

## On the work of Thouless, Haldane, and Kosterlitz

“Topological” phases and phase transitions of matter

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# Boyle and Newton in the 1600s

- ▶ Boyle's gas law:

$$P \propto \frac{1}{V} \text{ at fixed } T$$

- ▶ Newton's law(s) of motion:

$$m \frac{dy}{dt} = F$$

$$\text{Force of gravity: } F_{12} = G \frac{m_1 m_2}{r_{12}^2}$$

Planetary motion understood...

Beginnings of the systematic study of physical properties of materials...  
& the science of mechanics...

# 1750-1850: Bernoulli, Dalton, Avogadro, Carnot, and Kelvin

- ▶ Bernoulli & Dalton: Gases made of invisible particles with definite mass (**atoms**)
- ▶ Avogadro: Some gases made of **molecules**  
**Ideal gas equation of state:  $PV = Nk_B T$**
- ▶ Carnot's Thermodynamics: Connecting heat content to work output (engines)  
**absolute temperature, free-energy  $F$ , entropy of substances...**

# Dynamics of atoms vs thermodynamics of gases

- ▶ Trajectories of  $10^{23}$  particles predicted by Newton's laws  
vs  
Thermodynamic concepts heat, temperature, entropy,  
free-energy?

Where is thermodynamics “hiding” inside the mechanistic view?

# Waterston\*, Maxwell, Boltzmann, Gibbs: Statistical mechanics (1850–1920s)

- ▶ Statistical description of macroscopic aggregates of atoms  
Each microscopic configuration  $C \equiv \{v_i, x_i\}$  arises with probability

$$\text{Probability}(C) = \frac{\exp(-E(C)/k_B T)}{Z},$$

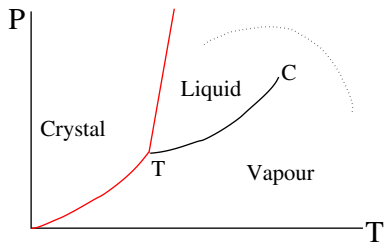
$$\text{where } Z = \sum_C \exp(-E(C)/k_B T)$$

- ▶ Free energy  $F = -k_B T \log(Z)$   
(For ideal of atoms :  $E = \sum_i \frac{mv_i^2}{2} + \sum_{i,j} V(x_i - x_j)$ )



\* Grant College Bombay, circa 1860

# Ordered phases and phase transitions of matter



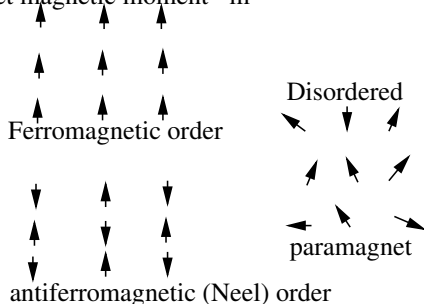
- ▶ Phase transformation from fluid to ordered crystalline phases
- ▶ Always involves crossing line of singular thermodynamic behaviour

Can statistical mechanics describe such ordering phenomena?

# Another example: Ordering of magnetic moments in ionic solids

Intrinsic spin angular momentum of ions quantized in half-integer units ( $|\vec{S}| = k/2$ ). Magnetic moment  $\vec{m}_{ion} = 2\mu_B\vec{S}$

Net magnetic moment  $\vec{m}$



Apparent “paradox”:  $\text{Prob}(C_{\vec{m}=\uparrow}) = \text{Prob}(C_{\vec{m}=\downarrow})$  by **symmetry** of  $E$   
( $E = J \sum_{rr'} \vec{S}_r \cdot \vec{S}_{r'} - A \sum_r (\vec{S} \cdot \hat{n})^2$ )

$\langle \vec{m} \rangle = 0$  by **Gibbs prescription**

# Onsager, Anderson: Spontaneously broken symmetry and fluctuation modes

- ▶ Resolution of “paradox”: Timescale to change direction of  $\vec{m}$  diverges with system size.  
“Spontaneous symmetry breaking” and long-range order in “thermodynamic limit”
- ▶ Real question: Do small-angle, long-wavelength fluctuations destabilize order?

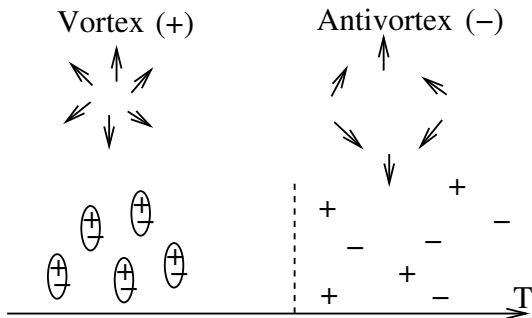


# Peierls, Mermin-Wagner: Role of spatial dimension and magnetic anisotropy

- ▶ Peierls: In easy-axis limit ( $A > 0$ ), long-range order possible in planar structures ( $d = 2$ ), and three-dimensional materials, but not in chain-like structures ( $d = 1$ )
- ▶ Mermin-Wagner: Without anisotropy ( $A = 0$ ), or with easy-plane anisotropy ( $A < 0$ ), long-range order possible in  $d = 3$ , but not  $d = 2$  or  $d = 1$

Long-range magnetic order only possible in sheet-like materials if magnetic moments can only point up or down along fixed axis (eliminates small-angle fluctuations)

# Kosterlitz-Thouless: Vortex-binding transition in $d = 2$ easy-plane case



$\langle \vec{m}(r) \cdot \vec{m}(r') \rangle \sim \exp(-|r - r'|/\xi)$  for  $T > T_{KT}$  (paramagnet)

$\langle \vec{m}(r) \cdot \vec{m}(r') \rangle = \frac{C}{|r - r'|^\eta}$ ,  $\eta \in (0, \frac{1}{4})$  for  $T < T_{KT}$  (Power-law ordered)

# Distinction is “topological”

- ▶ KT transition is transition between “ionized plasma” of single vortices and neutral gas of vortex-pairs
- ▶ Distinction has a “topological” flavour to it:  
Can count number of isolated vortices (signed sum) in region by simply looking at winding of moments along the boundary

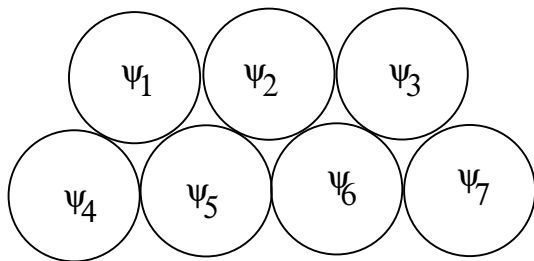
Connection to superfluid/superconducting thin films?

# Enter: Quantum mechanics

- ▶ **Linear superposition of alternatives:**  $a|\uparrow\rangle + b|\downarrow\rangle$
- ▶ Trajectories replaced by sum over paths, weighted by  $\exp(iS)$  for each path  $S = \int dt \left( \frac{m}{2} \left( \frac{dx}{dt} \right)^2 - V(x) \right)$
- ▶ Particles behave like waves in some ways

# From Superfluids/superconductors to magnets with easy-plane anisotropy

Superfluid grains



Each grain  $r$  is in state  $|\psi_r\rangle \sim \sum_{n=0}^{\infty} \frac{\psi_r^n}{\sqrt{n!}} |n\rangle$

$|n\rangle$ : State with exactly  $n$  particles in grain

$$E = -J \sum_{rr'} (\psi_r^* \psi_{r'} + \psi_{r'}^* \psi_r)$$

$\psi = |\psi| e^{i\theta} \rightarrow \vec{m}$  with easy-plane anisotropy

# Consequence: Thin-film superfluidity

- ▶  $\langle \psi^*(\mathbf{r})\psi(\mathbf{r}') \rangle \sim 1/|\mathbf{r} - \mathbf{r}'|^\eta$
- ▶ Superfluid fraction  $\rho_s \propto \eta$
- ▶  $\rho_s/(k_B T_{KT}) = 2m^2/\pi\hbar^2$   
Observable universal jump in superfluid fraction  
(Nelson-Kosterlitz)

# Haldane: Quantum mechanics of linear chains of magnetic moments:

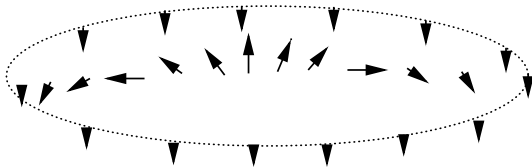
- ▶  $E = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1}$  with  $J > 0$

Recall: Intrinsic spin angular momentum of ions quantized in half-integer units ( $|S| = k/2$ ). Magnetic moment  $\vec{m}_{ion} = 2\mu_B \vec{S}$

- ▶ Quantum-mechanics: Trajectories replaced by sum over histories
- ▶ Best formulated in terms of Neel vector  $\vec{N}_i \propto \vec{S}_i - \vec{S}_{i+1}$  with  $|\vec{N}_i| = 1$   
 $\vec{N}$  varies slowly with  $i$ : Continuum approximation valid  $\vec{N}_i \rightarrow \vec{N}(x)$
- ▶ Weight of trajectory is  $\exp(iS)$  with 
$$S = \int dt \int dx \left[ \left( \frac{d\vec{N}}{dt} \right)^2 - \left( \frac{d\vec{N}}{dx} \right)^2 \right] + S_B$$

$S_B$ : Depends only on “topology” of  $\vec{N}(x, t)$

‘Wrapping number’ of  
Maps from  $(x, t)$  to  $N$



$S_B = \pi k Q[\vec{N}]$ , where  $Q = \frac{1}{4\pi} \int dx dt \vec{N} \cdot \left( \frac{d\vec{N}}{dx} \times \frac{d\vec{N}}{dt} \right)$  counts “wrapping number” of configuration



# Consequences

- ▶ Chains with  $S = 1$  (e.g.  $\text{Ni}^{2+}$ ) have exponentially small low-temperature susceptibility and specific heat
- ▶ Chains with  $S = 1/2$  (e.g.  $\text{Cu}^{2+}$ ) have much higher susceptibility and specific heat  
In fact, power-law ordered
- ▶ “Topologically protected” boundary spin  $S = 1/2$  moments in integer spin chains cut by non-magnetic impurities: Seen directly in NMR experiments.  
“Topological protection” Presence of free spin  $S = 1/2$  at chain-ends is totally independent of details of crystal structure and energetics

# Thouless-Nightingale-Kohmoto-Den Nijs, Haldane: Winding of wavefunctions

- ▶ Electron waves in “diffraction grating” created by regular crystalline arrangement of ionic cores
- ▶ Described by wavefunctions arranged in groups called bands
- ▶ **Winding number of band “wavefunction”  $u$  of electrons determines Hall-voltage**

- ▶ **Result: Hall conductivity  $\sigma_H = ne^2/h$**

$$n = \frac{1}{2\pi} \int d^2k B(\vec{k}) \text{ where } B = \frac{dA_y}{dk_x} - \frac{dA_x}{dk_y} \text{ with } A_j = i \langle u_k | \frac{d}{dk_j} | u_k \rangle$$

Not pictorially obvious: But counts “winding number”  $n$  of wavefunction

# Impact

- ▶ Inspiration for sustained efforts to expand our classification of phases of matter, beyond “obvious” distinctions of spontaneously broken symmetry and long-range order
- ▶ Much known by now about topologically distinct phases of matter and transitions between them
- ▶ **Most remarkably: Purely theoretical ideas playing key role in understanding new materials**  
e.g. “topological insulators” with “protected” surface states