

Condensed Matter Physics 3

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Part I

Symmetry, Structure, and Excitations

Lecture 1

use alongside lecture notes given

Chapters in this don't always coincide to lectures - missed a few

- Solid:
 - ➡ Can support shear stress
 - ➡ Doesn't flow
- Liquid:
 - ➡ Incompressible
 - ➡ Can't support shear stress
 - ➡ Flows the fill volume, subject to remaining pressure
 - ➡ Weaker forces ($\approx k_B T$)
 - ➡ Less dense atoms/molecules

A gas, liquid, or amorphous solid is rotationally invariant

N particles in a shell, what is $g(r)$?

$$g(r) = \frac{N}{4\pi r^2 \delta r \langle n \rangle} \quad (1.1)$$

For an ideal gas (point particles), $g(r)$ is just 1:

- $\int_V \langle n \rangle g(r) dV = (N' - 1)$
- $\langle n \rangle V g(r) = (N' - 1) \implies g(r) = 1 - \frac{1}{N'}$
- Despite rigidity of ice, it can be seen to flow.
- For enough stress, it will plastically deform (creep).
- "Enough" is about 5 orders of magnitude less than expected for a perfect crystal.
- Ice flows due to the motion of topological defects called dislocations. Electrons can scatter off them too.
- The pdf does not enable us to easily distinguish between a liquid and amorphous solid. The difference is one of timescale for flow.
- Therefore an arbitrary definition: "A solid is a material whose shear viscosity exceeds $10^{13.6} N s m^{-2}$ "
- this corresponds to a relaxation time of about a day

Lecture 2

2.1 Bonding in Condensed Matter

In general, inter-particle interactions produce a potential with the same type of form, usual potential well plot with repulsive and attractive forces. **image here from notes**

2.1.1 van der Waals bonding

Fluctuations (instantaneous in time) can lead to instantaneous dipole moments. Such dipoles create an electric field:

$$E = \frac{p_1}{4\pi\epsilon_0 r^3}, \quad (2.1)$$

where p_1 is the fluctuating dipole. On a neighbouring atom, this field induces a dipole,

$$p_2 = \alpha|E| \quad (2.2)$$

$$p_2 = \alpha \frac{p_1}{4\pi\epsilon_0 r^3} \quad (2.3)$$

where α is the atomic polarisability. We have a dipole-dipole potential:

$$U(r) = \frac{|p_1||p_2|}{4\pi\epsilon_0 r^3} = \frac{\alpha|p_1|^2}{(4\pi\epsilon_0)^2 r^6} \quad (2.4)$$

Note that $|p_1|^2$ does not average to zero even though p does, which implies that $U(r) \neq 0$.

If we have attractive interactions alone, our solid would collapse into a singularity. We need repulsion as well. Repulsion arises from the Pauli exclusion principle - no electrons (fermions) can have the same set of quantum numbers. Born and Mayer parameterised this repulsion as

$$U_{rep} = B_{ij} \exp -\frac{r_{ij}}{p_{ij}} \quad (2.5)$$

where r_{ij} is distance between atom i and j . p_{ij} and B_{ij} are constants.

Buckingham potential - Historically, a potential varying as r^{-n} is easier to deal with and reasonably reproduces f^n form. Lennard-Jones potential constants ϵ and σ - parameters which can be found by experiment

2.1.2 Ionic Bonding

When it's energetically favourable to transfer one or more electrons to a neighbour to achieve a closed shell configuration.

$U_{Madelung}$ is attractive interaction per mole of formula unit.

Born-Mayer is very short-ranged

2.1.3 Metallic bonding

Metallic bonding results from delocalisation of electrons.

The coulomb energy (attractive) can be found from a lattice sum (with negative charge background) and is $\propto \frac{1}{r}$. Two results from FoP2B are required to understand the electronic contribution to energy. The average energy electron is

$$\frac{E}{n} = \frac{3}{5} E_F = \frac{3\hbar^2 k_F^2}{10m_e} \quad (2.6)$$

$$k_F = \left(3\pi^2 \frac{N}{V}\right)^{1/3} \quad (2.7)$$

$$k_F \propto V^{-1/3} \quad (2.8)$$

$$\implies \frac{E}{n} \propto r_0^{-2} (\because V \propto r_0^3) \quad (2.9)$$

$$U_{metal} = U_{coul} + U_{kin} \quad (2.10)$$

$$= -\frac{a}{r_0} + \frac{b}{r_0^2} \quad (2.11)$$

Metallic crystal cohesive energy is of order of a few eV per atom.

Lecture 3

check DUO for these

Lecture 4

Thomson formula:

$$\frac{d\sigma}{d\Omega} = r_e^2 \frac{1 + \cos^2 \theta}{2} \quad (4.1)$$

Scattering amplitude

$$\langle k' | V | k \rangle = \langle k' | r_e(r) | k \rangle \quad (4.2)$$

- Introduce $q = k' - k$, note vector relation, the scattering wavevector
- Fourier transforms used - atomic scattering factor (scattering potential of each atom, summed over all)
- $I(q)$ depends on structure, $|f_a|^2$ depends on atoms
- $\frac{I(q)}{N} = S(q)$ - the target structure factor

4.1 Xray scattering and pair distribution

- Assume homogeneous material, translationally variant
- There is a '-1' due to avoidance of counting "oneself" - reference atom
- $\langle n(x_i) \rangle = \langle n(x_2) \rangle = n$

4.2 Xray scattering in periodic lattice

The expression

$$I(q) = \sum_{j,l} \langle e^{iq \cdot R_{jl}} \rangle \quad (4.3)$$

$R_{jl} = R_j - R_l$. Summing over all atoms yields N^2 terms. If $R_j - R_l$ is random, this sums to 0 as $N \rightarrow \infty$. Therefore, for non-zero $I(q)$, we must have $q \cdot R_{jl} = 2m\pi$ where m integer.

We can express the lattice points in terms of three basis vectors.

$$R_{jl} = U\underline{a} + V\underline{b} + W\underline{c} \quad (4.4)$$

Since $R_j - R_l$ must be a lattice vector.

For non-zero $I(q)$, let's define a set of vectors $\underline{a}^*, \underline{b}^*, \underline{c}^*$.

Atoms in the unit cell for the convolution

Written Fourier transform of lattice. For electrons in an atom, we have shown above that F.T. is atomic scattering amplitude, f_j . An atom at position r_j in a unit cell can be represented as delta fn, which has F.T. exp. For more than one atom in unit cell, can sum over them so last two terms in F(structure) become

$$\sum_j f_j e^{iq \cdot r_j} \quad (4.5)$$

We can write position of atoms within the unit cell in fractional coordinates.

Lattice is only non-zero when $q = G_{hkl}$. We can therefore write the lattice structure factor

$$F(hkl) = \sum_j f_j(q) e^{2\pi i(hx + ky + lz)} \quad (4.6)$$

Lecture 5

$$\underline{k} \cdot \underline{G} = \sin \theta = -\underline{k}' \cdot \underline{G} \quad (5.1)$$

$$G = \frac{2\pi}{\lambda} \Delta k \quad (5.2)$$

$$|G| = \frac{2\pi}{\lambda} (2 \sin \theta) \quad (5.3)$$

$$\lambda = 2 \left(\frac{2\pi}{|G|} \right) \sin \theta \quad (5.4)$$

$$= 2d \sin \theta \quad (5.5)$$

Lecture 6

- Neutron scattering factors can allow access to information complementary to xray scattering (very little angular dependence in b_i due to small size of nucleus)
- Point symmetry operations are those carried about a point, they do not involve translation
- The identity operation is given the symbol 1 in "International Notation". [However, in Schoenflies Notation, it has the symbol E.]
- An n-fold rotation axis exists if a rotation of $360/n$ brings an object back into coincidence with itself.
- *see notes for images of rotation axes*
- *see notes for various rotation stuff*
- Rotoinversion axes consist of two steps:
 1. Rotation, followed by
 2. Inversion

An n-fold rotoinversion axis is given the symbol \bar{n} . The simplest rotoinversion axis is $\bar{1}$ - the centre of inversion symmetry.
- In practice, we find that we need to combine symmetry operations. Consider a mirror plane which is perpendicular to a 2-fold rotation axis.
- Combinations can generate other symmetry operations.
- Note that you don't need commutativity - AB not necessarily equal to BA

Lecture 7

7.1 Lattices and Symmetry

Recall from section 2.1.5, Lecture 4, we can define translation vectors $\underline{a}, \underline{b}, \underline{c}$ and that these enable us to mathematically define a lattice.

$$\mathcal{L}(\underline{r}) = \sum_{u,v,m} \delta(\underline{r} - (U\underline{a} + V\underline{b} + W\underline{c})) \quad (7.1)$$

We can use these vectors to define a parallelepiped with sides a, b, c (moduli of vectors) and angles α, β, γ .

Symmetry imposes constraints on our choice of basis, or lattice, vectors $\underline{a}, \underline{b}, \underline{c}$. In the above case the 4-axis (conventionally along c) means that $a = b$ and $\alpha = \beta = \gamma = 90^\circ$.

For a lattice with mirror plane:

One axis must be perpendicular to mirror plane (let's define as \underline{c}). Other two axes must be in the plane of the mirror. This constrains us to $\alpha = \beta = 90^\circ$.

Once we build a 3D crystal by stacking planes something something something he moved the slides away

7.2 The 14 Bravais Lattices

It's often useful to consider non-primitive unit cells (cells with more than one lattice point) so that we can group structures of similar defining symmetry. The complete set of lattices which can be derived from our 7 crystal systems are the 14 Bravais lattices.

These lattices are labelled as followed:

- P - primitive
- I - body-centred
- F - face-centred (for all faces)
- R - rhombohedral
- A,B,C - face-centred (on one face A, B, or C only)

A crystal structure is generated by placing a group of atoms or molecules - a motif (or basis) - at each lattice point. This is a convolution.

$$\mathcal{L}(\underline{r}) * \text{motif} \quad (7.2)$$

Motif being the positions given by fractional co-ordinates within cell.

7.3 Translation Symmetry and Space Groups

A screw axis involves a $\frac{360^\circ}{n}$ rotation followed by translation along the axis by a fraction of a lattice vector, $\frac{1}{t}$. This is labelled

$$n_m, m = \frac{n}{t}, n = \text{rotation axis} \quad (7.3)$$

Screw axis shown is a 2_1 axis.

We can have a,b,c glide planes where the label indicates the direction of translation. We can also define an n-glide which involves translation along $\frac{1}{2}(\underline{a} + \underline{b})$ and a d-glide (diamond glide) which involves translation along the diagonal of the unit cell.

We label the space group of a crystal by combining the symbol for the conventional lattice with the symbols for the symmetry operations, e.g. the face-centred cubic structure with full symmetry would

be:

$$Fm\bar{3}m \quad (7.4)$$

Consider a rhombohedral crystal, with: an n-glide plane along (100); a mirror with reflection in (010); and an a glide with reflection in (001). This would have space group

$$Pnma. \quad (7.5)$$

7.4 Symmetry and Diffraction

Recall our expression for the lattice structure factor (Lecture 4, Section 2.1.5)

$$F(hkl) = \sum_{\text{unit cell}} f_j(\underline{q}_{hkl}) e^{2\pi i(hx_j + ky_j + lz_j)} \quad (7.6)$$

By inspection, for real f_j , $F(\bar{h}, \bar{k}, \bar{l}) = F^*(hkl)$. In a scattering experiment, we detect $|F|^2$, and $|F(hkl)|^2 = |F(\bar{h}\bar{k}\bar{l})|^2$, i.e. all diffraction patterns (where there's no anomalous scattering) have a centre of symmetry. This means that the point group symmetry measured - the Laue symmetry is the real symmetry plus a centre of inversion.

Note: several further lectures after this that I didn't attend, check duo

Part II

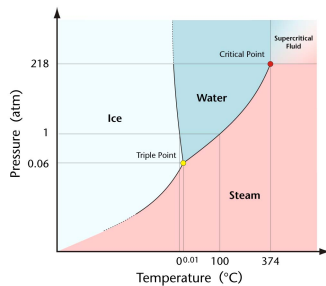
Broken Symmetry

Lecture 1 Introduction to Broken Symmetry

- Standard Tom Lancaster style - take note of what he does on visualiser, also check slides but not as important

1.1 Phase diagram of water

1. Solid to liquid - symmetry is changed
 2. liquid to gas - no change in symmetry (can avoid discontinuity)
- Distinguish two types of transition - no critical end point on melting curve
 - For many phenomena, symmetry is broken (lowered) at a critical temperature, T_c



Make this side on

1.2 Landau Theory of Phase Transitions

Free energy:

$$F = U - TS \quad (1.1)$$

$$M = \text{magnetization} \frac{\text{magnetic moment}}{\text{volume}} \quad (1.2)$$

$$F = F_0 + aM^2 + bM^4 + \dots \quad (1.3)$$

With no odd powers, this has a symmetry

$$M \rightarrow -M \quad (1.4)$$

$$F(M) = F(-M) \quad (1.5)$$

This is a symmetry - a Z_2 symmetry

Plot a graph of it in either a rough parabola or cubic function centred on 0, depending on whether $a, b, M >, <, = 0$.

$$\frac{\partial F}{\partial M} = 2aM + 4bM^3 = 0 \quad (1.6)$$

$$\text{Minima at } M = 0 \quad (1.7)$$

$$\text{Minima at } M^2 = \frac{-a}{2b} \quad (1.8)$$

Take $a = a_0(T - T_c)$, changes sign at T_c :

$$a_{+ve} \rightarrow T > T_c \quad (1.9)$$

$$a_{-ve} \rightarrow T < T_c \quad (1.10)$$

$$M = \pm \left[\frac{a_0}{2b} (T_c - T) \right]^{1/2} \quad (1.11)$$

Model has predicted a phase transition at T_c .

- We define the 'order parameter':

$$\text{Order parameter} = \begin{cases} 0 & T > T_c \\ \neq 0 & T < T_c \end{cases} \quad (1.12)$$

(Magnetization for a magnet)

- Impossible to change symmetry gradually - phase transitions are too sharp
- System can break symmetry in > 1 way(s).
- Consequences of broken symmetry:
 - ➡ Phase transitions
 - ➡ Rigidity
 - ➡ Excitations
 - ➡ Defects

Lecture 2

Lecture 3

3.1 Models and Dimensionality

- Model a system as spins on a lattice
- Hamiltonian,

$$H = \sum_{\langle ij \rangle} (-J_{ij}) \underline{S}_i \cdot \underline{S}_j \quad (3.1)$$

- $J > 0$: ferromagnetism is most likely
- D - dimensionality of the spin
- $D = 1$, $S_z = \pm 1$ - known as Ising models
- $D = 2$, S_x, S_y - XY model
- $D = 3$, S_x, S_y, S_z - Heisenberg model
- d - dimension of the lattice
- **Example:** $d = 1, D = 1$ (1d Ising model)
 N spins, up - each one has $-J/4$, if $S = 1/2$ - $F_0 = -(N-1)J/4$, entropy $S = 0$
- Put in mistake, of down state too - Energy cost $J/2$, entropy gain $k_B \ln(N-1)$, $N-1$ places to put the wall

$$F_1 = -(N-1)\frac{J}{4} + \frac{J}{2} - k_B T \ln(N-1) \quad (3.2)$$

Now let $N \rightarrow \infty$: energy cost is constant, entropy gain $\rightarrow \infty$. $F_1 < F_0$ when $k_B T \ln(N-1) > \frac{J}{2}$.
 So we conclude, No LRO for $T > 0$, no phase transition \rightarrow no ferromagnetism

- General result, $d = 1$ systems don't show a phase transition.
- 2d Ising model ($D = 1, d = 2$) - Can be solved, there is a phase transition. (Onsager, 1940s)

3.2 Critical Exponents

Most things in Physics depend on scale, e.g. $e^{-t/\tau}$, $e^{-x/L}$. It's remarkable when they don't, e.g. t^δ - a power law.

Example: Phase transitions

$$M = \alpha(T_c - T)^\beta \quad (3.3)$$

In general, β will depend on d, D . Consider the Landau theory from Lecture 1, $\beta = \frac{1}{2}$ in mean field theory.

3.2.1 Other critical exponents

- Consider magnet in an applied field, H ,

$$F = F(M) - \mu_0 M H \quad (3.4)$$

$$M \propto (T_c - T)^\beta, \quad T < T_c, \quad H = 0 \quad (3.5)$$

- Specific heat,

$$C \propto |T_c - T|^{-\alpha}, \quad T \rightarrow T_c, \quad H = 0 \quad (3.6)$$

- Susceptibility,

$$\left. \frac{M}{H} \right|_{H \rightarrow 0} = \chi \propto |T - T_c|^{-\gamma}, \quad T \rightarrow T_c, \quad H = 0 \quad (3.7)$$

➤

$$M \propto H^{1/\delta}, T = T_c \quad (3.8)$$

➤ Coherence length,

$$\zeta \propto |T - T_c|^{-\nu}, H = 0 \quad (3.9)$$

➤ These are often written in terms of 'reduced T':

$$T = \frac{T - T_c}{T_c} \quad (3.10)$$

➤ Universality is the notion that critical exponents depend on d, D, and whether interactions are long or short range

3.3 Scaling Relations

Consider 4 exponents, $\alpha, \beta, \gamma, \nu$ - only 2 are independent.

➤ Widom hypothesis

$$\alpha + 2\beta + \gamma = 2 \quad (3.11)$$

➤ Kadanoff relation

$$\alpha = 2 - \nu d \quad (3.12)$$

Lecture 4

Sort another lecture

Lecture 5 Excitations

5.1 Spin waves in a magnet

- Two "modes" in "wine bottle"
 1. Goldstone mode - rolling in the gutter
 2. Climbing the walls
- Goldstone's theorem - *whenever you break a continuous global symmetry, it's possible to make an excitation for vanishingly small energy costs*

For a $D = 3$ model:

$$H = - \sum_{\langle ij \rangle} J \underline{S}_i \cdot \underline{S}_j = -J \sum_i \hat{\underline{S}}_i \cdot \hat{\underline{S}}_{i+1} \quad (5.1)$$

$$= -J \sum_i S_i^z S_{i+1}^z + \frac{1}{2} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) \quad (5.2)$$

- Rules:

$$S^z | \uparrow \rangle = \frac{1}{2} | \uparrow \rangle \quad S^z | \downarrow \rangle = -\frac{1}{2} | \downarrow \rangle \quad (5.3)$$

$$S^+ | \uparrow \rangle = 0 \quad S^+ | \downarrow \rangle = | \uparrow \rangle \quad (5.4)$$

$$S^- | \uparrow \rangle = | \downarrow \rangle \quad S^- | \downarrow \rangle = 0 \quad (5.5)$$

- Ground state

$$| \Phi \rangle = | \uparrow \uparrow \uparrow \uparrow \rangle, \quad E = -\frac{NJ}{4} \quad (5.6)$$

- Flip a spin:

$$| j \rangle = | \uparrow \uparrow \uparrow \uparrow \downarrow \uparrow \uparrow \rangle = S_j^- | \Phi \rangle \quad (5.7)$$

$$H | j \rangle = \left(-\frac{NJ}{4} + J \right) | j \rangle \quad (5.8)$$

$$= -\frac{J}{2} | j+1 \rangle - \frac{J}{2} | j-1 \rangle \quad (5.9)$$

- Conclusion: $| j \rangle$ is not an eigenstate of H .
- Try a different ansatz: spin wave

$$| q \rangle = \frac{1}{\sqrt{N}} \sum_j e^{iqja} | j \rangle \quad (5.10)$$

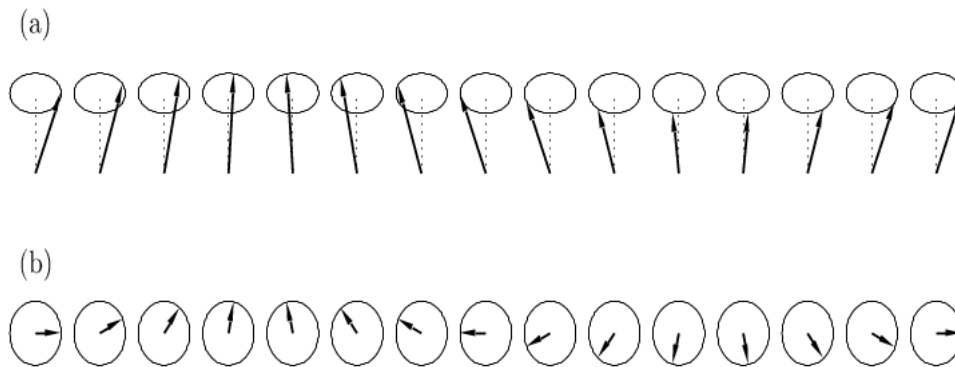
- ➡ a - lattice spacing
- ➡ q - wave vector
- ➡ j - number
- ➡ 1 spin flip, shared between N spins

$$H | q \rangle = \frac{1}{\sqrt{N}} \sum_j e^{iqja} H | j \rangle \quad (5.11)$$

$$= \left(-\frac{NJ}{4} + J - \frac{J}{2} e^{iqa} - \frac{J}{2} e^{-iqa} \right) | q \rangle \quad (5.12)$$

$$= \left[-\frac{NJ}{4} + J(1 - \cos(qa)) \right] | q \rangle \quad (5.13)$$

Therefore $| q \rangle$ is an eigenstate.



5.2 Energy above the ground state

$$\hbar\omega(q) = J(1 - \cos(qa)) \quad (5.14)$$

- *Plot graph here*
- $\omega \approx q^2$ for small q
- Spin waves are quantised into magnons
 - ➡ At low T, only small ω, q are important
 - ➡ The number of states in general in 3D is

$$N(q) \approx q^3 \quad (5.15)$$

- ➡ Density of states:

$$g(q) dq \approx q^2 dq \quad (5.16)$$

- ➡ For magnons,

$$g(\omega) d\omega \approx \omega^{1/2} d\omega \quad (5.17)$$

5.3 Remarks

- $S = 1$ spin (1 spin flipped)
- Bosons
- "massless" - $\omega \rightarrow 0, q \rightarrow 0$
- "Goldstone modes"
- Goldstone's theorem - *whenever a continuous symmetry is broken, we get a new massless excitation*
- Conclusions:
 - ➡ Breaking a continuous symmetry gives rise to a new mode of excitation
 - ➡ These "Goldstone modes" can be excited for vanishing energy cost
 - ➡ Magnons are the Goldstone bosons of the ferromagnet
 - ➡ Some cases will not have these bosons due to Higgs mechanism

Lecture 6 *Lecture 9*

- Consider standard cubic about zero, wells for v and $-v$
- Broken symmetry potential

$$f = \frac{1}{2}(\nabla\phi)^2 U(\phi) \quad (6.1)$$

$$U(\phi) = \frac{\lambda}{4}(v^2 - \phi^2)^2 \quad (6.2)$$

$$v^2 = \frac{u^2}{\lambda} \quad (6.3)$$

- Most systems break symmetry in the same way, i.e. whole system will sit at v
- Alternatively if sitting in both wells, field plots between the two - called a wall, kink, or soliton
- Suppose a kink is of size l (in 1D) - Energy cost:

$$\int \frac{1}{2} \left(\frac{\partial\phi}{\partial x} \right)^2 dx \approx l \left(\frac{v}{l} \right)^2 \quad (6.4)$$

$$\approx \frac{v^2}{l} \quad (6.5)$$

- To reduce the cost, we smear out the wall
- However, there's a second term

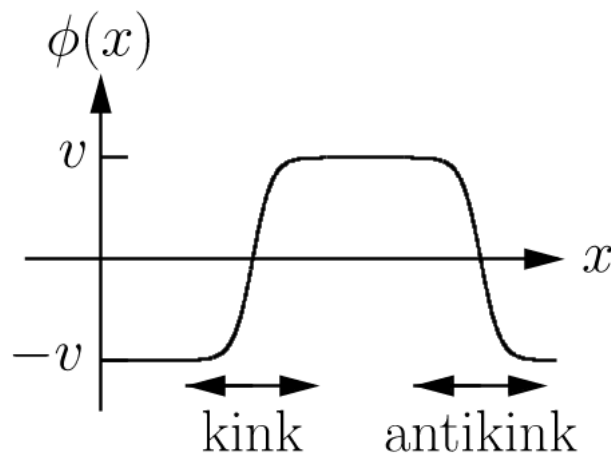
$$\int U dx = \lambda v^4 l \quad (6.6)$$

$$E = \frac{v^2}{l} + \lambda v^4 l \quad (6.7)$$

$$\frac{\partial E}{\partial l} = -\frac{v^2}{l^2} + \lambda v^4 = 0 \quad (6.8)$$

$$l = \left(\frac{1}{\lambda v^2} \right)^{1/2} \approx \frac{1}{\mu} \quad (6.9)$$

- $E(x)$ forms like a Gaussian, kink is localised in a region of size l
- Center can be anywhere
- It costs a (semi-)infinite energy to remove it
 - ➡ it's stable



- Can unwind for only a finite energy cost
- What about vortices?

- Swirly at $r \rightarrow \infty$
- Costs a huge amount of energy
- Derrick's theorem: *Time-independent topological objects are impossible to realise in greater than one spatial dimension for this theory*
- Contradictions to this:
 - ➡ time dependence
 - ➡ vortex-antivortex pairs
 - ➡ add a field that cancels the effects of the swirliness