**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**
  2. Icosahedral Packings in Viral Shells
  3. Disclination buckling
  4. Multi-electron bubbles -- an experimental realization of the Thomson problem

- **Continuum elastic treatment of defects and icosahedral ground states**
  - Euler's Theorem \( \Rightarrow N_5 - N_7 = 12 \)

- **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 Travesset & Mark Bowick
- Jack Lيدmar

**Related work**
- Alar Toomre (unpublished)
- M. Dodgson, M. Moore, A. Pérez-Garrido
**Motivation:**

* SV40, Polyomavirus

- 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 B and B' 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:
Dense-Packed Arrays

Two Dimensions:

- maximize density via equilateral triangles

Ground state of a 2d crystal

[Diagram of a hexagon formed by six triangles leading to a triangular lattice]
NUCLEATION AND GROWTH ON A SPHERE

\( a = \text{particle diameter} \)
\( R = \text{radius of sphere} \)

polar projection about north pole

\( \frac{R}{a} = 10, N \approx 1314 \text{ particle} \), M. Rubinstein

5 = five near neighbors
7 = seven near neighbors

\( N_5 - N_7 = 12 \)

\( N_0 M = 1314 \)
\( \text{DIAM}=0.1000 \)
South Polar Projection...

\[ \frac{R}{a} = 10, \quad N \approx 1400 \]

\[ N_5 - N_7 = 12, \text{ exactly!} \]
What is the ground state of many identical particles interacting on the surface of a sphere? $\frac{R}{a} \gg 1$

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

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

Monte Carlo simulations with

$$\frac{e^2}{k_B T} \equiv \text{Gamma} = 140 \ldots .$$

2048 particles.

Defect distribution in ground state?
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, P.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. 

"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:** Multi-electron bubbles in He$^4$


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**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.

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\[ \varepsilon(R) = 4 \pi R^2 \rho_0 + \frac{Z(Z-1) e^2}{2 \varepsilon R} \]

\[ R = \left( \frac{Z^2 e^2}{16 \pi \varepsilon_0 \varepsilon} \right)^{\frac{1}{3}} \]

\[ R \approx 10 - 100 \text{ \mu m} \]

\[ Z \approx 10^5 - 10^7 \text{ electrons}! \]

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

\[ \frac{R}{a} >> 1 \]
Motivation:

Colloidosomes

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
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 ($\alpha$, $\alpha'$, $\alpha''$) form a threefold interaction, the subunits labeled $\beta$ and $\beta'$ form one sort of twofold interaction, and the $\gamma$ subunits form another kind of twofold interaction across an icosahedral twofold axis. (Adapted from Salunke et al., 1986.)
Ground states for moderate $N \sim (R/a)^2$: Icosahedra

Euler's Thm: $F - E + \mathcal{V} = 2 \Rightarrow \sum_j (6 - x_j) = 12$

$Icosahedron$:

$F = 20$
$E = 30$
$\mathcal{V} = 12$
$(p, q) = (1, 0)$

"Magic" Numbers:

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

$(1, 1), N = 32$
$(2, 1), N = 72$
$(3, 1), N = 132$

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

$(14, 14), N = 5882$
Figure 1. Baker, Olson and Fuller - right page
Reproduced at 100% final size
Figure 1 Baker, Olson and Fuller - left page
Reproduced at 100% final size

(4,0) N = 162
(5,0) N = 252
(2,0) N = 42
Self-assembly of icosahedral bilayers

Museum piece
PCR identifies ‘Irish famine’ pathogen
X-ray astronomy
Polarimetry sees the light
Potassium channels’ Mechanism of inactivation

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

See also: Blaurock/Gamble faceted lecithin vesicles... E. Sackmann et al. ....
DEFECTS IN MONOLAYERS = flat space

disclinations

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

\[ Y_0 = \frac{4\mu (\mu + \lambda)}{2\mu + \lambda} = 4\mu \]

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

\[ E = \frac{Y_0 s^2}{R^2} \frac{R^2}{32\pi} \]

\[ S = \pm \frac{2\pi}{6} = \pm 60^\circ \]

\[ \text{"} + 1 \text{"} \]

\[ \text{"} - 1 \text{"} \]
\[ E = \sum_{\langle ij \rangle} V(|\mathbf{r}_i - \mathbf{r}_j|) - \kappa \sum_{\langle \alpha \beta \rangle} \mathbf{n}_\alpha \cdot \mathbf{n}_\beta \]

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

\[ Y_0 = \text{Young's Modulus} = \frac{2\sqrt{3}}{3} \varepsilon \]

\[ s = \frac{2\pi}{6} \]

The buckling radius is given by:

\[ R_b \approx \frac{R^2}{\kappa} \approx 160 \]

"von Karman number"

Before buckling:

\[ E(R) \approx Y_0 \left( \frac{2\pi}{6} \right)^2 R^2, \quad R < R_b \]

After buckling:

\[ E(R) \approx \text{const.} \times \kappa \ln \left( \frac{R}{a} \right), \quad R > R_b \]
Virus Buckling
(Jack Lidmar)

Buckling Transition

\[ r_c \propto R \left( \frac{h}{R} \right)^{\frac{1}{3}} \]

"ridge scaling"

Lobkovsky, Witten, et al.
Buckling Transition on a Sphere: Spherical Harmonic Expansion

**Expand radial coord.**

\[ R(\theta, \phi) = \sum_{l} \sum_{m=-l}^{l} Q_{lm} Y_{lm}(\theta, \phi) \]

\[ T = P^2 + PQ + Q^2 \]

\[ N = 10T + 2 \]

\[ l = 0, 6, 10, 12, 16, 18, \ldots \]

for icosahedral symmetry

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

**Test of Ridge Scaling**

\[ H_R = \frac{R}{r_c} = \left( \frac{R}{h} \right)^{1/3} \]

\[ \alpha \left( YR^3/k \right)^{1/6} \]

\[ r_c \]

\[ H_R \text{ (at midpoint of ridges)} \]

\[ YR^3/k \]

\[ \text{slope} = 1/6 \]
COLLOIDS ON WATER DROPLETS...

SCREENING OF DISCLINATIONS
BY A DISLOCATION CLOUD

(flattened space)

\[
E_{\text{tot}} = \frac{4\mu(\mu+\lambda)}{2\mu+\lambda} \frac{s^2}{32\theta} R^2
\]

\[
E_{\text{tot}} \approx 5 \times \left( \frac{R}{d} \right) E_c
\]
SCREENING: DISCLINATION IN A SQUARE LATTICE ON A SPHERE ...

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

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

Effective disclination charge at radial distance r:

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

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

$$s_{\text{eff}} = 0 \text{ for } \frac{r}{R} = \frac{a}{R} = \cos\left(\frac{\pi}{6}\right) = 0.5$$
Assume $m$ grain boundaries arrayed around dislocation with $s = 2\pi l$...

\[ n_d = \frac{1}{l} = \frac{s}{ma_0} = \text{constant.} \]

\[ n_d(r) = \frac{1}{l} = \frac{Seff(r)}{ma_0} \]

\[ n_d(r) = \frac{1}{ma_0} \left[ \frac{\pi}{3} - 4\pi \sin^2 \left( \frac{r}{2R} \right) \right] \]

\[ l(r) = \frac{ma_0}{Seff(r)} \]

\[ \gamma_c = \cos \frac{\gamma}{2} \]

\[ \Rightarrow \text{Grain boundary eventually terminates on a sphere} \]
\[
E = K_0 \int d^2 x \sqrt{g(x)} \int d^2 y \sqrt{g(y)} \left[ K(x) - s(x) \right] \frac{1}{\Delta^2} \left[ K(y) - s(y) \right] + N_4 E_{\text{core}}
\]

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

\[
s(x) = \frac{1}{\sqrt{g(x)}} \sum_{j=1}^{N_4} s_j \delta(x - \tilde{x}_j) = \text{distribution of disclination charge}
\]

\[
g(x) = \det g_{ij}(x), \quad g_{ij}(x) = \text{metric tensor}
\]

Specialize to the sphere:

\[
\tilde{x} = (\theta, \phi)
\]

\[
\int d^2 \tilde{x} \sqrt{g(\tilde{x})} \Rightarrow R^2 \int_0^\pi \sin \theta \, d\theta \int_0^{2\pi} d\phi
\]

\[
\frac{1}{\Delta^2} = \sum_{k=1}^{\infty} \sum_{m=-k}^{k} \frac{Y_{km}(\theta_0, \phi_0) Y_{km}^*(\theta_1, \phi_1)}{l^2 (l+1)^2}
\]

\[
4\pi = \frac{\pi}{3} (N_5 - N_7) \Rightarrow \quad N_5 - N_7 = 12
\]

\[
\Rightarrow l = 0 \text{ mode must vanish:} \quad R^2 \int_0^\pi \sin \theta \, d\theta \int_0^{2\pi} d\phi \left[ K - s(\theta, \phi) \right] = 0
\]
Consider $N = N_5 + N_7$ disclination "charges"

$$N_5 - N_7 = 12$$

$$E(K_0) = \frac{1}{36} R^2 \sum_{i=1}^{N} \sum_{j=1}^{N} q_i q_j \chi(\theta^i, \phi^i; \theta^j, \phi^j) + N E_{\text{core}}.$$

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

Where $\ldots$

$$\chi(\beta) = \text{disclination interaction potential}$$

$$\beta = \text{geodesic distance between} \ (\theta^a, \phi^a) \ \text{and} \ (\theta^b, \phi^b):$$

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

$$\chi(\beta) = R^2 (1 + \frac{1}{4} \beta^2 \ln \beta) \quad \beta \ll 1$$

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

* Icosahedral Ground State Energy

(12 disclinations at the vertices of an icosahedron)

$$E = 0.604 \left( \frac{N \chi_0 R^2}{36} \right) + 12 E_{\text{core}}$$
Ground state with grain boundaries

\[ E = 0.17 \left( \frac{\pi K_0 R^2}{36} \right) + 252 E_{\text{core}} < 0.604 \left( \frac{\pi K_0 R^2}{36} \right) + 12 E_{\text{core}} \]

Result for icosadeltahedron

132 5-fold disclinations
120 7-fold disclinations

252 defects

\[ \text{Ground state for } N \approx 23,000 \text{ particles!} \]
\[ N_c \approx 400 \] (state unstable for \( N \geq N_c \))
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]

$N_c = 400$, $(R/a)_c \approx 5-6$
Defect Constellations for 3D different colloid coated droplets...
(Ming Hsu & Andreas Bausch)

\[ R/a \approx 15.6 \]

Defect Screening as a Function of \( R/a \)

\[ N_d = m_c n a = m_c \left( \frac{2\pi}{6ma} \right) \]

\[ = \frac{\pi}{3} \cos^{-1}(5/6) \left( \frac{R}{a} \right) \]

\[ \approx 0.61 \frac{R}{a} \]

\[ (N_c \approx 230) \quad R_c/a \]
$\text{Euler: } E - V + N = 0 \implies N_5 = N_7$


**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.
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:

\[ \int_0^\frac{\pi}{2} d\phi \int_0^\frac{\pi}{2} d\theta \sqrt{g'} K_G(\theta, \phi) = \frac{2\pi}{6} \]

\[ = 60^\circ \]

\[ \sqrt{g'} = 1 + \frac{R_b}{R_a} \cos \theta \]

\[ \Rightarrow \psi = 30^\circ \Rightarrow \frac{360^\circ}{30^\circ} = 12 \text{ 5-fold disclinations on outer rim of torus!} \]

* Euler's Theorem \( \Rightarrow \) 12 7-fold disclinations (or Gauss-Bond Thm) on inner rim of torus
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 $R_2 = 6.3662$ ($\alpha = 1$, $\beta = 1.1$).