# PURE AND APPLIED MATHEMATICS EIGHTSQUAREDCON 2013

Nicholas Jackson

Easter 2013

Nicholas Jackson Pure and Applied Mathematics

## PURE VS APPLIED





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Mathematics, with its three-foot-long equations trying to describe the movement of water down a bath plug, as a grovelling and unwieldy subject getting dangerously close to engineering. The aim of pure mathematics is to get beautiful results on paper by ignoring real life; the shorter and more compact the result, the better. Hence, pure mathematicians tend to look down on Applied Mathematics, with its three-foot-long equations trying to describe the movement of water down a bath plug, as a grovelling and unwieldy subject getting dangerously close to engineering.

[Applied mathematics] aims to produce models describing how things work and by trying to describe systems more and more accurately gets longer and longer equations so that they frequently spill over several pages. Applied mathematicians look down on pure mathematicians as ivory tower dreamers. The aim of pure mathematics is to get beautiful results on paper by ignoring real life; the shorter and more compact the result, the better. Hence, pure mathematicians tend to look down on Applied Mathematics, with its three-foot-long equations trying to describe the movement of water down a bath plug, as a grovelling and unwieldy subject getting dangerously close to engineering.

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- Robert Ainsley, The Bluffer's Guide to Maths (1988)

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If useful knowledge is, as we agreed provisionally to say, knowledge which is likely, now or in the comparatively near future, to contribute to the material comfort of mankind, so that mere intellectual satisfaction is irrelevant, then the great bulk of higher mathematics is useless. Modern geometry and algebra, the theory of numbers, the theory of aggregates and functions, relativity, quantum mechanics no one of them stands the test better than another, and there is no real mathematician whose life can be justified on this ground. If this be the test. then Abel, Riemann, and Poincaré wasted their lives; their contribution to human comfort was negligible, and the world would have been as happy a place without them.

– G H Hardy, A Mathematician's Apology (1940)

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### NO APOLOGY NECESSARY



G H Hardy (1877–1947)

- Graduate and Fellow of Trinity College, Cambridge (fourth Wrangler 1898), elected FRS in 1910
- Savilian Professor of Geometry, Oxford (1919–1931)
- Sadleirian Professor of Mathematics, Cambridge (1931–1944)
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But...

- Group theory: molecular chemistry, particle physics
- Geometry: CAD, computer graphics
- Number theory: cryptography
- Relativity: GPS
- Quantum mechanics: lasers, microelectronics, MRI scanners

#### KNOTS IN THE ÆTHER



- Sir William Thomson OM GCVO PC PRS, Lord Kelvin (1824–1907) proposes that atoms are knots in the field lines of the luminiferous æther.
- Theory killed by Michelson–Morley experiment (1887) that disproves existence of the æther.
- But sparks off study and classification of knots as a mathematical problem in its own right.



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- Discovered in 1869 by Friedrich Miescher (1844-1895)
- Crystal structure determined by Francis Crick (1916–2004), James Watson, Rosalind Franklin (1920–1958) and others.



- Double helix structure: two strands of alternating sugar and phosphate groups.
- Each sugar molecule has one of four bases attached:



- Average of about 10.5 base pairs per full twist.
- More twisting induces supercoiling:





• With closed loops of DNA, too:





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Meanwhile, in knot theory... A knot is an embedded circle in 3–space. A link is an embedding of more than one circle in 3–space.





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The linking number measures how linked two components are:



#### LINKING NUMBER

Each crossing in an oriented link is positive or negative:



Let  $K_1$  and  $K_2$  be two components of a link L. Then

$$\mathsf{lk}(K_1, K_2) = \mathsf{lk}(K_2, K_1) = \frac{1}{2} \sum_{\text{crossings } c} \mathsf{sign}(c)$$

involving  $K_1, K_2$ 

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So, for



we have  $lk(red, blue) = \frac{1}{2} \times 6 = 3$ .

### LINKING NUMBER

For the Whitehead link



#### lk(red, blue) = 0.

For the Borromean rings



lk(red, blue) = lk(blue, green) = lk(red, green) = 0.

- A class of enzymes that change the linking number of DNA strands (and hence the twisting of the double helix).
- Break one strand, pass other strand through and reattach.
- Changes linking number by  $\pm 1$ .



- A related class of enzymes that knot and unknot DNA.
- Cut both strands, pass other strands through and reattach.
- Changes linking number by  $\pm 2$ .



• Type-II topoisomerase can lead to knotted DNA:



## $3_1$ (trefoil)

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- Can use techniques from knot theory to understand the action of topoisomerase and other enzymes.
- Ernst and Sumners (1995) applied Conway's tangle calculus to devise a model for the topology of Tn3 resolvase, one of a number of enzymes involved in site-specific recombination.

 The Jones polynomial V(K), Alexander polynomial Δ(K) and Kauffman bracket (K) can be defined recursively by skein relations:

$$\begin{aligned} (t^{1/2} - t^{-1/2})V(\Diamond \zeta) &= t^{-1}V(\leftthreetimes) - tV(\leftthreetimes) \\ (t^{1/2} - t^{-1/2})\Delta(\Diamond \zeta) &= \Delta(\leftthreetimes) - \Delta(\leftthreetimes) \\ & \bigotimes \rangle &= A(\leftthreetimes) + A^{-1}\langle \rangle \langle \rangle \end{aligned}$$

- Certain enzymes called recombinases act in a similar way when performing site-specific recombination.
- Tyrosine recombinases act like  $\succeq \longrightarrow$
- Serine recombinases act like  $\succsim \longrightarrow \leftthreetimes$  or  $\succsim \longrightarrow \leftthreetimes$

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What about simpler molecules?



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#### Schoenflies notation

Sn

- Ε Identity
- $\begin{array}{cc} C_n & n \text{fold rotation around an axis} \\ \sigma (\sigma_v, \sigma_h) & \text{Reflection in a plane} \end{array}$ 

  - *i* Inversion in a point
    - *n*-fold improper rotation around an axis



- Can use symmetry to understand charge distribution across a molecule.
- A molecule is polar if the bond polarities don't cancel each other out.
- A molecule with an inversion (*i*) symmetry can't be polar.
- A molecule with a  $C_n$  symmetry can't be polar except along that axis.
- A molecule with a  $\sigma_h$  symmetry can't be polar along that axis

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### Polarity



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Some molecules are chiral and have left-handed and right-handed forms (enantiomers):



L-(+)-lactic acid

D-(-)-lactic acid

A molecule can't be chiral if it has:

- improper rotational symmetry  $(S_n)$
- inversion symmetry (i)
- reflective symmetry ( $\sigma$ )

Together, all the symmetries of a molecule form its point group. Ammonia  $(NH_3)$  has six symmetries:

- identity *E*
- $\bullet$  clockwise and anticlockwise 120° rotations  $C_3^+$  and  $C_3^-$
- three reflections  $\sigma_{\rm v}^1,\,\sigma_{\rm v}^2$  and  $\sigma_{\rm v}^3$



$C_{3v}$	Ε	$C_v^+$	$C_v^-$	$\sigma_v^1$	$\sigma_v^2$	$\sigma_v^3$	
E	Ε	$C_v^+$	$C_v^-$	$\sigma_v^1$	$\sigma_v^2$	$\sigma_v^3$	
$C_v^+$	$C_v^+$	$C_v^-$	Ε	$\sigma_v^2$	$\sigma_v^3$	$\sigma_v^1$	
$C_v^-$	$C_v^-$	Ε	$C_v^+$	$\sigma_v^3$	$\sigma_v^1$	$\sigma_v^2$	
$\sigma_v^1$	$\sigma_v^1$	$\sigma_v^3$	$\sigma_v^2$	Ε	$C_v^-$	$C_v^+$	
$\sigma_v^2$	$\sigma_v^2$	$\sigma_v^1$	$\sigma_v^3$	$C_3^+$	Ε	$C_v^-$	
$\sigma_v^3$	$\sigma_v^3$	$\sigma_v^2$	$\sigma_v^1$	$C_3^{-}$	$C_v^+$	Ε	

Now use heavy mathematical machinery called representation theory

symmetry	$\longrightarrow$	matrix	$\xrightarrow{\text{trace}}$	character
E		$\left[\begin{smallmatrix}1&0\\0&1\end{smallmatrix}\right]$		2
$C_3^+$		$rac{1}{2} \left[ egin{array}{c} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{array}  ight]$		-1
$C_3^-$		$rac{1}{2} \left[ egin{array}{c} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{array}  ight]$		-1
$\sigma_v^1$		$\left[ \begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}  ight]$		0
$\sigma_v^2$		$\frac{1}{2} \left[ \begin{array}{c} -1 & -\sqrt{3} \\ -\sqrt{3} & 1 \end{array} \right]$		0
$\sigma_v^3$		$\frac{1}{2} \begin{bmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{bmatrix}$		0

Can use this information to calculate vibrational modes of molecular bonds, which tells us about spectroscopic behaviour.

• Physical state of a system represented by a state vector  $|\psi\rangle$  belonging to a Hilbert space *H*.

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• Heisenberg's uncertainty principle:

$$\sigma_{\mathsf{A}}\sigma_{\mathsf{B}} \geqslant \frac{1}{2} |\langle [\widehat{\mathsf{A}}, \widehat{\mathsf{B}}] \rangle|$$

where  $[\widehat{A}, \widehat{B}] = \widehat{A}\widehat{B} - \widehat{B}\widehat{A}$ .

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$$\sigma_x \sigma_p \geqslant \frac{1}{2} |\langle [\hat{x}, \hat{p}] \rangle| = \frac{\hbar}{2}$$

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- Measure relative to different axes via operators  $J_x$ ,  $J_y$  and  $J_z$ .
- These operators don't commute:

$$\begin{split} [J_x, J_y] &= J_x J_y - J_y J_x = J_z \\ [J_x, J_z] &= J_x J_z - J_z J_x = J_y \\ [J_y, J_z] &= J_y J_z - J_z J_y = J_x \end{split}$$

• This generates the Lie algebra  $\mathfrak{su}_2$  from which we can recover the Lie group  $SU_2$ 

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Wolfgang Pauli (1900–1958)

#### Pauli spin matrices

 Representation of the spin operators for spin-<sup>1</sup>/<sub>2</sub> particles (like electrons, protons, neutrons):

$$\sigma_{x} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$
$$\sigma_{y} = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$
$$\sigma_{z} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

• The fundamental representation of  $SU_2$ .

•  $m_p = 938 \text{MeV}, \ m_n = 939 \text{MeV}.$ 

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- Three-dimensional representation of  $SU_2$  leads to triplets: ( $\Sigma^-, \Sigma^0, \Sigma^+$ ), ( $\pi^-, \pi^0, \pi^+$ ) and ( $\rho^-, \rho^0, \rho^+$ )

#### QUARKS: STRANGENESS AND CHARM

- New particles discovered with property dubbed strangeness
- Murray Gell-Mann postulated that all of these particles are composed of two or three quarks: p = uud, n = udd, Ξ<sup>0</sup> = uss, Ξ<sup>-</sup> = dss, π<sup>+</sup> = ud̄, π<sup>0</sup> = 1/√2(uū + dd̄), ...

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- Used knowledge of representation theory to organise particles into *SU*<sub>3</sub> multiplets:





#### The Eightfold Way.

• Successfully predicted existence of  $\Omega^-$ .

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"If I have seen further than others, it is because I have been surrounded by dwarves." – Murray Gell-Mann (attributed) • The division between "pure" and "applied" mathematics is not as well-defined as I was told at A-level.

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- Group theory: abstract algebraic machinery originally devised in early 19th century to understand solutions of polynomial equations, effective at describing symmetry, can be used to predict chemical and physical properties of molecules.
- Representation theory of Lie groups: devised in late 19th and early 20th century to understand groups and algebras with continuous structure, is exactly what particle physicists needed to formulate and understand the Standard Model.