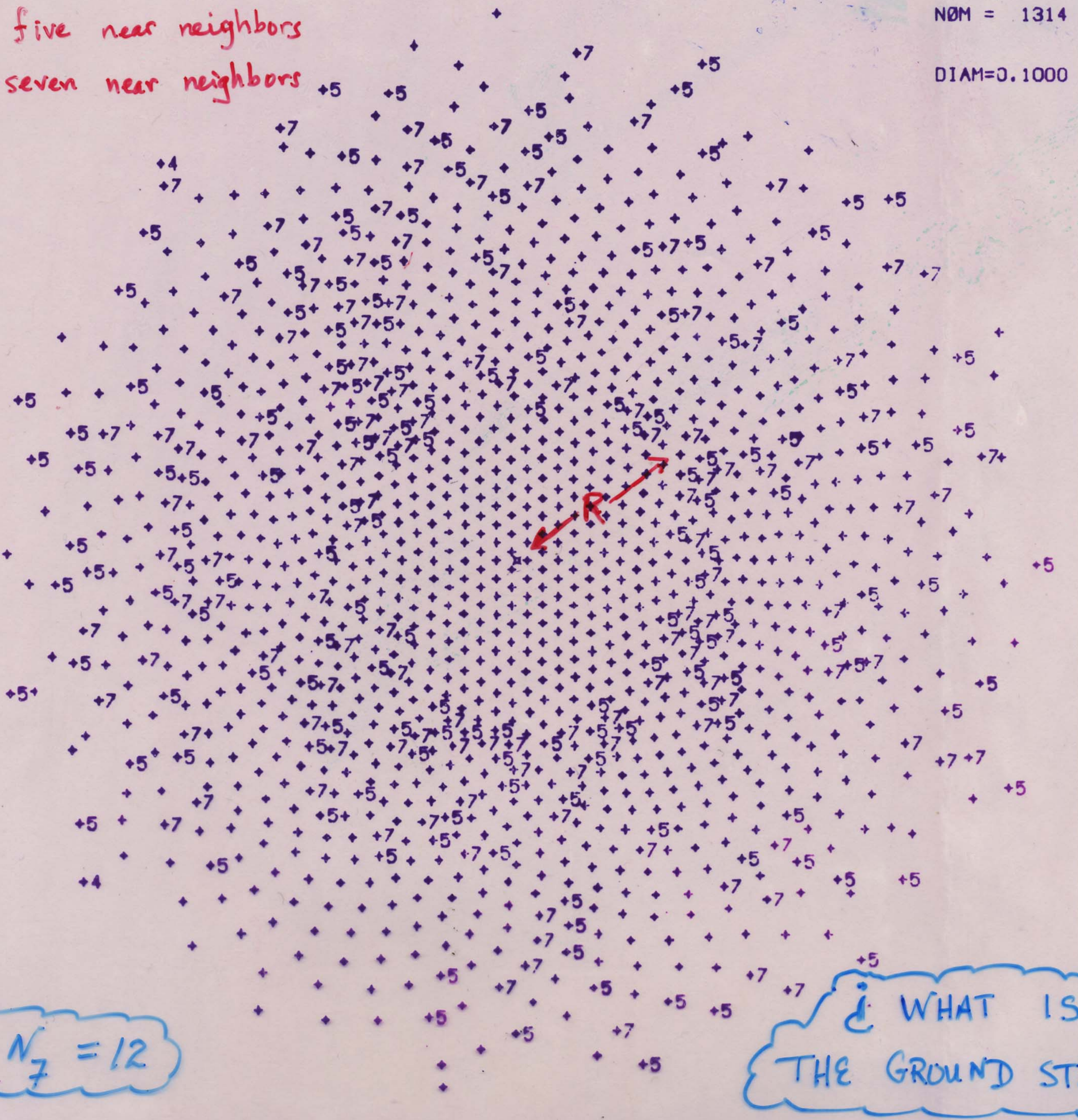
R = radius of sphere

polar projection about north pole

$\frac{R}{a} = 10$, $N \approx 1314$ particles, M. Rubinstein

5 = five near neighbors

7 = seven near neighbors



$N_5 - N_7 = 12$

¿ WHAT IS THE GROUND STATE?

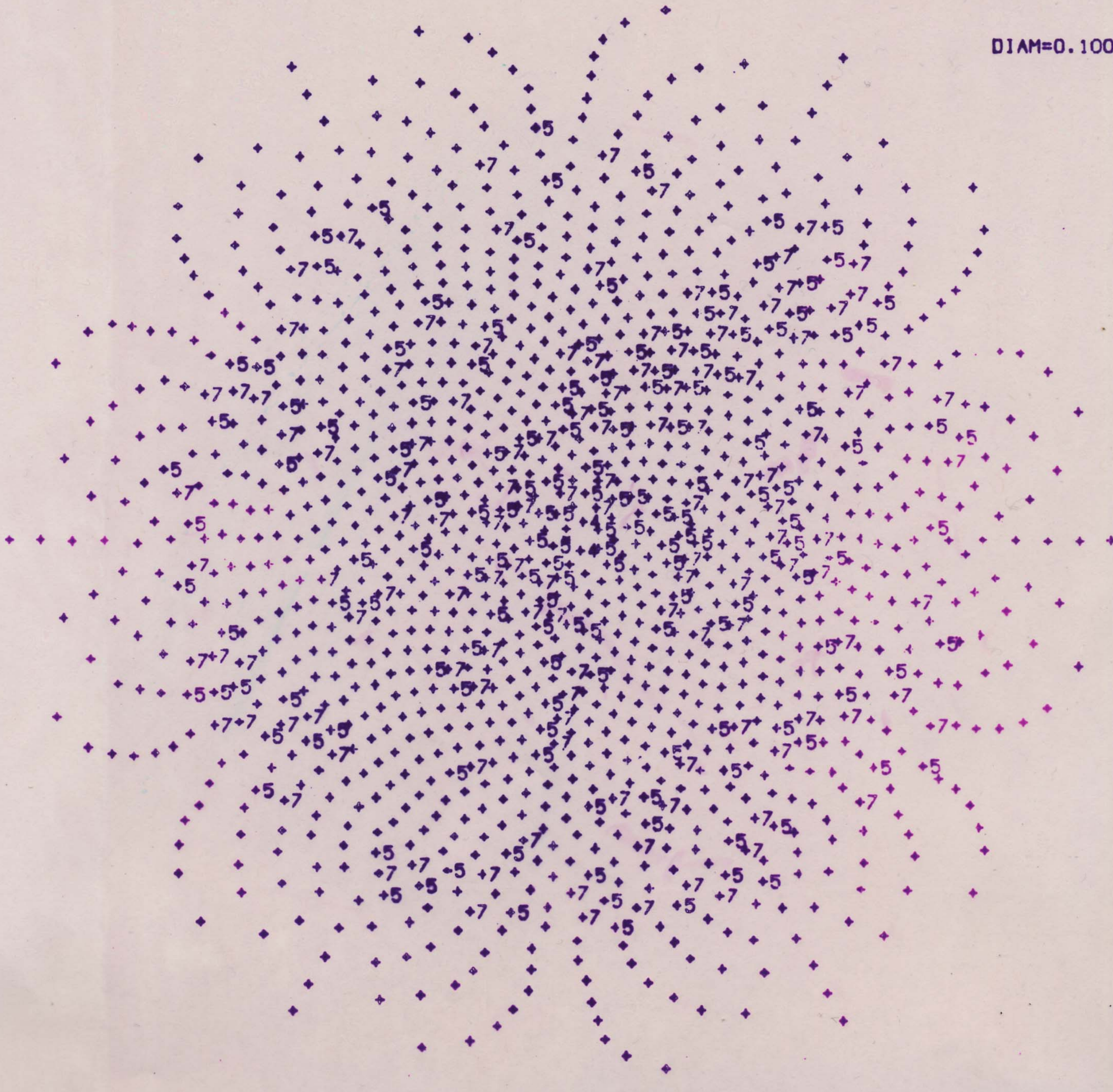
SOUTH POLAR PROJECTION . . .

$\frac{R}{a} = 10$, $N \approx 1400$

$N_5 - N_7 = 12$, exactly !

NØM = 1314

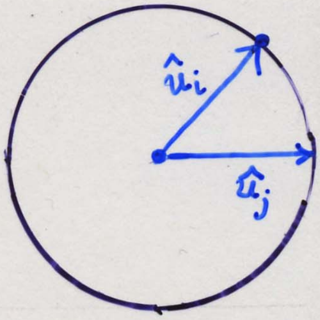
DIAM=0.1000



¿ WHAT IS THE GROUND STATE OF MANY IDENTICAL PARTICLES INTERACTING ON THE SURFACE OF A SPHERE ? $\frac{R}{a} >> 1$

See, e.g., D. Levesque, J.-J. Weis & J. L. Lebowitz, preprint

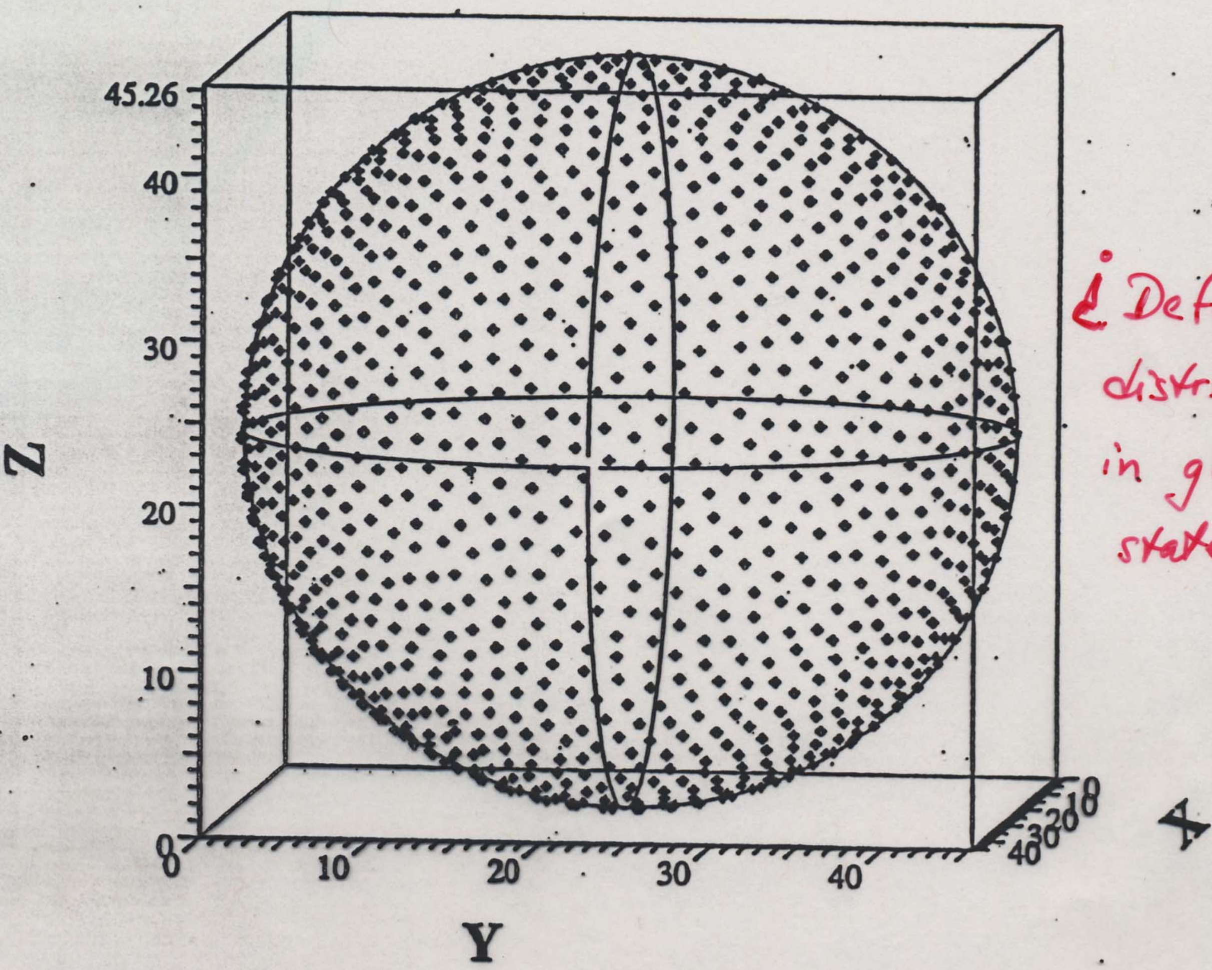
$$V(\hat{u}_1, \ldots, \hat{u}_N) = -\frac{e^2}{2} \sum_{i>j} \ln \left[\frac{2R^2}{a^2} (1 - \hat{u}_i \cdot \hat{u}_j) \right]$$



Monte Carlo simulations with

$$\frac{e^2}{k_B T} \equiv \textbf{Gamma = 140} \quad \ldots$$

2048 particles.



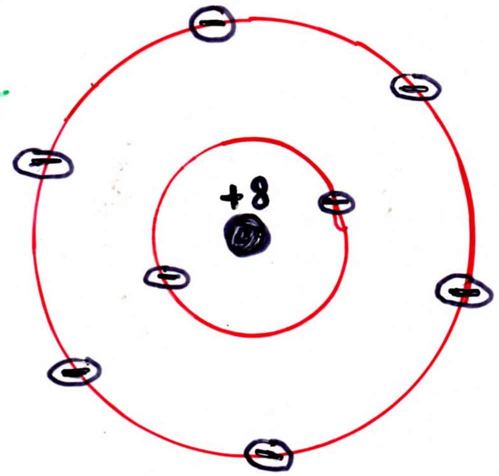
¿ Defect distribution in ground state ?

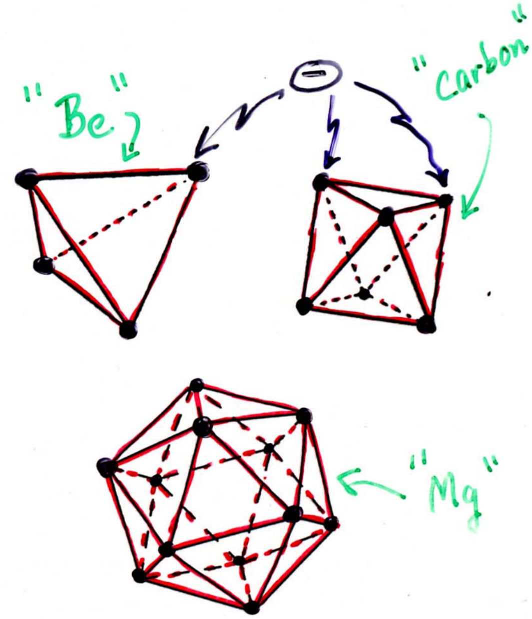
FREEZING ON CURVED SURFACES

The "Thomson Problem"

shell model of atomic structure ...

2d.





3d

[quantum mechanics makes this problem irrelevant for electrons in atomic orbitals!]

PHILOSOPHICAL MAGAZINE

AND

JOURNAL OF SCIENCE.

[SIXTH SERIES.]

MARCH 1904.

XXIV. *On the Structure of the Atom: an Investigation of the Stability and Periods of Oscillation of a number of Corpuscles arranged at equal intervals around the Circumference of a Circle; with Application of the results to the Theory of Atomic Structure. By* J. J. THOMSON, *F.R.S., Cavendish Professor of Experimental Physics, Cambridge* *.

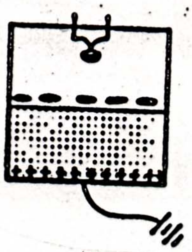
THE view that the atoms of the elements consist of a number of negatively electrified corpuscles enclosed in a sphere of uniform positive electrification, suggests, among other interesting mathematical problems, the one discussed in this paper, that of the motion of a ring of n negatively electrified particles placed inside a uniformly electrified sphere. S

"The analytical and geometrical difficulties of the problem of the distribution of the corpuscles when they are arranged in shells are much greater than when they are arranged in rings, and I have not as yet succeeded in getting a general solution."

MOTIVATION : Multielectron bubbles in He^4

U. Albrecht & P. Leiderer, J. Low Temp. Phys. 86, 131 (1992)

P. Leiderer, Zeitschrift. für Physik B 98, 303 (1995)



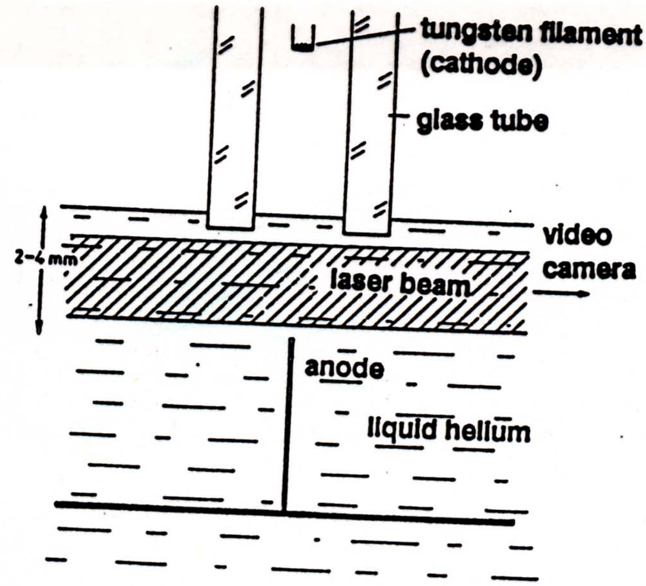
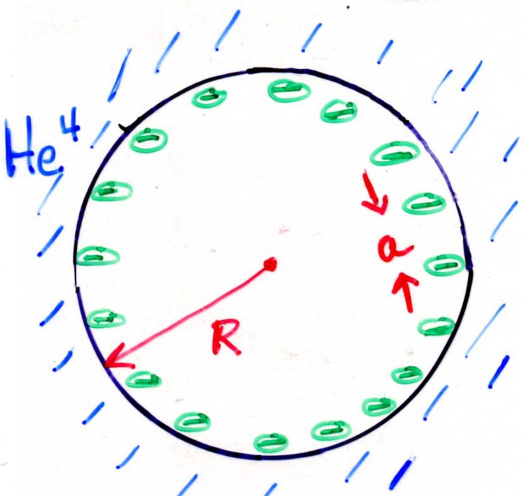


Fig. 4. Schematic set-up for electrical and optical detection of multi-electron bubbles. The video camera for the optical measurement was focussed on the volume between anode tip and glass tube, at an angle of 30° with respect to the laser beam, to pick up light scattered from the bubbles in nearly forward direction



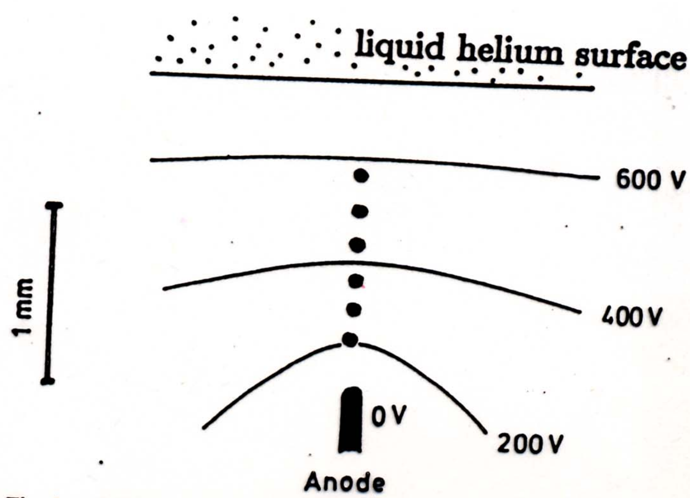


Fig. 1. (a) Displacement current induced in the anode by motion of a MEB with $Z = 1.4 \cdot 10^6$ electrons towards it through the liquid helium. (b) shows a sketch of the corresponding videopicture at chopped laser illumination (period $\tau = 3.7$ ms).

$$E_c(R) = 4\pi R^2 \sigma + \frac{Z(Z-1)e^2}{2\varepsilon R}$$

$$\Rightarrow \quad R \approx \left(\frac{Z^2 e^2}{16\pi \sigma \varepsilon}\right)^{1/3}$$

$R \approx 10 - 100\ \mu m$!

$Z \approx 10^5 - 10^7$ electrons!

$$\frac{R}{a} \gg 1$$

Colloidosomes

Motivation:

latex spheres adsorbed onto lipid bilayer vesicles

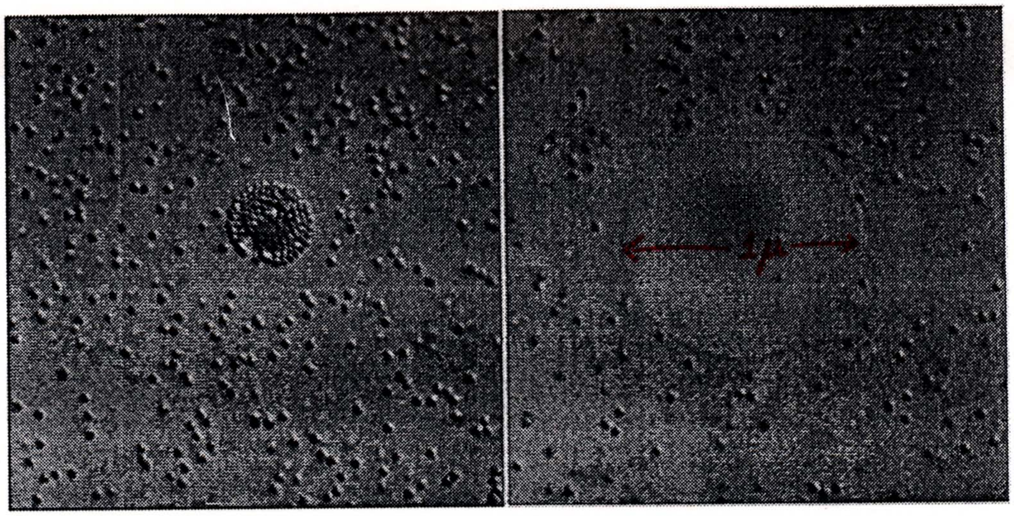
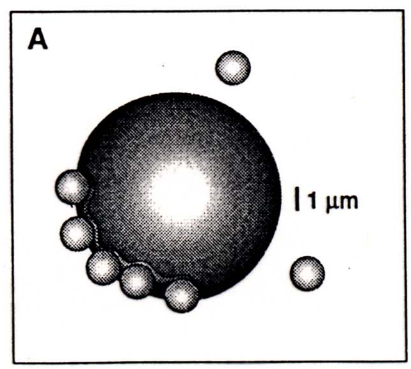


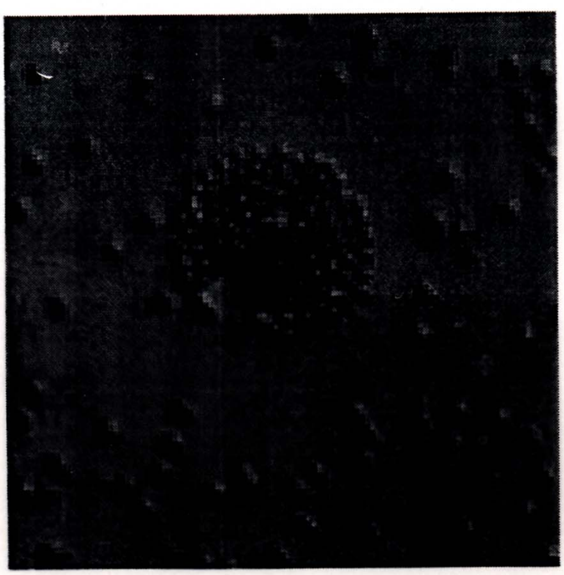
Fig. 1. A self-limited array of latex spheres on a charged surfactant vesicle at room temperature (3). The spheres are on the surface of a vesicle viewed in differential interference microscopy, focusing on the array itself (left) or on the vesicle equator (right). The membrane is a mixture of cationic and neutral surfactants (DDAB and Triton X, respectively, with octanol added to stabilize bilayer structures). The sphere diameter is 1 µm; the sphere volume fraction is 0.004.

H. Aranda-Espinoza et. al.
Science 285, 394 (1999)

Fig. 2. **(A)** Schematic of the geometry. A vesicle of mixed neutral and cationic surfactants



D. Weitz
A. Dinsmore
A. Bausch
⋮

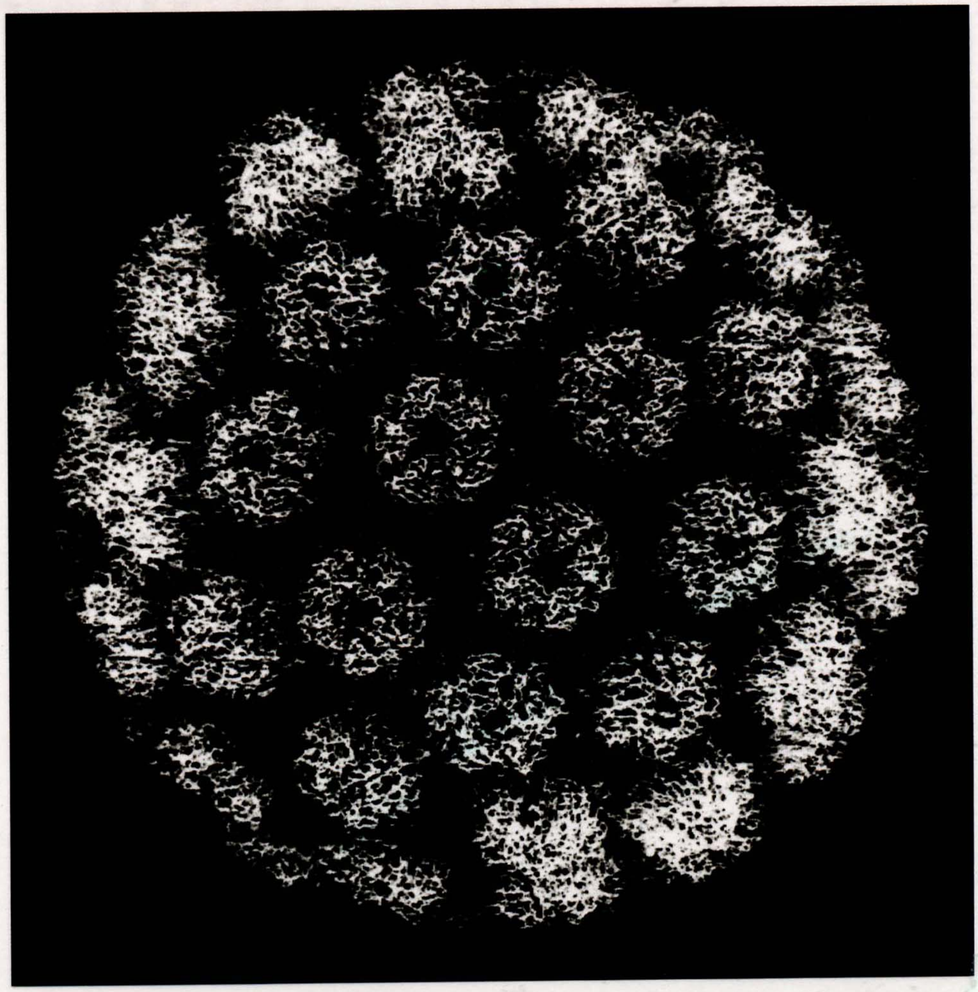


* encapsulation of flavors & fragrances
* targeted drug delivery
* protection of cells from immune system

VIRUSES

Motivation:

SV40, POLYOMAVIRUS (Steve Harrison)

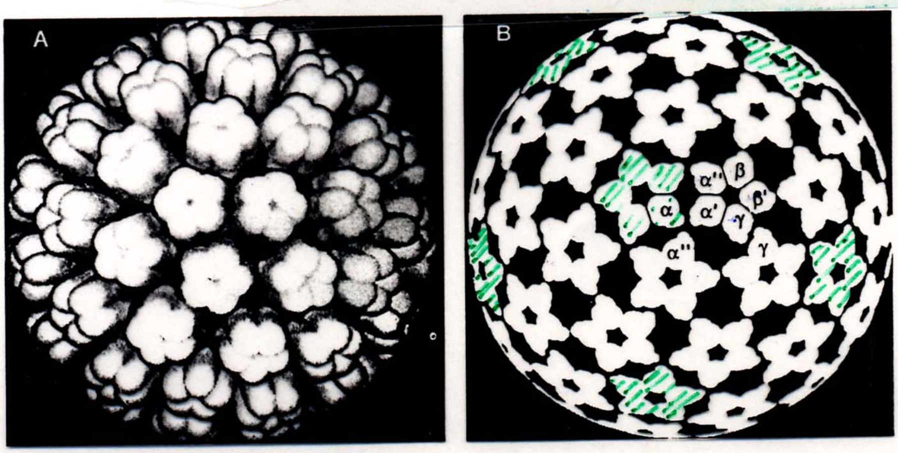


* 12 pentamers in a 5-fold environment

* 60 pentamers in a 6-fold environment

* overall icosahedral symmetry

* it's chiral!



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Crystallography on the sphere:

D. Caspar & A. Klug, Cold Spring Harbor Symp. on Quant. Biology 27, 1-24 (1962)

GROUND STATES FOR MODERATE $N \sim (R/a)^2$: ICOSADELTAHEDRA

Euler's Thm: $F - E + N = 2 \Rightarrow \sum_{j=1} (6 - z_j) = 12$

$= N_5 - N_7$

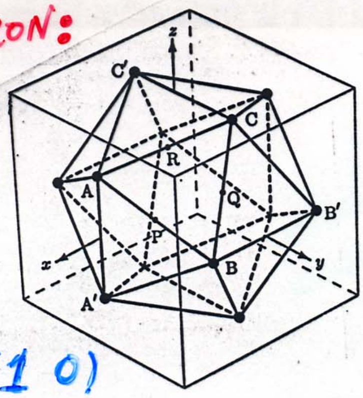
ICOSAHEDRON:

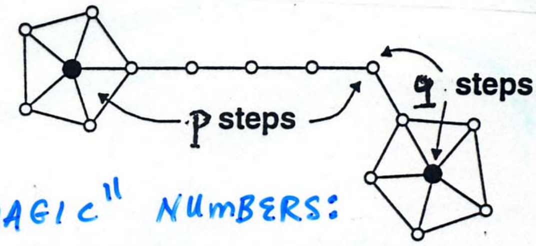
$F = 20$

$E = 30$

$N = 12$

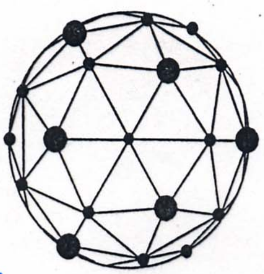
$(p, q) = (1\ 0)$



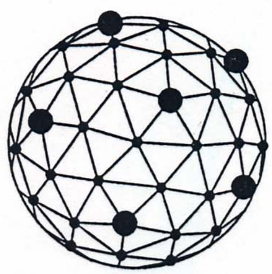


"MAGIC" NUMBERS:

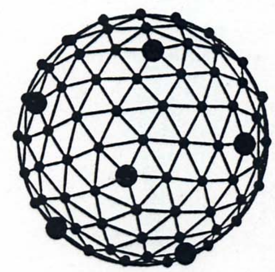
$N = 10(p^2 + pq + q^2) + 2$



$(1,1)$, $N = 32$

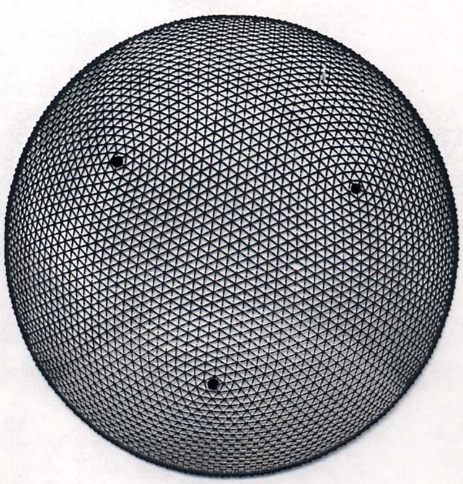


$(2,1)$, $N = 72$

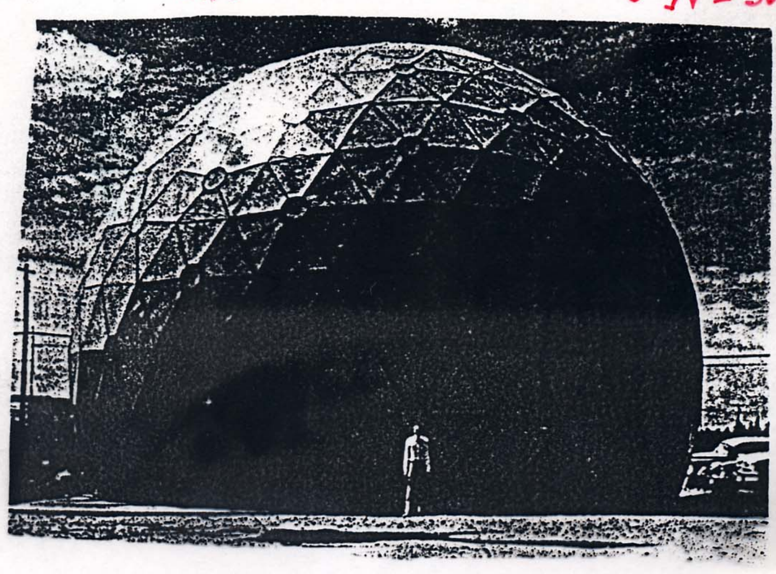


$(3,1)$, $N = 132$

c.f. Geodesic Dome! $(6,0)$ $N = 362$



$(14, 14)$, $N = 5882$



GALLERY OF VIRUSES

(1, 2) N = 72

(1, 1) N = 32

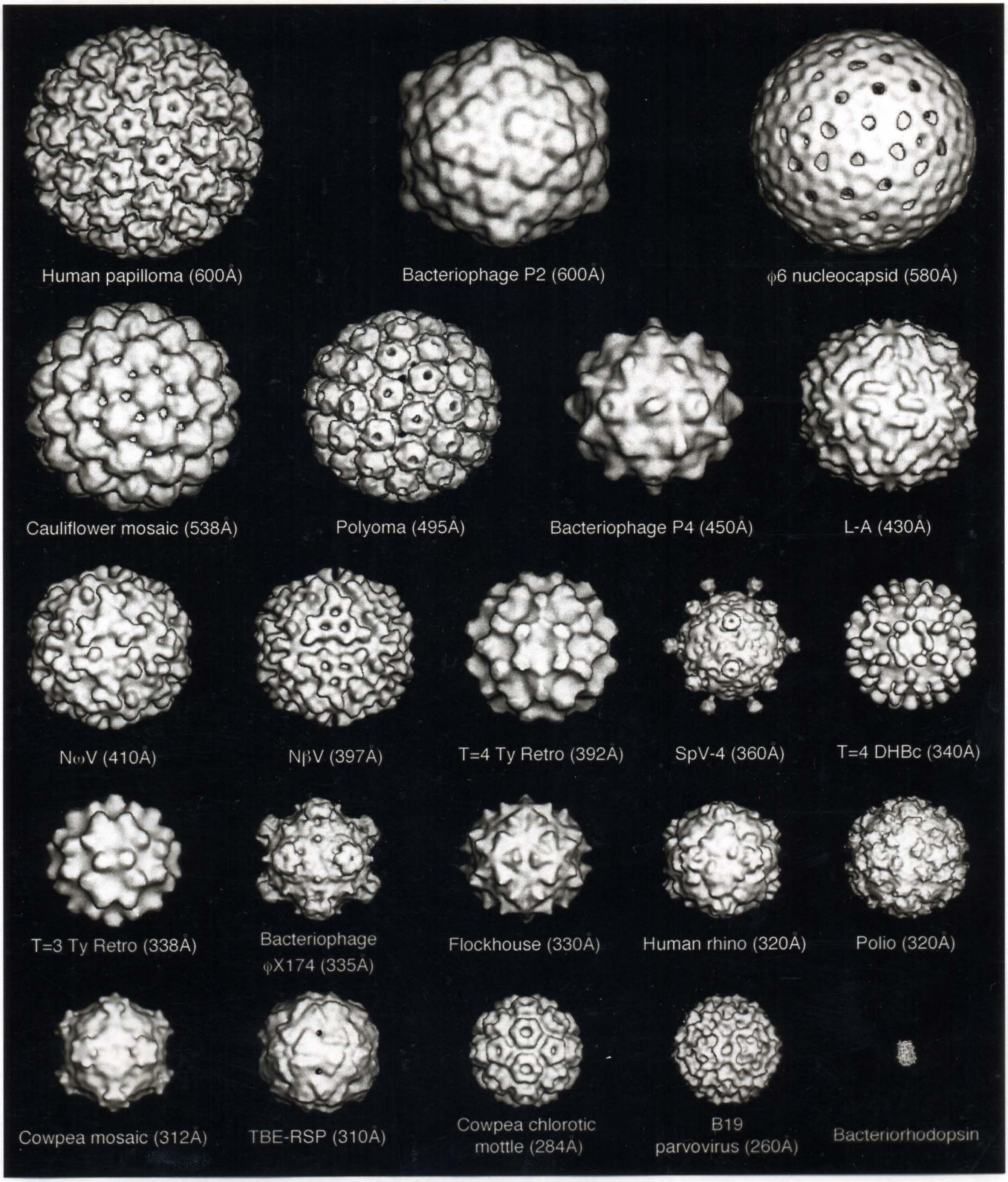


Figure 1. Baker, Olson and Fuller - right page
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(4,0)

N = 162

(5,0)

N = 252

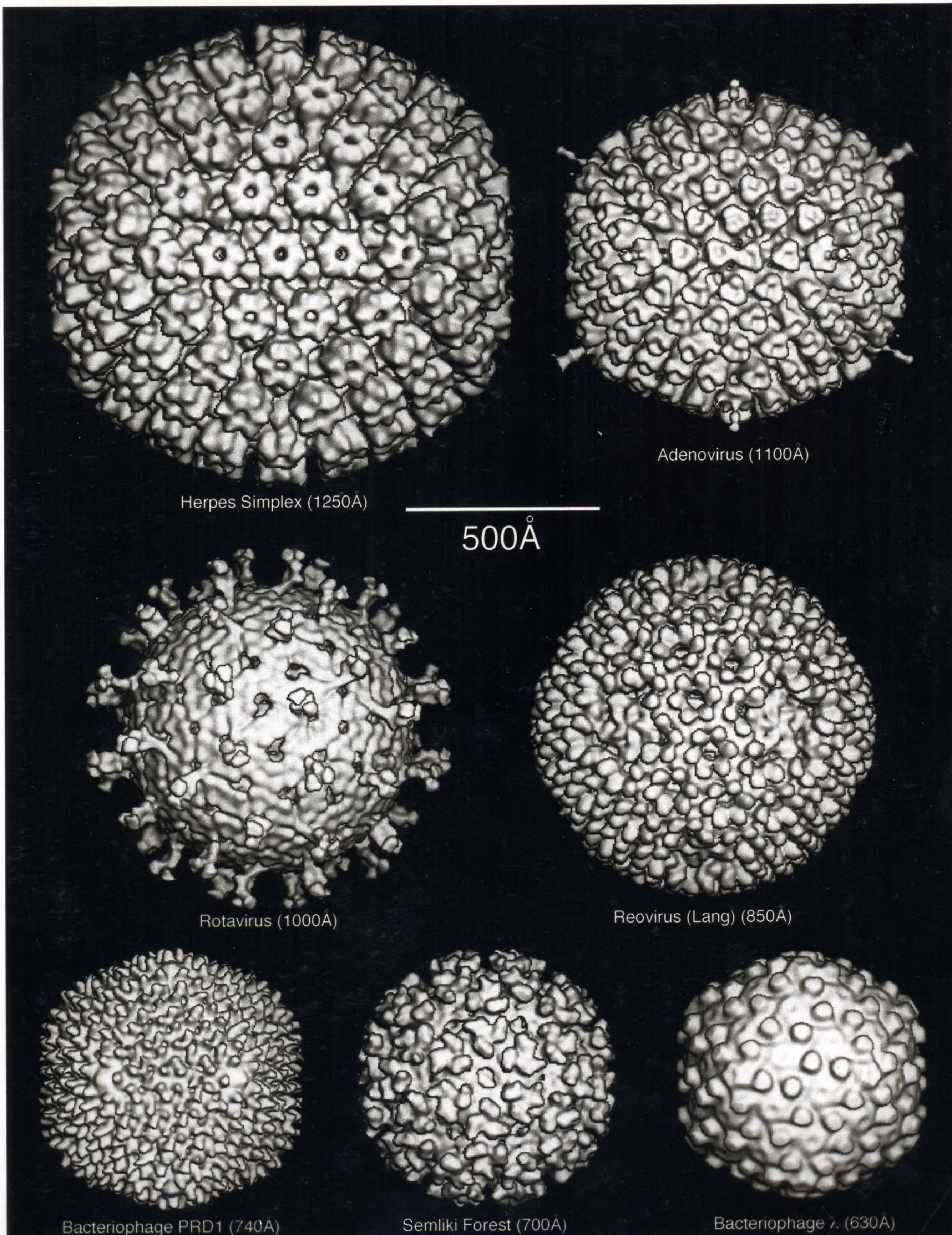

Figure 1. Baker, Olson and Fuller - left page
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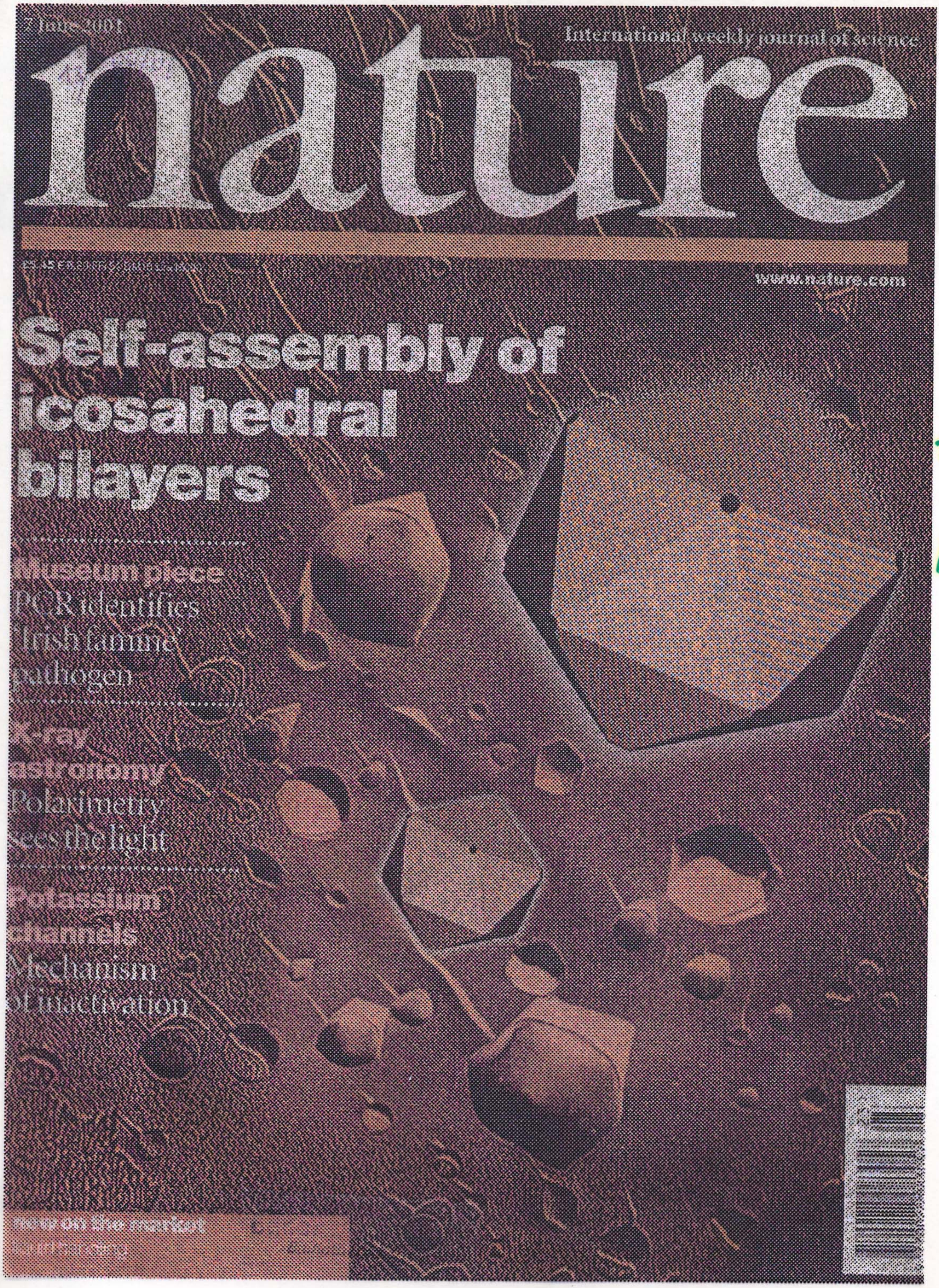
(2, 0) N = 42



See also:
Blaurock/Gamble
faceted lecithin vesicles . . .
E. Sackmann
et. al. . . .

<u>Motivation</u>: Salt-Free mixtures of anionic & cationic bilayers
M. Dubois, T. Zemb et. al. Nature <u>411</u>, 672 (2001)

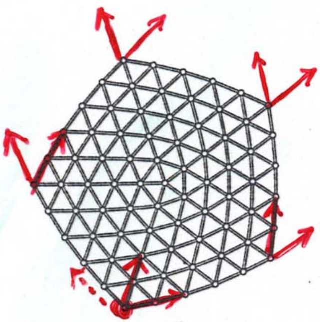
DEFECTS IN MONOLAYERS = flat space

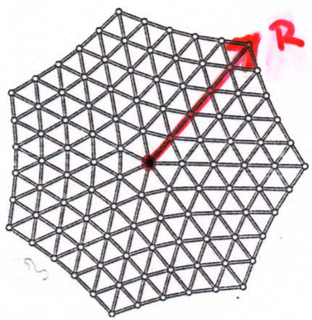
$$E = \frac{1}{2}\int d^2x \left[2\mu u_{ij}^2 + \lambda u_{kk}^2\right]$$

$$Y_0 = \frac{4\mu(\mu+\lambda)}{2\mu+\lambda} \approx 4\mu$$

$$u_{ij} = \frac{1}{2}\left[\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right]$$

<u>disclinations</u>





$$E \underset{R\to\infty}{\approx} \frac{Y_0 s^2}{32\pi} R^2$$

$s = \frac{+2\pi}{6} = +60^\circ$

"+1"

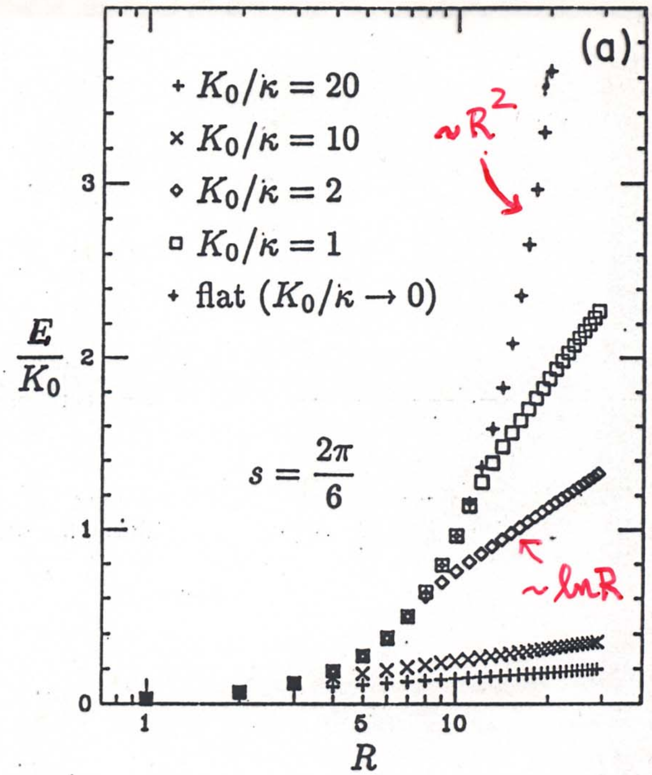
$s = \frac{-2\pi}{6} = -60^\circ$

"-1"

Disclination Buckling Transition

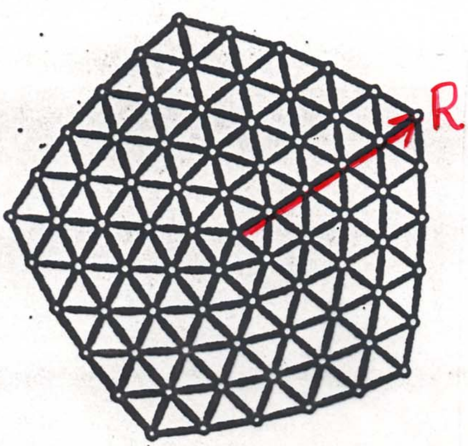
L. Peliti, S. Seung
drn
(flat space)

$$E = \sum_{\langle ij \rangle} V(|\vec{r}_i - \vec{r}_j|) - \kappa \sum_{\langle \alpha\beta \rangle} \hat{n}_\alpha \cdot \hat{n}_\beta$$



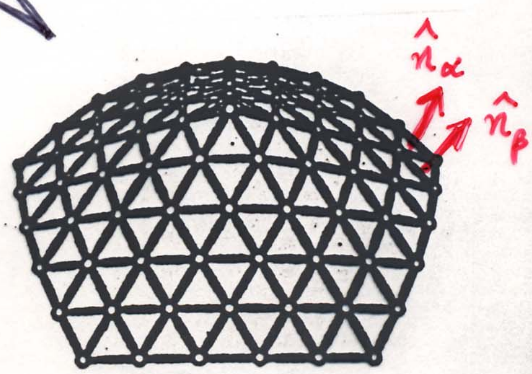
$$V(r) = \frac{1}{2}\varepsilon(r-a)^2$$

$$\cancel{K}Y_0 = \text{Young's Modulus} = \frac{2\sqrt{3}}{3}\varepsilon$$



buckling radius: $\frac{\cancel{K}Y_0 R_b^2}{\kappa} \approx 160$

"von Karman number"

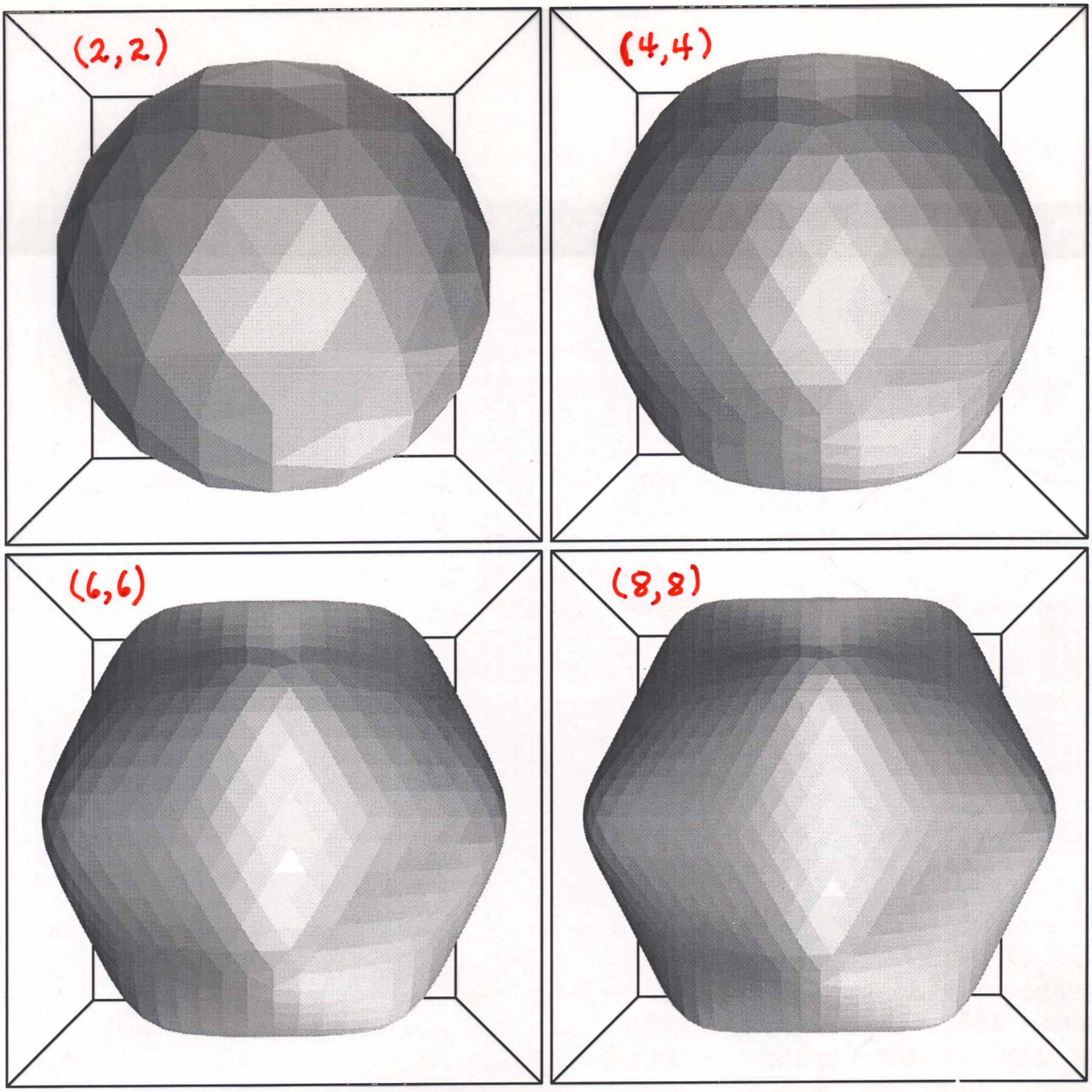


before buckling:

$$E(R) \approx \frac{\cancel{K}Y_0}{32\pi}\left(\frac{2\pi}{6}\right)^2 R^2 \quad , \quad R < R_b$$

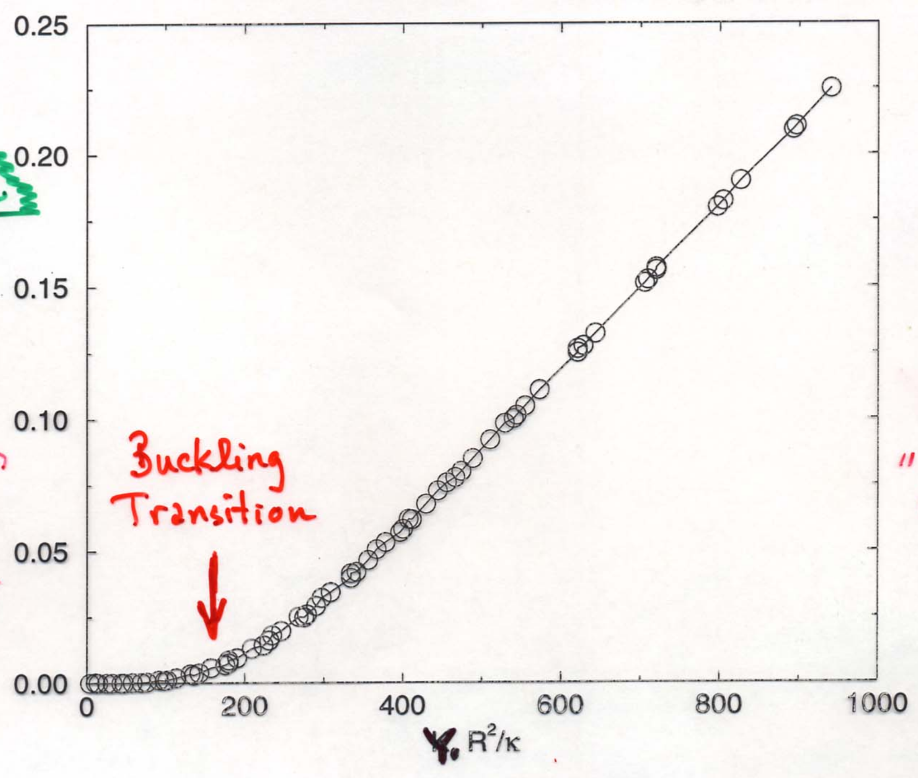
after buckling:

$$\boxed{E(R) \underset{R\to\infty}{\approx} \text{const.} \times \kappa \ln(R/a), \quad R > R_b}$$



Virus Buckling

(Jack Lidmar)



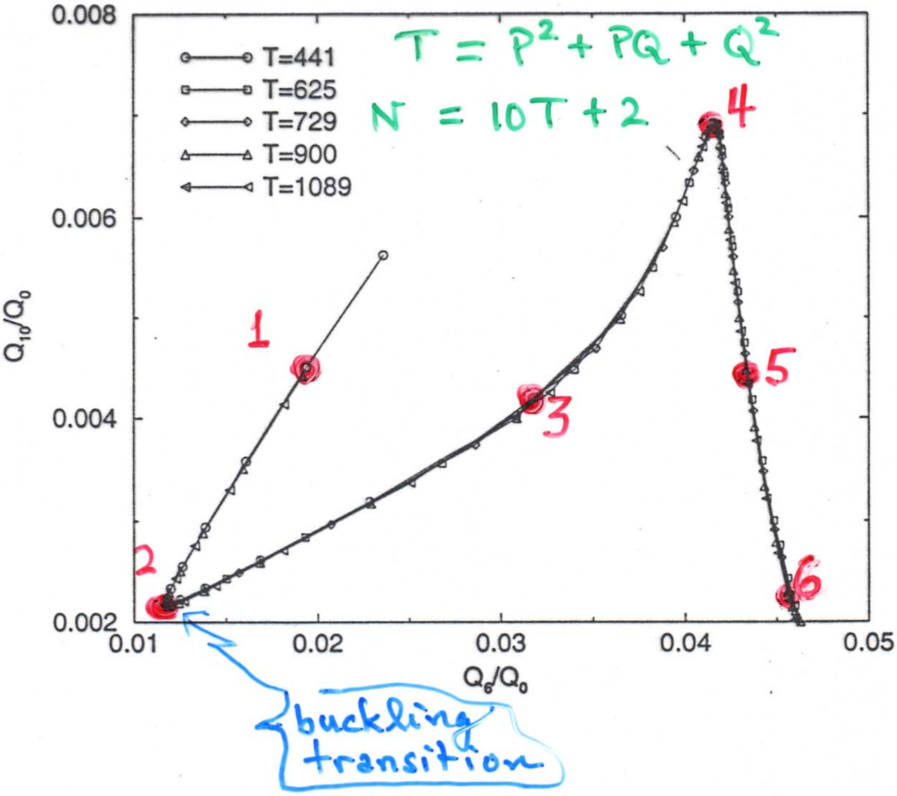
$$r_c \propto R\left(\frac{h}{R}\right)^{1/3}$$

"ridge scaling"

Lobkovsky, Witten, et. al.

BUCKLING TRANSITION ON A SPHERE: SPHERICAL HARMONIC EXPANSION

expand radial coord.: $R(\theta,\phi) = \sum_{l} \sum_{m=-l}^{l} Q_{lm} Y_{lm}(\theta,\phi)$



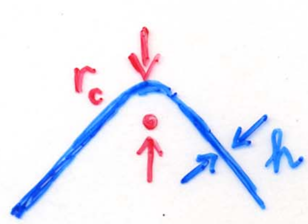
$l = 0, 6, 10, 12, 16, 18, \ldots$ for icosahedral symmetry

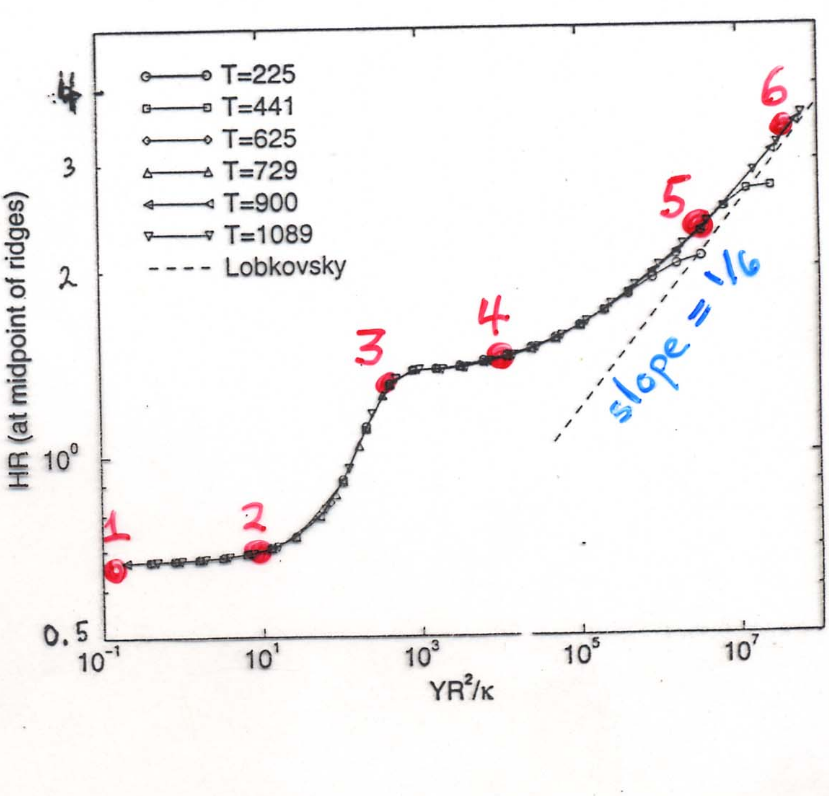
$$Q_l^2 = \frac{1}{2l+1} \sum_{m=-l}^{l} |Q_{lm}|^2$$

TEST of "RIDGE SCALING"

$$H\bar{R} = \frac{\bar{R}}{r_c} = \left(\frac{\bar{R}}{h}\right)^{1/3}$$

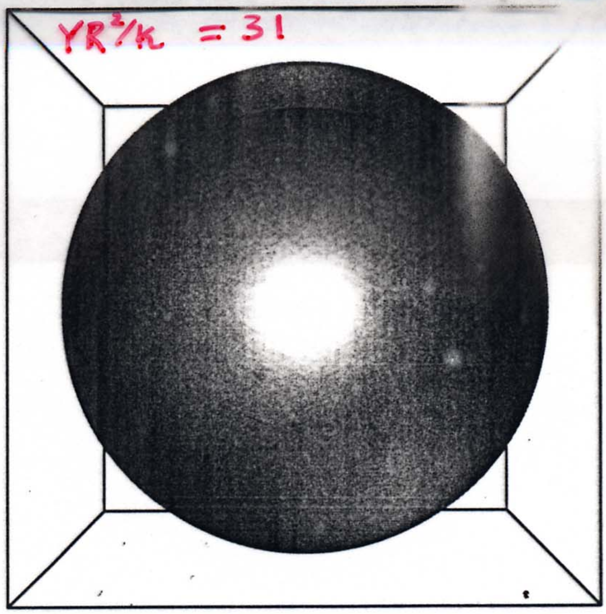
$$\propto \left(Y\bar{R}^2/\kappa\right)^{1/6}$$





→ N = 10,892 particles in ICOSDELTAHERON ON THE SPHERE

1



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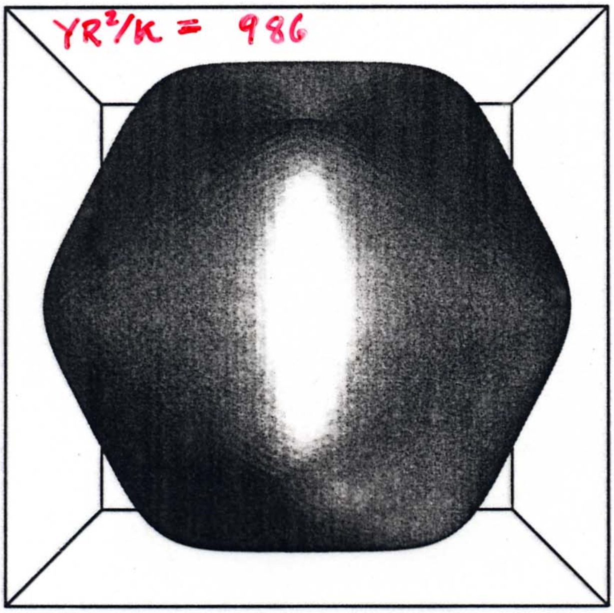

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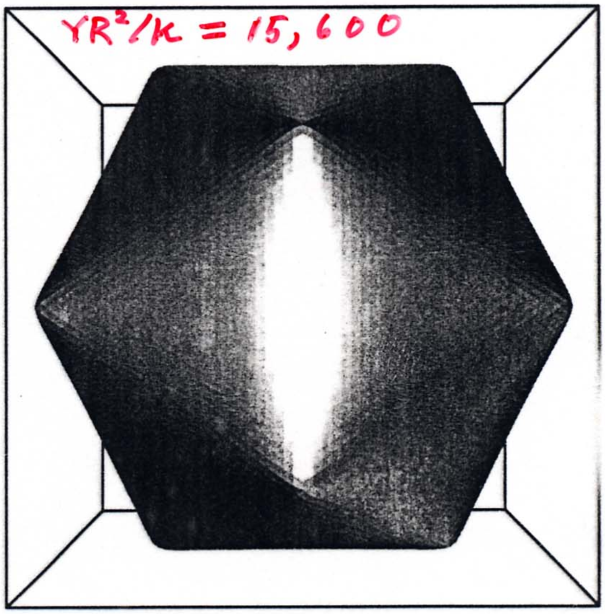
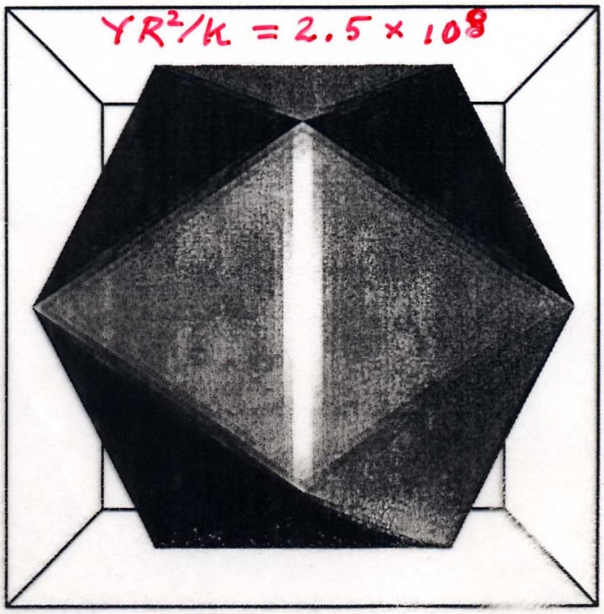


4

5

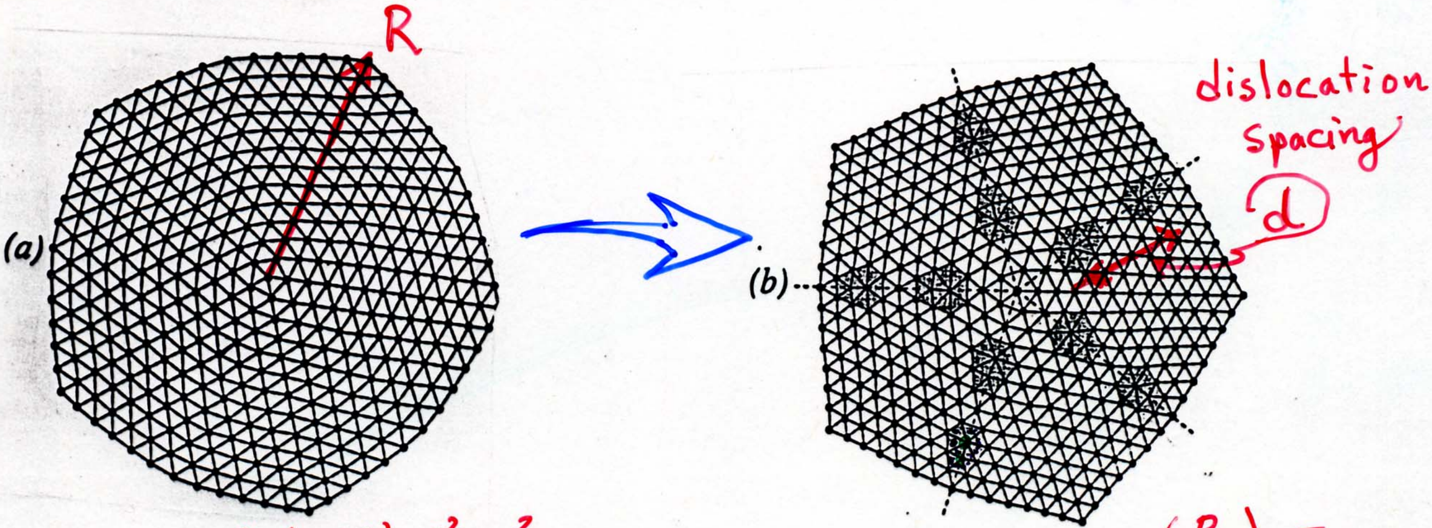


6

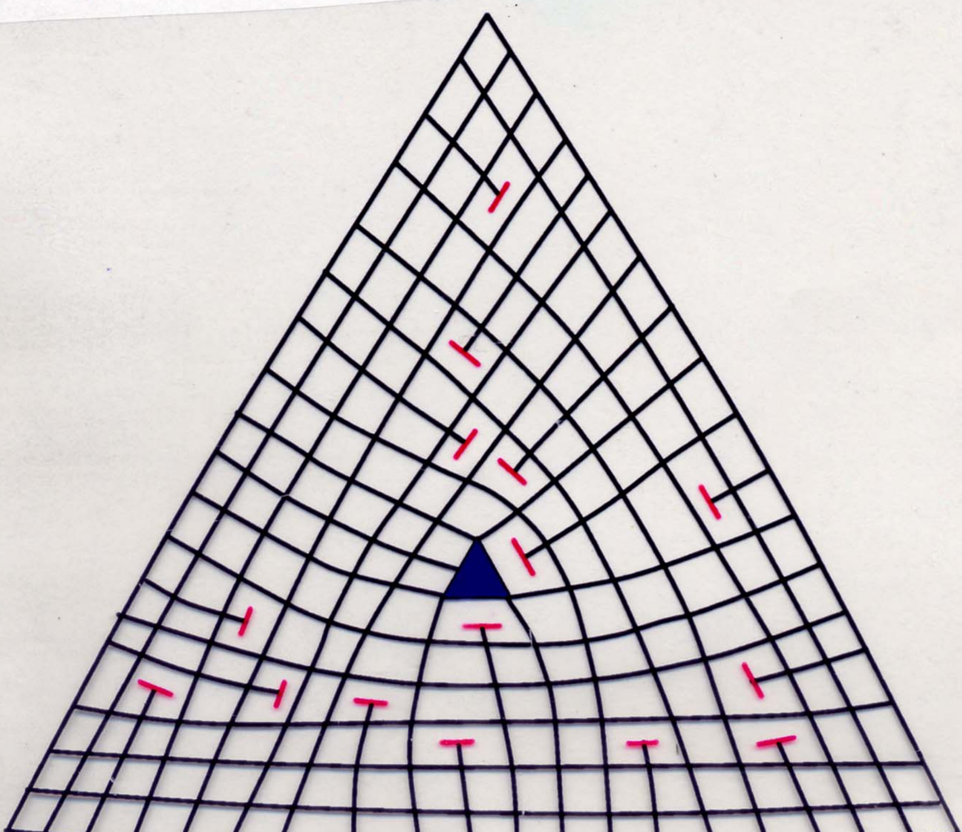
Colloids on Water Droplets . . .

SCREENING OF DISCLINATIONS BY A DISLOCATION CLOUD

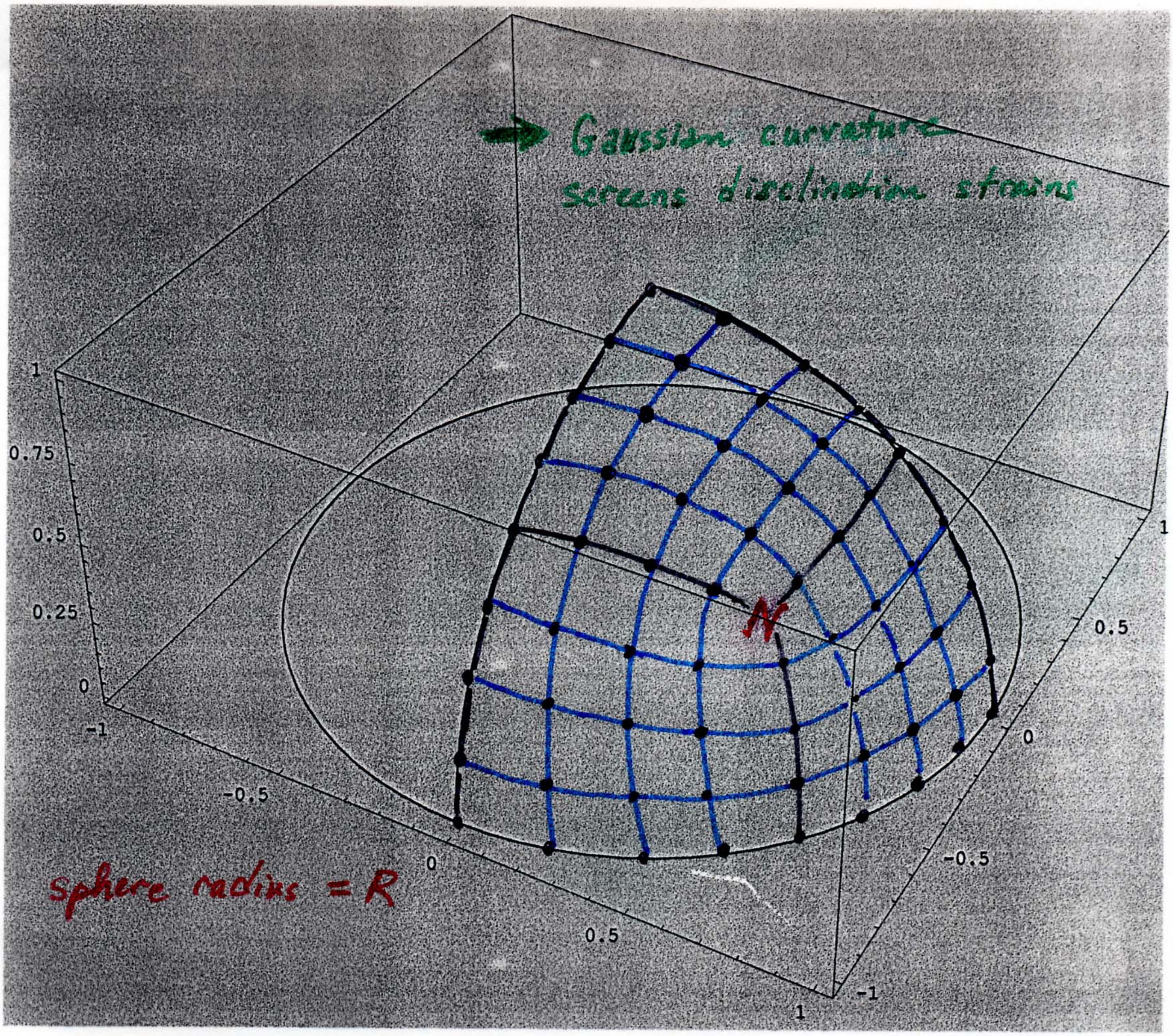
(flat space)



$$E_{TOT} = \frac{4\mu(\mu+\lambda)}{2\mu+\lambda}\,\frac{s^2}{32\pi}\,R^2 \qquad\qquad E_{TOT} \approx 5 \times \left(\frac{R}{d}\right) E_c$$

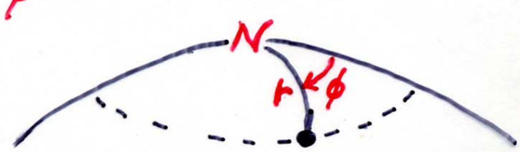


SCREENING : DISCLINATION IN a SQUARE LATTICE ON a SPHERE ...



→ Use spherical polar coordinates about the "north pole" N

$$d^2s = d^2r + R^2 \sin^2\left(\frac{r}{R}\right) d^2\phi$$



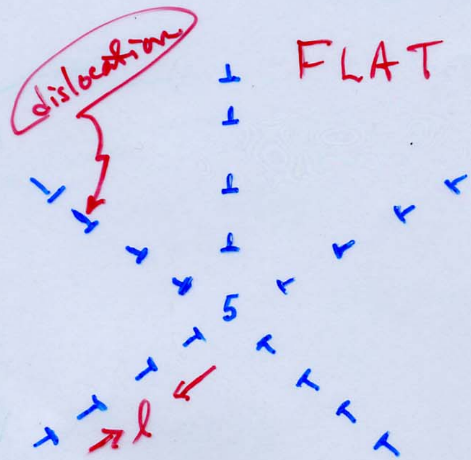
Effective disclination charge at radial distance r :

$$s_{eff}(r) = s - \int_0^{2\pi} d\phi \int_0^r R \sin\left(\frac{r'}{R}\right) dr' K$$

$$\boxed{s_{eff}(r) = \frac{\pi}{3} - 4\pi \sin^2\left(\frac{r}{2R}\right)}$$

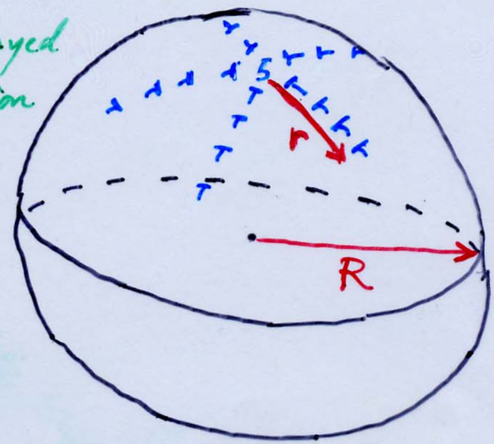
$\left(s_{eff} = 0 \text{ for } \frac{r}{R} = \frac{r_c}{R} = \cos^{-1}\left(\frac{5}{6}\right) \doteq 0.59 \right)$

FLAT



CURVED

Assume m grain boundaries arrayed around disclination with $s = 2\pi/6 \ldots$



$$l = \frac{m a_0}{s}$$

$$l(r) = \frac{m a_0}{s_{eff}(r)}$$

$$r_c = \cos^{-1}\frac{5}{6}$$

$$\boxed{n_d \equiv \frac{1}{l} = \frac{s}{m a_0} = \text{constant.}}$$

$$n_d(r) \equiv \frac{1}{l} = \frac{s_{eff}(r)}{m a_0}$$

$$\boxed{n_d(r) = \frac{1}{m a_0}\left[\frac{\pi}{3} - 4\pi \sin^2\left(\frac{r}{2R}\right)\right]}$$

$\Longrightarrow$ Grain boundary eventually terminates on a sphere!!

DEFECT INTERACTIONS & GAUSSIAN CURVATURE

$$\boxed{E = K_0 \int d^2\vec{x}\sqrt{g(\vec{x})}\int d^2\vec{y}\sqrt{g(\vec{y})}\left[K(\vec{x}) - s(\vec{x})\right]\frac{1}{\Delta^2}\bigg|_{\vec{x},\vec{y}}\left[K(\vec{y}) - s(\vec{y})\right] + N_d E_{core}}$$

with $K_0 = \dfrac{4\mu(\mu+\lambda)}{2\mu+\lambda}$, $K(\vec{x}) =$ Gaussian curvature $= \dfrac{1}{R_1 R_2}$, $E_{core} =$ core energy

$$\boxed{s(\vec{x}) = \frac{1}{\sqrt{g(\vec{x})}}\sum_{j=1}^{N_d} s_j\,\delta(\vec{x}-\vec{x}_j) = \text{distribution of disclination charge}}$$

$s_j = \pm\pi/3$

$g(\vec{x}) = \det g_{ij}(\vec{x})$, $g_{ij}(\vec{x}) =$ metric tensor

Specialize to the sphere: $\vec{x} \equiv (\theta, \phi)$

$$\int d^2\vec{x}\,\sqrt{g(\vec{x})} \rightarrow R^2\int_0^{\pi}\sin\theta\,d\theta\int_0^{2\pi}d\phi$$

$$\boxed{\frac{1}{\Delta^2}\bigg|_{\vec{x},\vec{y}} = \sum_{l=1}^{\infty}\sum_{m=-l}^{l}\frac{Y_{lm}(\theta_a,\phi_a)\,Y^*_{lm}(\theta_b,\phi_b)}{l^2(l+1)^2}}$$

$\Rightarrow$ $l=0$ mode must vanish: $R^2\displaystyle\int_0^{\pi}\sin\theta\,d\theta\int_0^{2\pi}d\phi\left[\overset{1/R^2}{K} - s(\theta,\phi)\right] \equiv 0!$

$$4\pi = \frac{\pi}{3}(N_5 - N_7) \Rightarrow \boxed{N_5 - N_7 = 12}$$

Interacting Disclinations on a Sphere

* Consider $N = N_5 + N_7$ disclination "charges"

$$N_5 - N_7 = 12$$

$$E(K_0)=\frac{\pi \cancel{K}_0}{36}R^2\sum_{i=1}^{N}\sum_{j=1}^{N} q_i q_j \chi(\theta^i,\phi^i;\theta^j,\phi^j)+NE_{core}. \qquad Y_0 = \frac{4\mu(\mu+\lambda)}{2\mu+\lambda}$$

where . . .

$$\chi(\theta^a,\phi^a;\theta^b,\phi^b)\equiv\chi(\beta)=R^2\sum_{l=1}^{\infty}\frac{2l+1}{l^2(l+1)^2}P_l(\cos\beta) = R^2\left(1+\int_0^{(1-\cos\beta)/2} dz\,\frac{\ln z}{1-z}\right)$$

β = geodesic distance between (θ^a, ϕ^a) & (θ^b, ϕ^b):

$$\cos\beta = \cos\theta^a \cos\theta^b + \sin\theta^a \sin\theta^b \cos(\phi^a-\phi^b)$$

$$\chi(\beta) \underset{\beta \ll 1}{\approx} R^2\left(1 + \tfrac{1}{4}\beta^2 \ln\beta\right)$$

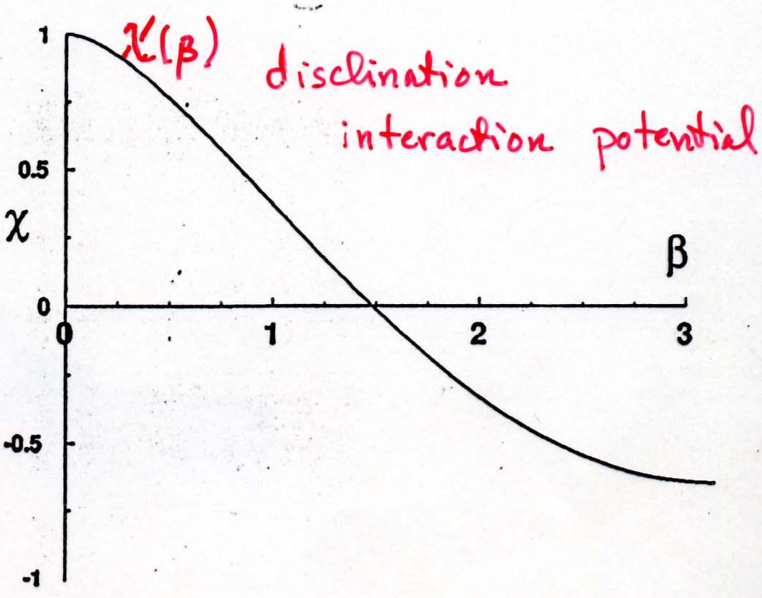


FIG. 2. Plot of χ/R^2 as a function of the geodesic angle β. Only the interval $\beta\in[0,\pi]$ is plotted.

* Icosadeltahedral Ground State Energy
(12 disclinations at the vertices of an icosahedron)

$$E = 0.604\left(\frac{\pi Y_0}{36}R^2\right) + 12\,E_{core}$$

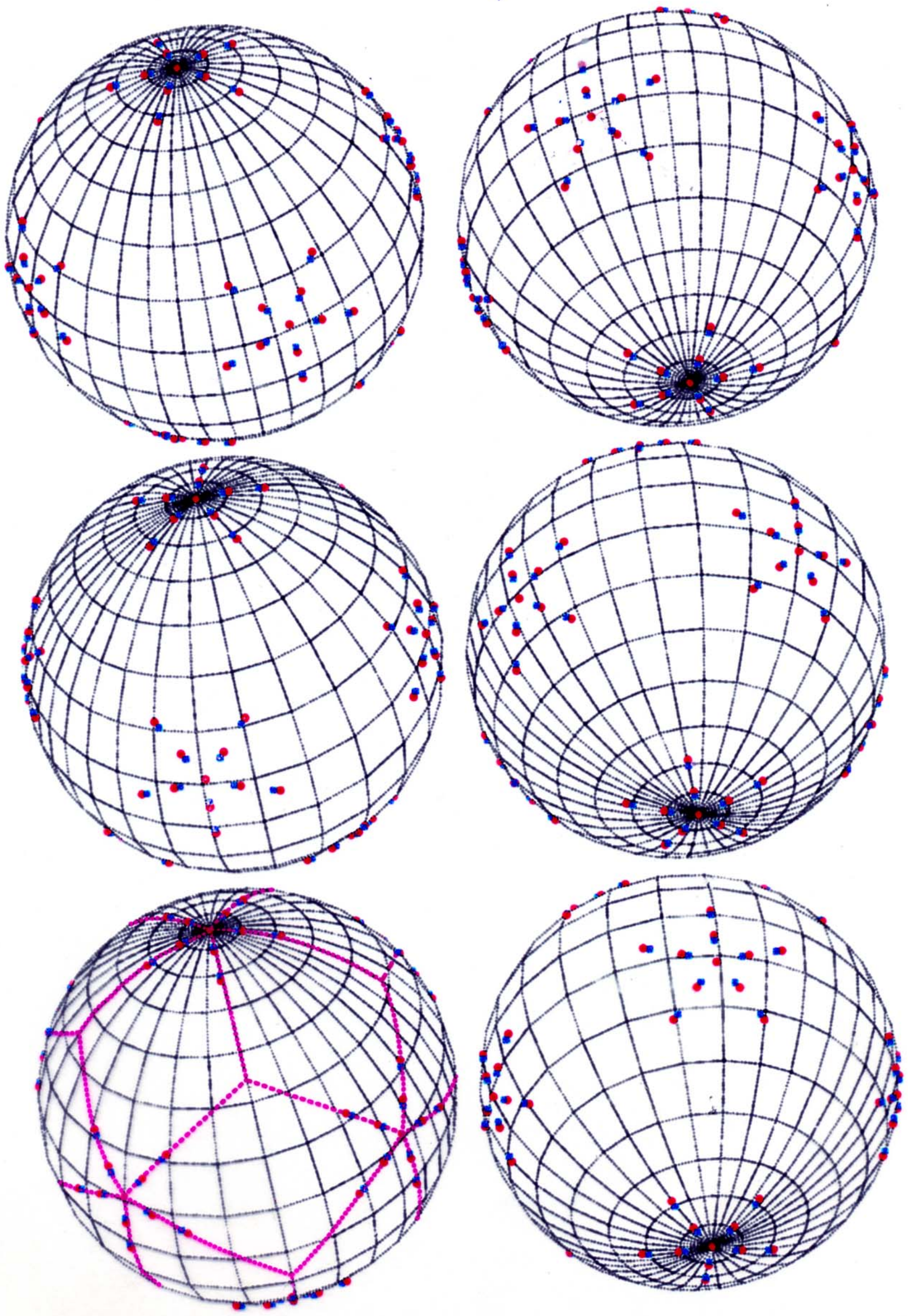
GROUND STATE WITH GRAIN BOUNDARIES

$$E = \underset{\sim}{0.170}\left(\frac{\pi K_0}{36}R^2\right) + 252\,E_{core} < \underset{\sim}{0.604}\left(\frac{\pi K_0}{36}R^2\right) + 12\,E_{core}$$

result for icosadeltahedron

132 5-fold disclinations

120 7-fold disclinations



• = 5

• = 7

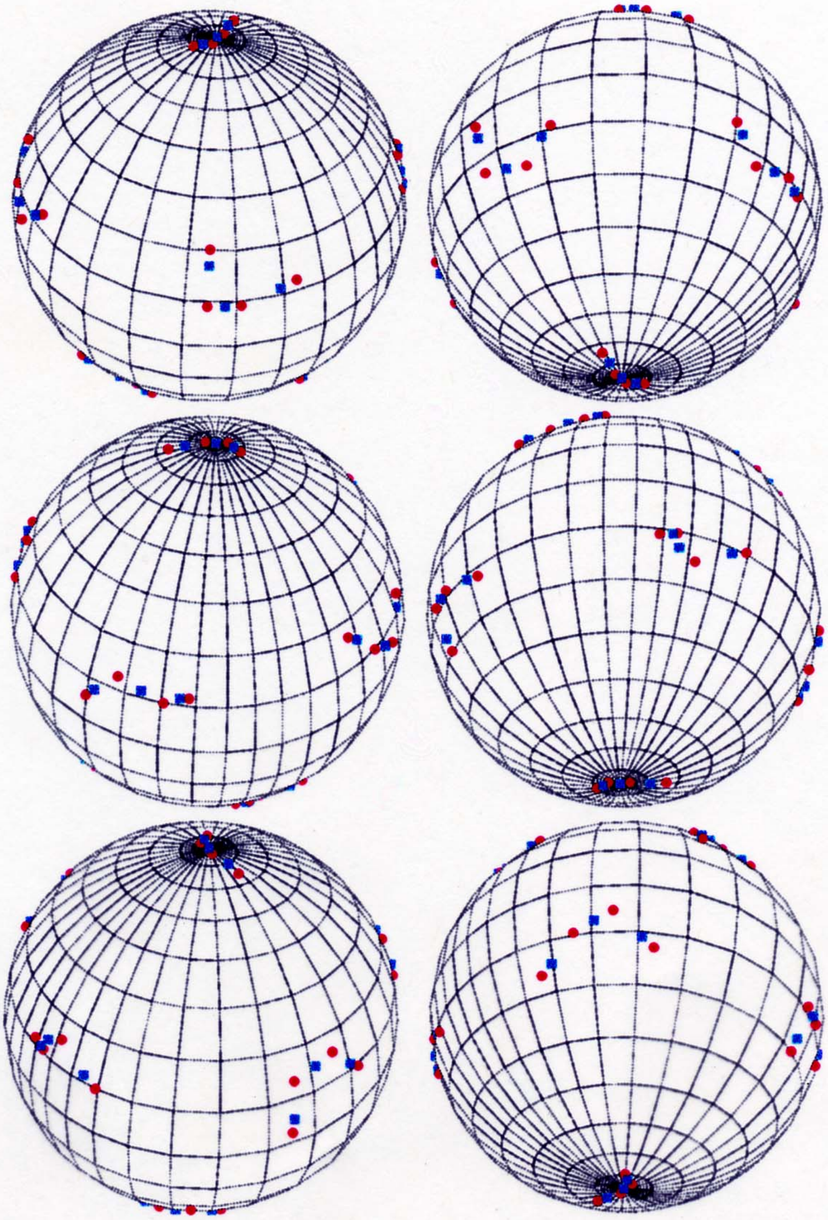
• = dislocation

252 defects . .

[Ground STATE for $N \sim 23{,}000$ particles!

$N_c \approx 400$ (icosadeltahedral ground state unstable for $N \gtrsim N_c$)

LINEAR grain boundaries are also possible in the ground state . . .



48 5-fold disclinations

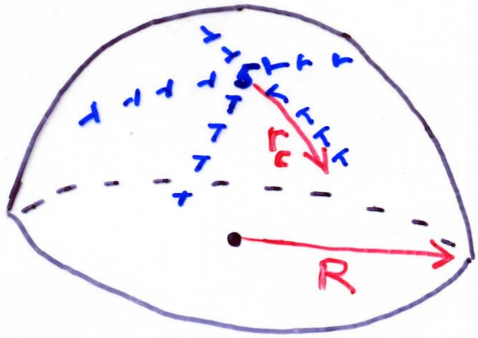
36 7-fold disclinations

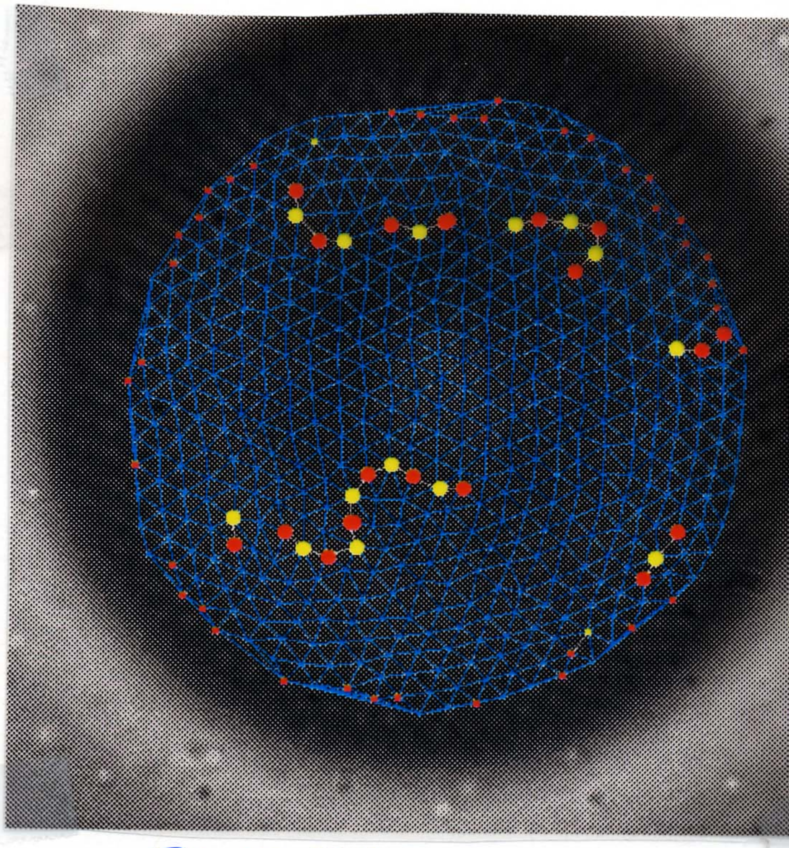
84 DEFECTS . . .

[GROUND STATE FOR $N \approx 16{,}000$ PARTICLES]

$N_c \approx 400$, $\left(\frac{R}{a}\right)_c \approx 5\text{-}6$

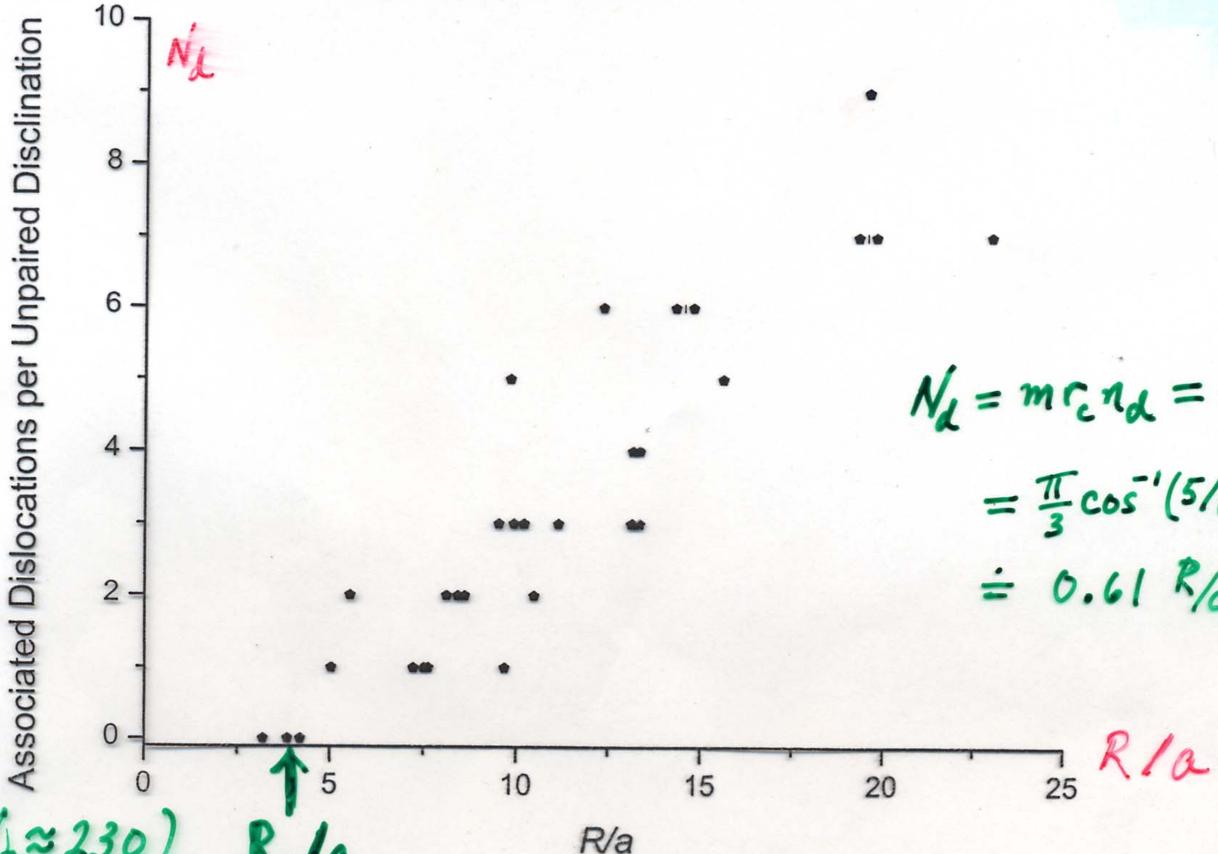
Defect Constellations for 30 different colloid coated droplets . . . (Ming Hsu & Andreas Bausch)





$R/a \simeq 15.6$

Defect Screening as a Function of *R/a*

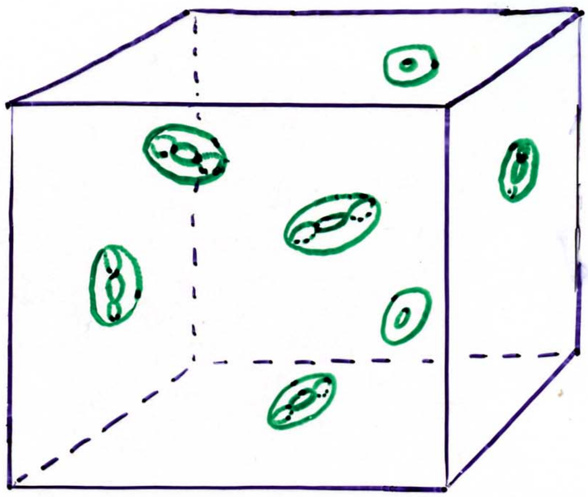


$$N_d = m r_c n_d = m r_c \left(\frac{2\pi}{6ma}\right)$$
$$= \frac{\pi}{3}\cos^{-1}(5/6)\,(R/a)$$
$$\doteq 0.61\, R/a$$

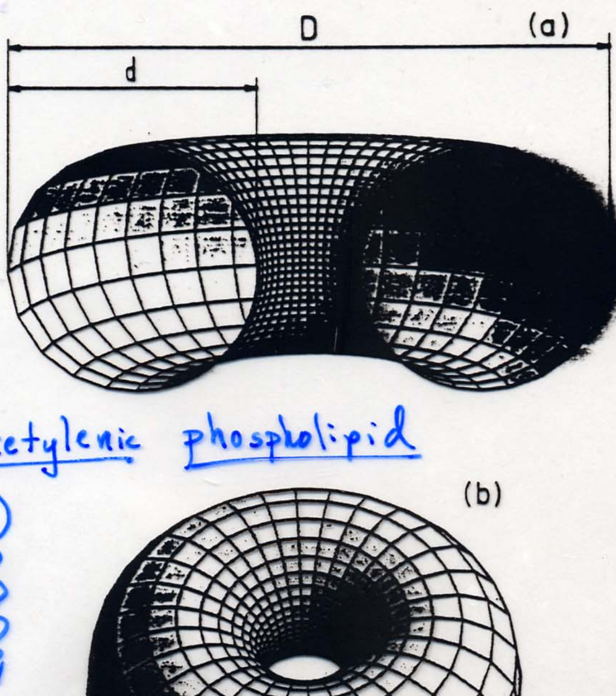
$(N_c \approx 230)$ R_c/a

Try: **TOROIDAL VESICLES!**

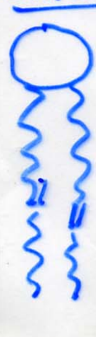
Euler: $E - V + N = 0 \Rightarrow N_5 = N_7$



M. Mutz & D. Bensimon, Phys. Rev. A $\underline{43}$, 4525 (1991)



diacetylenic phospholipid



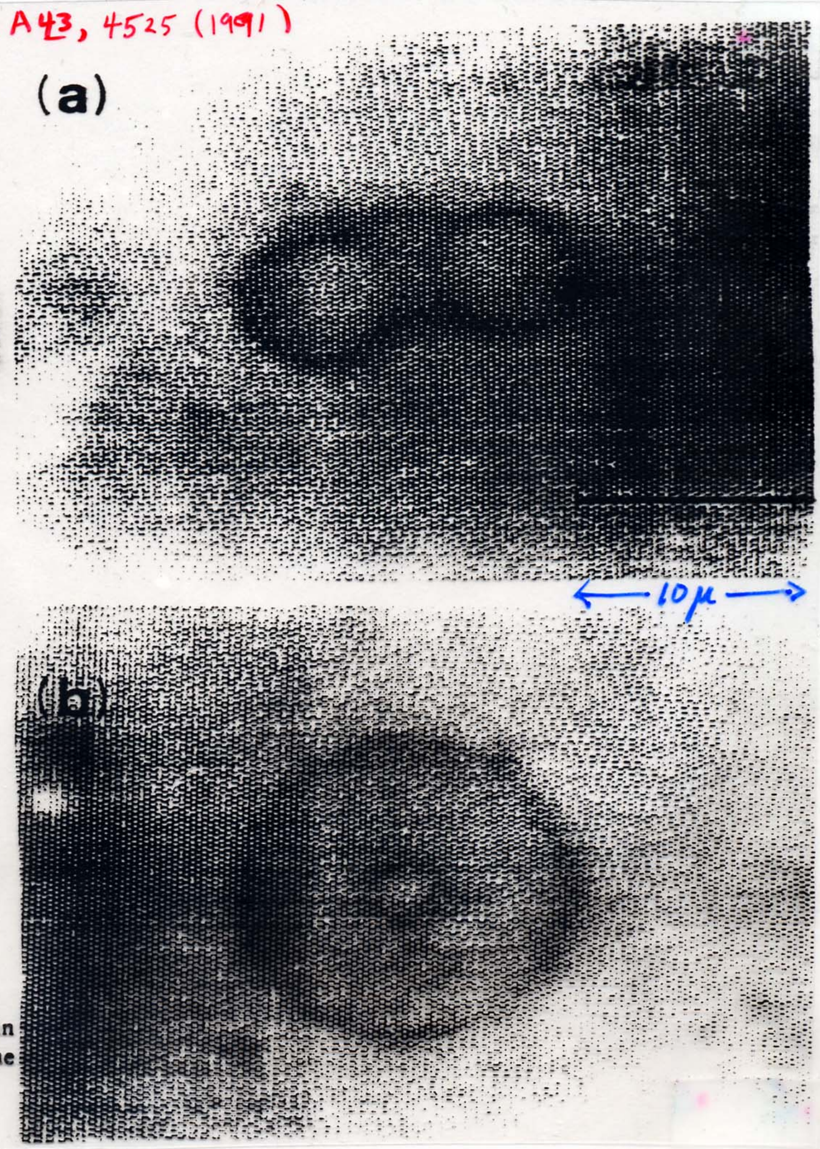
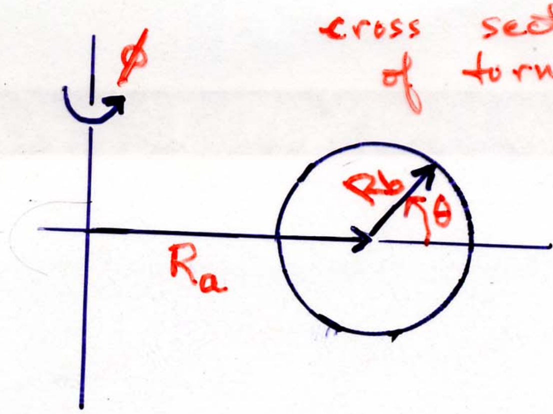
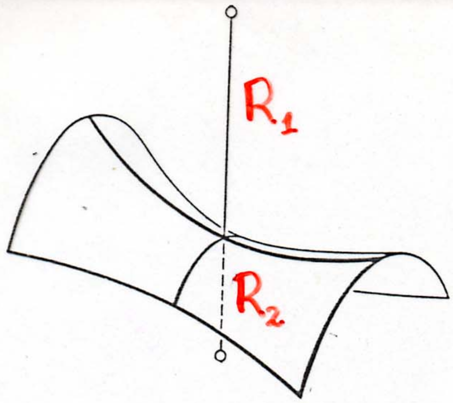


FIG. 1. Two views of a ring vesicle with generating radii in the ratio $1/\sqrt{2}$. D represents the outer diameter and d the width of the ring.

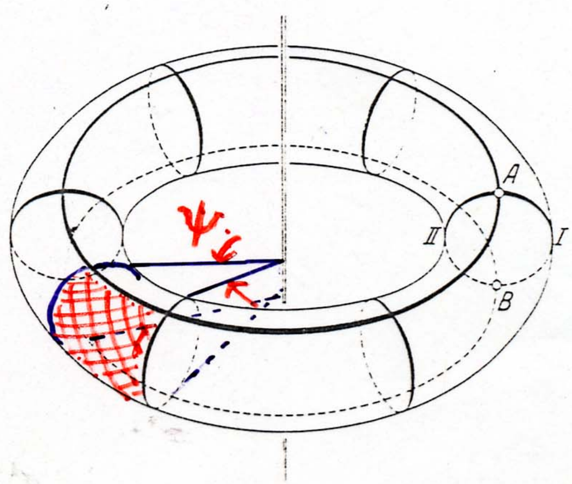
DISCLINATIONS ON A TORUS

cross section of torus





Integrate Gaussian Curvature:



$$K_G(\theta,\phi) = \frac{1}{R_1 R_2} = \frac{1}{R_a R_b}\,\frac{\cos\theta}{1 + \frac{R_b}{R_a}\cos\theta}$$

Set $\displaystyle\int_0^{\psi} d\phi \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} d\theta\,\sqrt{g}\,K_G(\theta,\phi) \equiv \frac{2\pi}{6} = 60^\circ$

$$\sqrt{g} = 1 + \frac{R_b}{R_a}\cos\theta$$

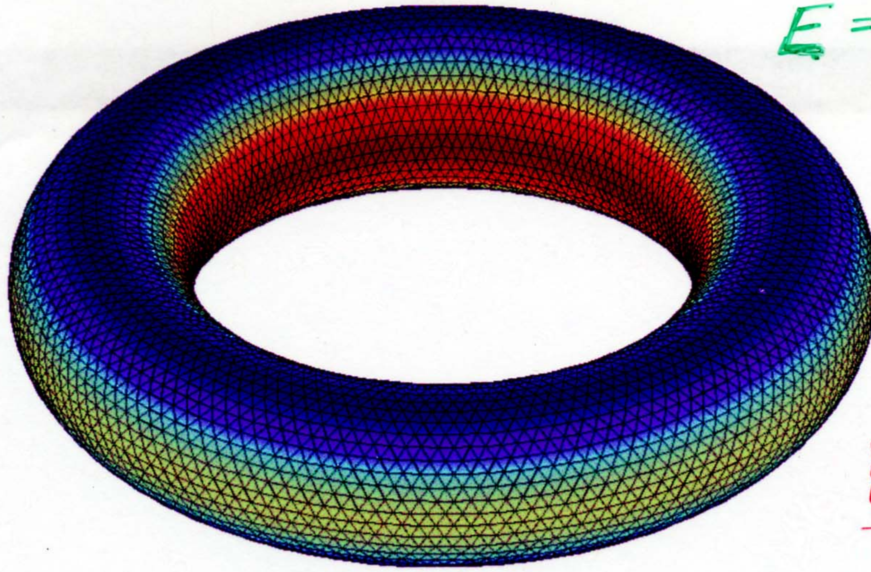
$\Rightarrow$ $\psi = 30^\circ$ $\Rightarrow$ $\dfrac{360^\circ}{30^\circ} = 12$ 5-fold disclinations on outer rim of torus!

* Euler's Theorem (or Gauss-Bonnet Thm) $\Rightarrow$ 12 7-fold disclinations on inner rim of torus

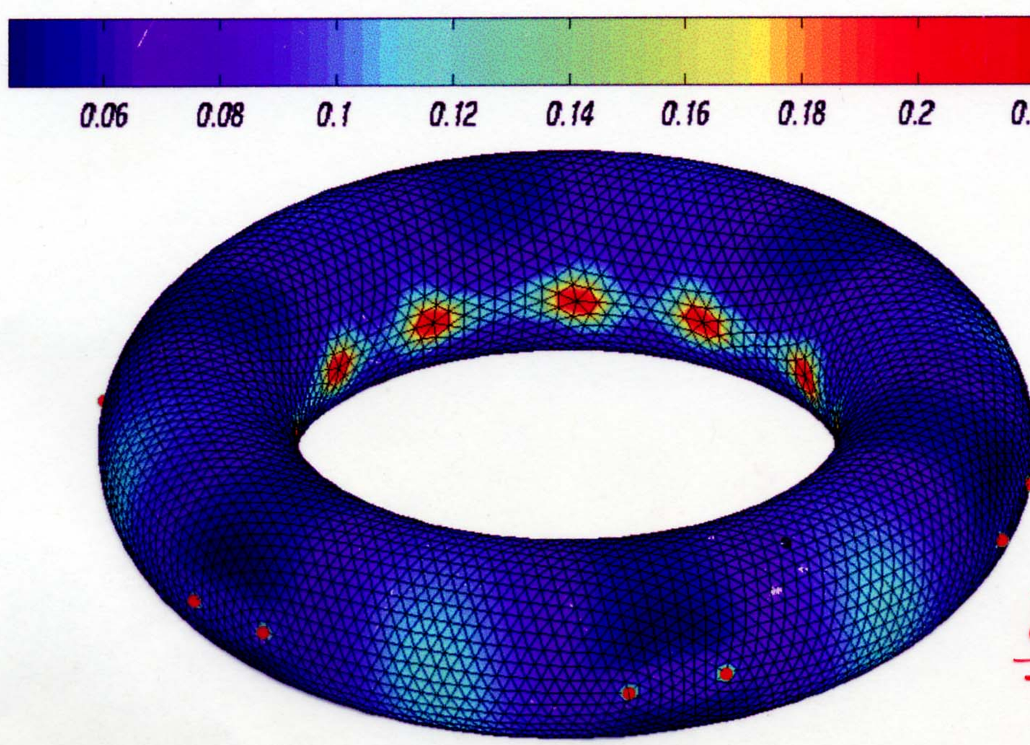
TRIANGULAR LATTICE ON A TORUS

$$E = \frac{\varepsilon}{2}\sum_{a,b}\left(|\vec{r}_a-\vec{r}_b|-a\right)^2$$

Defect-free



$E = 187.87\ \varepsilon a^2$



12 fives

&

12 sevens

$E = 71.87\ \varepsilon a^2$

Figure 1: Elastic energy of the Regular triangulation vs ($q = 8, l = 8, p = 20$) defected one. $N_{tri} = 12480$, $N_E = 18720$ and $N_V = 6240$, $R_1 = 23.652$ and $R_2 = 6.3662$ ($\alpha = 1$, $\beta = 1.1$).