Notes on Introduction to Condensed Matter Physics

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1 Basic Introduction

1. Condensed Matter: $\sim 10^{23}\ /cm^3$
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 <u>Normal</u> Metals: • Ductile • Excellent electrical conductor • Excellent thermal conductor • Most are weak paramagnet, some ferromagnet • Opaque
   • At low T: ρ increases with T $\quad \chi \sim Const.$ $\quad c_V \propto T$
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: $c_V = \frac{3}{2} n k_B = Const.$ • The susceptibility puzzle: χ 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: $E_F \sim 7\ eV$, $k_F \sim 1 \times 10^8\ cm^{-1}$, $T_F \sim 8 \times 10^4\ K$, $v_F \sim 2 \times 10^8\ cm/s$ • DOS In 3D: $D(\varepsilon) \sim \varepsilon^{1/2}$ • Linear T Heat Capacity at Low T

   • Pauli Paramagnetism (at low T): $\chi = \mu_B^2 D(E_F) = const.$

   • Successes: • Realized the importance of Fermi distribution • Established the k-space language for electrons • Introduced Fermiology • Resolved the Pauli susceptability 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 • $\varepsilon = \frac{\hbar^2 k^2}{2m^*}$ • $c_V = \frac{1}{3} \frac{m^* k_F}{\hbar^2} k_B^2 T$ • $\chi = \frac{m^* k_F}{\hbar^2 \pi^2} \frac{1}{1+F_0^a} \mu_B^2$ • Landau parameter: m^*, F_0^a • Wilson ration: $R_W = \frac{\pi^2 k_B^2}{3\mu_B^2} \frac{\chi}{\gamma}$ • 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, $\psi_{nk}(\boldsymbol{r}) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} u_{nk}(\boldsymbol{r})$, where $u_{nk}(\boldsymbol{r}) = u_{nk}(\boldsymbol{R}+\boldsymbol{r})$ • 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: $\varepsilon_k^1 = \overline{V}$ • Second order (non-degenerate): $\varepsilon_k^2 = \sum_{g \neq 0} \frac{|V_g|^2}{\varepsilon_K^0 - \varepsilon_{k-g}^0}$ • Second order (degenerate): $\varepsilon_k^2 = \pm |V_n|$ • 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. • $\psi_k(\boldsymbol{r}) = \sum_{\boldsymbol{R}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \psi_a(\boldsymbol{r} - \boldsymbol{R})$ • Overlap integral: $t_{\boldsymbol{R}} = \int \psi_a^*(\boldsymbol{r}+\boldsymbol{R})(\Delta V)\psi_a(\boldsymbol{r}) \mathrm{d}\boldsymbol{r} \rightarrow$ 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: $V(a+\delta x) = V_0 + \frac{1}{2}\beta(\delta x)^2$ • $\varepsilon = \sum_k (n_k + \frac{1}{2})\hbar\omega$ • Phonons: The quantum of the lattice vibration, $n_k = \frac{1}{\mathrm{e}^{\hbar\omega/kT}-1}$ • 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

• $T \to 0$ $c_V \sim T^3$ ⇐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, Flecibility • 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 ⇐ $V = 0$ when $r \to \infty$ • Phonon-phonon interaction: No longer independent excitations ⇒ 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 → 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 → 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 • $\boldsymbol{J} = L \cdot \boldsymbol{F}$

   • 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 ~ 10 mK

   • Superconducting magnet: up to 20 tesla ⇐ critical field

   • Super high megnetic field: Florida-Bitter resistive magnet, Hybrid magnet

4. The Boltzmann Transport Equation: • $\left.\frac{\partial f_k}{\partial t}\right|_{\text{diffusion}} + \left.\frac{\partial f_k}{\partial t}\right|_{\text{field}} + \left.\frac{\partial f_k}{\partial t}\right|_{\text{scattering}} = 0$ • $\left.\frac{\partial f_k}{\partial t}\right|_{\text{diffusion}} = -\dot{\boldsymbol{r}} \cdot \nabla_{\boldsymbol{r}} f_k$ • $\left.\frac{\partial f_k}{\partial t}\right|_{\text{field}} = -\dot{\boldsymbol{k}} \cdot \nabla_{\boldsymbol{k}} f_k$ • $\left.\frac{\partial f_k}{\partial t}\right|_{\text{scattering}} = -\frac{f_k - f_k^0}{\tau}$

5. Electrical Transport: •$\boldsymbol{J}_e = \sigma \boldsymbol{E}$ • Measurements: Four-probe, Low frequency ac lock-in method

   • Drude model: $\sigma = \frac{ne^2\tau}{m}$ • Semi classical: $\delta \boldsymbol{k} = \frac{e\tau \boldsymbol{E}}{\hbar}$ • Only the surface of the FS changed !

   • Ignore the diffusion effect, Complexity of the FS

   • The Boltzmann transport equation: $\overleftrightarrow{\sigma} = \frac{1}{4\pi^3}\frac{e^2\tau}{\hbar}\int \frac{\boldsymbol{v}_k \boldsymbol{v}_k \mathrm{d}S_F}{v_k}$

   • Cubic symmetry: $\sigma_{x,y,z} = \frac{e^2}{3} v_F l D(\varepsilon_F)$

   • Matthiessen's rule: Different scattering mechanisms don't interfere each other $\Rightarrow \frac{1}{\tau} = \frac{1}{\tau_{imp}} + \frac{1}{\tau_{ph}} + \cdots$

   • 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: •$\boldsymbol{J}_Q = \kappa(-\nabla T)$ • Measurement: One-heater, Two-thermometer

   • Drude: $J_{Qe,x} = \frac{1}{2} n v_x [\varepsilon(T_{x-v\tau} - T_{x+v\tau})] = \frac{1}{3} c_V v l$ • $\boldsymbol{J}_Q = 2\int f_k(\varepsilon_k - \mu)\boldsymbol{v}_k \mathrm{d}\boldsymbol{k}$ • $\kappa_e = \frac{\pi^2}{3}\frac{k_B^2}{e^2} T\sigma$

   • Phonon Thermal Conductivity: Good metals ~ 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 ε_F • $S = \frac{\pi^2}{3}\frac{k_B}{e} k_B T \left.\left(\frac{\partial \ln \sigma(\varepsilon)}{\partial \varepsilon}\right)\right|_{\varepsilon=\mu}$ • Reveal abrupt change of electronic stucture

   • Study novel electronic phases and phase transitions, But poorly understood

   • Thermal couple: $V = (S_B - S_A)(T_x - T_0)$ • Thermoelectric power generation: Π-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: Π-junction consisting of N type & P type material • $J_Q = J_e(|\Pi_N| + |\Pi_P|)$

8. Peltier Effect: •$\boldsymbol{J}_Q = \Pi \boldsymbol{J}_e$

9. Onsager reciprocal relations: • $\begin{pmatrix} \boldsymbol{J}_e \\ \boldsymbol{J}_Q \end{pmatrix} = \begin{pmatrix} \sigma & \sigma S T \\ \sigma\Pi & -\kappa T \end{pmatrix} \begin{pmatrix} \boldsymbol{E} \\ \frac{\nabla_{\boldsymbol{r}} T}{T} \end{pmatrix}$ • $\Pi = ST$

10. The Thermoelectric Figure of Merit: •$ZT = \frac{\sigma S^2 T}{\kappa}$ • $ZT \sim 3$, for applilcation, Now $ZT \sim 1$

    • Now focusing on heavily doped narrow-band semiconductors, $n \sim 10^{19} - 10^{20}/cm^3$, Not promising because of W-F law • Minimize phonon thermal conductivity ⇒ Low Dimension, Amorphous, Nano-materials • Bi_2Se_3 & Bi_2Te_3: Quasi-2D system (Quintuple-layer) • Future focus: Considering Spin, Strong-correlation system

11. Magnetic Field: • Free electron gas: • No magnetoresistance • Hall coefficeint: $R_H = \frac{1}{ne}$
• 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 ∇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 ⇒ impurity bands
• Pressure: Structure change ⇒ Overlap ⇐ 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 ⇒ δV ⇒ $\delta n = -D(\varepsilon_F)\delta V$ ⇒ $\nabla^2(\delta V) = k^2\delta V$ • Yukawa Potential: $\delta V = \frac{e^2}{r}\mathrm{e}^{-kr}$ • Screening length: $\lambda = \frac{1}{k}$, $k = \sqrt{\frac{4me^2k_F}{\pi\hbar^2}} \propto n^{1/6}$ for 3D FEG • Good metals ⇒ 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%) ⇐ 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 $t = \int \varphi_j^*\left[V(r) - v_i(r)\right]\varphi_i dr$
$U = \int\left|\varphi_i(r_1)\right|^2 \frac{e^2}{r_{12}}\left|\varphi_i(r_2)\right|^2 dr$ 1^{st} tern: Hopping tern, 2^{nd} tern: on-site Coulomb repulsion tern
• 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 ~ 10-30 meV • Bonding angle: W is the largest for straight bond ($Ni^{3+} - O^{2-} - Ni^{3+}$ 180°) 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: $H = \sum_i \varepsilon_i n_i + \sum_{i,j} t_{ij} c_i^\dagger c_j$ • $V = 0$, as ε_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: $\pm\varepsilon_c$: $0 < \frac{V}{W} < 1$, Separating localized and non-localized states • Tuned by changing the level of disorder. • MIT: ε_F tuned by doping level or pressure • Trait: • No energy gap in DOS near ε_F (Psesdogap) • The electron number need not be integer • Coulomb repulsion in 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: $\frac{\hbar}{e^2}G(L) = g(L) \approx \frac{\Delta E}{\Delta V}$ •$\beta(g) = \frac{\mathrm{d}\ln g}{\mathrm{d}\ln L}$ • 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, ξ 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: τ_ϕ , Loss of phase coherence will destroy weak localization

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

• 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: $H = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k,\sigma} c_{k,\sigma} + \sum_q \hbar\omega_q b^\dagger_q b_q + \sum_{k,\sigma,q} g(k) c^\dagger_{k+q,\sigma} c_{k,\sigma} \left(b_q + b^\dagger_{-q} \right)$ • CDW gap: $\Delta = 2W\mathrm{e}^{-1/g}$ • CDW transition T: $T_P = \frac{\Delta(0)}{1.76k_B}$, From BCS theory

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: $E_g = 5.5eV$, good insulator

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