The XY model, the Bose Einstein Condensation and Superfluidity in 2d (I)

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LABORATORY FOR SIMULATION IN PHYSICS

A Guide to Monte Carlo Simulations in Statistical Physics”
by Landau & Binder


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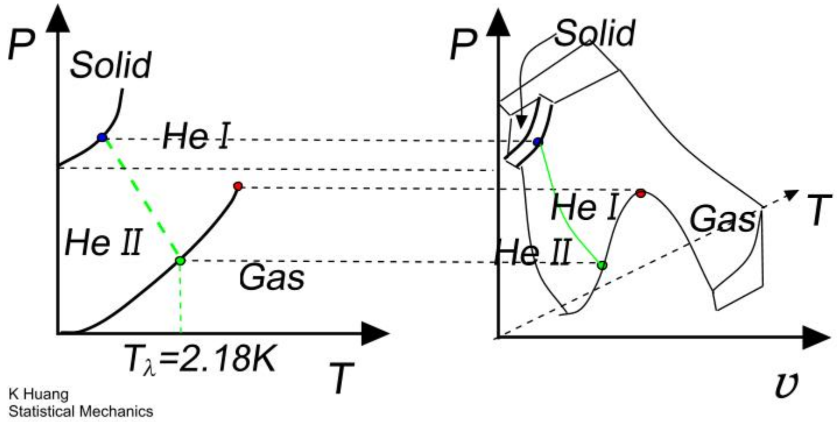
Outline

- Short introduction
- A 3d Ferromagnetic Model
  - Phase transition
- The ideal Bose gas
- The two dimensional world



Historic

The first superconductivity microscopic theory appeared in 1947 in a paper by Boliubov. The connection between BEC and superfluidity was stablished by Penrose and Onsager in 1956.

During the following decades, apart from the superfluidity in liquid Helium, the quest for new system with BEC was unsuccessful until the end of the 20th century when a fascinating series of experiments on Rubidium and Sodium demonstrated the existence of BEC in some materials. (Ketterle 2001 and Cornell and Wieman, 2002) .

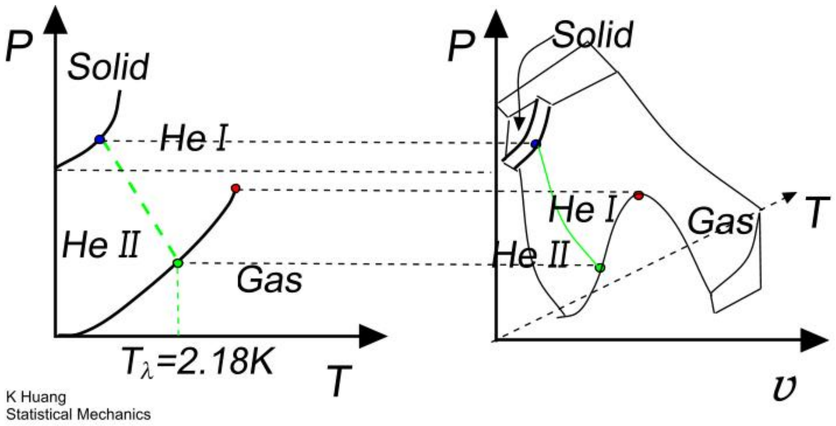
The realizations of BEC opened up the doors for new possibilities like dimensional transitions, crossover from BEC to BSC pair condensation and many others.

What is a Superfluid?

As the temperature is lowered, a many particle system generally undergoes a phase transition to a more ordered state. The existence of such ordered state requires the existence of an **order parameter**. Below the transition, certain fluctuations are correlated at long distances, and additional long-wavelength collective modes appear. To a broken symmetry is associated a Goldstone mode (A collective mode of low frequency for large wavelength).

Liquid Helium ($He^4 + He^3$) boils, under atmospheric pressure at 4.2K. It undergoes a phase transition from gas to liquid fase I . The temperature can be further lowered and the gas pressure reduced.

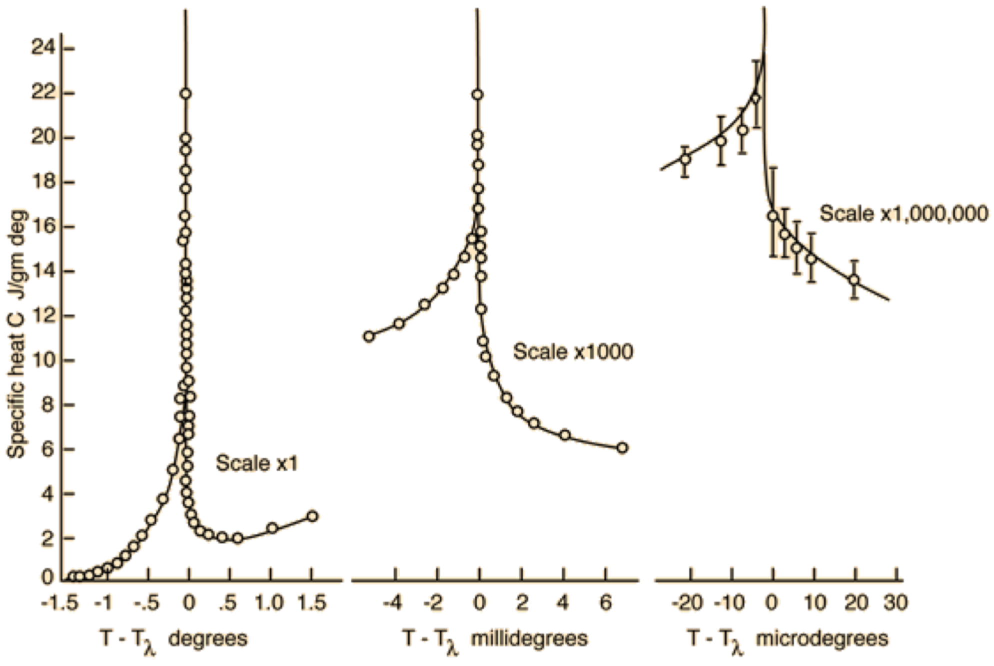
Initially we see the liquid bubbling wildly as temperature is lowered. Then, abruptly, there is no more bubbles! He^4 has underwent a transition to superfluid fase II at T_λ.



What is a Superfluid

Below a temperature $T_\lambda = 2.18K$, He^4 looks clear despite the pressure continuously is decreased. At T_λ He^4 becomes superfluid.

Below T_λ the bubbling stops because in He II temperature fluctuations propagates in waves, named a second sound. Second sound is a much more efficient way of spreading out local fluctuations of temperature than the slow heat diffusion process which acts in normal liquids. Therefore, superfluidity doesn't overheat locally, and thus there are no bubbles. All evaporation takes place at the surface.



Ferromagnetic Model

Before we start discussing the Bose condensate, we will make a digression to briefly discuss the 3d ferromagnetic Heisenberg model.

Let us consider an initially fully magnetized ferromagnet with spin S. Without lose of generality we assume the magnetization in the z direction.

For an isotropic ferromagnet the Heisenberg model with first neighbor is enough for us.

$$H = -J \sum_{\langle i,j \rangle} \hat{S}_i \cdot \hat{S}_j \quad ; \quad \mathrm{J} > 0$$

$$\hat{S}_i \cdot \hat{S}_j = S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z$$

$$= \frac{1}{2}\left(S_i^+ S_j^- + S_j^+ S_i^-\right) + S_i^z S_j^z$$

This system can be described in terms of the occupancy number $\hat{n}_i$

Ferromagnetic Model

In terms of the occupancy number $\hat{n}_i$

$$\langle n_i|S^x|n_{i+1}\rangle = \frac{1}{2}[(n_i+1)\ (2s-n_i)\ ]^{1/2}$$

$$\langle n_i|S^y|n_{i+1}\rangle = \frac{i}{2}[(n_i+1)\ (2s-n_i)\ ]^{1/2}$$

$$\langle n_i|S^z|n_{i+1}\rangle = s-n_i \qquad ,\ 0\ \leq n_i \leq 2s\ \ ,\ \hbar \equiv 1$$

The total number of states is $n_1 + n_2 + \cdots = (2s+1)^N$

In the low occupancy limit ($n_i \ll s$) we can make a harmonic approach…

Ferromagnetic Model
Harmonic Approach

The connection with the harmonic oscillator is obtained if we observe that an operator can be represented as

$$\mathcal{O}_{mn} = \int \psi_m^*(x_i)\,\hat{O}\psi_n(x_i)dx_i$$

Such that,

$$\langle n_i|x_i|n_i+1\rangle = \left[\frac{\hbar}{2m\omega}(n_i+1)\right]^{1/2}$$

$$\langle n_i|p_i|n_i+1\rangle = -i\left[\frac{\hbar m\omega}{2}(n_i+1)\right]^{1/2}$$

The quantum number is defined as the eigenvalue of the energy operator

$$\left\{\frac{1}{2m}p_i^2 + \frac{m\omega^2}{2}x_i^2 - \frac{1}{2}\hbar\omega\right\}|n_i\rangle = n_i\hbar\omega|n_i\rangle$$

Ferromagnetic Model
Harmonic Approach

Reescaling $x_i \; and \; p_i$ as

$$Q_i = x_i \left(\frac{m\omega}{\hbar}\right)^{1/2} \; ; P_i = x_i \left(\frac{1}{\hbar m\omega}\right)^{1/2} \; ; \; [P_i, Q_i] = -i\delta_{i,j}$$

So that,

$$\langle n_i | Q_i \sqrt{s} | n_{i+1} \rangle = \frac{1}{2}[(n_i + 1)\, 2s]^{1/2}$$

$$\langle n_i | P_i \sqrt{s} | n_{i+1} \rangle = \frac{i}{2}[(n_i + 1)\; 2s]^{1/2}$$

$$\left\langle n_i \middle| s - \frac{1}{2}\left(P_i^2 + Q_i^2 - 1\right) \middle| n_{i+1} \right\rangle = s - n_i$$

Those equations are the limit of the ferromagnet equations in the low occupancy limit.

Ferromagnetic Model Harmonic Approach

If we write

$$S_i^x = Q_i\sqrt{s} \quad ; S_i^y = P_i\sqrt{s} \quad ; \quad S_i^z = s - \tfrac{1}{2}\left(P_i^2 + Q_i^2 - 1\right) \quad ;$$

and substitute in the original Hamiltinian we get

$$H = E_0 - Js\sum\left(P_iP_j + Q_iQ_j\right) \quad ; \; where\; E_0 = -\frac{1}{2}NzJs^2$$

The operators can be written in terms of plane waves as

$$Q_i = \tfrac{1}{\sqrt{N}}\textstyle\sum_k Q_k\, e^{\boldsymbol{ik\cdot r}} \quad ; \quad P_i = \tfrac{1}{\sqrt{N}}\textstyle\sum_k P_k\, e^{\boldsymbol{ik\cdot r}} \quad ; \quad [Q_k, P_{k'}] = i\delta_{kk'}$$

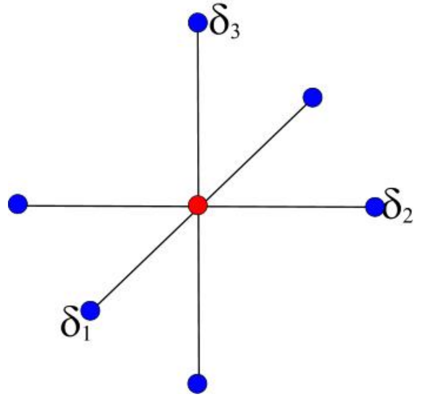
$$\boldsymbol{k} = k_x, k_y, k_z \quad ; \; k_m = \frac{2\pi}{L}m \quad ; \quad m = 0,1,2\ldots$$

Ferromagnetic Model
Harmonic Approach

With this transformation the Hamiltonian is diagonalized

$H = E_0 + \sum_k \frac{1}{2}(P_k P_k^+ + Q_k Q_k^+)\hbar\omega = \sum_k n_k \hbar\omega \quad ; n_k \, is\ the\ number\ operator\ and$

$\hbar\omega = Js\sum_\delta(1 - \cos \boldsymbol{k}\cdot\boldsymbol{\delta}) \cong Jsa^2k^2$



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$\boldsymbol{k} = k_x, k_y, k_z \quad ; \; k_m = \frac{2\pi}{L}m \quad ; \quad m = 0,1,2 \ldots$

Ferromagnetic Model Harmonic Approach

The order parameter (Magnetization, m) is estimated as

$$m = \sum_k m_k = Ns - s\left(\frac{L}{2\pi}\right)\int d^3k n\,(k) = Ns - s2\pi\left(\frac{L}{2\pi}\right)^3\left(\frac{1}{Jsa}\right)^{3/2}\int d\varepsilon\varepsilon^{1/2}n(\varepsilon) =$$

$$V\int d\varepsilon\rho(\varepsilon)n(\varepsilon) \quad ; \quad where\ \ \rho(\varepsilon)\ is\ the\ density\ of\ states$$

$$\rho(\varepsilon) = \left(\frac{1}{2\pi}\right)^2\left(\frac{1}{Jsa}\right)^{3/2}\varepsilon^{1/2}, which\ is\ the\ characteristic\ behavior\ in\ 3d.$$

Ferromagnetic Model
Harmonic Approach

A phase transition occurs when the symmetry is spontaneously broken

$$m = Ns - sV\int d\varepsilon\rho(\varepsilon)n(\varepsilon)\begin{cases}\neq 0 \; T < T_c \\ = 0 \; T \geq T_c\end{cases}$$

Using $n(k) = \frac{1}{(e^{\beta\varepsilon} - 1)}$ and integrating

$m = Ns\left[1 - \left(\frac{T}{T_c}\right)^{3/2}\right]$, Bloch's law (Valid only if $T \ll T_c$)

There are several sources of errors in this mean field approximation. In particular the magnon-magnon interaction completely destroy long range order in $d \leq 2$.

In 2 dimensions the situation is far more interesting!

We will turn back to this point latter.

The ideal Bose gas

The Hamiltonian for an ideal Bose gas can be written in second quantization as

$$H = \sum_k \left(\frac{\hbar^2 k^2}{2M} - \mu \right) c_k^+ c_k + \mu N$$

We observe that it has the same structure as the Ferromagnetic model except for the introduction of the chemical potential $\mu(\beta)$.

Let us consider N particles inside a box of volume $V = L^3$ so that,

$N = V \int d\varepsilon \rho(\varepsilon) \frac{1}{(e^{\beta(\varepsilon_k - \mu)} - 1)}$, $\rho(\varepsilon)$ has a typical 3d behavior: $\rho(\varepsilon) = \frac{1}{(2\pi)^2} \left(\frac{2M}{\hbar^2}\right)^{3/2} \varepsilon^{1/2}$

Bose–Einstein Condensation and Superfluidity
Lev Pitaevskii and Sandro Stringari, Oxford University Press.

The ideal Bose gas

Above T_c the occupation number is

$$N = C \int d\varepsilon (\varepsilon)^{1/2} \frac{1}{(e^{\beta(\varepsilon_k - \mu)} - 1)}$$

At T_c , $\mu = 0$

$N = \mathrm{C}(k_B T_c)^{3/2} I_{1/2}$ (Here C is a constant)

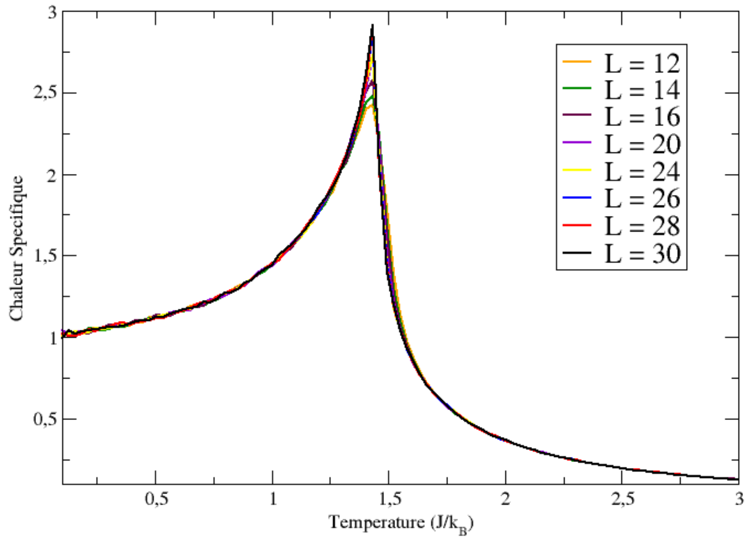
At low T we expect the state $k = 0$ becomes more populated as $T \rightarrow 0$.

A reasonable order parameter is the relative density of occupied states $\frac{n_0}{N}$ that behaves as

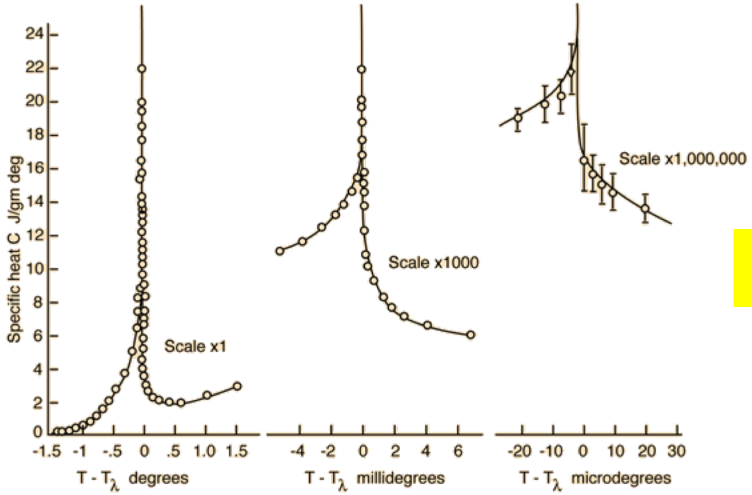
$$\sigma \equiv \frac{n_0}{N} = \left[1 - \left(\frac{T}{T_c}\right)^{3/2}\right]$$

The ideal Bose gas (superfluid)

The specific heat can be calculated above and below T_c



Heisenberg 3d. Simulation



Superfluid

Same universality class

The ideal Bose gas (superfluid)

Soon after the first observations, Fritz London proposed that Bose-Einstein condensation—the phenomenon in which bosons below a transition temperature accumulate into a single one-particle quantum state—might be responsible for superfluidity of liquid helium. Several decades elapsed before London's hypothesis got a direct experimental verification from the measurement of the momentum distribution by means of neutron scattering experiments: even at the lowest temperatures where the superfluid fraction is almost 100%, the strong correlations between the atoms forming the liquid deplete the population of the Bose-Einstein condensate state to only 10% of the total mass.

Iacopo Carusotto
https://physics.aps.org/articles/v3/5

Two Dimensions

What happens in two dimensions?

In this case we have $N = \mathrm{C}(k_B T_c) I_0$; $k_B T_c = \frac{N}{C I_0}$; $I_0 \; is \; a \; divergent \; integral$

This ensure that at finite T the system is in its normal phase, which is in accordance with the Mermin-Wagner theorem

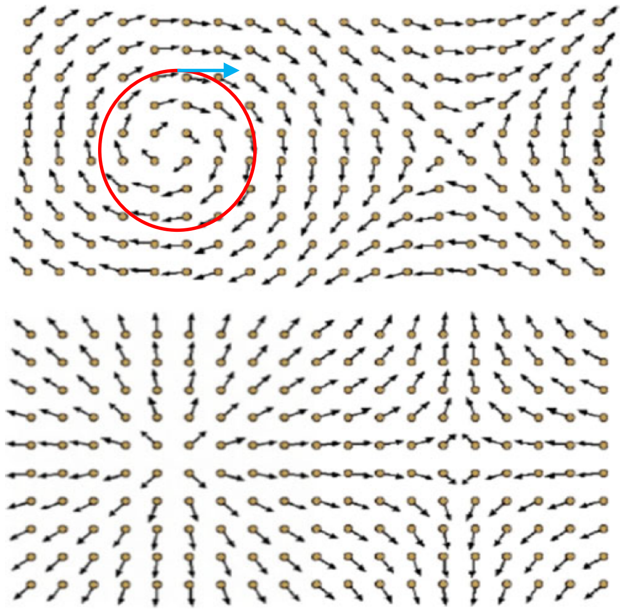
"In one and two dimensions, continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions."

Mermin, N. D., and Wagner, H. Absence of ferromagnetism or antiferromagnetism in one- or two-dimensional isotropic heisenberg models. Phys. Rev. Lett. 17, 22 (Nov 1966), 1133–1136.

Two Dimensions

Kosterlitz and Thouless made the supposition that a two dimensional system could support vortex excitations

V_1



V_2

Typical pair vortex-antivortex

Vorticity
$$\begin{cases} v_1 = \dfrac{1}{2\pi R}\oint \vec{S}.d\vec{s} = \pm 1 \\ v_2 = \dfrac{1}{2\pi R}\oint \left(\vec{S}\times d\vec{s}\right)_z = \pm 1 \end{cases}$$

Using the Stokes theorem

$$v_1 = \frac{1}{R}\int_0^R \left[\nabla\times\vec{S}\right]_z rdr$$

$$v_2 = \frac{1}{R}\int_0^R \left(\nabla\cdot\vec{S}\right) rdr$$

Two Dimensions

$$v_1 = \frac{1}{R}\int_0^R [\vec{\nabla}\times\vec{S}]_z\, r dr \;\rightarrow [\vec{\nabla}\times\vec{S}]_z = \pm\frac{1}{r} \rightarrow \frac{\partial S_x}{\partial y} - \frac{\partial S_y}{\partial x} = \pm\frac{1}{r}$$

$$v_2 = \frac{1}{R}\int_0^R (\vec{\nabla}\cdot\vec{S})\, r dr \rightarrow \vec{\nabla}\cdot\vec{S} = \pm\frac{1}{r} \rightarrow \frac{\partial S_x}{\partial x} + \frac{\partial S_y}{\partial y} = \pm\frac{1}{r}$$

$$\vec{S}^2 = S_x^2 + S_y^2 \;\rightarrow \frac{\partial S_x}{\partial x}\frac{\partial S_y}{\partial y} = \frac{\partial S_x}{\partial y}\frac{\partial S_y}{\partial x}$$

Considering the Planar Rotator Hamiltonian and its continuum version

$$\mathcal{H} = -J\sum \vec{S}_i\vec{S}_j \rightarrow -J\int h(x,y)\, dxdy$$

$$h = 1 - \frac{1}{4}\left[\left(\frac{\partial S_x}{\partial x}\right)^2 + \left(\frac{\partial S_x}{\partial y}\right)^2 + \left(\frac{\partial S_y}{\partial x}\right)^2 + \left(\frac{\partial S_y}{\partial y}\right)^2\right] = 1 - \frac{1}{4}[v_1^2 + v_2^2]$$

$$\rightarrow \quad \mathcal{H} - \mathcal{H}_0 = \pi lnR$$

Two Dimensions

The energy of a vortex is $\pi J lnR$

The entropy is just the number of ways the vortex can be distributed in the system lnR^2

The cost in free energy to create a vortex is

$$F = \pi J lnR - \mathrm{T} lnR^2 = (\pi J - T) lnR$$

The phase transition occurs when vortices are spontaneously created

$$(\pi J - T_{BKT}) = 0 \rightarrow T_{BKT} = \pi J$$

That is the essence of the BKT transition.

Of course there are corrections due to vortex-vortex, vortex-antivortex, vortex-magnons … interactions.

In the next lecture we will explore this in more details.

Thank you for your attention

Special thanks for this kind invitation

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