Electronic Structure of Condensed Matter
Fudan University - April 2010

Lecture 8
Summary and Conclusions

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Last slide from Lect. 1

Goal of Course

Understanding of the role of electrons in condensed matter

• **Practical, useful knowledge of methods that are working tools of theorists, experimentalists, and researchers in many fields**
Without the burden of heavy math, many-body theory, …..

• **Appreciation for the real many-body problems presented by electrons in condensed matter**
Understanding when to expect correlation to be important
The grand challenges of condensed matter physics today

For those who are interested

• **Practical, useful knowledge of many-body methods that are becoming more and more important for quantitative predictions and understanding the grand challenges in condensed matter**

Basis of Most Modern Calculations
Density Functional Theory

- **Why is Density Functional Theory so widely used?**
- **A new approach to the many-body interacting electron problem**
  - **In principle DFT is exact**
  - **Kohn and Sham introduced the idea of an auxiliary system that in principle gives the exact ground state density and energy - but NOT other properties.**
  - **In practice, DFT allows useful approximations**

The Car-Parrinello Advance

- **Car-Parrinello Method – 1985**
  - Simultaneous solution of Kohn-Sham equations for electrons and Newton's equations for nuclei
- **A revolution in the power of the methods**
  - Relaxation of positions of nuclei to find structures
  - "First principles" molecular dynamics simulations of solids and liquids with nuclei moving thermally
  - Chemical reactions, . . .
- **Stimulated further developments . . . .**

Contents of a typical solid state physics text (Kittel, Ashcroft and Mermin, ….)

From Lect. 1

- **Structures of crystals**
  - Definitions of structures
  - Typical bonding and structures
  - Structural phase transitions
- **Mechanical Properties**
  - Lattice vibrations – phonons
  - Elastic constants
  - Piezoelectric constants
  - Effective charges
- **Thermal Properties**
  - Heat capacity, heat conduction
- **Electronic properties**
  - Definition of bands
  - Metals vs. insulators
  - Conductivity, dielectric functions
  - Magnetism

Properties that can be described without knowing anything about electrons

Did we answer the question: Why are they a part of electronic structure?

Properties that can only be understood in terms of the electrons?

So what is left to do?

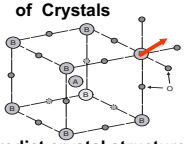
- **Failures of present density functional approximations in important cases!**
- **Electronic excitations**
  - The "band gap problem" . . .
- **Strongly interacting systems**
  - Magnetic insulators, metal-insulator transitions, . . .
- **Example of "Failure" that has been solved!**
  - Weak Van der Waals bonds
  - Development of non-local functional has the right distance dependence and is accurate enough for real materials
- **Very brief presentation in special lectures**

From Lect. 1 modified

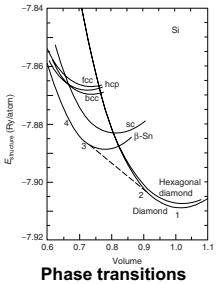
Useful!

Treat many types of materials in a unified way from the basic equations

Calculate properties of Crystals

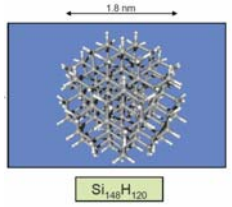


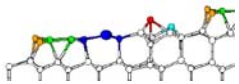
Predict crystal structures
Example – atomic positions in a ferroelectric



Phase transitions under pressure

Predict properties of nanostructures

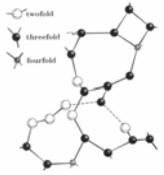




Structures of surfaces

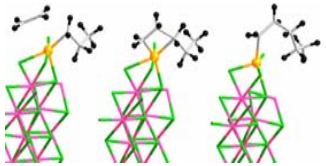
Many other examples!

Simulation of Liquids – example Carbon at high T



"snapshot" of liquid

Reactions – catalysis at a surface



Not covered due to time constraint

Magnetism

Wannier functions – transformation from extended Bloch states to localized orbitals

Linear scaling methods – using Wannier functions

Electric polarization in solids – using Wannier functions (or Berry phases)

Excitations and time dependent density functional theory

Discussion is class

Magnetism

The good thing about magnetism

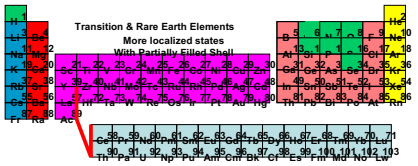
- Simple models give the right qualitative understanding
- Atom-like magnetic moments
- Ordered for T < Tc -- disordered for T > Tc

Another good thing about magnetism

- Simple models give the right qualitative understanding
- Electrons in bands
- Magnetic moment is $n_{up} - n_{down}$

The hard thing about the theory of magnetism

To understand both these pictures at the same time!



Discussion is class

"Order N"

Quantum Mechanics is not "local"

- Eigenstates extend over entire system
- Interference of states is essential to understanding quantum behavior

Effect in theoretical calculations for materials

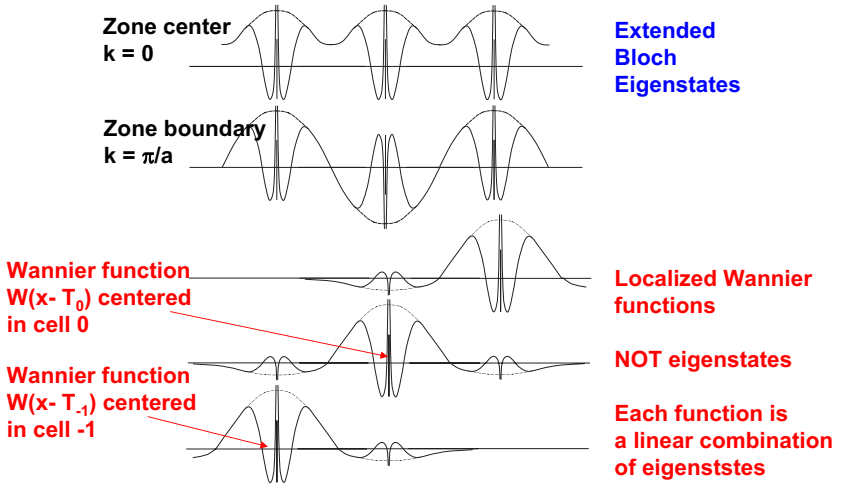
- Exact calculations - Computer time scales exponentially with N = number of electrons
- In DFT – scales as N^3 (The time to diagonalize a matrix)

Is it possible to do accurate calculations with computational time linear in N?

Discussion is class

Wannier functions

Transformation from an entire band of Bloch states to a set of Wannier functions



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