Modeling in Physics

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Lecture 1

The scientific method and its application to very hard problems
Symmetries in nature
Crystals

Solids with a periodic pattern
Scientists try to make sense of patterns in nature.

Bad news: nature can be quite complicated!
Good news: there is a systematic method to uncover the reality of nature...
Scientific Method

Observations

Question

Hypothesis

Prediction

Test does not support hypothesis: revise hypothesis or pose new one

Test: experiment or additional observation

Test supports hypothesis: make additional predictions and test them

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Posing a question:

Do all four feet of a galloping horse ever off the ground?
Answer: Yes!
Solid crystals can have a variety of properties, for instance the way they conduct electricity.

- **metals**
- **semiconductors**

Elements:
- Tungsten (W)
- Copper (Cu)
- Silicon (Si)
- Germanium (Ge)
Metals dissipate when they conduct electricity
Drude model

\[ J = \left( \frac{ne^2 \tau}{m} \right) E \]

Conductivity

Hypothesis: the electrons form an ideal gas of classically impenetrable particles, with the scattering rate set by the mean free path between ionic collisions.
Drude model

\[ J = \left( \frac{ne^2\tau}{m} \right) E \]

Conductivity (Ohm's law)

The motion of the electrons is governed by the classical equation:

\[ \frac{dp}{dt} = e \left( E + \frac{p \times B}{m} \right) - \frac{p}{\tau} \]

Lorentz force

Mean free time
Drude model

DC and AC conductivity of metals

Hall effect

Thermal transport
But we know that electrons are not classical objects. They interact strongly with ions and with other electrons by long range Coulomb interactions.

Why can we successfully describe them in metals as classical particles bouncing between the ions?
Lesson 1: Models are effective descriptions of reality.

Bare in mind that sometimes, they hide our ignorance about the underlaying physics.
Lesson 1: Models are effective descriptions of reality.

One way to learn about the underlaying physics is to explore limits where these models break down.
Lord Kelvin predicted that the resistivity of metals should diverge at very low temperature due to the freezing of the electrons at the atoms.

In 1909, he convinced a dutch physicist, K. Onnes to make the experiment.
Onnes found that Drude’s law indeed fails at low temperatures but in a rather unexpected way...

This property is known as superconductivity!
The Nobel Prize in Physics 1913
Heike Kamerlingh Onnes

Heike Kamerlingh
Onnes

The Nobel Prize in Physics 1913 was awarded to Heike Kamerlingh Onnes "for his investigations on the properties of matter at low temperatures which led, inter alia, to the production of liquid helium".
100 years of superconductivity

Heike Kamerlingh
Onnes

The Nobel Prize in Physics 1913 was awarded to Heike Kamerlingh Onnes "for his investigations on the properties of matter at low temperatures which led, inter alia, to the production of liquid helium."

Photos: Copyright © The Nobel Foundation
A superconductor expels external magnetic fields!
Meissner effect
Phase diagram of superconductivity

Superconductivity occurs only if one cools down the material below $T_c$. 
Why does superconductivity exist?

When an experiment challenges our understanding, physicists have to work hard to understand why it happens.

A successful theory must explain the current experiments (can be falsified) and should make valid predictions about future experiments!
Why does superconductivity exist?

Over 50 years, they all had failed attempts to explain superconductivity.

J. Schmalian, arXiv:1008.0447v2
Superconductivity was discovered 15 years before the advent of quantum mechanics...
In 1922, Einstein proposed a classical model of closed molecular conduction chains, where the electrons would carry the supercurrent.
Prediction

A supercurrent cannot be transmitted across a junction between different superconductors, since the junction behaves and the termination of classical chains.
Prediction

A supercurrent cannot be transmitted across a junction between different superconductors, since the junction behaves and the termination of classical chains.

Experiment: the supercurrent does travel across the junction. Einstein's theory is wrong!
Lesson 2: solving a problem can be very hard (if not impossible) if you don’t have the right tools. Make sure you have them.
**Other attempts**

Hypotnesis: at low temperatures, the electrons crystalize in a lattice and move coherently in an electric field.
Other attempts

Hypothetical: at low temperatures, the electrons crystallize in a lattice and move coherently in an electric field.

Bloch showed that this state cannot be the ground state unless the current is zero.
After the discovery of the Meissner effect (1933), it was realized that superconductors are NOT perfect conductors, but perfect diamagnets!

A superconductor is a non-trivial macroscopic quantum coherent state!
Other attempts

Heisenberg: Finding bound states near the Fermi energy due to Coulomb interactions

Meissner effect? No

Feynman: Perturbation theory. No

And several others...
Bloch’s (in)famous second theorem, that “every theory of superconductivity can be disproved” was often cited by other theorists.

In 1956 (47 years after the Onnes experiment) Feynman declared that physicists could not figure out superconductivity because of lack of imagination.
Why does superconductivity exist?

As the electrons diffuse in a metal:

Dissipative motion ($T>T_c$)

Coherent motion ($T<T_c$)

Coherent motion requires that a macroscopic fraction of the particles occupies the same quantum state!
Superfluidity

Something similar happens with liquid helium: superfluidity = flow with zero viscosity
Bose-Einstein condensation

When the lowest quantum state is occupied by a macroscopic fraction of the particles, there is superflow!
In quantum mechanics, a state of a free electron is defined by its “velocity” and spin.

Coherent motion ($T<T_c$)

spin down state

spin up state
The problem is that electrons satisfy the Pauli exclusion principle: “Two electrons cannot occupy the same quantum state”

A given state with velocity $v$ can only have two electrons!

spin up  spin down

Free electrons cannot form a condensate!
Coherent pairs of electrons can condense!

Work around: Electron pairs

when the center of mass of all pairs is at rest,

\[ v + (-v) = 0 \]

macroscopic condensate of pairs!

\[ T = T_{\text{critical}} \]

Coherent pairs of electrons can condense!
The glue to form the pairs comes from lattice vibrations of the solid crystal where the electrons diffuse!
Meissner effect follows from diamagnetic supercurrents which expel the magnetic field!
A theory of superconductivity is presented, based on the fact that the interaction between electrons resulting from virtual exchange of phonons is attractive when the energy difference between the electrons states involved is less than the phonon energy, $\hbar \omega$. It is favorable to form a superconducting phase when this attractive interaction dominates the repulsive screened Coulomb interaction. The normal phase is described by the Bloch individual-particle model. The ground state of a superconductor, formed from a linear combination of normal state configurations in which electrons are virtually excited in pairs of opposite spin and momentum, is lower in energy than the normal state by amount proportional to an average $\langle \hbar \omega \rangle^{2}$, consistent with the isotope effect. A mutually orthogonal set of excited states in one-to-one correspondence with those of the normal phase is obtained by specifying occupation of certain Bloch states and by using the rest to form a linear combination of virtual pair configurations. The theory yields a second-order phase transition and a Meissner effect in the form suggested by Pippard. Calculated values of specific heats and penetration depths and their temperature variation are in good agreement with experiment. There is an energy gap for individual-particle excitations which decreases from about $3.5k_{B}T_{c}$ at $T=0^\circ K$ to zero at $T_{c}$. Tables of matrix elements of single-particle operators between the excited-state superconducting wave functions, useful for perturbation expansions and calculations of transition probabilities, are given.
The Nobel Prize in Physics 1972
John Bardeen, Leon N. Cooper, Robert Schrieffer

BCS theory (1957)
(superconductivity for metals)

The Nobel Prize in Physics 1972 was awarded jointly to John Bardeen, Leon Neil Cooper and John Robert Schrieffer "for their jointly developed theory of superconductivity, usually called the BCS-theory".

Photos: Copyright © The Nobel Foundation

The Nobel Prize in Physics 1913
Heike Kamerlingh Onnes

Experimental discovery (1911)
BCS results

Explain the energy required to break a Cooper pair (gap energy) as a function of temperature.
Explained the gap energy as a function of the critical temperature as well.
BCS results

\[ Q = cm\Delta T \]

- heat added
- specific heat
- mass change in temperature

Explain the specific heat jump at the phase transition
BCS results

\[ Q = cm\Delta T \]

- heat added
- specific heat
- mass
- change in temperature

\[ C = Ae^{-b/kT} \]

Vanadium heat capacity approaching its critical temperature from below.

\[ T_c = 5.4 \text{ K} \]

Explained the exponential scaling of the specific heat at low temperatures
BCS results

Also explained the Meissner effect...
Time line of superconductor temperatures ($T_c$)

Experimental discovery

Theoretical explanation
Discovery of high temperature superconductivity in insulators!
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<th>Transition temperature (in celsius)</th>
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The Nobel Prize in Physics 1987
J. Georg Bednorz, K. Alex Müller

J. Georg Bednorz     K. Alexander Müller

The Nobel Prize in Physics 1987 was awarded jointly to J. Georg Bednorz and K. Alexander Müller "for their important break-through in the discovery of superconductivity in ceramic materials"

Photos: Copyright © The Nobel Foundation
The standard theory does not explain superconductivity in insulators!
Phase diagram of cuprates
Applications for superconductivity?

Ultra sensitive magnetic sensors

Powerful electromagnets
This is a hard problem. Physicists have a lot of work ahead...
Soliton excitations in polyacetylene

W. P. Su,* J. R. Schrieffer,* and A. J. Heeger
Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania 19174
(Received 3 December 1979)

A theoretical analysis of the excitation spectrum of long-chain polyenes is presented. Because of the twofold degeneracy of the ground state of the dimerized chain, elementary excitations corresponding to topological solitons are obtained. The solitons can have three charge states \( Q = 0, \pm e \). The neutral soliton has spin one-half while the charged solitons have spin zero. One electronic state is localized at the gap center for each soliton or antisoliton present. The soliton's energy of formation, length, mass, activation energy for motion, and electronic properties are calculated. These results are compared with experiment.

Sometimes wrong theories can inspire successful theories in different contexts!

[Image of Einstein]