Basic Training in Condensed Matter Physics

Module 1: Crystals

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* No class Friday (Jan 28)
* Two more weeks ( W 29, F 31, W 5, F 7)
* One teaser homework per lecture

Feb 12-28  Practical DFT Arias

Mar 8-12  Continuum Quantum Urrygo
         -28  Monte Carlo

Apr 9- May 7  Geometry in QM Mueller
I. What are crystals?

- Regular lattice of atoms?

  - Face Centered Cubic (Cu, Al, Ar, ...)
  - Body Centered Cubic (bcc: Mo, Fe, Na)
  - Diamond HCP Hexagonal Triclinic

- Rigid?

  Push on one end of table: 
  \(10^{10}\) atoms away atoms move?

- Broken Symmetries?

  - Sphere
  - Cube

Which is more symmetric
Liq uid  Crystal

Which is more symmetric?

Snapshot of liquid has no symmetry (nor does snapshot of single crystal)

Ensemble of liquid has translational symmetry: \( x \rightarrow x + \Delta \)

Crystal has only discrete translational symmetry \( x \rightarrow x + \text{maximal} \)

Different symmetry \( \rightarrow \) different phase (phase transition when symmetry shifts)

- Which define the crystal? Not the reverse.
  - [Boring, language, nomenclature]

How do these properties relate?
Rigidity

Ligo: mirrors held fixed to

$$4 \times 7500 \text{ atomic size}$$

$$\frac{10^{-13}}{m} =$$

$$L \sim 4 \text{ km}$$

strain $$\varepsilon = \frac{2 \mu \varepsilon_1}{E} + \frac{\partial u}{\partial x} \frac{\partial u}{\partial y} \frac{1}{E}$$

Potential Energy $$\varepsilon = \int \frac{1}{2} C \left( \frac{\partial u}{\partial x} \right)^2 \, dx$$

One dimension $$\frac{\partial u}{\partial x} \sim \frac{\Delta x}{L}$$

$$\varepsilon = \frac{1}{2} C \left( \frac{\Delta x}{L} \right)^2$$

$$= \frac{1}{2} \frac{C}{L} \Delta x^2$$

Temperature $$T \Rightarrow$$

Boltzmann distribution $$P(\Delta x) = e^{-\frac{\varepsilon}{k_B T}}$$

Ginzburg criterion

RMS fluct.

at melting, $$\sigma = 0.1a$$

$$\sigma = \sqrt{\langle (\Delta x)^2 \rangle} = \sqrt{\frac{L \cdot k_B T}{c}}$$

Di-dimensions?

A one dimensional system at finite forces at non-zero temperature cannot have a phase transition $$d$$-dimensions?
\[ z = \frac{1}{2} C (\frac{\Delta x}{L})^2 \]

\[ \rho(\Delta x) = e^{-\frac{1}{2} \left( \frac{C \Delta x}{k_B T} \right)^2} \]

\[ \Delta x \sim \frac{a}{\sqrt{n}} \approx \frac{a}{\sqrt{0.01 a}} = 0.1a \]

\[ d = 3 \Rightarrow \Delta x \text{ goes like } \frac{1}{\sqrt{n}} \]

\[ \Delta x \text{ at } L = \text{ atomic size } = a \Rightarrow a \sim \frac{1}{100} a \]

(Mostly unexplained, e.g. melting)

\[ \Delta x \sim (0.01 a) \sqrt{n} \]

\[ a \in (0.01 a, 0.1a) \]

Molecules vibrate less when further apart? *Yes*

Average over \( \langle (\Delta x)^2 \rangle \) is \( N \) if each were \( \frac{1}{100} \)

\[ \text{average } (\frac{1}{100}) \text{ random fluxes } \Rightarrow \langle \Delta x^2 \rangle \text{ at } a \]

\[ \langle \Delta x^2 \rangle \approx \frac{a^2}{100 L} \]

Better test: look for distance between two \( \text{atoms} \)

\[ \langle (\Delta x(x) - \Delta x(x+n))^2 \rangle \approx \Delta u^2 \]

Straight forward long calculation?

\[ 1d \Delta x \approx \frac{a}{\sqrt{n}} \]

(same: only one boundary atom)

\[ 3d \Delta x \approx \frac{a}{n^{\frac{1}{3}}} \] (\[ \text{constant } n^{\frac{1}{3}} a \rightarrow \text{ long range order} \]

\[ L \rightarrow \infty \]

Know one atom position and crystal orientation \( \Rightarrow \text{all} \)
Peierls Argument

1. Rigidity needed for precise quantum measurement?
   - crystals
   - Josephson
   - Pound-Rebka
   - QHE
   - Ligo

2. Crystal rigidity necessary?

3. What about 2D?

\[ \Delta x \approx \sqrt{\frac{k_B T}{c}} \quad \text{independent of } L \]

Distance between pairs of atoms:
\[ \left\langle \left( \hat{u}(x) - \hat{u}(x+\vec{r}) \right)^2 \right\rangle \sim 1/n^2 \quad \eta > 0, \text{ depends on temperature} \]

\[ \Rightarrow \text{no long range order} \]

\[ \Rightarrow \text{no broken symmetry (translations)} \]

(Can't tell if shift of crystal to right by \( \epsilon \), if \( \epsilon \) in 2D.)
Mermin-Wagner Theorem:

Paraphrased:

"A two dimensional system with short-range forces cannot break a continuous symmetry."

Hohenberg & Long wavelength fluctuations (earlier) → Power laws (like here)

Ising Model? OK - discrete symmetry

- XY model, Heisenberg model?
  - Power-law decays in 2D at best
  - Low T, exponential decay

- Rotation modes in crystals?
  - Continuous rotation symmetry

Long-wavelength rotation? No. Low temperatures
in rotations in 2D.

Crystals violate technical qualifications on theorem, dropped in Paraphrasing.