

Vibrational Quantisation of Skyrmions

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Topological Solitons, Nonperturbative Gauge Dynamics and Confinement 2

18-20 June 2019

Based on work with Will Grummitt

- 1 The Skyrme Model
- 2 Rigid Body Quantisation
- 3 Vibrational Quantisation
- 4 Oxygen-16
- 5 Summary and Outlook

The Skyrme Model

- The standard Skyrme Model is Lagrangian is

$$L = \int \left(-\frac{1}{2} \text{Tr}(R_\mu R^\mu) + \frac{1}{16} \text{Tr}([R_\mu, R_\nu][R^\mu, R^\nu]) + m^2 \text{Tr}(U - I_2) \right) d^3x,$$

where $R_\mu = (\partial_\mu U)U^\dagger$ and $U \in SU(2)$ is the Skyrmon field. We also include a pion mass term.

- We can write U in terms of pion fields as $U = \sigma + i\boldsymbol{\pi} \cdot \boldsymbol{\tau}$ where $\boldsymbol{\pi}$ is a triplet of pion fields, $\boldsymbol{\tau}$ are the Pauli matrices and σ is an additional scalar field.
- Since $U \in SU(2)$ the pion fields satisfy the constraint

$$\sigma^2 + \boldsymbol{\pi} \cdot \boldsymbol{\pi} = 1.$$

The Skyrme Model

- At spatial infinity we impose the boundary conditions that the fields tend to the limits $\sigma = 1$ and $\pi_i = 0$ for $i = 1, 2, 3$, equivalent to imposing $U \rightarrow I_2$.
- Hence we can do a one-point compactification and think of physical space $\mathbb{R}^3 \cup \{\infty\}$ as the 3-sphere S^3 .
- Effectively, we have a map from physical space to target space $S^3 \rightarrow S^3$. It is known that such a map is indexed by an integer which we shall call B , and which counts the number of Skyrmions.
- The baryon number B can be calculated as an integral of the topological density

$$B = \int \mathcal{B} d^3x.$$

Visualising Skyrmions

- The topological density provides a good way of visualising Skyrmions, by plotting level sets of \mathcal{B} . Some examples are given below: from left to right we have the minimal energy configurations for $B = 1$ to $B = 4$: a sphere, a torus, a tetrahedron and a cube.



- Note that $B = 1$ has spherical symmetry, $B = 2$ has toroidal symmetry, $B = 3$ has tetrahedral symmetry and $B = 4$ has cubic symmetry.

- In quantum field theory, there are two types of particles: **Bosons** and **Fermions**.
- When a **Boson** wavefunction is rotated by 2π , it remains invariant. However, if a **Fermion** wavefunction is rotated by 2π , then it changes by a factor of (-1) .
- If two identical particles are exchanged then nothing happens to **Bosons**, whereas the wavefunction of the **Fermions** changes by a factor of (-1) .
- In quantum field theory, **Bosons** are usually described by scalar, vector or tensor fields, whereas **Fermions** are represented by spinors.
- Atomic nuclei are fermions, so we must build the fermionic constraint into our quantisation scheme.

Finkelstein-Rubinstein constraints

- Key observation:

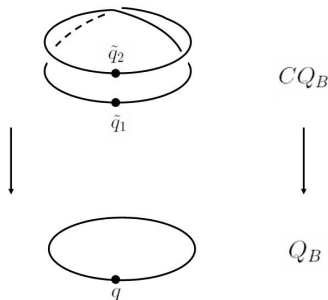
$$\pi_1(Q_B) = \mathbb{Z}_2,$$

where Q_B is the space of Skyrme configurations with charge B .

- Define wavefunctions ψ on the covering space of configuration space:

$$\psi : CQ_B \rightarrow \mathbb{C}.$$

- Impose $\psi(\tilde{q}_1) = -\psi(\tilde{q}_2)$.
- Symmetries of Skyrmions induce loops in configuration space.



Finkelstein-Rubinstein constraints

- Induced action of $SO(3) \times SO(3)$ symmetries on ψ :

$$\exp(-i\alpha \mathbf{n} \cdot \mathbf{L}) \exp(-i\beta \mathbf{N} \cdot \mathbf{K}) \psi(\tilde{\mathbf{q}}) = \chi_{FR} \psi(\tilde{\mathbf{q}}),$$

$$\text{where } \chi_{FR} = \begin{cases} 1 & \text{if the induced loop is contractible,} \\ -1 & \text{otherwise.} \end{cases}$$

- This is a rotation by α around axis \mathbf{n} in space and a rotation by β around axis \mathbf{N} in target space (called an isorotation).
- Here \mathbf{L} and \mathbf{K} are the body-fixed angular momentum operators in space and target space, respectively.
- Can we calculate the Finkelstein-Rubinstein constraint $\chi_{FR} \in \pi_1(Q_B)$?

Finkelstein-Rubinstein constraints

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- Here \mathbf{L} and \mathbf{K} are the body-fixed angular momentum operators in space and target space, respectively.
- Can we calculate the Finkelstein-Rubinstein constraint $\chi_{FR} \in \pi_1(Q_B)$?
- Yes, there is a simple formula:

$$\chi_{FR} = (-1)^{\mathcal{N}} \quad \text{where } \mathcal{N} = \frac{B}{2\pi} (B\alpha - \beta).$$

Rigid Body Quantization — Key idea

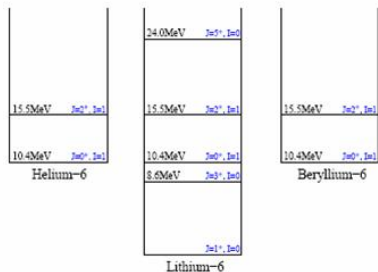
- Calculate a minimal energy Skyrmion for a given charge B .
- Derive its symmmetries.
- Use Finkelstein-Rubinstein constraints to find allowed states with given spin J and isospin I .
- Compare these states $|J\rangle|I\rangle$ with experiment

Rigid Body Quantization - Results

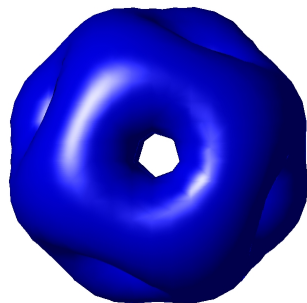
B	$ J\rangle I\rangle_0$	$ J\rangle I\rangle_1$	$ J\rangle I\rangle_2$	Experiment	$ J\rangle I\rangle_{\text{Exp.}}$	Match
1	$ \frac{1}{2}\rangle \frac{1}{2}\rangle$	$ \frac{3}{2}\rangle \frac{3}{2}\rangle$	$ \frac{5}{2}\rangle \frac{5}{2}\rangle$	^1_1H	$ \frac{1}{2}\rangle \frac{1}{2}\rangle$	✓
2	$ 1\rangle 0\rangle$	$ 3\rangle 0\rangle$	$ 0\rangle 1\rangle$	^2_1H	$ 1\rangle 0\rangle$	✓
3	$ \frac{1}{2}\rangle \frac{1}{2}\rangle$	$ \frac{5}{2}\rangle \frac{1}{2}\rangle$	$ \frac{3}{2}\rangle \frac{3}{2}\rangle$	^3_2He	$ \frac{1}{2}\rangle \frac{1}{2}\rangle$	✓
4	$ 0\rangle 0\rangle$	$ 4\rangle 0\rangle$	$ 2\rangle 1\rangle$	^4_2He	$ 0\rangle 0\rangle$	✓
5	$ \frac{1}{2}\rangle \frac{1}{2}\rangle$	$ \frac{3}{2}\rangle \frac{1}{2}\rangle$	$ \frac{1}{2}\rangle \frac{3}{2}\rangle$	^5_2He	$ \frac{3}{2}\rangle \frac{1}{2}\rangle$	✗ $^5_2\text{He}^*$
5*	$ \frac{5}{2}\rangle \frac{1}{2}\rangle$	$ \frac{7}{2}\rangle \frac{1}{2}\rangle$	$ \frac{3}{2}\rangle \frac{3}{2}\rangle$	^5_2He	$ \frac{3}{2}\rangle \frac{1}{2}\rangle$	✗ $^5_2\text{He}^{**}$
6	$ 1\rangle 0\rangle$	$ 3\rangle 0\rangle$	$ 1\rangle 1\rangle$	^6_3Li	$ 1\rangle 0\rangle$	✓
7	$ \frac{7}{2}\rangle \frac{1}{2}\rangle$	$ \frac{13}{2}\rangle \frac{1}{2}\rangle$	$ \frac{3}{2}\rangle \frac{3}{2}\rangle$	^7_3Li	$ \frac{3}{2}\rangle \frac{1}{2}\rangle$	✗ $^7_3\text{Li}^{**}$
8	$ 0\rangle 0\rangle$	$ 2\rangle 0\rangle$	$ 0\rangle 1\rangle$	^8_4Be	$ 0\rangle 0\rangle$	✓
9	$ \frac{1}{2}\rangle \frac{1}{2}\rangle$	$ \frac{3}{2}\rangle \frac{1}{2}\rangle$	$ \frac{1}{2}\rangle \frac{3}{2}\rangle$	^9_4Be	$ \frac{3}{2}\rangle \frac{1}{2}\rangle$	✗ $^9_4\text{Be}^{**}$
9*	$ \frac{1}{2}\rangle \frac{1}{2}\rangle$	$ \frac{5}{2}\rangle \frac{1}{2}\rangle$	$ \frac{3}{2}\rangle \frac{3}{2}\rangle$	^9_4Be	$ \frac{3}{2}\rangle \frac{1}{2}\rangle$	✗ $^9_4\text{Be}^{**}$

S. Krusch *Homotopy of Rational Maps and the Quantization of Skyrmions*, Ann. Phys., **394**, (2003) 103

Predictions of the Skyrme model for $B = 6$



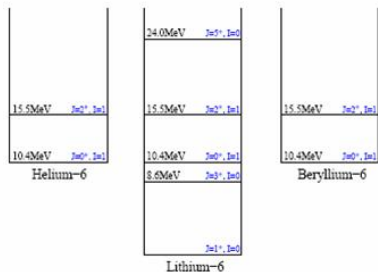
(a) Skyrme data



(b) Experiment

Figure: Energy level diagram for nuclei with $B = 6$.

Predictions of the Skyrme model for $B = 6$



(a) Skyrme data



(b) $B = 6$ Skyrmin

Figure: Energy level diagram for nuclei with $B = 6$.

- We see that the approach is successful for calculating the ground states for small nuclei, in particular for $B = 1$ to $B = 4$ and also for larger even nuclei.
- It is also known that even excited spectra can be produced fairly well for some nuclei such as Lithium-6 and other small even nuclei.
- For Carbon-12 the ground state and first excited state (Hoyle state) have both been calculated as compositions of $B = 4$ cubes, the ground state as a triangular arrangement and the Hoyle state as a chain.
- For odd nuclei however, the method is largely unsuccessful.

General Idea of Vibrational Quantization

- Starting from our original Lagrangian, we can construct a reduced Lagrangian by restricting the Skyrmion configuration to some finite dimensional manifold.
- For zero-mode quantisation we only allow rotations and isorotations to change the kinetic energy and leave the static energy invariant.
- Now we go one step further and introduce deformations that change the static energy, which are parameterised by \mathbf{s} .
- The reduced Lagrangian becomes

$$L = \frac{1}{2} g_{ij}(\mathbf{s}) \dot{y}_i \dot{y}_j - V(\mathbf{s}),$$

where the \dot{y}_i are shorthand for the velocities of the deformations $\dot{\mathbf{s}}$ and the angular velocities \mathbf{a} and \mathbf{b} , and g_{ij} is the metric on the manifold.

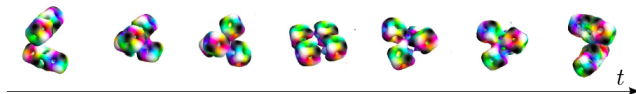
- A 2015 paper by Chris Halcrow looks at quantising the Lithium-7 nucleus with the inclusion of a vibrational mode.



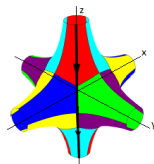
- The results are very promising. Not only does the paper predict the ground state to be a spin $3/2$ state which is already an improvement on the rigid body approach, but it also predicts a spectrum for Lithium-7.
- It predicts excited spin $1/2$, $7/2$ and $5/2$ states which are experimentally known to exist, and are correctly ordered although the precise values of the energies are not perfect.

Oxygen-16

- A 2016 paper by Chris Halcrow, Chris King and Nick Manton looks at quantising the Oxygen-16 nucleus, which they treat as being composed of four $B = 4$ blocks and again a vibrational mode.

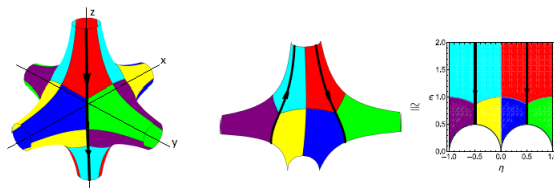


- The restricted manifold is the 6-punctured sphere which we call M , here the solid black line is the scattering mode shown. There are in fact three copies of this mode corresponding to the three symmetry axes of the tetrahedron.



Properties of the 6-punctured Sphere

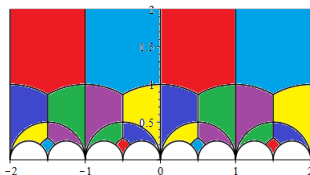
- M has $O/D_2 \cong S_3$ symmetry.
- We need only consider one quarter of the 6-punctured sphere which we map onto a region of the complex upper half plane \mathbb{H} , which we call F . Note $F = \mathbb{H}/\Gamma(2)$, where $\Gamma(2)$ is a modular subgroup whose fundamental domain can be chosen to coincide with F .



- We will define a complex coordinate $\xi = \eta + i\epsilon$ on F .
- The colouring is done such that tetrahedrons are at positions where 3 colours meet and squares are at positions where 4 colours meet.

Properties of the 6-punctured Sphere

- As an aside we can visualise the whole 6-punctured sphere. It is related to the domain of the modular subgroup $\Gamma(4)$.



- We can identify the four quarters and six punctures quite easily.
- $\Gamma(4)$ is generated by the matrices $A = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$ and $B = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$, and combinations of these matrices and their inverses allow us to map between all of the coloured regions.
- So, if we know the solution in one region, we can construct it in all of the others.

The Schrödinger Equation on F

- The Schrödinger equation in general form is

$$\left(-\frac{\hbar^2}{2}\Delta + V\right)\psi = E\psi. \quad (1)$$

where $\xi = \eta + i\epsilon$ are coordinates of $F \in \mathbb{H}$.

- We split the operator Δ into a rotational and a vibrational part as $\Delta = \Delta_\xi + \nabla^2$ with $\psi = \phi|\Theta\rangle$ and $\nabla^2|\Theta\rangle = E_J|\Theta\rangle$.
- On F the vibrational part becomes $\Delta_\xi = \epsilon^2 \left(\frac{\partial^2}{\partial \eta^2} + \frac{\partial^2}{\partial \epsilon^2} \right)$, which is invariant under all Möbius transformations.
- Using the Möbius transformation $\xi \mapsto \frac{\xi - 1}{\xi}$ and parity $\xi \mapsto -\bar{\xi}$, we only need to solve (1) in the red region.

The Schrödinger Equation on F

- We can now separate out and solve the vibrational part of the equation for the vibrational wavefunction ϕ

$$\left(-\epsilon^2 \left(\frac{\partial^2}{\partial \eta^2} + \frac{\partial^2}{\partial \epsilon^2} \right) + V(\eta, \epsilon) \right) \phi = (E - E_J) \phi$$

where a convenient choice of the potential is

$$V(\eta, \epsilon) = \epsilon^2 \left(\omega^2 \left(\eta - \frac{1}{2} \right)^2 + \mu^2 \right)$$

which attains its global minimum at the tetrahedron $(\eta, \epsilon) = (1/2, \sqrt{3}/2)$. The formula applies only in the red region.

- The term E_J is related to the rotational energy (the ξ dependence of E_J can be treated with perturbation theory.)

The Different Representations of S_3

- The region F has S_3 symmetry, and the group S_3 has three irreducible representations called the trivial, sign and standard representations.
- In the trivial representation vibrational wavefunctions are invariant under any element of S_3 , and in the sign representation they are invariant under 3-cycles but change sign under transpositions.
- The standard representation is two dimensional and more complicated, and we will not discuss this here.
- The potential is invariant under all elements of S_3 so all vibrational wavefunctions can be labelled completely by their representation and parity.

Constraints for the trivial and the sign representation

- The transposition $(1, 2)$ corresponds to a $\pi/2$ rotation around the z -axis, so the wave function $\psi = \phi|\Theta\rangle$ is invariant provided that

$$(-1)^s \phi|\Theta\rangle = \phi e^{\frac{\pi i}{2} L_3} |\Theta\rangle,$$

where s is 0 and 1 for the trivial and sign representations respectively.

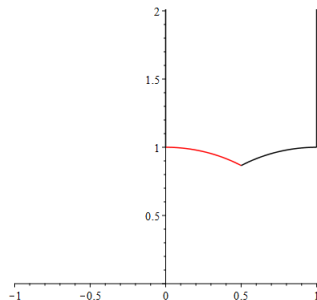
- Since ϕ is invariant under the 3-cycles $(1, 2, 3)$ which corresponds to a $2\pi/3$ rotation, we also have

$$\phi|\Theta\rangle = \phi e^{\frac{2\pi i}{3} \frac{1}{\sqrt{3}} (L_1 + L_2 + L_3)} |\Theta\rangle.$$

- These are essentially Finkelstein-Rubinstein constraints as we have met earlier. Allowed spin states for the trivial representation are $J = 0, 4, 6, \dots$, and for the sign representation they are $J = 3, 6, \dots$
- (The standard representation gives $J = 2, 4, 5, 6, \dots$)

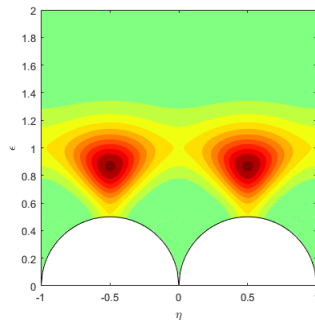
Boundary conditions

- We can deduce the boundary conditions on the red region by looking at how points on either side of boundary curves are related by symmetry.
- For the vertical lines, states with positive parity require the derivative normal to the boundary to be zero, whereas negative parity requires the function to vanish on the boundary (for both trivial and sign rep).
- On the red curve, either the normal derivative or the function has to vanish (depending on parity and representation).
- Furthermore, the function vanishes at infinity.



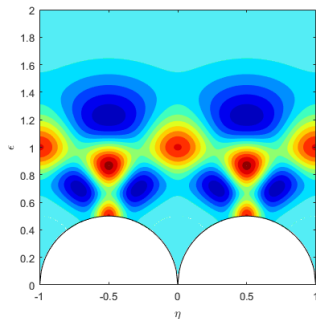
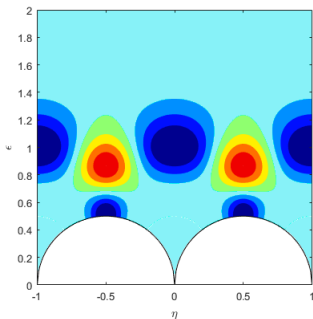
The Ground State

- The equation for ϕ now has to be solved subject to suitable boundary conditions on the red region. Then the solution is mapped to the other regions using parity and $\xi \mapsto \frac{\xi - 1}{\xi}$.
- The ground state is a 0^+ state with $\partial_{\perp}\phi(\xi) = 0$ on the boundary.
- The wave function ψ has its maximum at the tetrahedron and no nodal lines.
- This state is consistent with the zero-mode quantisation.



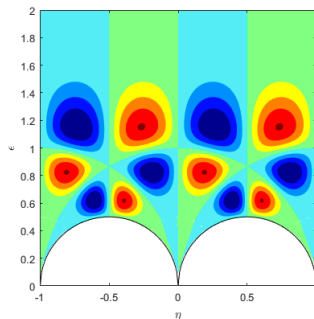
Excited 0^+ States

- These states have the same boundary conditions, parity and spin as the ground state but a higher energy.
- Note that for the first excited state $|\psi|^2$ has maxima at the tetrahedrons and the squares which are minima and saddle points of V , respectively.



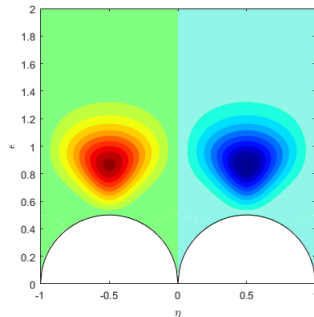
The first 0^- State

- This state has the opposite boundary conditions due to having negative parity, name $\phi = 0$ on the boundary of the red region.
- This forces the maxima of $|\psi|^2$ away from tetrahedron and square. The nodal lines are in fact the attractive channel. Therefore, this state has much higher energy.



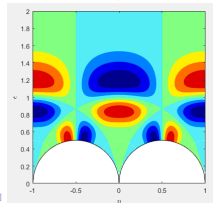
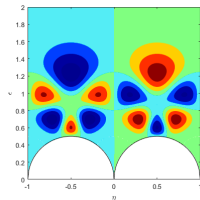
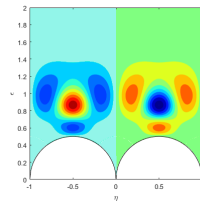
The Lowest State in the Sign Representation (3^-)

- In the sign representation with negative parity, $\phi = 0$ on the vertical lines $\eta = 0$ and $\eta = \pm 1$. On the curved boundary we have $\partial_{\perp}\phi(\xi) = 0$.
- The square of the wave function $|\psi|^2$ has its maximum at the tetrahedrons and nodal lines on the vertical lines.



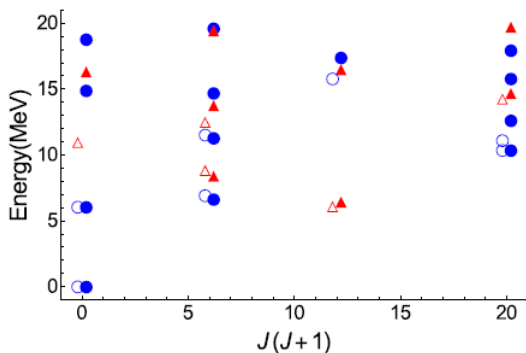
Excited 3^- States and the first 3^+ State

- The 3^- states have the same boundary conditions, parity and spin as the previous state but a higher energy.
- The 3^+ has the “opposite” boundary conditions. It vanishes on the attractive channel and in particular the square and the tetrahedron. It therefore has much higher energy.
- Note that states with opposite parity are not captured by a vibrational quantisation that only takes the attractive channel into account whereas the remaining states can be calculated.

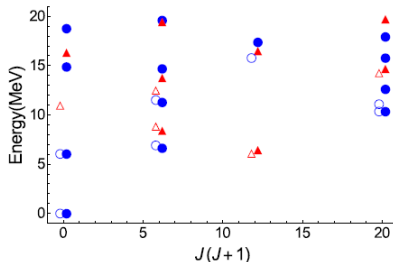


The O-16 Spectrum

- Halcrow, King and Manton produced the following spectrum



- Solid shapes are predicted states and hollow shapes are experimental states. Circles are states of positive parity and triangles are states with negative parity.



- Note that the ground state, first excited 0^+ state and first 4^+ state are fixed to experiment by the calibration.
- The lowest lying $J = 2$ states have the correct order and approximately the correct energy gaps.
- The energy of the 0^- state is much too high.

The potential

- In their original paper Halcrow, King and Manton make a simple choice of potential that allowed them to solve the Schrödinger equation using separation of variables and hence 1D numerics.
- However in general the Schrödinger equation is not separable, and requiring that it be so imposes severe restrictions on the potential that we can choose, specifically it must be of the form

$$V(\eta, \epsilon) = \epsilon^2(f_1(\epsilon) + f_2(\eta)).$$

- Observe that this potential is guaranteed to blow up at infinity due to the ϵ^2 factor, rather than tend to a constant.
- It also turns out that this potential will be continuous but not smooth across the boundaries when mapped into the other coloured regions.

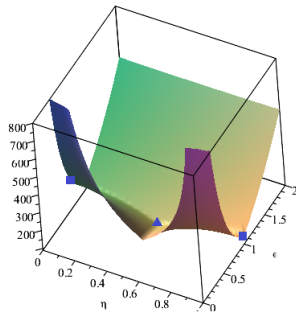
More general potentials

- In order to avoid these restrictions on the potential, we implemented a 2D numerical scheme using a finite element method in FreeFEM++.
- As a proof of concept, we will first apply the potential used by Halcrow, King and Manton, specifically

$$V(\eta, \epsilon) = \epsilon^2 \left(\omega^2 \left(\eta - \frac{1}{2} \right)^2 + \mu^2 \right).$$

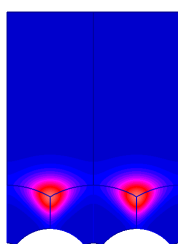
This formula is only valid in the red region.

- Note that this potential has a global minimum at the tetrahedron. It also has saddle points at the squares.

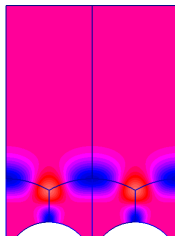


Results (trivial rep)

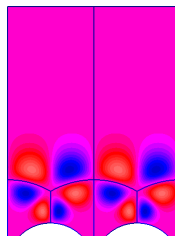
- Here we show the ground state, first excited trivial state, and the first trivial state with negative parity (much higher energy), in agreement with earlier calculations.



0.13007
0.11097
0.09093
0.07460
0.06094
0.04909
0.03874
0.03007
0.02402
0.01918
0.01505
0.01151
0.00846
0.00582
0.00307
0.00124

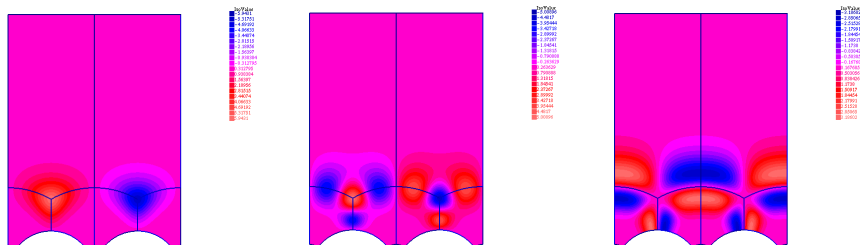


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- We also show the lowest energy sign state, the first excited sign state and the first sign state with positive parity:



A more general potential

- We would like our potential to satisfy the following conditions:
 - Global minimum at the tetrahedron.
 - Other stationary points at the squares.
 - Smooth across the boundaries of the coloured regions.
 - Flattens off to a finite value at infinity.
- These latter two conditions were previously impossible to satisfy, but we now have the scope to do this.
- The key idea is to solve the Schrödinger equation with zero potential, and then find one state that is localised entirely around the tetrahedron and one which is localised entirely around the squares.
- We then construct a potential as a linear combination of these wavefunctions and it will satisfy all of our requirements.

$$V = \omega^2 (V_{tet} + \lambda V_{sq}) + \mu^2$$

- Then fit ω , λ and μ to obtain best fit with experimental spectrum.
Work in progress!

- We have reviewed the rigid body quantization of Skyrmions
- We then introduced vibrational quantization and how it improves on rigid body quantization
- We have recapped the existing work on Oxygen-16
- We reproduced the Oxygen-16 spectrum using a finite element method
- We are currently fitting parameters for a more general potential.

Outlook

- We discussed how the 6-punctured sphere can be used to parametrises an important O -symmetric vibrational manifold and quantize oxygen-16
- The 3-punctured sphere is related to the shape space of triangles. We are currently working on a vibrational quantization of carbon-12 on this space
- The figures show visualisations of the 3-punctured and 6-punctured sphere using the Poincare disk model:

