Challenges in computational quantum mechanics

Simen Kvaal

Centre of Mathematics for Applications
University of Oslo

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Outline

Overview of computational QM at CMA

- QM – a crash course
- Bose-Einstein condensates

Outline

Overview of computational QM at CMA

QM – a crash course

Bose-Einstein condensates

The Skyrme model

Description and topology of the model

Discretization of the Skyrme model

Simulated annealing

Quantum mechanics (QM)

- Non-relativistic QM is a microscopic model
- Extremely diverse range of applications
  - Semi-conductor physics and quantum dots
  - Bose-Einstein condensation (BEC)
  - Quantum computing, cryptography
  - Nuclear physics, shell model computations
- Basic formulation in terms of linear operators in abstract Hilbert space
- Typically, PDE and/or eigenvalue problems

Quantum mechanics II

$\mathcal{H}$ – The Hilbert space; a subspace of $\left[L^2(\mathbb{R}^d,\mathbb{C})\otimes\mathbb{C}^{2s+1}\right]^{\otimes n}$.

Ψ – The "state", or "wave function". We write

$$\Psi(\underbrace{x_1\ x_2\ \ldots\ x_n}_{\text{spatial coordinates}};\underbrace{\sigma_1\ \sigma_2\ \ldots\ \sigma_n}_{\text{spin coordinates}})$$

$\hat{H}$ – The Hamiltonian; a linear operator on $\mathcal{H}$. Models interactions with world.

$$\hat{H} = \underbrace{\sum_i \hat{h}(i)}_{\text{interactions with world}} + \underbrace{\sum_{i<j}\hat{v}(i,j)}_{\text{inter-particle interactions}}$$

The Schrödinger equation

Dynamics is governed by the Schrödinger equation:

$$i\Psi_t = \hat{H}\Psi$$

Typical example:

$$\begin{aligned} i\Psi_t(t, x_1, x_2, \ldots) &= \left[-\Delta + V(t, x_1, x_2, \ldots)\right]\Psi(t, x_1, x_2, \ldots) \\ &\quad + \left(\sum_{i<j} \frac{1}{|x_i - x_j|}\right)\Psi(t, x_1, x_2, \ldots) \end{aligned}$$

This is a very difficult problem!

Curse of dimensionality

- Adding more particles $\Rightarrow$ exponential growth in complexity
- Example: Finite difference approximation with N points in each direction gives

$$k = N^{nd} \quad \text{total grid points!}$$

- Six particles, three dimensions, 10 grid points:

$$k = 10^{18}$$

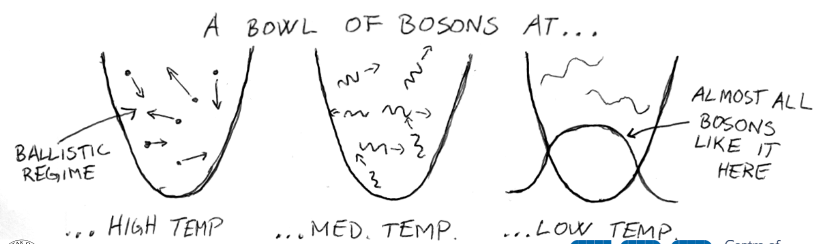
- Most systems have hundreds of particles ...

Bose-Einstein condensates

- At low temperature, a dilute gas of bosons *condense into the ground state*
- A much-used model is the Gross-Pitaevski equation:

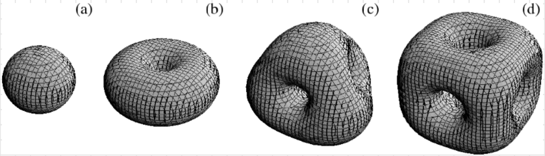
$$i\Psi_t(x,t) = \left[-\Delta + V(x,t) + c|\Psi(x,t)|^2\right]\Psi(x,t)$$

- Inter-particle interaction and many dimensions $\longrightarrow$ nonlinearity and few dimensions



The Skyrme model

- In the 60's, T. Skyrme proposed an effective model for nucleons
- Today considered as low-energy limit of QCD
- Very challenging nonlinear PDE problem
- Challenging geometric aspects of model
- Solitons in 3D

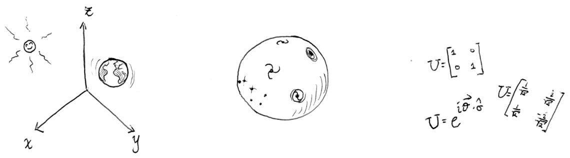


The primary unknown

Primary unknown is an $SU(2)$ map

$$U : \mathbb{R}^3 \cup \{\infty\} \longrightarrow SU(2)$$

Topological identifications:



$$\mathbb{R}^3 \cup \{\infty\} \qquad S^3 \subset \mathbb{R}^4 \qquad SU(2)$$

Hence, possible interpretations:

$$U : SU(2) \longrightarrow SU(2) \quad \text{or} \quad U : S^3 \longrightarrow S^3$$

Winding number

- Since $\pi_3(S^3) = \mathbb{Z}$, we have homotopy classes characterized by winding number $B[U]$
- Conserved under continuous deformations, including propagation in time

Winding number 2 map on S^2

The Lagrangian

- The Lagrangian $\mathcal{L}(U, \partial_\mu U)$ of the model:

$$\mathcal{L} = -\frac{1}{2}\,\mathrm{Tr}\left(L_\mu L^\mu\right) + \frac{1}{16}\,\mathrm{Tr}\left([L_\mu, L_\nu][L^\mu, L^\nu]\right)$$

where

$$L_\mu = U^\dagger \partial_\mu U$$

- *Lorentz invariant*, relativistic model
- Euler-Lagrange equations:

$$\partial_\mu R^\mu = \partial_\mu \left(L^\mu + \frac{1}{4}[L_\nu, [L^\nu, L^\mu]] \right) = 0$$

Skyrmions

- Visualizations of energy minimizing stationary solutions with winding numbers (left to right) $B = 1, 2, 3$ and 4

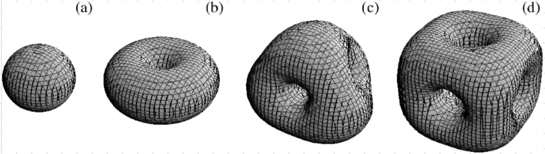


Figure taken from Hale *et al.* (2000)

These are isosurfaces of constant "winding number density"

- Bound groups of nuclear particles/baryons

Challenge

Our problem is now:

- Numerical computation of "Skyrmions": energy minimizing solutions in a given topological sector
- These are solitons: Particle-like solutions
- Solve the time-dependent model numerically: collision processes, . . .
- All this in a geometric way, due to limited resolution and complexity of model

Lie Algebra vs. group representation

As in all studies in the literature, we may represent U by a point on S^3:

$$\phi = [\phi^0, \vec{\phi}] \in \mathbb{R}^4, \qquad \phi \cdot \phi = 1$$

Really important drawbacks:

- The constraint must be maintained explicitly
- The space of maps $\phi : \mathbb{R}^3 \to S^3$ is not linear $\Rightarrow$ difficult to use variational methods, FEM, . . .
- Discrete winding number ill-defined

Lie Algebra vs. group representation II

Or we can use an element in the Lie algebra $su(2)$:

$$\vec{\theta} \in \mathbb{R}^3, \qquad U = e^{i\vec{\theta}\cdot\hat{\sigma}}$$

Hence, $\vec{\theta}$ are angles on S^3. The *Pauli matrices* are given by

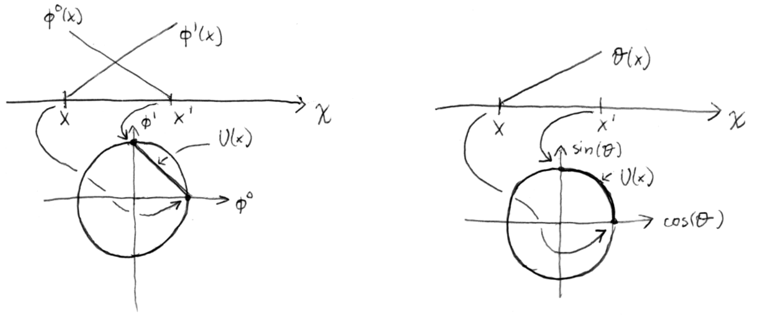
$$\hat{\sigma} = (\sigma_1, \sigma_2, \sigma_3) = \left(\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \right)$$

Really important benefits:

- No constraint!
- The space of maps $\theta : \mathbb{R}^3 \to \mathbb{R}^3$ is linear
- Discrete winding number well-defined
- But: Difficult boundary conditions introduced

Picture this ...

The difference can easily be pictured by considering $U : \mathbb{R} \to S^1$.



Group element *vs.* Lie algebra element

Discretization

- We employ trilinear finite elements over a uniform grid
- We truncate the domain as a box

$$\Omega = [-L, L]^3 \subset \mathbb{R}^3$$

- We use the Lie algebra model, resulting in

$$\vec{\theta} : \Omega \to \mathbb{R}^3, \qquad U = \exp(i\vec{\theta} \cdot \hat{\sigma})$$

$$\mathcal{L} = \mathcal{L}(\vec{\theta}, \partial_\mu \vec{\theta}) = \text{complicated stuff, but nice}$$

Minimization approach

Solving the Euler-Lagrange eqns $\Leftrightarrow$ minimization of energy:

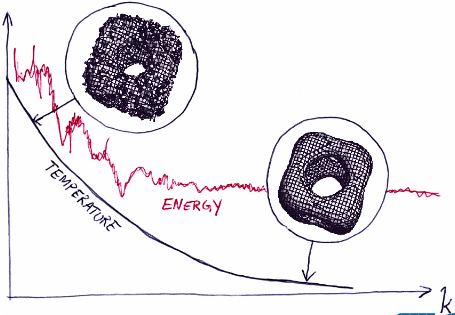
- We seek global minimum of energy functional $E[U]$ in given sector $n \in \mathbb{Z}$, i.e., $B[U] = n$:

$$E[U] = \int_{\mathbb{R}^3} \mathcal{E}(U, \partial_\mu U)\; d^3x$$

- Discrete Euler-Lagrange (Newton-Rhapson iteration) useless due to huge number of local minima
- We minimize using simulated annealing

Simulated annealing

- SA is a Monte Carlo method
- Slow convergence, very expensive
- Global minimum always found
- Basic SA has intuitive appeal



Simulated annealing II

Rough (!) overview of algorithm:

1. Choose initial configuration $\vec{\theta} : \Omega \to \mathbb{R}^3$
2. Pick initial temperature T_0, and compute energy E. Set $k = 0$.
3. Repeat until $\vec{\theta}$ has converged
   3.1 Randomly perturb $\vec{\theta}$ at random grid point
   3.2 Compute change $\Delta E = E' - E$ in energy
   3.3 If $\Delta E \leq 0$, accept the move
   3.4 If $\Delta E > 0$, accept the move with probability $p = \exp(-\Delta E / T_k)$ (Metropolis algorithm)
   3.5 If E is stabilized, lower temperature $T_{k+1} = \alpha T_k$, $k \mapsto k + 1$

Geometry of FEM discretization

- All FEM maps with $\vec{\theta}(x) = 0$ on $\partial\Omega$ are homotopic to the identity mapping ($\vec{\theta} \equiv 0$, or $U \equiv \mathbf{1}$)
- Consequence: Boundary conditions define $B[U]$
- Problem: How to define proper conditions
- Problem: Homotopy classes become *disconnected*

Current status

Research by others have established:

- Non-geometric discretization, $N \sim 200$, $B[U] \sim 20$.
- Big body of conjectures, few answered questions
- Only crude dynamical simulations

Our research (S. Kvaal, P.C. Moan and J.B. Thomassen):

- We believe geometric discretization is important, and it is within reach
- Simulated annealing for $N \sim 100$, $B[U] = 1$
- $B[U] > 1$ requires BC analysis and/or use of constrained SA
- Attempt at multisymplectic formulation