Physics 503

5/1 - Administrative matters
- Introduction & Course Contents

- Name, email, office
- Hamed Karimi, HA 414, hamed@phas.ubc.ca
- office hour: Wed 3-4
- feel free to come and see me!
- web site up soon
- No textbook but several useful books on reserve in library & important review article
- Ashcroft-Mermin [review of CM I material]
- Mahan - 2nd quantization notation, Green's functions, Kubo formula.
- A G D - diagram notation, terms liquid theory
- Hewson - Kondo model

Yamanishi - interacting fermions in 1 dimension
- Shankar RMP 66, 129-192 (1994)
- Renormalization Group approach to Fermi liquid theory.
- I will assign readings

Grading Scheme

Problem sets (biweekly) 30%

Mid-term Exam 30%

Grad presentation to class 40%

- one hour presentation/work in pairs
- topics assigned later - will be related to lecture material - must be ready on time
- homework - OK to discuss with class-mates but write up your own solutions
ASK QUESTIONS!

Course ~~Objectives~~ Learning Goals

- to be able to solve problems in advanced CMP
- to be able to apply techniques of CMT ~~to~~ [Green's functions, Feynman diagrams, path integrals, RG---] to various situations
- to be able to read and understand

CMT papers & explain them to your colleagues.

- Introduction & Course Contents
- each branch of Physics may have a defining result
- QED - g-2 of electron
- atomic physics - exact sol'n of H-atom
- what it is for CMP?
- arguably free electron [Fermi gas] model of metals
- many metals obey free electron prediction quite well
  - linear specific heat at low T $C = \gamma T$
  - T-independent magnetic susceptibility at low T.
  - including periodic potential ⇒ band structure
  - including impurities ⇒ resistivity

- but this approach ignores e-e [e-p] interactions - why is this justified?

- a simple estimate suggest they are important

- kinetic energy per particle $\sim \frac{\hbar^2 k_F^2}{2m}$

[will set $\hbar = 1$]

density $n \sim k_F^3$ or $E_K \sim \frac{n^{2/3}}{m}$

- e-e Coulomb energy/particle $\sim \frac{e^2}{r_0} \sim E_K$

where $r_0 \sim n^{-1/3}$ is average distance to closest electron [actually this is exchange energy - read Mahan, Chap 5 if not familiar]

$$E_K \sim \frac{1}{m r_0^2}$$

$$\frac{E_C}{E_K} \sim e^2 m \cdot r_0 \sim \frac{r_0}{a_0}$$

where $a_0 = \frac{1}{e^2 m}$ = Bohr radius $\sim .5 \text{ Å}$

- this number is typically ~ 1 for a metal

- separation of atoms ~ a, about 1 electron/atom
- perturbation theory in Coulomb interaction doesn't work for metals! [unless density is very high]
- expansion is very complicated due to long-range nature of Coulomb interaction
$E_0 \sim E_K + O(e^2) + O(e^4 \ln e) + \cdots$?
- Landau proposed a more subtle explanation:
- interaction can be ignored, in a sense, at low T only
- actually, even at low T they have important consequences: $C \to \gamma T$, $\gamma = \frac{m}{3} (3\pi^2 n)^{1/3}$
[& set $k_B = 1$ also] - see A-M.

m = electron mass

- while $C \to \gamma T$ holds with interactions,

$m \to m^*$ [NB - in addition to band-structure effect - this is from interactions]

- basic form of free electron result holds but with modified parameters

- i.e., even at low T, Coulomb interaction turn m into m^*

- how low is low T? $T \ll E_F$

- fortunately $E_F \sim 1eV \sim 10^4 K$ for most metals so room temperature is low

- why does low T simplify things?

= consider an electron excited above the Fermi energy by an amount ΔE (at $T=0$)

(1111) $\Delta k \cdot \Delta E \sim V_F \Delta k$

- ~~At low~~ it can decay into 2 electrons & a hole due to Coulomb interaction

- but both final state electrons must have energies (measured from E_F) $< \Delta E$ and so must hole
- energy & momentum must be conserved
- reduced phase space at low ΔE
  ⇒ decay rate $\propto (\Delta E)^2$ - will show later
- $\Rightarrow$ electrons [holes] near E_F are only weakly affected by e-e interaction despite large r_0/a_0
- at low T only electrons near E_F are "active" - it costs too much energy to excite other ones
- Landau's reasoning foreshadowed RG
- eliminate high energy degrees of freedom [far from Fermi surface] to obtain

~~low energy~~ effective Hamiltonian for low energy ones

- this H_{eff} may have strongly renormalized parameters in it (eg m^2) but interactions in it may be weak
- we need to understand "eliminate" (RG)
- this approach (RG) is basis of modern theory of critical phenomena (Phys 5(d))
- near a critical point, (2nd order phase transition) correlation length becomes big & we may eliminate short distance degrees of freedom [sum over them in classical Boltzmann sum]
- in metals, we attempt to take advantage of $E \ll E_F$ (for $E \sim T$ or other

energy scale of interest] to eliminate high energy degrees of freedom
[NB - high energy corresponds to large wave vector (measured from RF) OR short distances]

- important that T_N, T_c << EF
- the RG approach is useful for understanding:
  - superconductivity
  - 1D metals
  - dilute magnetic impurities (Kondo effect)
- in last 25 years people are trying to apply RG to hi-T_c superconductors, heavy fermions, frustrated magnets...
- still at an early stage!
- we will discuss several of these topics

In Phys 503 to illustrate RG approach

- some needed techniques
  - Green's function
  - path integral & Feynman diagrams for eliminating high energy degrees of freedom
  - RG

- reading - review free electron theory of metals [eg A-M chap 2]
  - check that low T properties only depend on states near E_F
  - review 2nd quantization & exchange energy [Mahan]

- next topic: Green's functions
  - see eg. Mahan chap 2, 3

10/1 (course goals) questions? (Hw Th.)

- notation, Hamiltonians, Kubo formula and retarded Green's functions
- Mahan's notation is pretty standard in CMP, Shankar's a bit less so - will follow Mahan thru most of course but switch to Shankar's when we cover his article

$c_{\vec{k}\sigma}$ annihilates electron of wave-vector $\vec{k}$, spin $\sigma = \pm$ [$\Leftrightarrow \pm\frac{1}{2}$] [$\Leftrightarrow \uparrow, \downarrow$]

$$\{c_{\vec{k}\sigma}, c^{+}_{\vec{k}'\sigma'}\} = \delta_{\vec{k},\vec{k}'}\,\delta_{\sigma,\sigma'}$$

Kronecker-delta normalization

$\delta_{\vec{k},\vec{k}'} = 1$ if $\vec{k} = \vec{k}'$, 0 otherwise

- $\vec{k}$'s discrete - box of side L $k_i = 2\pi n_i/L$, $n_i = 0, \pm 1, \ldots$
- take $L \to \infty$ at end

vacuum $|0\rangle$: $c_{\vec{k}\sigma}|0\rangle = 0$

$|\vec{k}\sigma\rangle = c^{+}_{\vec{k}\sigma}|0\rangle$ is single-particle state

- en Continuum model (jellium)

$\frac{L}{2\pi} k_i \in \mathbb{Z}$, position space annihilation op defined at arbitrary pt $\vec{r} \in \mathbb{R}^3$

$$\psi_\sigma(\vec{r}) = \frac{1}{V^{1/2}} \sum_{\vec{k}} e^{i \vec{k} \cdot \vec{r}} a_{\vec{k}\sigma}$$

where $V = L^3$ = volume of space

$$\{ \psi_\sigma(\vec{r}), \psi^+_{\sigma'}(\vec{r}') \} = \frac{1}{V} \sum_{\vec{k}} e^{i \vec{k} \cdot (\vec{r} - \vec{r}')} \delta_{\sigma,\sigma'}$$

$$\sum_{\vec{k}} \to \frac{V}{(\Delta k)^3} \int \frac{d^3k}{(\Delta k)^3} = V \int \frac{d^3k}{(2\pi)^3} \quad \text{at } V \to \infty$$

$\Rightarrow \{ \} = \delta_{\sigma,\sigma'} \delta^3(\vec{r} - \vec{r}')$ - Dirac δ-function

electron density operator $\rho(\vec{r}) = \sum_\sigma \psi^+_\sigma(\vec{r}) \psi_\sigma(\vec{r})$

$$= \frac{1}{V} \sum_{\vec{k}, \vec{k}', \sigma} c^+_{\vec{k}\sigma} c_{\vec{k}'\sigma} \exp\left[i (\vec{k}' - \vec{k}) \cdot \vec{r} \right]$$

Hamiltonian

$$H = \int d^3r \, \psi^+ \left[-\frac{\nabla^2}{2m} \right] \psi + \frac{1}{2} \int d^3r \, d^3r' \, \rho(\vec{r}) \, V(\vec{r} - \vec{r}') \, \rho(\vec{r}')$$

where $V(\vec{r})$ is inter-electron interaction

$V(r) = e^2/r$ or might used short-range screened interaction

$$H = \sum_{\vec{k},\sigma} \epsilon_{\vec{k}} C^+_{\vec{k}\sigma} C_{\vec{k}\sigma} + \frac{1}{2V} \sum_{\vec{q},\vec{k},\vec{k}',\sigma\sigma'} V_{\vec{q}}$$

$$C^+_{\vec{k}+\vec{q},\sigma} C^+_{\vec{k}'-\vec{q},\sigma'} C_{\vec{k}'\sigma'} C_{\vec{k}\sigma}$$

$\propto V_q = 4\pi e^2/q^2$

- I moved $C_{\vec{k}\sigma}$ to right of $C^+_{\vec{k}'-\vec{q},\sigma'} C_{\vec{k}'\sigma'}$

this produces a term $\frac{1}{2V}\sum_{\vec{q}} V_q \cdot \sum_{\vec{k},\sigma} C^+_{\vec{k}\sigma} C_{\vec{k}\sigma}$

$= \frac{1}{2} V(\vec{r}=0) \cdot N_e$ [N_e = # electrons]

where $V(\vec{r}) = \frac{1}{V} \sum_{\vec{q}} e^{i\vec{q}\cdot\vec{r}} V_{\vec{q}}$

- this is self-interaction of electrons - we drop this term which is actually u-v divergent: $V(0) = \infty$

- elementary particle physics issue!

[we actually also drop $\vec{q}=0$ term from sum which is i.r. divergent

this is $\frac{1}{2} N \rho_0 \int d^3 r\, V(\vec{r})$ – it is cancelled by interaction of electrons with uniform positive charge density ρ_0 in jellium model, and by interaction of (+)ve charge with itself]

- we sometimes consider instead a periodic potential from (+)ve ions

$$\int H = \int d^3 \vec{r}\, \rho(\vec{r})\, U(\vec{r})$$

$$U(\vec{r}) = U(\vec{r} + \vec{q}_i) \qquad i = 1, 2, 3$$

- it is then often convenient to work in basis of eigenstates of kinetic energy + lattice potential energy

$|\vec{k}, \sigma\rangle$ where now $\vec{k}$ is restricted to 1st Brillouin zone

$e[i = 1, 2, 3, \ldots]$ labels bands

We will sometimes consider simplified tight-binding model which keeps only a single band.

$$H_0 = -t \sum_{\vec{R}, \vec{\delta}, \sigma} C^{+}_{\vec{R}\sigma} C_{\vec{R}+\vec{\delta}, \sigma}$$

where $\vec{R}$ is summed over discrete lattice points [eg simple cubic or square in 2D with spacing a] and $\vec{\delta}$ are vectors to all nearest neighbours [eg $\vec{\delta} = a(\pm 1, 0, 0), a(0, \pm 1, 0), a(0, 0, \pm 1)$]

t is hopping amplitude

$C_{\vec{R}\sigma}$ annihilates an electron at site $\vec{R}$, $\{ C_{\vec{R}'\sigma}, C^{+}_{\vec{R}''\sigma'} \} = \delta_{\sigma\sigma'} \delta_{\vec{R}, \vec{R}''}$

- Kronecker δ-fnc in position space

in lattice model

here $C_{\vec{R}\sigma} = \frac{1}{N^{1/2}} \sum_{\vec{k} \in BZ} e^{i\vec{k}\cdot\vec{R}} C_{\vec{k}\sigma}$

N = # of lattice sites in a large volume → $\vec{k}$ restricted to BZ

$$H_0 = \sum_{\vec{k}\sigma} \epsilon_{\vec{k}} C^{\dagger}_{\vec{k}\sigma} C_{\vec{k}\sigma}$$

$\epsilon_{\vec{k}} = -2t [\cos k_x a + \cos k_y a + \cos k_z a]$

for simple cubic case

- interaction term is often approximated as nearest neighbour repulsion only [highly screened]

$$H_{INT} = U \sum_{\vec{R}} n_{\vec{R}\uparrow} n_{\vec{R}\downarrow}$$

where $n_{\vec{R}\sigma} \equiv C^{\dagger}_{\vec{R}\sigma} C_{\vec{R}\sigma}$ = number operator on site $\vec{R}$ for spin σ electrons $= 0, 1$ only.

- more realistic models take into account

longer-range hopping & interactions
- questions?

Kubo formula for Conductivity &
Retarded GF's

- apply external electric field $\vec{E}(\vec{r},t)$
to system [will often consider
$\vec{E}(\vec{r},t) = E_0 \, \mathrm{Re}\, e^{i\omega t}$ and take $\omega \to 0$]

$$\vec{E} = -\frac{1}{c}\frac{\partial \vec{A}}{\partial t} + \nabla \phi$$

- use $\nabla \cdot \vec{A} = 0$ gauge and assume $\nabla \cdot \vec{E} = 0$ $\Rightarrow$ $\phi = 0$
[no "external charges" in sphd]

vector potential $\vec{A}$ added to Hamiltonian

$$H_K \to \frac{1}{2m}\sum_\sigma \int d^3\vec{r}\; \psi_\sigma^+(\vec{r})\left[-i\nabla - \frac{e}{c}\vec{A}\right]^2 \psi_\sigma(\vec{r})$$

$(e<0)$

Current operator $\vec{J}(\vec{r},t) = \frac{e}{m}\sum_\sigma \psi_\sigma^+(\vec{r})\left[-i\nabla - \frac{e}{c}\vec{A}\right]\psi_\sigma(\vec{r})$

$$H = H_0 - \frac{1}{c}\int d^3\vec{r}\; \vec{j}(\vec{r})\cdot\vec{A} + O(A^2)$$

where $\vec{j}(\vec{r}) = \frac{e}{m}\sum_\sigma \psi^+ (-i\nabla)\psi$

[current operator at $O(A^0)$]

- can ignore A^2 term in H at weak fields - we calculate linear response

current $\langle \vec{J} \rangle \propto \vec{E}$

$\vec{J} = \langle \vec{J}(r,t) \rangle = \langle \vec{j} \rangle - \frac{e^2}{mc} \langle \vec{\rho}(\vec{r},t) \rangle \vec{A}$

$\langle \rho \rangle = \rho$ evaluated at $\vec{A}=0$ but

$\langle \vec{j} \rangle$ calculated to 1st order in $\vec{A}$

$\langle \vec{j} \rangle = 0$ at $\vec{A}=0$ we assume

[H_0 above includes Coulomb interaction]

$H = H_0 + H'(E)$

NB: H' is E-dependent but small

- Convenient to use interaction picture of quantum mechanics

Schroedinger picture

$$i\frac{d}{dt}|\psi\rangle_S = H|\psi\rangle_S,$$

$$\Rightarrow |\psi\rangle_S(t) = e^{-iHt}|\psi\rangle_S(0)$$

(if H is t-independent, which it usn't here)

- for t-dependent H, $|\psi\rangle_S(t)$ given by a complicated time-integral
- observables given by $\langle\psi(t)|O_S|\psi(t)\rangle_S$ (depend on time), O_S operators often t-independent (not H)
- for simple case of constant H,

$$\langle\psi(t)|O_S|\psi(t)\rangle_S = \langle\psi(0)|e^{iHt}O_S e^{-iHt}|\psi(0)\rangle_S$$

- in Heisenberg picture, for t-independent H,

$$|\psi\rangle_H = |\psi(0)\rangle_S = \text{constant}$$

$$O_H(t) = e^{iHt}O_S e^{-iHt} \quad \text{depends on } t$$

$$\langle\psi|O_H(t)|\psi\rangle_H = \langle\psi(t)|O_S|\psi(t)\rangle_S$$

interaction picture - we transfer only some of time dependence to operator
- that coming from H_0 (t- independent)

$|\psi(t)\rangle_I$ ~~=~~ $\mathcal{O}_I(t) \equiv e^{iH_0 t} \mathcal{O}_S e^{-iH_0 t}$

[NB- H_0 constant] $|\psi(t)\rangle_I$ defined by $\langle \psi(t)|_I \mathcal{O}_I(t) |\psi(t)\rangle_I = \langle \psi(t)|_S \mathcal{O}_S |\psi(t)\rangle_S$

$\Rightarrow |\psi(t)\rangle_I = e^{iH_0 t} |\psi(t)\rangle_S$

- N.B - this "removes" some of t-dependency of $|\psi\rangle_S = e^{-iHt} |\psi(0)\rangle_S$ (for constant H)
- we want explicit formula for $|\psi(t)\rangle_I$ when $H = H_0 + H'$, $H' = H'(t)$
- NB- when no subscript is written operators are "original" ones in Schroedinger rep