Statistical Mechanics and Dynamics of Multicomponent Quantum Gases

Austen Lamacraft

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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
Boson pairing and unusual criticality

- Yifei Shi, Austen Lamacraft and Paul Fendley
  arXiv:1108.5744
- Also Andrew James and Austen Lamacraft
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Statistical Mechanics of Boson Pairs

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Boson pair condensates
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Dynamics of Spinor Condensates

Geometry of phase space
Mechanics of the Mexican hat
Connection to spinor condensates
Why study phase transitions?

Amazingly, there is a sense in which the two problems are the same.
Why study phase transitions?

Amusingly, there is a sense in which the two problems are \textit{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 \( \langle M(x)M(y) \rangle = \frac{C}{|x-y|^{2\Delta}} \)
- Behavior is characteristic of *scale invariance*
From scale invariance to simple models
From scale invariance to simple models

Studying simple models is *a really good idea!*

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

\[
\beta \mathcal{H}_{\text{Ising}}[\sigma] = -J \sum_{\langle ij \rangle} \sigma_i \sigma_j
\]
Universality classes

Characterized by *broken symmetry* of order parameter\(^1\)
e.g. XY model

\[ \beta \mathcal{H}_{XY}[\theta] = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j) \]

\(^1\)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, $\lambda$-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

<table>
<thead>
<tr>
<th>Ising class</th>
<th>XY class</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Liquid-gas, binary mixtures,</td>
<td>• Easy plane magnets, (\lambda)-transition in (^4)He, superconductors, BEC,...</td>
</tr>
<tr>
<td>uniaxial magnetic systems,</td>
<td></td>
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<td>micellization,…</td>
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Beautiful classification…
Examples of 3D universality classes

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Beautiful classification...

Let’s try to break it!
Bose condensates and superfluids are XY systems

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

- Wavefunction $\Psi(r)$ 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 $q$)

$$v = \frac{\hbar}{m} \nabla \theta = \frac{\hbar}{m} \hat{e}_\theta$$
Vortices give a twist in 2D

Logarithmic interaction between vortices of charge $q_1$, $q_2$

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

2D density $n$
The Kosterlitz–Thouless transition

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

$$Z_{\text{pair}} = \int dx dy \exp \left[ -\beta V_{1,-1}(x - y) \right]$$

$$= \int \frac{dx dy}{|x - y|} \frac{\beta \pi \hbar^2}{2m}$$

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

- **Pair dissociates for**
  $$k_B T > k_B T_{\text{KT}} \equiv \frac{\pi n \hbar^2}{2m}$$

- **Pair bound for**
  $$T < T_{\text{KT}}$$
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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 $\rightarrow$ condensate breaks an Ising symmetry!$^2$

A simple model

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

Korshunov (1985), Lee & Grinstein (1985)

- \( \Delta = 0 \) is usual XY; \( \Delta = 1 \) is \( \pi \)-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)
Radzihovsky et al. (2004)
Geng & Selinger (2009)
James & AL (2011)
Ejima et al. (2011)
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How things change on the Ising critical line

Redo KT argument accounting for string

Domain wall terminates at *disorder operator* $\mu(x)$
How things change on the Ising critical line

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

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

$$Z_{\text{pair}} = \int dx dy \langle \mu(x)\mu(y) \rangle \exp \left[ -\beta V_{1/2,-1/2}(x - y) \right]$$

$$= \int \frac{dx dy}{|x - y|^{1/4} + \frac{\beta \pi n \hbar^2}{8m}}$$

Dissociation at higher temperatures than for ‘free’ half vortices
How things change on the Ising critical line

\[ T \]

\[ \langle \mu \rangle \text{ nonzero} \]

Pair condensate

Condensate

Ising

\[ 1/2 \, KT \]

\[ KT \]
Numerical simulation using worm algorithm

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

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

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

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

$$V(\theta_{ij})$$

$$J_* = J^{-1}$$
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 \textit{microcondensates}

Manifesto

- The order parameter of a BEC is a *macroscopic variable*
- For a BEC with spin, it should be some kind of *pendulum*
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A very simple system
Periodic boundary conditions $=$ motion on a torus

Quasiperiodicity: asteroid always hits spaceship!
Description of phase space

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

Not as special as it seems!
Action angle variables

Hamilton’s equations for \( H = E(p_1, p_2) \)

\[
\begin{align*}
\dot{x}_1 &= \frac{\partial H}{\partial p_1} = v_1 \\
\dot{x}_2 &= \frac{\partial H}{\partial p_2} = v_2
\end{align*}
\]

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

\[
\theta_i = \frac{2\pi v_i}{L_i} t + \text{const}_i
\]

Simplest example of action \((p_1 L_1, p_2 L_2)\) angle \((\theta_1, \theta_2)\) variables
Quantizing the system
Other choices are possible

\[ a(p_1 L_1) + b(p_2 L_2) \quad a, b \in \mathbb{Z} \]

(1, 0) \hspace{1cm} (0, 1) \hspace{1cm} (1, 1)
Different actions = different unit cells

\[
\begin{pmatrix}
  l_1 \\
  l_2
\end{pmatrix} = 
\begin{pmatrix}
  2 & 1 \\
  1 & 1
\end{pmatrix}
\begin{pmatrix}
  p_1 L_1 \\
  p_2 L_2
\end{pmatrix}
\]
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It's Sombrero Time!
The Mexican hat

Consider the Hamiltonian for two dimensional motion

\[ H = \frac{p^2}{2} - \frac{r^2}{2} + r^4 \]
A natural approach – separate angular motion

\[ H = \frac{p^2}{2} - \frac{r^2}{2} + r^4 \]

\[ = \frac{p_r^2}{2} + \frac{\ell^2}{2r^2} - \frac{r^2}{2} + r^4 \]

\[ \ell = xp_y - yp_x \quad p_r = \frac{p_x x + p_y y}{r} \]

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

\[ V(r) \]
Phase space of integrable systems

This is an *integrable* system:

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

\[ \dot{\theta} = -\frac{\partial H}{\partial \ell} = -\frac{\ell}{r^2} \]

(Note that $\theta$ motion is not trivial)

- The motion at fixed $(E, \ell)$ lies on a *torus*. 

\[ \dot{p}_\theta = 0 \implies p_\theta = \ell, \text{ const} \]
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
Action angle variables, and the Liouville–Arnold theorem

Liouville–Arnold theorem

• For a system \textit{integrable} in the above sense, can find \( N \) conjugate pairs of action-angle variables \((I_i, \phi_i)\), 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 \((\ell, E)\) plane, there is a special point \((0, 0)\) where torus *pinches*

\[
\begin{align*}
\ell & \quad E \\
\text{p} & \quad \text{r}
\end{align*}
\]
At a pinch...

In the \((l, E)\) plane, there is a special point \((0, 0)\) where torus *pinches*
Rotation angle in the Mexican hat
Dynamics of Spinor Condensates

In our case (an element of the group \( M \) where \( i \) is written as single-valued. The mapping of the period lattice vectors by Eq. (24) corresponds to angle variables that are not single-valued (though logarithmically diverging as we pass through the origin).

Each of these regions action-angle coordinates can be introduced without difficulty, although there are two regions that are distinguished by the presence of a singular limit (see Fig. 13). In each of these regions the phase space for \( \tilde{q} < 0 \) the action-angle coordinates may be expressed as an element of the 3-torus: we evolve for a time \( 2\pi \) and return to its original form, but after shifting the lattice one period of the reduced motion (see Fig. 14). Conversely the period lattice divides the phase space into two disjoint regions (see Fig. 13).

Rotation angle

![Rotation angle diagram](image)

The non-trivial mapping of the period lattice into itself is called the monodromy \( \Phi \). From Eq. (54), varying the overall phase of \( \Omega \) tells us how to execute a single period of the reduced motion on the pinched torus, the two components corresponding to the stable and unstable branches respectively. These correspondences are then associated with the three circles of the three-dimensional complex oscillator, as may be seen by defining \( \chi \equiv -\Phi \). What is special about the point \( \chi = 0 \) this corresponds to an 'inverted' focus-focus singularity – known as a focus-focus singularity – which is invariant under the action-angle coordinates.

By contrast the period lattice \( T \) may be expressed as an element of the 3-torus: we evolve for a time \( 2\pi \) and return to its original form, but after shifting the lattice one period of the reduced motion (see Fig. 14). Conversely the period lattice divides the phase space into two disjoint regions (see Fig. 13).

![Rotation angle diagram](image)
Hamiltonian monodromy in a nutshell

Rotation angle increases by $2\pi$ 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.
Experimental Demonstration of Classical Hamiltonian Monodromy in the 1:1:2 Resonant Elastic Pendulum


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Spin 1 Bose condensates

Bose condensation: *macroscopic occupancy* of single-particle state
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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 $\implies$ Oscillators are (close to) classical
Spin-1 gas in the single mode approximation

\[ H_{\text{SMA}} = \frac{c_0}{2V} : N^2 : + \frac{c_2}{2V} : \mathbf{S} \cdot \mathbf{S} : + H_Z. \]

\[ N = \sum_{m=-1}^{1} a_m^* a_m \quad \mathbf{S} = \sum_{m,m'} a_m^* \mathbf{S}_{mm'} a_{m'} \]

\( \mathbf{S}_{mn} \) spin-1 matrices, and \( H_Z = \sum_m a_m^* \left[ p m + q m^2 \right] a_m \)

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

\( \tilde{q} = q/c_2 n. \) \( h \) is energy per particle in units of \( c_2 n \).
Classical mechanics of the spin-1 gas

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

\[
2|0\rangle \rightarrow |+\rangle + |-\rangle
\]

\[
|+\rangle + |-\rangle \rightarrow 2|0\rangle
\]
Classical mechanics of the spin-1 gas

There are three conserved quantities

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

For a range of parameters this system displays monodromy!
Single mode dynamics in experiment

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