Statistical Mechanics and Dynamics of Multicomponent Quantum Gases

Austen Lamacraft

October 26, 2011

UNIVERSITY of VIRGINIA
RESEARCH CORPORATION for SCIENCE ADVANCEMENT
A foundation dedicated to science since 1912.
NSF

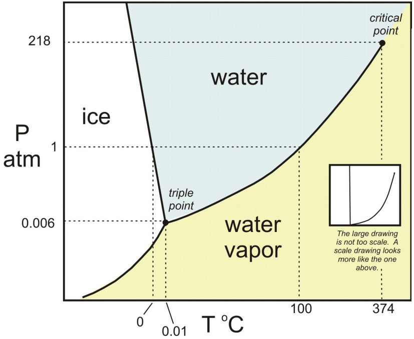
Outline

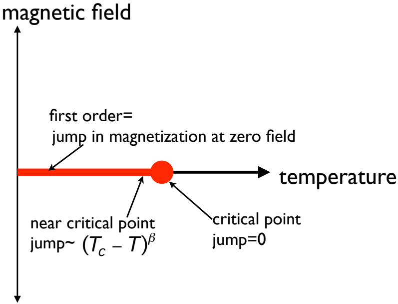
Boson pairing and unusual criticality

- Yifei Shi, Austen Lamacraft and Paul Fendley
  arXiv:1108.5744
- Also Andrew James and Austen Lamacraft
  Phys. Rev. Lett. **106**, 140402 (2011)

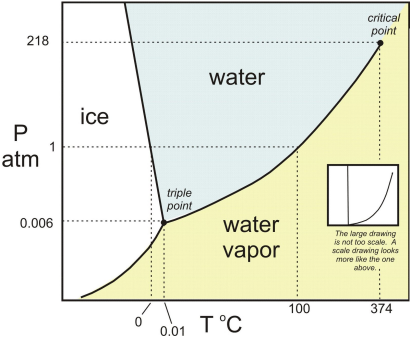
Outline

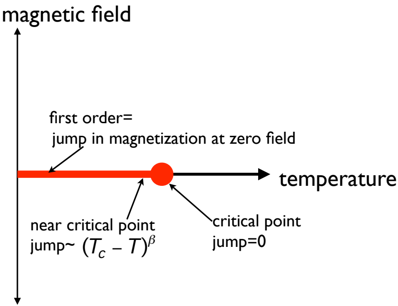
Why study phase transitions?





Why study phase transitions?





Amazingly, there is a sense in which the two problems are *the same*.

Universality: pick your battles

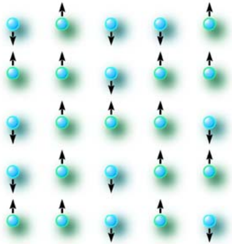
- Forget phase diagram and focus on *phase transitions*
- *Continuous* transitions characterized by *critical exponents*
  - $M \propto (T - T_c)^{\beta}$, $C \propto (T - T_c)^{-\alpha}$
  - At $T = T_c$ correlation functions $\langle M(\mathbf{x})M(\mathbf{y})\rangle = \frac{C}{|\mathbf{x}-\mathbf{y}|^{2\Delta}}$
- Behavior is characteristic of *scale invariance*

From scale invariance to simple models

(Scale invariance)

From scale invariance to simple models

Studying simple models is *a really good idea!*

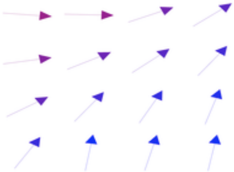


$$\mathcal{Z} = \sum_{\{\sigma\}} e^{-\beta\mathcal{H}_{\text{Ising}}[\sigma]}, \qquad \sigma_i = \pm 1$$

$$\beta\mathcal{H}_{\text{Ising}}[\sigma] = -J \sum_{<ij>} \sigma_i \sigma_j$$

Universality classes

Characterized by *broken symmetry* of order parameter[1]
e.g. XY model



$$\beta\mathcal{H}_{\mathsf{XY}}[\theta] = -J\sum_{<ij>}\cos(\theta_i - \theta_j)$$

[1] Also spatial dimension

Examples of 3D universality classes

Ising class

- Liquid-gas, binary mixtures, uniaxial magnetic systems, micellization,...
- $C \propto (T - T_c)^{-0.11}$
- $\xi \propto (T - T_c)^{0.63}$

XY class

- Easy plane magnets, λ-transition in ^{4}He, superconductors, BEC,...
- $C \propto (T - T_c)^{-0.01}$
- $\xi \propto (T - T_c)^{0.67}$

Examples of 3D universality classes

Ising class

- Liquid-gas, binary mixtures, uniaxial magnetic systems, micellization,...
- $C \propto (T - T_c)^{-0.11}$
- $\xi \propto (T - T_c)^{0.63}$

XY class

- Easy plane magnets, λ-transition in ^{4}He, superconductors, BEC,...
- $C \propto (T - T_c)^{-0.01}$
- $\xi \propto (T - T_c)^{0.67}$

Beautiful classification...

Examples of 3D universality classes

Ising class

- Liquid-gas, binary mixtures, uniaxial magnetic systems, micellization,...
- $C \propto (T - T_c)^{-0.11}$
- $\xi \propto (T - T_c)^{0.63}$

XY class

- Easy plane magnets, λ-transition in ^{4}He, superconductors, BEC,...
- $C \propto (T - T_c)^{-0.01}$
- $\xi \propto (T - T_c)^{0.67}$

Beautiful classification...

Let's try to break it!

Bose condensates and superfluids are XY systems

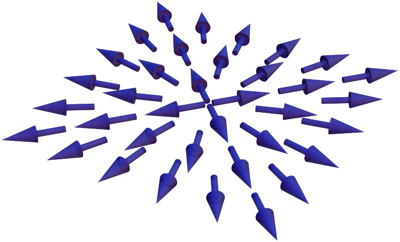
Bose condensation: *macroscopic occupancy* of single-particle state

- Wavefunction $\Psi(\mathbf{r})$ is *condensate order parameter*
- Free to choose phase: XY symmetry breaking
- Superfluid velocity $\mathbf{v} = \frac{\hbar}{m}\nabla\theta$

Vortices give a twist in 2D

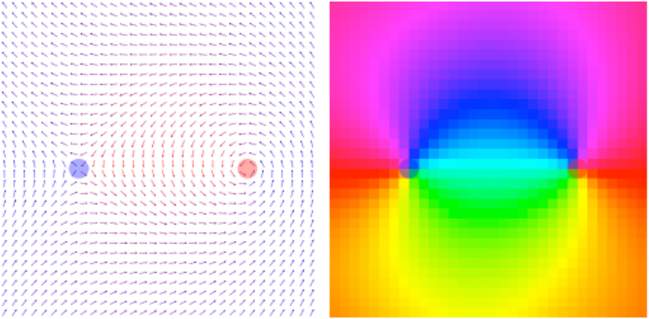
Quantized vortices: phase increases by $2\pi \times q$ (Integer q)

$$\mathbf{v} = \frac{\hbar}{m}\nabla\theta = \frac{\hbar}{m}\frac{\hat{\mathbf{e}}_\theta}{r}$$



Vortices give a twist in 2D

Logarithmic interaction between vortices of charge q_1, q_2



$$V_{q_1,q_2}(\mathbf{x}-\mathbf{y}) = -q_1 q_2 \frac{\pi n \hbar^2}{2m} \ln|\mathbf{x}-\mathbf{y}|$$

2D density n

The Kosterlitz–Thouless transition

Consider contribution to the partition function from a $q = \pm 1$ pair

$$\mathcal{Z}_{\text{pair}} = \int d\mathbf{x} d\mathbf{y} \, \exp\left[-\beta V_{1,-1}(\mathbf{x}-\mathbf{y})\right]$$
$$= \int \frac{d\mathbf{x} d\mathbf{y}}{|\mathbf{x}-\mathbf{y}|^{\frac{\beta \pi n \hbar^2}{2m}}}$$

Pair found at separation r with probability $\propto r^{1-\frac{\beta\pi n\hbar^2}{2m}}$

- Pair dissociates for

$$k_{\text{B}} T > k_B T_{\text{KT}} \equiv \frac{\pi n \hbar^2}{2m}$$

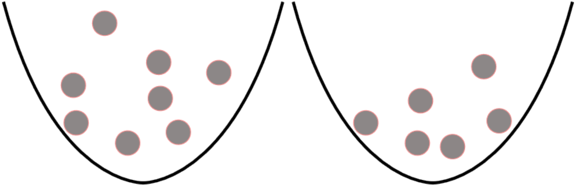
- Pair bound for

$$T < T_{\text{KT}}$$

Outline

Pair condensates: an Ising transition in an XY system

Two Bose condensates with a definite *phase*

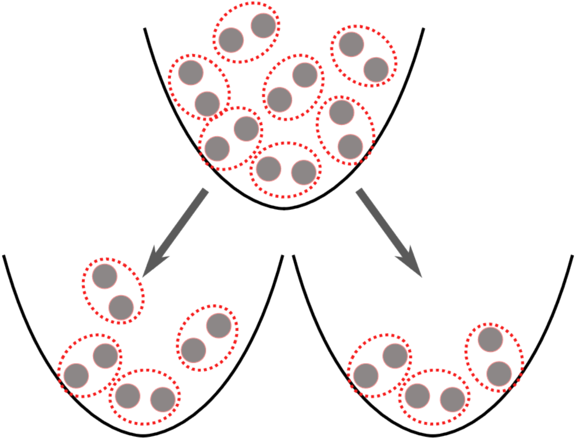


$$|\Delta\theta\rangle = \sum_{n=0}^{N} e^{in\Delta\theta} |n\rangle_L |N-n\rangle_R$$

Detect phase by interference

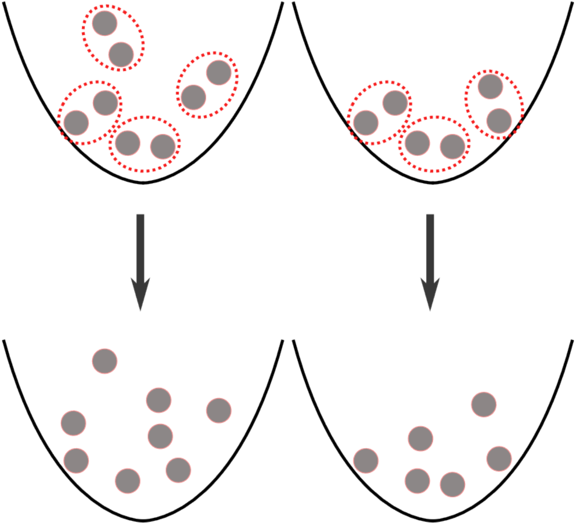
Pair condensates: an Ising transition in an XY system

Take a condensate of molecules and *split it*



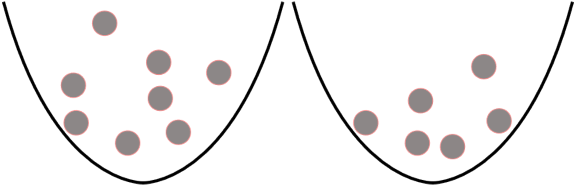
Pair condensates: an Ising transition in an XY system

Dissociate pairs



Pair condensates: an Ising transition in an XY system

What is the resulting state?



Superposition involves only *even* numbers of atoms

$$\sum_{n=0}^{N/2} |2n\rangle_L |N-2n\rangle_R = \frac{1}{2}\sum_{n=0}^{N} |n\rangle_L |N-n\rangle_R + \frac{1}{2}\sum_{n=0}^{N}(-1)^N |n\rangle_L |N-n\rangle_R$$

$$= |\Delta\theta = 0\rangle + |\Delta\theta = \pi\rangle$$

Pair condensates: an Ising transition in an XY system

Pair condensate $\longrightarrow$ condensate breaks an Ising symmetry![2]

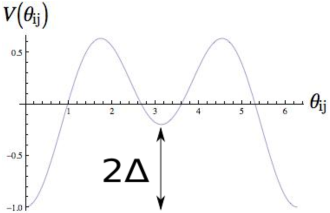
[2] Romans *et al* (2004), Radzihovsky *et al.* (2004)

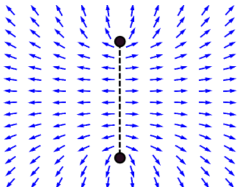
A simple model

$$H_{\mathrm{GXY}} = -\sum_{\langle ij \rangle} \left[(1-\Delta)\cos(\theta_i - \theta_j) + \Delta \cos\left(2\theta_i - 2\theta_j\right) \right]$$

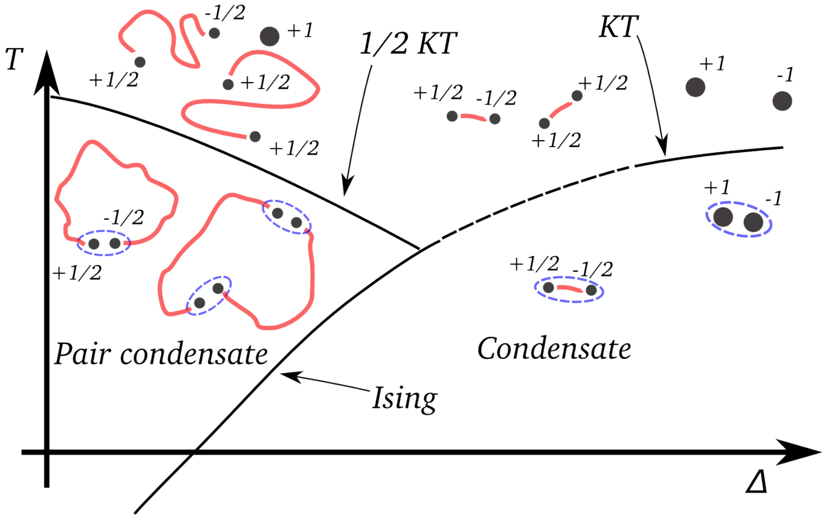
Korshunov (1985), Lee & Grinstein (1985)

- $\Delta = 0$ is usual XY; $\Delta = 1$ is π-periodic XY
- $\Delta < 1$ has metastable minimum





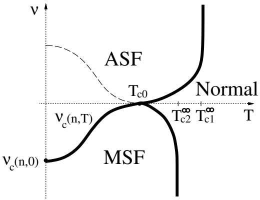
Schematic phase diagram

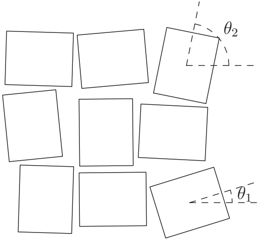


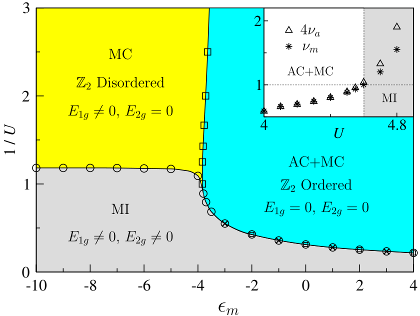
What is the nature of phase transition along dotted line?

An old problem with many guises

Korshunov (1985)
Lee & Grinstein (1985)
Sluckin & Ziman (1988)
Carpenter & Chalker (1989)
Romans *et al* (2004)
Radzihovsky *et al.* (2004)
Geng & Selinger (2009)
James & AL (2011)
Ejima *et al.* (2011)







Outline

Statistical Mechanics of Boson Pairs

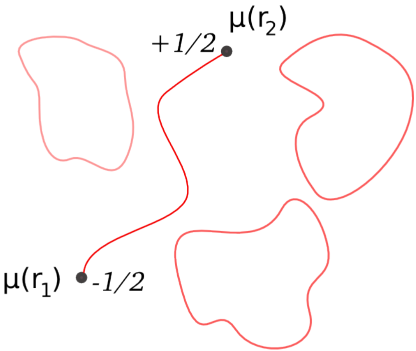
- Phase transitions and universality
- Boson pair condensates
- Interplay of strings and vortices

Dynamics of Spinor Condensates

- Geometry of phase space
- Mechanics of the Mexican hat
- Connection to spinor condensates

How things change on the Ising critical line

Redo KT argument accounting for string



Domain wall terminates at *disorder operator* $\mu(\mathbf{x})$

How things change on the Ising critical line

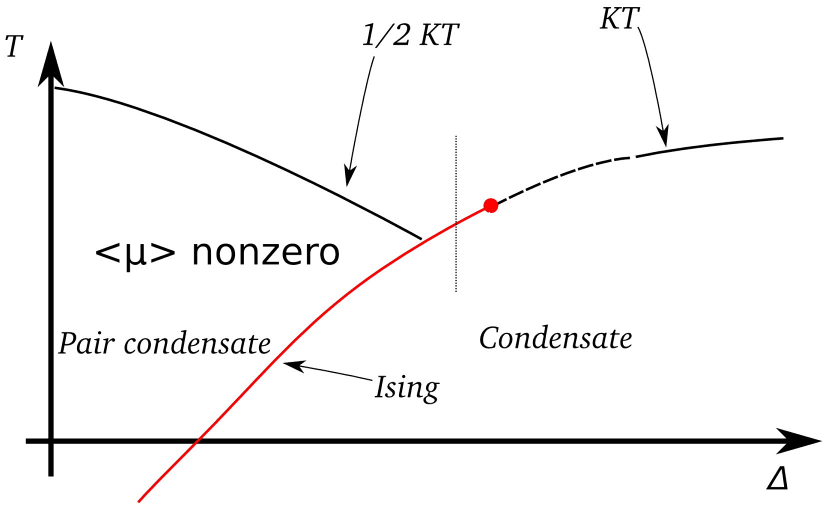
Disorder operators dual to $\sigma(\mathbf{x})$ of Ising model

$$\langle \sigma(\mathbf{x})\sigma(\mathbf{y})\rangle = \langle \mu(\mathbf{x})\mu(\mathbf{y})\rangle = \frac{1}{|\mathbf{x}-\mathbf{y}|^{1/4}}$$

$$\begin{aligned}\mathcal{Z}_{\text{pair}} &= \int d\mathbf{x}d\mathbf{y}\,\langle \mu(\mathbf{x})\mu(\mathbf{y})\rangle \exp\left[-\beta V_{1/2,-1/2}(\mathbf{x}-\mathbf{y})\right] \\ &= \int \frac{d\mathbf{x}d\mathbf{y}}{|\mathbf{x}-\mathbf{y}|^{\frac{1}{4}+\frac{\beta\pi n\hbar^2}{8m}}}\end{aligned}$$

Dissociation at higher temperatures than for ‘free’ half vortices

How things change on the Ising critical line



Numerical simulation using worm algorithm

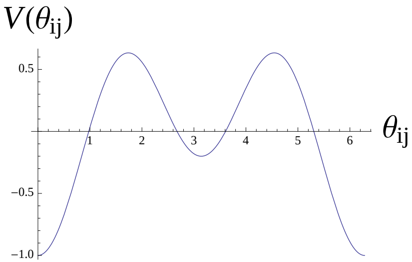
$$\mathcal{Z} = \prod_c \int_{-\pi}^{\pi} \frac{d\theta_c}{2\pi} \prod_{\langle ab \rangle} w(\theta_a - \theta_b),$$

$w(\theta)$ is written in terms of the Villain potential $w_V(\theta)$

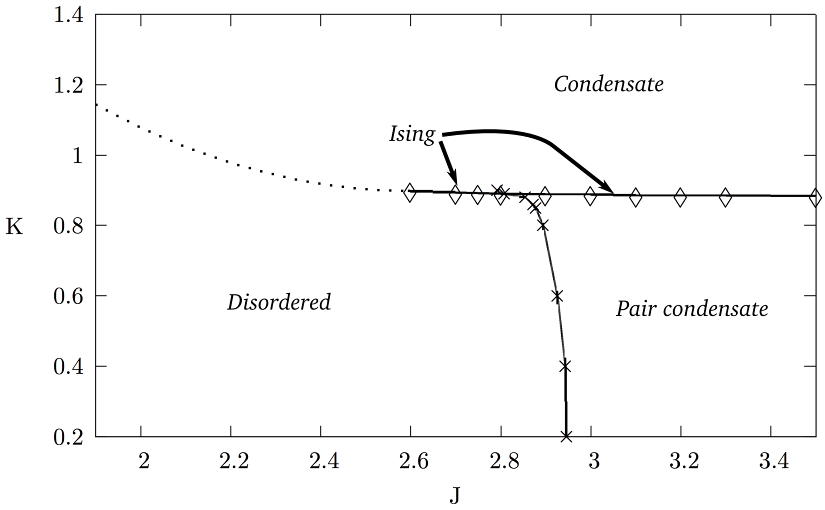
$$w(\theta) \equiv w_V(\theta) + e^{-K} w_V(\theta - \pi)$$

$$w_V(\theta) \equiv \sum_{p=-\infty}^{\infty} e^{-\frac{J}{2}(\theta + 2\pi p)^2} \propto \sum_{n=-\infty}^{\infty} e^{in\theta} e^{-\frac{J_*}{2} n^2}$$

$J_* = J^{-1}$

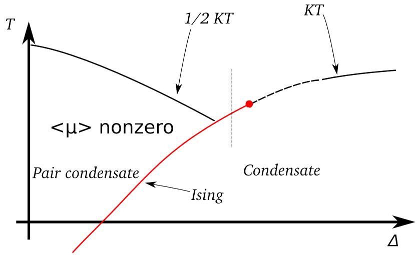


Numerical simulation using worm algorithm



Boson pairing and unusual criticality: summary

- We found an Ising transition where you'd expect an XY (KT) transition!



- The same phenomenon in 3D would be truly remarkable (true long-range XY order developing at an Ising transition)

Work underway

Spin 1 *microcondensates*

AL, Phys. Rev. A **83**, 033605 (2011)

Manifesto

- The order parameter of a BEC is a *macroscopic variable*
- For a BEC with spin, it should be some kind of *pendulum*

Outline

A very simple system

(Loading Asteroids)

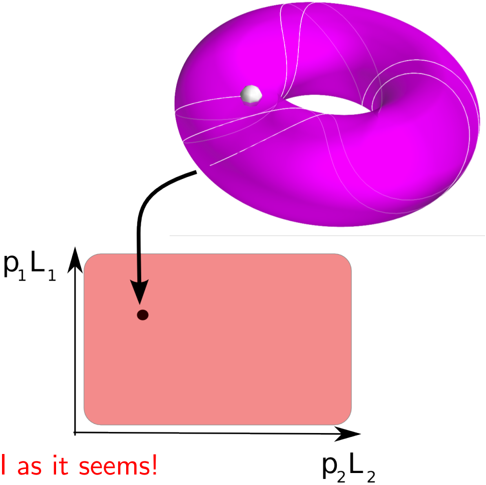
Periodic boundary conditions = motion on a *torus*

Quasiperiodicity: asteroid always hits spaceship!

(Loading torus)

Description of phase space

Phase space is a *product* $T^2 \times \mathbb{R}^2$



Not as special as it seems!

Action angle variables

Hamilton's equations for $H = E(p_1, p_2)$

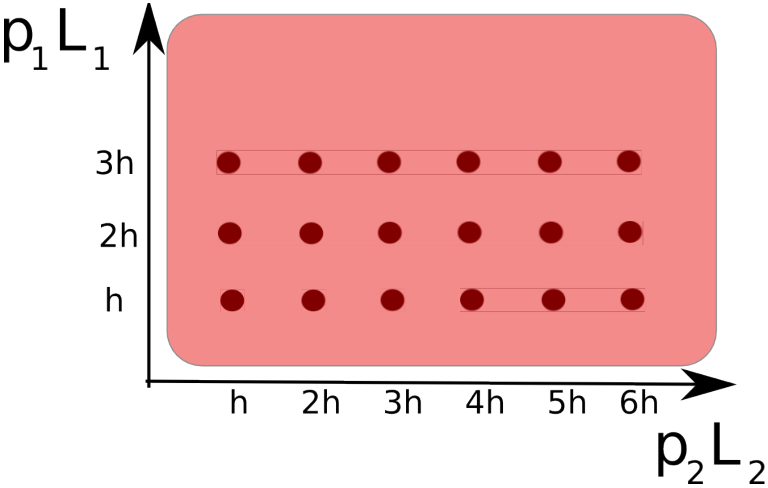
$$\dot{x}_1 = \frac{\partial H}{\partial p_1} = v_1$$
$$\dot{x}_2 = \frac{\partial H}{\partial p_2} = v_2$$

$\theta_i = \frac{2\pi x_i}{L_i}$ are angles on the torus obeying

$$\theta_i = \frac{2\pi v_i}{L_i} t + \mathrm{const}_i$$

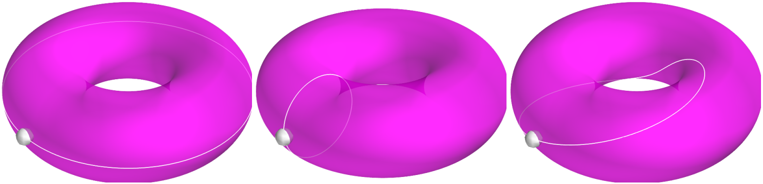
Simplest example of action $(p_1 L_1, p_2 L_2)$ angle (θ_1, θ_2) variables

Quantizing the system



Other choices are possible

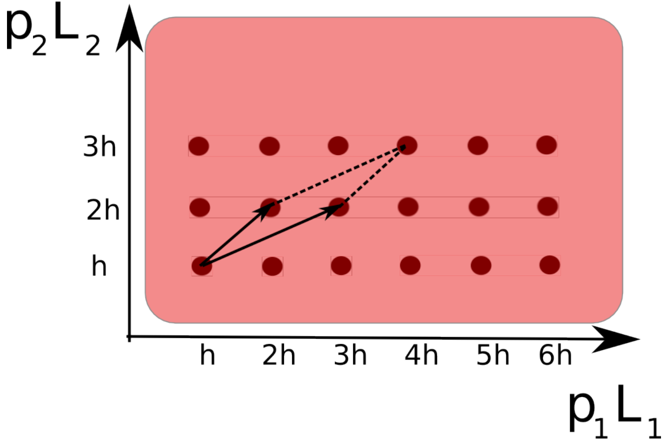
$$a(p_1 L_1) + b(p_2 L_2) \qquad a, b \in \mathbb{Z}$$



$(1,0)$ $(0,1)$ $(1,1)$

Different actions = different unit cells

$$\begin{pmatrix} l_1 \\ l_2 \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} p_1 L_1 \\ p_2 L_2 \end{pmatrix}$$



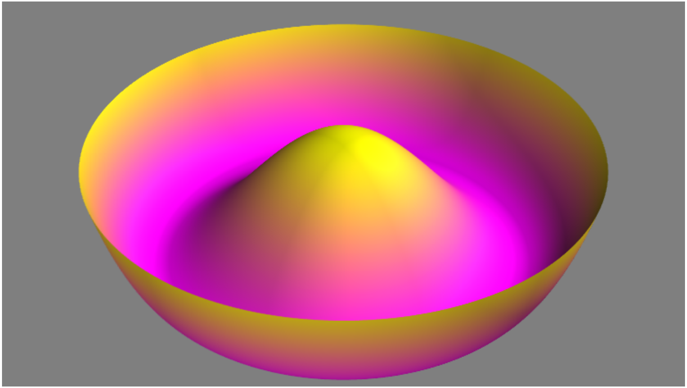
Outline


It's
Sombrero Time!

The Mexican hat

Consider the Hamiltonian for two dimensional motion

$$H = \frac{\mathbf{p}^2}{2} - \frac{\mathbf{r}^2}{2} + \mathbf{r}^4$$

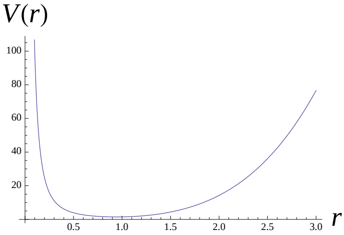


A natural approach – separate angular motion

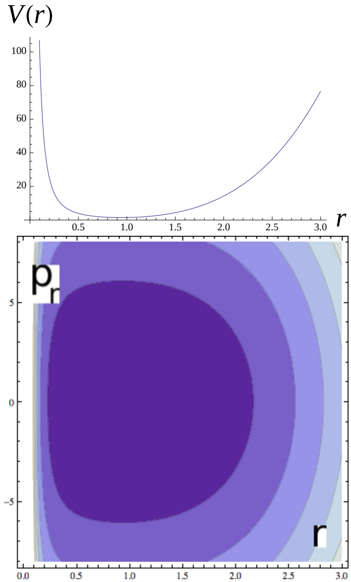
$$H = \frac{\mathbf{p}^2}{2} - \frac{\mathbf{r}^2}{2} + \mathbf{r}^4$$
$$= \frac{p_r^2}{2} + \frac{\ell^2}{2r^2} - \frac{r^2}{2} + r^4$$

$$\ell = xp_y - yp_x \qquad p_r = \frac{p_x x + p_y y}{r}$$

Defines potential for radial motion $V(r) = \frac{\ell^2}{2r^2} - \frac{r^2}{2} + r^4$



Phase plane for reduced motion



Phase space of integrable systems

This is an *integrable* system:

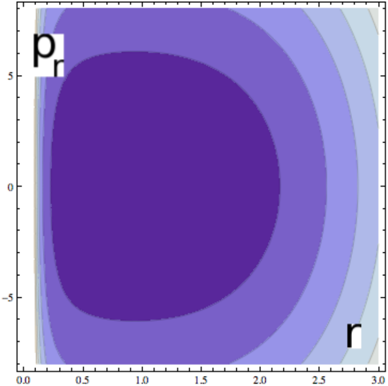
- 2 degrees of freedom and two integrals of motion (energy E, angular momentum ℓ). Motion lies on two dimension submanifold of four dimensional phase space.
- Closed trajectories for reduced motion in (r, p_r) plane, and angle θ in the (real) plane is cyclic coordinate

$$\dot{p}_\theta = 0 \longrightarrow p_\theta = \ell, \text{ const}$$
$$\dot{\theta} = -\frac{\partial H}{\partial \ell} = -\frac{\ell}{r^2}$$

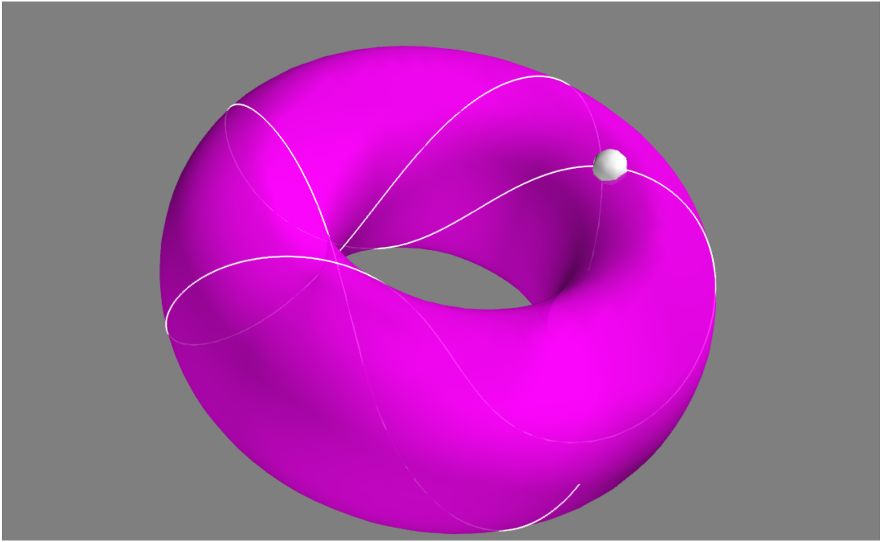
  (Note that θ motion is not trivial)
- The motion at fixed (E, ℓ) lies on a *torus*.

Motion on the torus

$$H_{\text{radial}} = \frac{p_r^2}{2} + \frac{\ell^2}{2r^2} - \frac{r^2}{2} + r^4$$



Motion on the torus



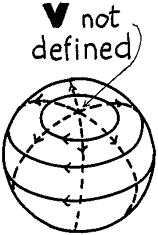
Quasiperiodic motion

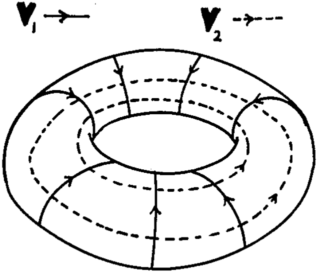
(Loading hat)

Action angle variables, and the Liouville–Arnold theorem

Liouville–Arnold theorem

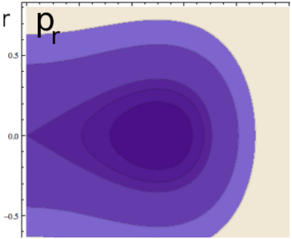
- For a system *integrable* in the above sense, can find N conjugate pairs of action-angle variables (I_i, ϕ_i), such that evolution of angles is trivial $\phi_i = \omega t + \phi_{i,0}$ $\dot{\phi}_i = \frac{\partial H}{\partial I_i}$
- Submanifold of phase space at fixed $\{I_i\}$ is N-Torus T^N

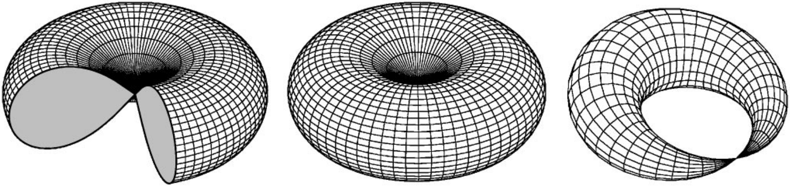




At a pinch...

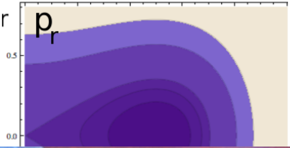
In the (ℓ, E) plane, there is a special point $(0, 0)$ where torus *pinches*

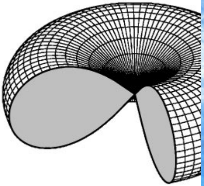


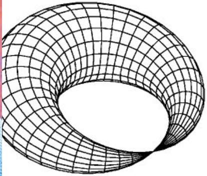


At a pinch...

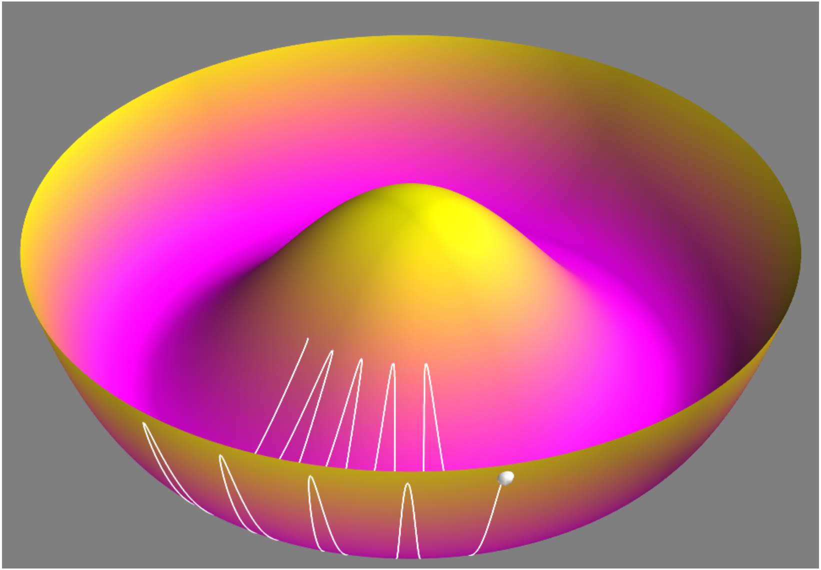
In the (ℓ, E) plane, there is a special point $(0, 0)$ where torus *pinches*



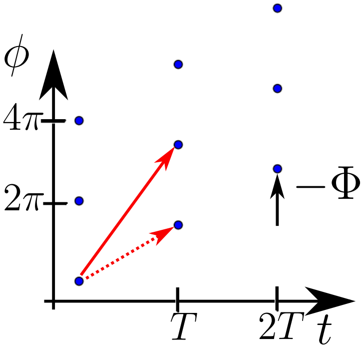


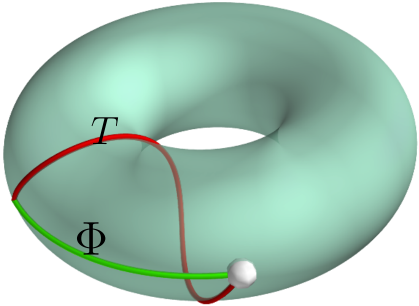


Rotation angle in the Mexican hat

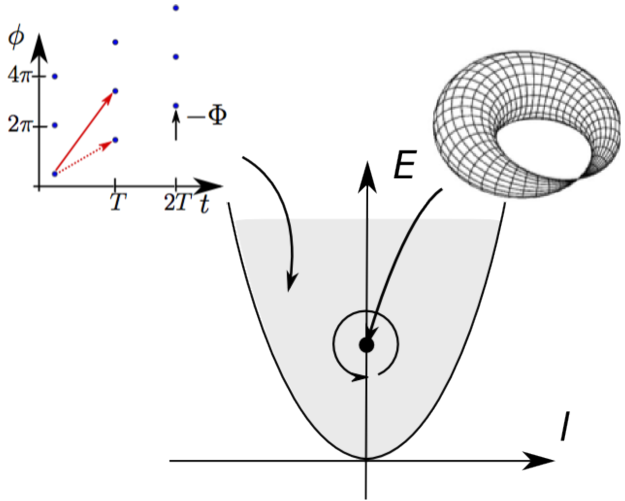


Rotation angle





Hamiltonian monodromy in a nutshell



Rotation angle increases by 2π as we circle the pinched torus

Some history

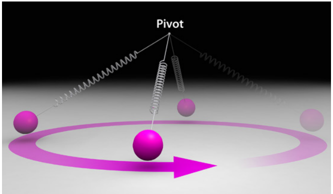
- 1673 Huygens finds period of spherical pendulum (20 years before Newton!)
- Classical mechanics: Newton, Euler, ... Hamilton ...
- 1980 Duistermaat discovers Hamiltonian monodromy, with the spherical pendulum a prominent example.
- 1988 Cushman and Duistermaat discuss signatures in quantum mechanics (no time today...)
- 1997 Molecular physicists become interested. Candidate systems are flexible triatomic molecules HAB, such as HCN, HCP, HClO.

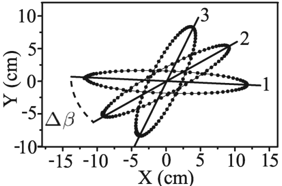
From another cold atom lab...

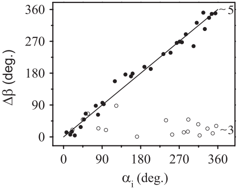
PRL **103,** 034301 (2009) PHYSICAL REVIEW LETTERS week ending 17 JULY 2009

Experimental Demonstration of Classical Hamiltonian Monodromy in the 1:1:2 Resonant Elastic Pendulum

N. J. Fitch,[1] C. A. Weidner,[1] L. P. Parazzoli,[1] H. R. Dullin,[2] and H. J. Lewandowski[1]
[1]*JILA and Department of Physics, University of Colorado, Boulder, Colorado 80309-0440*
[2]*School of Mathematics and Statistics, The University of Sydney, Sydney, NSW 2006, Australia*
(Received 7 April 2009; published 15 July 2009)







Outline

Spin 1 Bose condensates

Bose condensation: *macroscopic occupancy* of single-particle state

Spin 1 Bose condensates

Bose condensation: *macroscopic occupancy* of single-particle state

Q: But what if Bosons have spin?

Spin 1 Bose condensates

Bose condensation: *macroscopic occupancy* of single-particle state

Q: But what if Bosons have spin?

A: Macroscopic occupancy *and interaction* of different states

Spin 1 Bose condensates

Bose condensation: *macroscopic occupancy* of single-particle state

Q: But what if Bosons have spin?
A: Macroscopic occupancy *and interaction* of different states

Bosons just oscillator quanta
Macroscopic occupancy $\Longrightarrow$ Oscillators are (close to) classical

Spin-1 gas in the single mode approximation

$$H_{\mathrm{SMA}} = \frac{c_0}{2V} : \mathcal{N}^2 : + \frac{c_2}{2V} : \boldsymbol{\mathcal{S}} \cdot \boldsymbol{\mathcal{S}} : + H_{\mathrm{Z}}.$$

$$\mathcal{N} = \sum_{m=-1}^{1} a_m^* a_m \qquad \boldsymbol{\mathcal{S}} = \sum_{m,m'} a_m^* \mathbf{S}_{mm'} a_{m'}$$

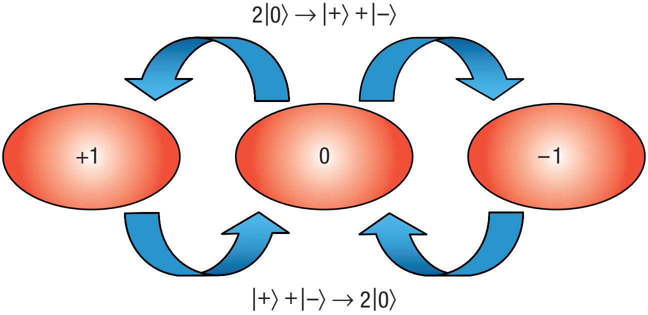
$\mathbf{S}_{mn}$ spin-1 matrices, and $H_{\mathrm{Z}} = \sum_m a_m^* \left[pm + qm^2\right] a_m$

$$h \equiv \frac{1}{2N^2}\left[\mathcal{S}_z^2 + 2\left(a_1^* a_{-1}^* (a_0)^2 + (a_0^*)^2 a_1 a_{-1}\right) + 2a_0^* a_0 \left(a_1^* a_1 + a_{-1}^* a_{-1}\right)\right] + \frac{\tilde{q}}{N}\left[a_1^* a_1 + a_{-1}^* a_{-1}\right].$$

$\tilde{q} = q/c_2 n$. h is energy per particle in units of $c_2 n$

Classical mechanics of the spin-1 gas

$$h \equiv \frac{1}{2N^2}\left[\mathcal{S}_z^2 + 2\left(a_1^* a_{-1}^* (a_0)^2 + (a_0^*)^2 a_1 a_{-1}\right) + 2a_0^* a_0 \left(a_1^* a_1 + a_{-1}^* a_{-1}\right)\right] + \frac{\tilde{q}}{N}\left[a_1^* a_1 + a_{-1}^* a_{-1}\right].$$



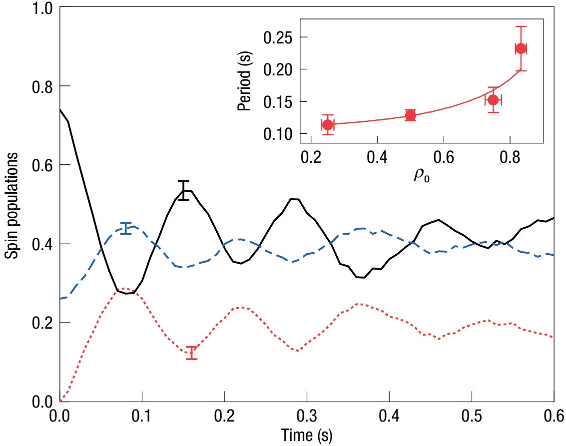
Classical mechanics of the spin-1 gas

There are three conserved quantities

1. The energy Nh
2. The angular momentum $\mathcal{S}^z$
3. The particle number $\mathcal{N}$

For a range of parameters this systems displays monodromy!

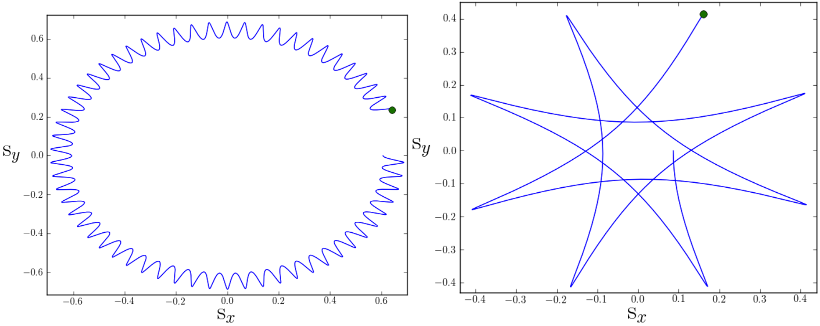
Single mode dynamics in experiment



Chapman group (GA Tech) with ^{87}Rb (2005)
Also Lett group (NIST) with ^{23}Na (2007)

Rotation angle in spinor condensates

Monitor evolution of perpendicular magnetization



Can be measured by Faraday rotation spectroscopy

Summary

In multicomponent quantum gases find *unusual phase transitions*

Yifei Shi, AL & Paul Fendley arXiv:1108.5744
Andrew James & AL PRL **106**, 140402 (2011)

...and *unusual dynamics*

AL, Phys. Rev. A **83**, 033605 (2011)