

# Notes on Introduction to Condensed Matter Physics

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## Contents

1	Basic Introduction	1
2	Conventional Metal Physics: Electrons and Phonons	1
3	Transport	3
4	Metal Insulator Transition (MIT)	5
5	Others	7

## 1 Basic Introduction

1. Condensed Matter:  $\sim 10^{23} / \text{cm}^3$
2. Major Study: Electrons, Phonons, The interactions between
3. Drives: New materials & New technologies

## 2 Conventional Metal Physics: Electrons and Phonons

1. Basic Properties of Normal Metals: • Ductile • Excellent electrical conductor • Excellent thermal conductor • Most are weak paramagnet, some ferromagnet • Opaque  
• At low  $T$ :  $\rho$  increases with  $T$   $\chi \sim \text{Const.}$   $c_V \propto T$
2. Drude Free Electron Model:
  - Assumptions: • Free electrons (Ignore interaction with lattice) • Independent electrons (Ignore interactions between electrons) • Electrons were treated as independent classical particles
  - Maxwell-Boltzmann distribution

- Successes: • Electrical conductivity and thermal conductivity • Wiedemann-Franz law (by luck!) • The Hall effect and magnetoresistance • AC conductivity and optical properties of metals
  - Problems: • Heat capacity puzzle:  $c_V = \frac{3}{2}nk_B = \text{Const.}$  • The susceptibility puzzle:  $\chi$  does not change with temperature, non-Curie like  $\chi \sim 1/T$
3. The Sommerfeld Model: • Free Electron Gas + Schrodinger Equation + Fermi Statistics
- The Fermi Surface: In 3D  $E_F \sim n^{2/3}$  • Typical Values:  $E_F \sim 7 \text{ eV}$ ,  $k_F \sim 1 \times 10^8 \text{ cm}^{-1}$ ,  $T_F \sim 8 \times 10^4 \text{ K}$ ,  $v_F \sim 2 \times 10^8 \text{ cm/s}$  • DOS In 3D:  $D(\epsilon) \sim \epsilon^{1/2}$  • Linear  $T$  Heat Capacity at Low  $T$
  - Pauli Paramagnetism (at low  $T$ ):  $\chi = \mu_B^2 D(E_F) = \text{const.}$
  - Successes: • Realized the importance of Fermi distribution • Established the k-space language for electrons • Introduced Fermiology • Resolved the Pauli susceptibility puzzle • Resolved the heat capacity puzzle • Resolved the thermopower puzzle • Explained the Wiedemann-Franz Law
4. Landau's Fermi Liquid Theory: • Quasi-particle: Same charge, spin, momentum as non-interacting electron
- Adiabatic Continuity, Only valid at low  $T$  and low energy • Qualitatively explain the susceptibility, heat capacity • Only require a Fermi sea • Entropy, distribution function unchanged • Energy modified by the effective mass & the Fermi interaction function • Low energy excitation like single particle •  $\epsilon = \frac{\hbar^2 k^2}{2m^*}$
  - $c_V = \frac{1}{3} \frac{m^* k_F}{\hbar^2} k_B^2 T$  •  $\chi = \frac{m^* k_F}{\hbar^2 \pi^2} \frac{1}{1+F_0^a} \mu_B^2$  • Landau parameter:  $m^*, F_0^a$  • Wilson ratio:  $R_W = \frac{\pi^2 k_B^2 \chi}{3 \mu_B^2 \gamma}$  • For non-interacting electron gas  $R_W = 1$  •  $T^2$  Law (Experimental Signature): qp-qp scattering • Scattering rate  $\frac{1}{\tau} \sim k_B T \cdot k_B T \propto T^2$  • But electron seems to be a wrong place to start for many novel phenomena • Spinon, holon, fractional charge: Collective mode looks like a fraction of an electron
5. Bloch Theory: • Bloch Theorem: For periodic potential,  $\psi_{nk}(\mathbf{r}) = e^{i\mathbf{k} \cdot \mathbf{r}} u_{nk}(\mathbf{r})$ , where  $u_{nk}(\mathbf{r}) = u_{nk}(\mathbf{R} + \mathbf{r})$
- Momentum is no longer a good quantum number • Band index  $n$
  - NFE model: Perturbation to the free electron plane wave states (maximum mixing) (highly delocalized)
  - First order:  $\epsilon_k^1 = \bar{V}$  • Second order (non-degenerate):  $\epsilon_k^2 = \sum_{g \neq 0} \frac{|V_g|^2}{\epsilon_k^0 - \epsilon_g^0}$  • Second order (degenerate):  $\epsilon_k^2 = \pm |V_n|$  • Energy gap: Level repulsion, Explains metal or insulator
  - +2 Metals: Band overlap
  - Tight Binding Model: (nearly localized) such as transition metal and rare earth metal with partially filled  $d$  and  $f$  orbitals. •  $\psi_k(\mathbf{r}) = \sum_{\mathbf{R}} e^{i\mathbf{k} \cdot \mathbf{R}} \psi_a(\mathbf{r} - \mathbf{R})$  • Overlap integral:  $t_{\mathbf{R}} = \int \psi_a^*(\mathbf{r} + \mathbf{R})(\Delta V) \psi_a(\mathbf{r}) d\mathbf{r} \rightarrow$  Nearest neighbor approximation • Band width:  $W \sim 2zt$ , where  $z$  is coordination number,  $t$  is overlap integral • Useful starting point
6. Lattice Vibrations: • Harmonic Approximation:  $V(a + \delta x) = V_0 + \frac{1}{2}\beta(\delta x)^2$  •  $\epsilon = \sum_k (n_k + \frac{1}{2}) \hbar \omega$  • Phonons: The quantum of the lattice vibration,  $n_k = \frac{1}{e^{\hbar \omega / kT} - 1}$  • Mono-atomic 1D Chain:  $\omega = 2 \sqrt{\frac{\beta}{m}} \left| \sin\left(\frac{aq}{2}\right) \right|$
- Di-atomic 1D Chain: Acoustic & Optical phonon • Phonon specific heat: Debye model: • Assume linear

dispersion • Define a cutoff in the integral: Debye frequency

•  $T \rightarrow 0$   $c_V \sim T^3 \Leftrightarrow$  Blackbody radiation

7. Specific Heat: • Directly related to internal energy • To extract important microscopic parameters • To study phase transition • **Calorimetry**: What, How, Better resolution and accuracy, Flexibility • **Adiabatic Nernst Calorimeter**: Slow, Heat leak problem, Need big sample
  - **Relaxation time calorimeter**:  $\Delta T = \Delta T_0 e^{-t/\tau}$ , where  $\tau = c_V l / \kappa S$  (with addenda)  
Advantage: Accurate, Fast, Microgram crystals, Small, Work in extreme conditions  
Disadvantage: The addenda
  - **Membrane calorimeter**: Nano-gram crystals, Measure in-situ evaporated thin films, Extreme conditions
  - **Heater**: Resistance stable with  $T$  • **Thermometer**: Resistance has Linear relationship with  $T$
8. Anharmonic Potential: • Universal  $\Leftrightarrow V = 0$  when  $r \rightarrow \infty$  • Phonon-phonon interaction: No longer independent excitations  $\Rightarrow$  Phonon heat conduction (low  $T$ , high  $T$ ) • Thermal Expansion: •  $\alpha = \frac{1}{l} \frac{\partial^2 l}{\partial T \partial p} = \frac{1}{3V} \frac{\partial^2 V}{\partial T \partial p}$  • Provide similar information as specific heat • Bad in engineering
  - **XRD**  $\rightarrow$  Measure  $l$  or  $V$ , High resolution, Hard to use in extreme physical conditions
  - **Capacitive dilatometer**: High resolution (capacitance bridge) (0.01 Å), ultra low  $T$  and large  $B$  (compact design)
    - Negative thermal expansion:  $ZrW_2O_8 \rightarrow$  Rigid Unit Modes
9. Main Frame: Landau Fermi Liquid Theory + Band Theory

### 3 Transport

1. Basic Notions: • Movement of Particles or Quantities • Non-equilibrium steady state •  $\mathbf{J} = L \cdot \mathbf{F}$ 
  - Very informative and instructive, esp. on Novel materials and in Extreme conditions
  - Normally the first to be carried out • Close relations to device applications
2. Fractional Quantum Hall Effect: • Ultra low  $T$ , Super strong  $B$ , Very clean • Strong electron correlations
  - Most precise method to measure  $h$
3. **Cryogenic Technology**: • **Dilution fridge method**: He-3 rich & He-3 poor phase at  $T < 0.87 K$ 
  - He-3 diffuse, absorb heat • Down to  $\sim 10$  mK
  - **Superconducting magnet**: up to 20 tesla  $\Leftarrow$  critical field
  - **Super high magnetic field**: Florida-Bitter resistive magnet, Hybrid magnet

4. The Boltzmann Transport Equation: •  $\frac{\partial f_k}{\partial t}\Big|_{\text{diffusion}} + \frac{\partial f_k}{\partial t}\Big|_{\text{field}} + \frac{\partial f_k}{\partial t}\Big|_{\text{scattering}} = 0$  •  $\frac{\partial f_k}{\partial t}\Big|_{\text{diffusion}} = -\dot{\mathbf{r}} \cdot \nabla_{\mathbf{r}} f_k$   
 •  $\frac{\partial f_k}{\partial t}\Big|_{\text{field}} = -\dot{\mathbf{k}} \cdot \nabla_{\mathbf{k}} f_k$  •  $\frac{\partial f_k}{\partial t}\Big|_{\text{scattering}} = -\frac{f_k - f_k^0}{\tau}$
5. Electrical Transport: •  $\mathbf{J}_e = \sigma \mathbf{E}$  • Measurements: Four-probe, Low frequency ac lock-in method  
 • Drude model:  $\sigma = \frac{ne^2\tau}{m}$  • Semi classical:  $\delta \mathbf{k} = \frac{e\tau \mathbf{E}}{\hbar}$  • Only the surface of the FS changed !  
 • Ignore the diffusion effect, Complexity of the FS  
 • The Boltzmann transport equation:  $\overleftrightarrow{\sigma} = \frac{1}{4\pi^3} \frac{e^2\tau}{\hbar} \int \frac{\mathbf{v}_k \mathbf{v}_k dS_F}{v_k}$   
 • Cubic symmetry:  $\sigma_{x,y,z} = \frac{e^2}{3} v_F l D(\epsilon_F)$   
 • Matthiessen's rule: Different scattering mechanisms don't interfere each other  $\Rightarrow \frac{1}{\tau} = \frac{1}{\tau_{imp}} + \frac{1}{\tau_{ph}} + \dots$   
 • Electron-electron scattering:  $\frac{1}{\tau} \sim T^2$   
 • Electron-lattice scattering:  $\rho \sim T$ , at high  $T$   $\rho \sim T^5$ , at low  $T$   
 • Electron-impurity scattering: • Roughly, Temperature-independent • Residual resistivity:  $\rho(T=0)$  •  
 Residual resistivity ratio (RRR):  $\frac{\rho_{300K}}{\rho_0}$  Higher the better
6. Thermal Transport: •  $\mathbf{J}_Q = \kappa(-\nabla T)$  • Measurement: One-heater, Two-thermometer  
 • Drude:  $J_{Qe,x} = \frac{1}{2} n v_x [\epsilon(T_{x-v\tau} - T_{x+v\tau})] = \frac{1}{3} c_V v l$  •  $\mathbf{J}_Q = 2 \int f_k (\epsilon_k - \mu) \mathbf{v}_k d\mathbf{k}$  •  $\kappa_e = \frac{\pi^2}{3} \frac{k_B^2}{e^2} T \sigma$   
 • Phonon Thermal Conductivity: Good metals  $\sim 1\%$
7. Thermoelectric Power: • Seebeck Coefficient:  $S = \frac{E}{\nabla T} = \frac{c_V}{3ne}$  • The piece of heat carried by each charge  $e$   
 • Inversely proportional to  $\epsilon_F$  •  $S = \frac{\pi^2}{3} \frac{k_B}{e} k_B T \left( \frac{\partial \ln \sigma(\epsilon)}{\partial \epsilon} \right) \Big|_{\epsilon=\mu}$  • Reveal abrupt change of electronic structure  
 • Study novel electronic phases and phase transitions, But poorly understood  
 • **Thermal couple**:  $V = (S_B - S_A)(T_x - T_0)$  • **Thermoelectric power generation**:  $\Pi$ -junction consisting of N type & P type material •  $V = (|S_N| + |S_P|)(T_h - T_c)$  • No moving part, reliable • Environmental friendly • Arbitrary Shape & Size • **Radioisotope thermoelectric generator**: For unmanned situations, Low power, Long durations • **Thermoelectric refrigeration**:  $\Pi$ -junction consisting of N type & P type material •  $J_Q = J_e(|\Pi_N| + |\Pi_P|)$
8. Peltier Effect: •  $\mathbf{J}_Q = \Pi \mathbf{J}_e$
9. Onsager reciprocal relations: •  $\begin{pmatrix} \mathbf{J}_e \\ \mathbf{J}_Q \end{pmatrix} = \begin{pmatrix} \sigma & \sigma S T \\ \sigma \Pi & -\kappa T \end{pmatrix} \begin{pmatrix} \mathbf{E} \\ \frac{\nabla_{\mathbf{r}} T}{T} \end{pmatrix}$  •  $\Pi = S T$
10. The Thermoelectric Figure of Merit: •  $ZT = \frac{\sigma S^2 T}{\kappa}$  •  $ZT \sim 3$ , for application, Now  $ZT \sim 1$   
 • Now focusing on heavily doped narrow-band semiconductors,  $n \sim 10^{19} - 10^{20}/\text{cm}^3$ , Not promising because of W-F law • Minimize phonon thermal conductivity  $\Rightarrow$  Low Dimension, Amorphous, Nano-materials •  $\text{Bi}_2\text{Se}_3$  &  $\text{Bi}_2\text{Te}_3$ : Quasi-2D system (Quintuple-layer) • Future focus: Considering Spin, Strong-correlation system

11. Magnetic Field: • Free electron gas: • No magnetoresistance • Hall coefficient:  $R_H = \frac{1}{ne}$   
 • Hall angle:  $\tan \theta = \frac{E_y}{E_x} = \frac{Be\tau}{m} = \omega_c \tau$  • Quantum oscillations:  $\omega_c \tau \gg 1$ , Shubnikov-de Haas oscillations
12. Thermo-magnetic Transport: • Thermal Hall effect: Heat current (x) produces  $\nabla T$  (y)  
 • Nernst effect:  $\nu = \frac{E_y}{\nabla T_x B_z}$ , Powerful technique for novel metals & superconducting vortices in type-II superconductors

## 4 Metal Insulator Transition (MIT)

1. I-M Transition within Band Theory: • Doping: Donors & Acceptors  $\Rightarrow$  impurity bands  
 • Pressure: Structure change  $\Rightarrow$  Overlap  $\Leftarrow$  Tight binding model • Wilson transition
2. Mott Insulator: • Mott's Gedanken Experiment: Increase the distance between atoms: Smaller hopping integral ( $t$ ) and carrier density ( $n$ )  
 • Thomas-Fermi Theory: A negative charge added to the Fermi Sea  $\Rightarrow \delta V \Rightarrow \delta n = -D(\epsilon_F) \delta V \Rightarrow \nabla^2(\delta V) = k^2 \delta V$  • Yukawa Potential:  $\delta V = \frac{e^2}{r} e^{-kr}$  • Screening length:  $\lambda = \frac{1}{k}$ ,  $k = \sqrt{\frac{4\pi e^2 k_F}{\hbar^2}} \propto n^{1/6}$  for 3D FEG • Good metals  $\Rightarrow$  Non-interacting FEG  
 • Mott Insulator: Coulomb energy cost will exceed the kinetic energy gain • Low dimensional materials with large lattice constant • IMT: Tune the  $U/W$  ratio; Change band filling by doping. • Pressure induced IMT: Lattice contraction at IMT ( $\sim 0.2\%$ )  $\Leftarrow$  Metallic bonds • Increase of  $m^*$  due to strong electron interaction in doped Mott insulator • Many transition metal oxides (TMO): Separated by O, small density; Inner d electrons, weak overlap  
 • The Hubbard Model:  $H = -t \sum_{\langle i,j \rangle, \sigma} c_{i\sigma}^\dagger c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$ , where  $t = \int \varphi_j^* [V(r) - v_i(r)] \varphi_i dr$   
 $U = \int |\varphi_i(r_1)|^2 \frac{e^2}{r_{12}} |\varphi_i(r_2)|^2 dr$  1<sup>st</sup> term: Hopping term, 2<sup>nd</sup> term: on-site Coulomb repulsion term  
 • Band split:  $U > W$  ( $W$  is the width of the original band) • Energy gap:  $E_g \sim (U - W)$   
 • Perovskite Structure:  $ABO_3$  • A only donates electronic charge and stabilizes the structure • For electronic properties, the  $BO_6$  octahedral is most relevant •  $RNiO_3$  system: Charge transfer insulators: O's  $p$  orbits and Ni's  $d$  orbits strongly hybridized. gap  $\sim 10-30$  meV • Bonding angle:  $W$  is the largest for straight bond ( $Ni^{3+} - O^{2-} - Ni^{3+}$   $180^\circ$ ) and smaller in distorted case. • Becomes better insulator with increasing  $R$  atomic number (smaller radius, more twisted bond of  $B - O - B$ ) • Different transition metal: Different  $d$ -electron configuration, Different  $p - d$  hybridization, Different  $U$  • Different A ions: Different ion size, Different bonding angle, Different  $W$  • Substitution of A: Different carrier density • Extra O or O deficiency: Different hole concentration • Substitution of B: Different on site configuration • Different dimensionality  
 • Magnetic Structure: Most have Antiferromagnetically ordered ground state

- Typical Strongly Correlated Materials: Incompletely filled  $d$  or  $f$  electron shells with narrow bands
- Wigner Crystal: Crystal of electrons • Potential  $\sim \frac{e^2}{r_0}$  Kinetic  $\sim \frac{\hbar^2}{mr_0^2}$  • when  $r_0$  is large

### 3. Anderson Localization • Dilute, Nonmagnetic Impurity, $T = 0$ , The distribution of the interaction

- The Spin Diffusion Puzzle: The relaxation time of donor electron spin is way longer at low concentrations
- Electron Spin Resonance (ESR): Unpaired electrons, Resonance frequency  $\rightarrow$  microwave ( $9GHz$  for  $0.3T$ ), challenging, Study electron spin dynamics. • Phase sensitive (lock-in) detector, The first derivative of absorption line.
- The Anderson Hamiltonian:  $H = \sum_i \epsilon_i n_i + \sum_{i,j} t_{ij} c_i^\dagger c_j$  •  $V = 0$ , as  $\epsilon_i$  is const, Tight-binding model
  - $t = 0$ , Atomic orbitals at each site •  $\frac{V}{W} \ll 1 \Rightarrow$  Impurity scattering of Bloch waves •  $\frac{V}{W} > 1 \Rightarrow$

#### Localization

- Mobility Edge:  $\pm \epsilon_c$ :  $0 < \frac{V}{W} < 1$ , Separating localized and non-localized states • Tuned by changing the level of disorder. • MIT:  $\epsilon_F$  tuned by doping level or pressure • Trait: • No energy gap in DOS near  $\epsilon_F$  (Pseudogap) • The electron number need not be integer • Coulomb repulsion is unnecessary

#### ► Near the localization transition – Still Controversy

- Mott's Minimum Conductivity: Localization transition is discontinuous. •  $lk_F > 1$ ,  $l \geq a$  •  $\sigma_{min}^{3D} \approx \frac{1}{3\pi^2} \frac{e^2}{\hbar} \frac{1}{a}$
- **Scaling Theory**:  $\frac{\hbar}{e^2} G(L) = g(L) \approx \frac{\Delta E}{\Delta V}$  •  $\beta(g) = \frac{d \ln g}{d \ln L}$  • The transition is continuous •  $\beta(g_c) = 0$ ,  $g_c \Rightarrow$  Unstable fixed point •  $g_0 > g_c \Rightarrow$  Conductor;  $g_0 < g_c \Rightarrow$  Insulator • No extended states for any degree of disorder in 1D and 2D. • Doesn't consider other effects can destroy the localization (Magnetic field, S-O coupling, E-E interaction ...)
- Weak Localization:  $l \ll l_i < L < \xi$ , where  $l$  is for elastic scattering,  $l_i$  is for inelastic scattering,  $L$  is the sample's scale,  $\xi$  is the localization length,  $k_F l \gg 1$  • Self-crossing loops:  $P = |A_1 + A_2|^2 = 2 \times 2|A|^2$ , decreases the conductivity, Localization • Dephasing length:  $\tau_\phi$ , Loss of phase coherence will destroy weak localization

$$\frac{\delta\sigma}{\sigma} = -\gamma_d \begin{cases} \left(\frac{\tau_\phi}{\tau}\right)^{1/2} & = T^{-\eta/2} & , d = 1 \\ \hbar \ln\left(\frac{\tau_\phi}{\tau}\right) & = \frac{\eta\hbar}{2} \ln \frac{\hbar}{k_B T} & , d = 2 \\ \hbar^2 \left(\frac{\tau_\phi}{\tau}\right)^{-1/2} & = \hbar^2 T^{\eta/2} & , d = 3 \end{cases}$$

- Wave Property: Reported for light waves, microwaves, sound waves, matter waves (BEC)
- Non-interacting theory, hard to ideally realize in Solid

### 4. Charge Density Wave (CDW):

- Peierls' Theorem: 1D materials are insulating • The distortion of lattice opens an energy gap around the original  $E_F$  • The lattice distortion induced a CDW with  $\lambda = \frac{\pi}{k_F}$ ,  $k = 2k_F$ ,  $\frac{\lambda}{a}$  can be irrational • Mechanism: e-ph coupling an electron-hole pair is created by a phonon • Kohn Anomaly: Electron-phonon interaction has a strong influence on the phonon spectrum near  $q = 2k_F \Rightarrow$  Phonon softening • 1D, Phonon Frequency

can drop to 0 • Hamiltonian:  $H = \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_q \hbar \omega_q b_q^\dagger b_q + \sum_{k,\sigma,q} g(k) c_{k+q,\sigma}^\dagger c_{k,\sigma} (b_q + b_{-q}^\dagger)$  • CDW gap:  $\Delta = 2W e^{-1/g}$  • CDW transition  $T$ :  $T_P = \frac{\Delta(0)}{1.76 k_B}$ , From BCS theory

- TTF (donor)-TCNQ (acceptor): • MIT:  $\sigma$  drops at 55K and 38K (superstructure with  $3.4a$ ), has a thermal activation behavior  $\Rightarrow$  Energy gap • Kohn anomaly: Neutron inelastic scattering • Fermi Surface Nesting: two pieces of parallel FS • Quasi-1D: FS as parallel planes  $\Rightarrow$  Warped, Still has FS nesting • Pressure: Pressure  $\uparrow \rightarrow T_{CDW} \uparrow \Leftarrow$  Imperfect nesting
- $NbSe_3$ : • Two sharp increases of  $\rho$  at 144K and 59K, remains metallic down to  $T = 0$  • 3 types of chains, 2 successive Peierls transitions
- $NbSe_2$ : Layered structure, can be grown to extremely high quality • A superstructure with  $3a$  • CDW state below 33K while being metallic, Superconductor below 7.2K • Multiband material

## 5. Jahn-Teller Theorem:

- Non-linear degenerate molecules cannot be stable. • Change of electronic structure  $\Rightarrow$  MIT
- Energy Gain: Electronic • Energy Cost: Elastic, Hund's rule coupling
- Octahedral complexes of the transition metals: Elongation along  $z$ , Lower  $d_{z^2}$ , Upper  $d_{x^2-y^2}$
- $K_xC_{60}$  Monolayers: MIT From  $K_3C_{60}$  to  $K_4C_{60}$  • Electrons in the LUMO orbital interact with certain vibrational mode of the  $C_{60}$  molecule and cause a permanent molecular distortion

## 5 Others

1. Topological Insulator: • Single electron model • Mainly spin-orbit interaction
2. Superfluidity: • Liquid He-4 & He-3: Low boiling  $T \Leftarrow$  Weak van der Waals force & low atomic mass
  - He-4 (Boson) < 2.17 K (BEC), He-3 (Fermion) < 2.49 mK (BCS)
3. Diamond: Indirect band gap:  $E_g = 5.5 eV$ , good insulator

