Introduction

In condensed matter the basic equation is relatively simple to write:

fundamental Hamiltonian: $H = H_e + H_i + H_{ei}$

$$H_e = \sum_i \frac{p_i^2}{2m_e} + \sum_{i \neq j} \frac{1}{2} V_{ee}(\vec{r}_i - \vec{r}_j)$$ here $V_{ee}(\vec{r}) = \frac{e_0^2}{4\pi\varepsilon_0 |\vec{r}|}$ $\vec{r}_i$ electron coordinate

$$H_i = \sum_\alpha \frac{P_\alpha^2}{2M_\alpha} + \sum_{\alpha \neq \beta} \frac{1}{2} V_{ii}(\vec{R}_\alpha - \vec{R}_\beta)$$ here $V_{ii}(\vec{R}_\alpha - \vec{R}_\beta) = \frac{Z_\alpha Z_\beta e_0^2}{4\pi\varepsilon_0 |\vec{R}|}$; R_α ion coordinate

$$H_{ie} = \sum_{i\alpha} V_{ei}(\vec{r}_i - \vec{R}_\alpha)$$ here $V_{ei}(\vec{r}_i - \vec{R}_\alpha) = - \frac{Z_\alpha e_0^2}{4\pi\varepsilon_0 |\vec{r}_i - \vec{R}_\alpha|}$

What is missing? Spin (very easy to add)

Spin-orbit interaction and other relativistic corrections because electron travel fast near nucleus

$$H_{soc} = \frac{\mu_B}{\hbar m_e e_0 c^2} \sum_i \frac{1}{r_i} \frac{\partial V}{\partial r_i} \vec{l}_i \times \vec{s}_i \quad \propto Z^4$$

Important for heavy ions

Fe : 20 meV

Ce : 0.3 eV

Pu : 1 eV

Ir : 0.5 eV

We usually treat ion & electron degrees of freedom differently because $M_\alpha >> m_e$.

$\frac{M_H}{m_e} = 1840$ $\frac{M_{Si}}{m_e} = 25760$ hence expansion in $\frac{m_e}{M_\alpha}$ is well justified.

Born-Oppenheimer approximation "almost" allways works

Exceptions: - conventional superconductors
- resistivity due to phonons
- electron-phonon coupling important

Because nuclei move much slower than electrons the nuclei positions can be frozen when computing the electron wave function.

Born Oppenheimer ansatz for separable wave function $|\Psi\rangle = |\Psi_{electron}\rangle \otimes |\Psi_{ion}\rangle$

Born – Oppenheimer

$$(H_e + H_{ie} + H_i)\,|\Psi_{electron}\rangle \otimes |\Psi_{ion}\rangle$$

Because $M_\alpha >> m_e$ we first neglect $\frac{P_\alpha^2}{2M_\alpha}$ term for the purpose of computing the electron wave function, i.e.,

How large is neglected term $\langle \Psi_{electron} | \sum_e \frac{P_e^2}{2M_e} | \Psi_{electron} \rangle$?

$$\vec{P}_{ion} \sim \vec{p}_{electron} \Rightarrow$$

$$\langle \Psi_{electron} | \sum_e \frac{P_e^2}{2M_e} | \Psi_{electron} \rangle \approx E^{kin}_{electron} \underbrace{\frac{m_e}{M_i}}_{10^{-4}}$$

should be small correction in most cases.

$$\underbrace{\Big[H_e + \underbrace{\sum_{ie} V_{ei}(\vec{r}_i - \vec{R}_e) + \sum_{l \neq m} \tfrac{1}{2} V_{ii}(\vec{R}_l - \vec{R}_m)}_{V_{ext}(\vec{r}_i)} \Big]}_{H_{electronic}} |\Psi_{electron}\rangle = E_{electron}[\{\vec{R}\}]\, |\Psi_{electron}\rangle$$

$\vec{R}_l$ are now fixed to the lattice sites and are parameters in electron sch. Eq.
They are not operators or physical observables.
We can still determine best possible low T structure by comparing

$$\underset{bcc}{E_{electron}[\{R\}_1]}, \quad \underset{fcc}{E_{electron}[\{R\}_2]}, \ldots \qquad \underset{\text{closest-packed hexagonal}}{cph} \quad \ldots$$

Finally we can consider small vibrations around the ground state lattice configuration

$$H\,|\Psi_{electron}\rangle \otimes |\Psi_{ion}\rangle = \Big[H_{electronic} + \sum_\alpha \frac{P_\alpha^2}{2M_\alpha} \Big] |\Psi_{electron}\rangle \otimes |\Psi_{ion}\rangle$$

$$\approx \underbrace{\Big[E_{electronic}[\{\vec{R}\}] + \sum_\alpha \frac{P_\alpha^2}{2M_\alpha} \Big]}_{\text{gives phonon dispersion at the second order expansion}} |\Psi_{electron}\rangle \otimes |\Psi_{ion}\rangle$$

<u>Adiabatic approximation</u>

as the nuclei move, electrons are always in the ground state wave function

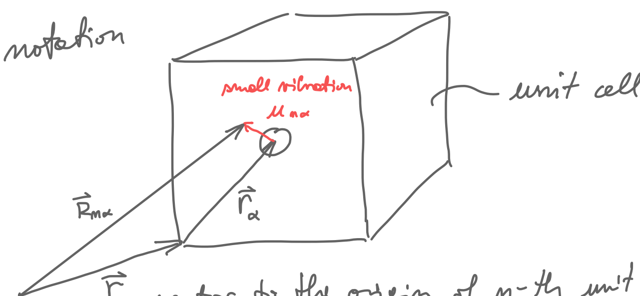
How do we obtain phonon dispersions?

We can expand $\vec{R}_\alpha = \vec{R}_\alpha^{equilibrium} + \vec{u}_\alpha$ ← small displacement

$$E_{electron}[\{\vec{R}\}] = \underset{\uparrow \text{ equilibrium}}{E^0_{electron}[\{R\}]} + \sum_\alpha \underset{\substack{\uparrow \\ \text{should vanish} \\ \text{because force} = 0 \text{ in} \\ \text{equilibrium}}}{\frac{\partial E^0_{electron}[\{\vec{R}\}]}{\partial \vec{R}_\alpha}} \vec{u}_\alpha + \frac{1}{2}\sum_{\alpha,\beta} \vec{u}_\alpha \underset{\substack{\uparrow \\ \boxed{\text{Matrix of force constants}}}}{\left(\frac{\partial^2 E^0_{electron}[\{\vec{R}\}]}{\partial \vec{R}_\alpha \partial \vec{R}_\beta}\right)} \vec{u}_\beta + \dots$$

If truncated here, we call it <u>harmonic</u> approximation

In periodic solids we will use more appropriate notation



$\vec{r}_m$ vector to the origin of m-th unit cell

$$\vec{R}_{m\alpha} = \vec{r}_m + \vec{r}_\alpha + \vec{u}_{m\alpha} \leftarrow \text{small vibration}$$

$\vec{r}_m = m_1\vec{a}_1 + m_2\vec{a}_2 + m_3\vec{a}_3$; $\vec{r}_\alpha$ ← Wyckoff position

$$E_{electron}[\{\vec{R}\}] = E^0_{electron}[\{R\}] + \frac{1}{2}\sum_{\substack{m,m,\\ \alpha,\beta,\\ i,j}} \underset{\nwarrow x,y,z}{u_{m\alpha i}} \underbrace{\frac{\partial^2 E^0[\{R\}]}{\partial R_{m\alpha i}\partial R_{m\beta j}}}_{\Phi^{m\beta j}_{m\alpha i}} \underset{\nwarrow x,y,z}{u_{m\beta j}}$$

then $H|\psi\rangle \Rightarrow \Big(\overbrace{\sum_{\substack{\alpha\\ m,i}} \frac{1}{2}\frac{\vec{P}_\alpha^2}{2M_\alpha} + \sum_{\substack{m\,m\\ \alpha\,\beta\\ i\,j}} \frac{1}{2} u_{m\alpha i}\, \Phi^{m\beta j}_{m\alpha i}\, u_{m\beta j}}^{\text{Harmonic oscillators}} + E^0_{electron}[\{R\}]\Big)|\psi_{ion}\rangle = E\,|\psi_{ion}\rangle$

$\boxed{\text{Solve in Lagrange formulation:}}$

Instead of $\sum_\alpha \frac{\vec{P}_\alpha^2}{2M_\alpha} \Rightarrow \sum_\alpha \frac{1}{2} M_\alpha \dot{\vec{u}}_{m\alpha}^2 \equiv T$

$H = T + V$; $\mathcal{L} = T - V$

We are solving classical Lagrangian: $\mathcal{L} = \sum_{\substack{\alpha\\ m,i}} \frac{1}{2} M_\alpha \dot{u}_{m\alpha i}^2 - \sum_{\substack{m\,m\\ \alpha\,\beta\\ i\,j}} \frac{1}{2} u_{m\alpha i}\, \Phi^{m\beta j}_{m\alpha i}\, u_{m\beta j}$

Equation of motion $\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{u}_{m\alpha i}}\right) = \frac{\partial \mathcal{L}}{\partial u_{m\alpha i}}$ gives $M_\alpha \ddot{u}_{m\alpha i} = -\sum_{m\beta j} \Phi^{m\beta j}_{m\alpha i}\, u_{m\beta j}$

stopped 9/6/2022

EOM: $$M_\alpha \ddot{u}_{m\alpha i} = -\sum_{m\beta j} \Phi^{m\beta j}_{m\alpha i}\, u_{m\beta j}$$

We search for the solution with ansatz:

$$u_{m\alpha i} = \underbrace{\frac{1}{\sqrt{M_\alpha}}}_{\text{for convenience}} \mathcal{E}^{\overset{\text{phonon polarization}}{p}}_{\alpha i}(\vec{q})\, e^{i(\vec{q}\vec{r}_m - \omega_p t)}$$

p: different branches; α: different atoms; i: x,y,z

$$-\frac{1}{\sqrt{M_\alpha}} \Big/ \quad -\sqrt{M_\alpha}\,\omega_p^2\, \mathcal{E}^p_{\alpha i}(\vec{q})\, e^{i(\vec{q}\vec{r}_m - \omega_p t)} = -\sum_{m\beta j} \Phi^{m\beta j}_{m\alpha i} \frac{1}{\sqrt{M_\beta}}\, \mathcal{E}^p_{\beta j}(\vec{q})\, e^{i(\vec{q}\vec{r}_m - \omega_p t)}$$

$$\sum_{\vec{r}_m} \frac{1}{\sqrt{M_\alpha M_\beta}}\, \underline{\Phi}^{m\beta j}_{m\alpha i}\, e^{i\vec{q}(\vec{r}_m - \vec{r}_m)} = \boxed{D_{\alpha i, \beta j}(\vec{q})}$$

matrix of force constants

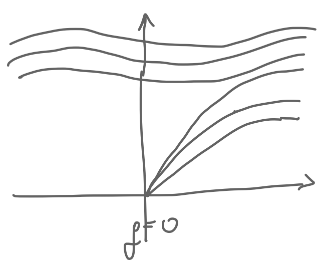
different atoms (α, β), xyz (i, j) — Dynamical matrix

D is essentially the Fourier transform of $\underline{\Phi}$.

$$\sum_{\beta j} \left[-\omega_p^2\, \delta_{\alpha\beta}\, \delta_{ij} + D_{\alpha i, \beta j}(\vec{q}) \right] \mathcal{E}^p_{\beta j}(\vec{q}) = 0$$

Is eigenvalue problem solved by $\mathrm{Det}\left[\underline{D}(\vec{q}) - \omega_p^2\, \underline{I} \right] = 0$

How many solutions $\omega_p(\vec{q})$? Dimension is $(\alpha, i) =$ # atoms in unit cell $\times 3$



$3\cdot(N-1)$ optical branches

3 acoustic branches

& $\omega_p(\vec{q})$ are eigenvalues of $\underline{D}$.

polarization $\mathcal{E}_{p\beta j}(\vec{q})$ are eigenvectors of $\underline{D}$.

Direct method of calculating phonons

Force: $\vec{F}_\ell \equiv -\dfrac{\delta E_{electron}[\{\vec{R}\}]}{\delta \vec{R}_\ell}$

any ion

This requires solution of $H_{electronic}$ and implementation of forces, which is usually done analytically.

In practice it is many times easier to calculate force, i.e., first derivative because:

$$\frac{\delta}{\delta \vec{R}}\langle\psi|H|\psi\rangle = \langle\frac{\delta\psi}{\delta\vec{R}}|H|\psi\rangle + \langle\psi|H|\frac{\delta\psi}{\delta\vec{R}}\rangle + \langle\psi|\frac{\delta H}{\delta\vec{R}}|\psi\rangle$$

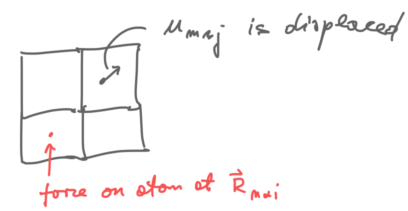
$$E\underbrace{\left(\langle\frac{\delta\psi}{\delta\vec{R}}|\psi\rangle + \langle\psi|\frac{\delta\psi}{\delta\vec{R}}\rangle\right)}_{\frac{\delta}{\delta\vec{R}}\langle\psi|\psi\rangle = 0} + \langle\psi|\frac{\delta H}{\delta\vec{R}}|\psi\rangle$$

because $\langle\psi[\{R\}]|\psi[\{R\}]\rangle = 1$

Hence in general force: $F_{m\alpha i} = -\dfrac{\delta E_{electronic}[\{R\}]}{\delta R_{m\alpha i}} = -\langle\psi_{elect}|\dfrac{\delta H_{electronic}}{\delta R_{m\alpha i}}|\psi_{electronic}\rangle$

is easier to compute.

We can create supercell and displace atom in different supercells and evaluate force $F_{m\alpha i}$



The matrix of force constants $\Phi^{m\beta j}_{m\alpha i} = \lim_{u\to 0}\left(-\dfrac{F_{m\alpha i}[u_{m\beta j}]}{u_{m\beta j}}\right)$ when using small displacement $u_{m\beta j}$

This is because $-F_{m\alpha i} = \dfrac{\delta E_{electronic}[\{R\}+u_{m\beta j}]}{\delta u_{m\alpha i}} \approx \dfrac{\delta^2 E_{electronic}}{\delta u_{m\alpha i}\,\delta u_{m\beta j}}\, u_{m\beta j}$

Most of this semester will be devoted to solving

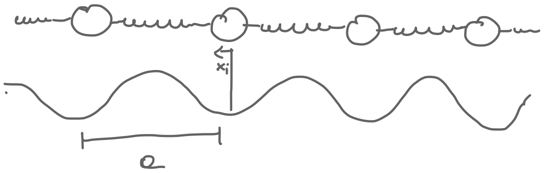
$$H_e |\Psi_e\rangle = E |\Psi_e\rangle \quad \text{with } 10^{23} \text{ electrons.}$$

We will try to

- look for universal behaviour of materials
  - Fermi liquid concept
  - Superconductivity & superfluidity
  - Collective low energy excitations such as phonons and magnons
- symmetries can greatly reduce the complexity
  - good momentum $\vec{k}$ in solids due to translational invariance
  - point group and space group symmetry of the lattice
  - SU(2) symmetry of the spin encoded in Pauli matrices

Simons 1.1.

Simple example of a field: 1D phonons



potential $V(x)$

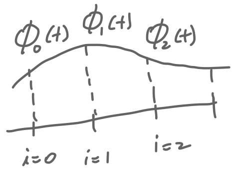
$$k = \left.\frac{\partial^2 V}{\partial x^2}\right|_{\substack{x = n\cdot a \\ \text{minimum}}}$$

$$H = \sum_i \frac{p_i^2}{2M} + \frac{k}{2}(x_{i+1} - x_i - a)^2 \qquad \text{Hamiltonian}$$

$$L = \sum_i \frac{1}{2} M \dot{x}_i^2 - \frac{k}{2}(x_{i+1} - x_i - a)^2 \qquad \text{Lagrangian}$$

The low energy excitations will be long wavelength waves. We do not need to care about the discreteness of the problem, but can define the theory in continuum.

$$x_i(t) = i a + \phi_i(t)\sqrt{a}$$



$\phi(x,t)$ continuum field
$\|$
$\phi^t(x)$

$$L = \sum_i \frac{1}{2} M \dot{\phi}_i^2 - \frac{k}{2}(\phi_{i+1} - \phi_i)^2$$

Transition to continuum: $\phi_i \to \sqrt{a}\,\phi(x,t)\Big|_{x=ia}$ has dimension of $\sqrt{\text{length}}$

$$\phi_{i+1} - \phi_i \to \sqrt{a}\cdot a \left.\frac{\partial \phi}{\partial x}\right|_{x=ia} \qquad -\!\!\!\;//\!\!\;-$$

$$\sum_i \longrightarrow \frac{1}{a}\int_0^L dx \qquad \text{has no dimension}$$

$$L = \frac{1}{a}\int_0^L dx \left[\frac{1}{2} M a \dot{\phi}^2 - \frac{k}{2} a^3 \left(\frac{\partial \phi}{\partial x}\right)^2\right] = \int_0^L dx \left[\frac{1}{2} M \dot{\phi}^2 - \frac{k a^2}{2}\left(\frac{\partial \phi}{\partial x}\right)^2\right]$$

Define Lagrangian density $\mathcal{L}[\phi, \frac{\partial \phi}{\partial x}, \dot{\phi}] = \frac{1}{2} M \dot{\phi}^2 - \frac{k a^2}{2}\left(\frac{\partial \phi}{\partial x}\right)^2$

Action is the functional of ϕ: $S[\phi] = \int dt \int_0^L dx\, \mathcal{L}[\phi, \frac{\partial \phi}{\partial x}, \dot{\phi}]$

S is classical action

ϕ is classical field $\phi(x,t)$

Eq of motion: EOM

The classical solution corresponds to the extremum of the action $\delta S = 0$.

$$S[\phi] = \int dt \int dx\, \mathcal{L}\left[\phi, \frac{\partial\phi}{\partial x}, \dot\phi\right]$$

If we add a small correction $\phi \to \phi + \eta$ and η is small $S[\phi+\eta] = S[\phi] + O(\eta^2)$

$$S[\phi+\eta] = \int dt\int dx\, \mathcal{L}\left[\phi+\eta, \frac{\partial\phi}{\partial x}+\frac{\partial\eta}{\partial x}, \dot\phi+\dot\eta\right] = ?$$

Note: $f[\phi+\eta] = f[\phi] + \int \frac{\partial f}{\partial\phi(x)}\,\eta(x)\,dx$

Follows from discrete analog: $f[\phi_1+\eta_1, \phi_2+\eta_2, \dots] = f[\phi_1,\phi_2 \dots] + \sum_i \frac{\partial f}{\partial \phi_i}\eta_i + \dots$

For above case

$$\sum_i \mathcal{L}\left[\phi_i+\eta_i, \frac{\partial\phi_i}{\partial x_i}+\frac{\partial\eta_i}{\partial x_i}, \dot\phi_i+\dot\eta_i\right] = \sum_i \mathcal{L}\left[\phi_i, \frac{\partial\phi_i}{\partial x_i}, \dot\phi_i\right] +$$

$$+\sum_i \frac{\partial\mathcal{L}[\dots]}{\partial\phi_i}\eta_i + \sum_i \frac{\partial\mathcal{L}[\dots]}{\partial\frac{\partial\phi_i}{\partial x_i}}\frac{\partial\eta_i}{\partial x_i} + \sum_i \frac{\partial\mathcal{L}[\dots]}{\partial\dot\phi_i}\dot\eta_i + O(\eta^2)$$

$$S[\phi+\eta] = \int dt\int dx\, \mathcal{L}\left[\phi+\eta, \frac{\partial\phi}{\partial x}+\frac{\partial\eta}{\partial x}, \dot\phi+\dot\eta\right] = S[\phi] + \int dt\int dx\, \frac{\partial\mathcal{L}[\phi, \frac{\partial\phi}{\partial x}, \dot\phi]}{\partial\phi}\eta(x) +$$

$$+\int dt\int dx\, \frac{\partial\mathcal{L}[\phi, \frac{\partial\phi}{\partial x}, \dot\phi]}{\partial\frac{\partial\phi}{\partial x}}\frac{\partial\eta}{\partial x} + \int dt\int dx\, \frac{\partial\mathcal{L}[\phi, \frac{\partial\phi}{\partial x}, \dot\phi]}{\partial\dot\phi}\dot\eta + \dots$$

by parts   by parts

$$-\int dt\int dx\, \frac{\partial}{\partial x}\left(\frac{\partial\mathcal{L}[\phi, \frac{\partial\phi}{\partial x}, \dot\phi]}{\partial\frac{\partial\phi}{\partial x}}\right)\eta(x) + \int dt\left[\frac{\partial\mathcal{L}[\;]}{\partial\frac{\partial\phi}{\partial x}}\cdot\eta(x)\right]_{-\infty}^{\infty} \to 0$$

The boundary conditions are satisfied by ϕ and $\phi(\pm\infty)+\eta(\pm\infty) = \phi(\pm\infty)$ because ϕ satisfy b.c.
It follows $\phi(\pm\infty)=0$

$$S[\phi+\eta] = S[\phi] + \int dt\int dx\, \eta(x)\underbrace{\left\{\frac{\partial\mathcal{L}}{\partial\phi} - \frac{\partial}{\partial x}\left(\frac{\partial\mathcal{L}}{\partial\frac{\partial\phi}{\partial x}}\right) - \frac{\partial}{\partial t}\left(\frac{\partial\mathcal{L}}{\partial\dot\phi}\right)\right\}} + O(\eta^2)$$

Has to vanish for any $\eta(x)$ variation, has the following Eq. have to be satisfied:

Lagrangian EOM: $$\frac{\partial\mathcal{L}}{\partial\phi} - \frac{\partial}{\partial x}\left(\frac{\partial\mathcal{L}}{\partial\frac{\partial\phi}{\partial x}}\right) - \frac{\partial}{\partial t}\left(\frac{\partial\mathcal{L}}{\partial\dot\phi}\right) = 0$$

We sometimes use $\partial_x\phi \equiv \frac{\partial\phi}{\partial x}$

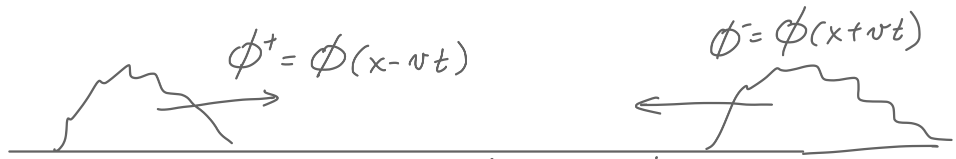
Example of 1D field: $\mathcal{L}[\phi, \frac{\partial \phi}{\partial x}, \dot\phi] = \frac{1}{2}M\dot\phi^2 - \frac{\kappa a^2}{2}\left(\frac{\partial \phi}{\partial x}\right)^2$ stopped 9/8/2022

$$\frac{\partial \mathcal{L}}{\partial \phi} = 0 \qquad \frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot\phi}\right) = M\ddot\phi \qquad \frac{\partial}{\partial x}\frac{\partial \mathcal{L}}{\partial(\partial_x \phi)} = -\kappa a^2 \frac{\partial^2 \phi}{\partial x^2}$$

EOM: $\left.\frac{\partial \mathcal{L}}{\partial \phi} - \frac{\partial}{\partial x}\left(\frac{\partial \mathcal{L}}{\partial \frac{\partial \phi}{\partial x}}\right) - \frac{\partial}{\partial t}\left(\frac{\partial \mathcal{L}}{\partial \dot\phi}\right) = 0\right\}$ $-M\ddot\phi + \kappa a^2 \frac{\partial^2 \phi}{\partial x^2} = 0$ or $\left(\frac{\partial^2}{\partial t^2} - \kappa a^2 \frac{\partial^2}{\partial x^2}\right)\phi = 0$

Solution is propagating wave $\phi(x \pm vt)$ because $\ddot\phi = v^2 \phi''$ and $\frac{\partial^2 \phi}{\partial x^2} = \phi''$

$(-Mv^2 + \kappa a^2)\phi''(x \pm vt) = 0$ and $v = a\sqrt{\frac{\kappa}{M}}$ is the velocity of propagating wave.



propagating sound waves

1.2. Hamiltonian formulation

generalized or canonical momentum: $\Pi(x,t) = \frac{\partial \mathcal{L}[\phi, \partial_x\phi, \dot\phi]}{\partial \dot\phi}$

$\Pi(x,t)$ is a continuous function of x just like field $\phi(x,t)$;

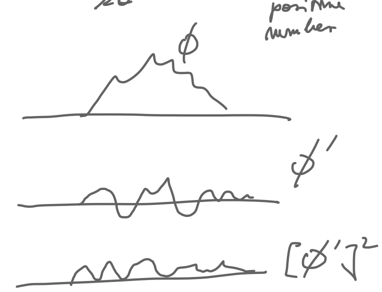
Hamiltonian density: $\mathcal{H}[\phi, \partial_x\phi, \Pi] = \Pi\dot\phi - \mathcal{L}[\phi, \partial_x\phi, \dot\phi]$

Our example: $\Pi(x,t) = M\dot\phi$ and $\mathcal{H}[\phi, \partial_x\phi, \Pi] = \frac{1}{2}M\dot\phi^2 + \frac{\kappa a^2}{2}(\partial_x\phi)^2 = \frac{1}{2M}\Pi^2 + \frac{\kappa a^2}{2}(\partial_x\phi)^2$

total $H[\phi, \Pi] = \int dx \left[\frac{1}{2M}\Pi^2 + \frac{1}{2}\kappa a^2 (\partial_x\phi)^2\right]$

What is energy contained in a sound wave? $\dot\phi = \pm v\,\phi'(x - vt)$ and $\Pi = \pm Mv\,\phi'(x - vt)$

Hence $H[\phi, \Pi] = \int_{-\infty}^{\infty} dx \left(\frac{1}{2}Mv^2 + \frac{1}{2}\kappa a^2\right)[\phi'(x - vt)]^2 = \underbrace{\left(\frac{1}{2}Ma^2\frac{\kappa}{M} + \frac{1}{2}\kappa a^2\right)}_{\kappa a^2} \underbrace{\int_{-\infty}^{\infty}[\phi'(x)]^2 dx}_{\text{positive number}}$



Exercise : Compute specific heat (for classical 1D chain of phonons)

We need energy density: $u = \frac{1}{L}\frac{\int d\Gamma\, e^{-\beta H} H}{\int d\Gamma\, e^{-\beta H}} = -\frac{1}{L}\frac{\partial}{\partial\beta}\ln\int d\Gamma\, e^{-\beta H}$

for discrete systems $d\Gamma = \prod_i dx_i\, dp_i$

this system can be discretized: $d\Gamma = \prod_i d\phi_i\, d\pi_i$

We will use the trick for quadratic Hamiltonians $\phi = \frac{1}{\sqrt{\beta}}\tilde{\phi}$

$\pi = \frac{1}{\sqrt{\beta}}\tilde{\pi}$

then $\beta H = \frac{1}{2M}\tilde{\pi}^2 + \frac{1}{2}\kappa a^2(\partial_x\tilde{\phi})^2 = \tilde{H}$

then $u = -\frac{1}{L}\frac{\partial}{\partial\beta}\ln\left(\left(\frac{1}{\beta}\right)^N \underbrace{\int d\tilde{\Gamma}\, e^{-\tilde{H}}}_{\text{Not } \beta \text{ dependent}}\right)$

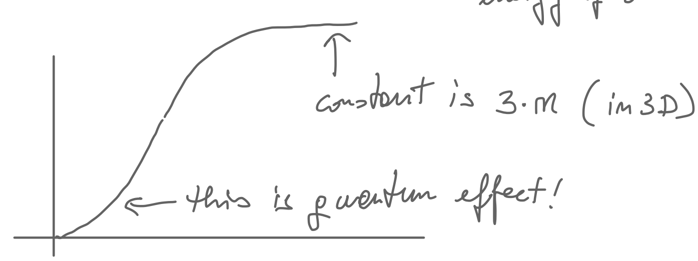
$u = \frac{N}{L}\frac{\partial}{\partial\beta}(\ln\beta) = \frac{N}{L}\frac{1}{\beta} = \frac{N}{L}\cdot T$

$C_V = \frac{\partial u}{\partial T} = \frac{N}{L} = n$ density of phonons

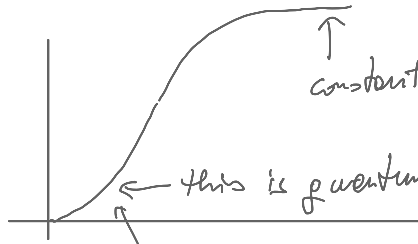
Equivalent to equipartition theorem $u = \underbrace{\frac{1}{2}k_B T}_{\text{kinetic}} + \underbrace{\frac{1}{2}k_B T}_{\text{potential}}$

energy of oscilator

But solids have $C_V \propto T^3$



Quantum chain of atoms



constant is $3\cdot n$ (in 3D)

← this is quantum effect!

Excitations are quantized and $\frac{1}{e^{\beta\omega}-1}$ are available at low T.

In Q.M. we have discrete states of harmonic oscilator available $E=\hbar\omega(n+\frac{1}{2})$

In quantum mechanics $[\hat{p}_i,\hat{x}_j]=-i\hbar\delta_{ij}$ when Classical conjugate variables satisfy $\{p_i,x_j\}=\delta_{ij}$
↑ poisson brackets

Since Π and ϕ are canonically conjugate variables they must satisfy

$$\{\Pi(x),\ \phi(x')\}=\delta(x-x')$$

In Quantum formulation we quantize the fields, hence $[\hat{\Pi}(x),\hat{\phi}(x')]=-i\hbar\,\delta(x-x')$
commutators

$\hat{\phi}(x)$ and $\hat{\Pi}(x)$ are now quantum fields

They are not just functions of x and t but Hermitian operators.

Classical hamiltonian $H[\phi,\Pi]\rightarrow$ is quantized to $\hat{H}[\hat{\phi},\hat{\Pi}]$

$$\hat{H}[\hat{\phi},\hat{\Pi}]=\int dx\left[\frac{1}{2M}\hat{\Pi}^2+\frac{1}{2}\kappa a^2(\partial_x\hat{\phi})^2\right]$$

How to solve quadratic Hamiltonian?

Derivatives can be avoided in Fourier space.

$$\hat{\phi}(x)=\frac{1}{\sqrt{L}}\sum_q e^{iqx}\hat{\phi}_q \quad\text{hence}\quad \hat{\phi}_q=\frac{1}{\sqrt{L}}\int_0^x dx\,\hat{\phi}(x)e^{-iqx}$$

First Brillouine zone only: $q=\frac{2\pi}{L}m=\frac{2\pi}{a}\frac{m}{N}$

$$\hat{\Pi}(x)=\frac{1}{\sqrt{L}}\sum_q e^{iqx}\hat{\Pi}_q$$

$$\hat{H}[\hat{\phi}_q,\hat{\Pi}_q]=\sum_{q_1q_2}\int\frac{dx}{L}e^{i(q_1+q_2)x}\left[\frac{1}{2M}\hat{\Pi}_{q_1}\hat{\Pi}_{q_2}+\frac{1}{2}\kappa a^2(iq_1\,iq_2)\hat{\phi}_{q_1}\hat{\phi}_{q_2}\right]=\sum_q\frac{1}{2M}\hat{\Pi}_q\hat{\Pi}_{-q}+\frac{1}{2}\kappa a^2q^2\hat{\phi}_q\hat{\phi}_{-q}$$

$$\int\frac{dx}{L}e^{i(q_1+q_2)x}=\delta_{q_1=-q_2}\int\frac{dx}{L}=\delta_{q_1=-q_2}$$

Define $\omega_q=v|q|=a\sqrt{\frac{\kappa}{M}}|q|$ hence $\frac{1}{2}\kappa a^2q^2=\frac{1}{2}\omega_q^2M$

Finally $\hat{H}[\hat{\phi}_q,\hat{\Pi}_q]=\sum_q\frac{1}{2M}\hat{\Pi}_q\hat{\Pi}_{-q}+\frac{1}{2}M\omega_q^2\hat{\phi}_q\hat{\phi}_{-q}$ like quantum harmonic oscilator

Recall algebra of quantum harmonic oscilator:

$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$ with spectrum $E_n = \omega(n+\frac{1}{2})$ here $\hbar \to 1$

equidistant energies

can be interpreted as n-particles in a state with energy ω.
These particles are bosons because the state can be occupied by many particles

transformation to ladder operators

$$a = \sqrt{\frac{m\omega}{2}}\left(\hat{x} + \frac{i}{m\omega}\hat{p}\right)$$

$$a^+ = \sqrt{\frac{m\omega}{2}}\left(\hat{x} - \frac{i}{m\omega}\hat{p}\right)$$

$[\hat{p}_i, \hat{x}_i] = -i\delta_{ij}$

hence $[a, a^+] = \frac{m\omega}{2}\left[\hat{x} + \frac{i}{m\omega}\hat{p}, \hat{x} - \frac{i}{m\omega}\hat{p}\right] = 1$ as needed for bosons

and $a^+ a = \frac{m\omega}{2}\left(\hat{x}^2 + \frac{1}{m^2\omega^2}\hat{p}^2 - \frac{1}{m\omega}\right) = \frac{m\omega}{2}\hat{x} + \frac{1}{2}\frac{1}{m\omega}\hat{P}^2 - \frac{1}{2}$

hence $H = \omega(a^+ a + \frac{1}{2})$

Back to solving phonon problem

$$\hat{H}[\hat{\phi}_q, \hat{\Pi}_q] = \sum_q \frac{1}{2M}\hat{\Pi}_q\hat{\Pi}_{-q} + \frac{1}{2}M\omega_q^2\hat{\phi}_q\hat{\phi}_{-q}$$

Define ladder operators

$$\boxed{\begin{aligned} a_q &= \sqrt{\frac{M\omega_q}{2}}\left(\hat{\phi}_q + \frac{i}{M\omega_q}\hat{\Pi}_{-q}\right) \\ a_q^+ &= \sqrt{\frac{M\omega_q}{2}}\left(\hat{\phi}_{-q} - \frac{i}{M\omega_q}\hat{\Pi}_q\right) \end{aligned}}$$

$\hat{\phi}_q^+ = \hat{\phi}_{-q}$ because $\phi(x)$ is real

Check $[a_q, a_q^+] = \frac{M\omega_q}{2}\left[\phi_q + \frac{i}{M\omega_q}\Pi_{-q}, \phi_{-q} - \frac{i}{M\omega_q}\Pi_q\right] = \frac{M\omega_q}{2}\frac{i}{M\omega_q}\left(\underbrace{[\Pi_{-q}, \phi_{-q}]}_{-i} - \underbrace{[\phi_q, \Pi_q]}_{i}\right) = 1$

$$a_q^+ a_q = \frac{M\omega_q}{2}\left(\hat{\phi}_{-q} - \frac{i}{M\omega_q}\hat{\Pi}_q\right)\left(\hat{\phi}_q + \frac{i}{M\omega_q}\hat{\Pi}_{-q}\right) = \frac{M\omega_q}{2}\left(\hat{\phi}_{-q}\hat{\phi}_q + \frac{1}{M^2\omega_q^2}\hat{\Pi}_q\hat{\Pi}_{-q} + \frac{i}{M\omega_q}(\phi_q\Pi_q - \Pi_q\phi_q)\right)$$

$$\sum_q \omega_q(a_q^+ a_q + \tfrac{1}{2}) = \sum_q \frac{1}{2}M\omega_q^2\hat{\phi}_{-q}\hat{\phi}_q + \frac{1}{2M}\hat{\Pi}_q\hat{\Pi}_{-q} + \underbrace{\omega_q\frac{i}{2}\underbrace{[\phi_q, \Pi_q]}_{i} + \frac{1}{2}\omega_q}_{0} = \sum_q \frac{1}{2M}\hat{\Pi}_q\hat{\Pi}_{-q} + \frac{1}{2}M\omega_q^2\hat{\phi}_q\hat{\phi}_{-q}$$

$$\hat{H}[\hat{\phi}_q, \hat{\Pi}_q] = \sum_{q\in 1BZ} \frac{1}{2M}\hat{\Pi}_q\hat{\Pi}_{-q} + \frac{1}{2}M\omega_q^2\hat{\phi}_q\hat{\phi}_{-q}$$

$$\Downarrow$$

Finally $\boxed{H = \sum_{q\in 1BZ}\omega_q\left(a_q^+ a_q + \frac{1}{2}\right) \text{ with } \omega_q = \sqrt{\frac{2}{M}}(|q|a)}$

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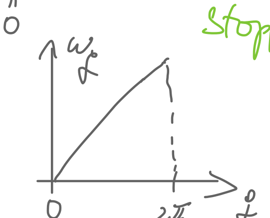

What is specific heat of a quantum chain?

$$Z = Tr(e^{-\beta H}) = \sum_m \langle m| e^{-\beta \sum_q \omega_q (a_q^+ a_q + \frac{1}{2})} |m\rangle \quad \text{where } |m\rangle = |m_{q_0}\rangle \otimes |m_{q_1}\rangle \otimes \dots |m_{q_N}\rangle$$

$|m_{q_0}\rangle$ can be $|0\rangle$

$|1\rangle = a_q^+ |0\rangle$

$|2\rangle = (a_q^+)^2 |0\rangle$

$\vdots$

$$Z = \prod_q \sum_{m_q = 0}^{\infty} \langle m_q | e^{-\beta\omega_q (m_q + \frac{1}{2})} | m_q \rangle = \prod_q \sum_{m_q=0}^{\infty} \left(e^{-\beta\omega_q}\right)^{m_q} e^{-\frac{1}{2}\beta\omega_q} = \prod_q \frac{e^{-\frac{1}{2}\beta\omega_q}}{1-e^{-\beta\omega_q}}$$

$$u = -\frac{1}{L}\frac{\partial}{\partial\beta}\ln Z = -\frac{1}{L}\frac{\partial}{\partial\beta}\sum_q \left(-\frac{1}{2}\beta\omega_q - \ln\left(1-e^{-\beta\omega_q}\right)\right) = -\frac{1}{L}\sum_q\left(-\frac{1}{2}\omega_q - \frac{e^{-\beta\omega_q}\omega_q}{1-e^{-\beta\omega_q}}\right)$$

$$= \sum_q \left(\frac{1}{2}\omega_q + \frac{\omega_q}{e^{\beta\omega_q}-1}\right)$$

Here generalize to any D:

$$u = \underbrace{\frac{1}{V}\sum_q \frac{1}{2}\omega_q}_{\text{zero point energy}} + \underbrace{\int_0^{2\pi}\frac{d^D q}{(2\pi)^D}\frac{v|q|}{e^{\beta v|q|}-1}}_{\text{generalized to D-dimensions}} = u_0 + \frac{1}{\beta(\beta v)^D}\int_0^{2\pi}\frac{d(\beta v q)^D}{(2\pi)^D}\frac{\beta v q}{e^{\beta v q}-1} = u_0 + \frac{T^{D+1}}{v^D}\int_0^{2\pi v\beta}\frac{d^D x}{(2\pi)^D}\frac{x}{e^x - 1}$$

$\beta v|q|$ is new variable

$\beta v|q| = x$

Note: $\sum_{q\in 1BZ} \to V\int\frac{d^D q}{(2\pi)^D}$

At low T: $u \approx u_0 + T^{D+1}\cdot\frac{1}{v^D}\int_0^{\infty}\frac{d^D x}{(2\pi)^D}\frac{x}{e^x-1}$

$$\underline{C_v = \frac{du}{dT} = c\cdot T^D}$$

At high T: $$u \approx u_0 + \frac{T^{D+1}}{v^D}\int_0^{2\pi v\beta}\frac{d\phi\, D^2 x^{D-1}\cdot x}{(2\pi)^D (x + \frac{1}{2}x^2)} \approx u_0 + \frac{T^{D+1}}{v^D}\cdot D^2\int_0^{2\pi v\beta}\frac{x^{D-1}}{(2\pi)^D}d\phi = u_0 + \frac{T^{D+1}}{v^D}\frac{D^2(2\pi v\beta)^D}{(2\pi)^D D} =$$

$$u_0 + T\cdot D$$

$C_v = k_B\cdot D$ classical result

should not be sphere but cube, hence this is only order of magnitude estimation.

Second quantization — Altland & Simons Chpt 2

- Let's start with the single particle wave function $\psi_\lambda(\vec{r})$: $\quad H^{(1)}\psi_\lambda = \varepsilon_\lambda \psi_\lambda$

$$\langle \underset{\underset{x}{\parallel}}{\vec{r}} / \lambda \rangle = \psi_\lambda(\vec{r})$$

- For 2 particles, the two possible wave functions are

$$\psi(x_1,x_2) = \frac{1}{\sqrt{2}}\left(\psi_{\lambda_1}(x_1)\psi_{\lambda_2}(x_2) \mp \psi_{\lambda_2}(x_1)\psi_{\lambda_1}(x_2)\right) \quad \begin{array}{l}\text{fermions } - \\ \text{bosons } +\end{array}$$

symmetric wave function for bosons
antisymmetric — //— for fermions

In Dirac notation we would write

$$|\lambda_1 \lambda_2\rangle = \frac{1}{\sqrt{2}}\left(|\lambda_1\rangle \otimes |\lambda_2\rangle \mp |\lambda_2\rangle \otimes |\lambda_1\rangle\right)$$

- For N-particles we can write:

$$|\lambda_1 \lambda_2, \dots \lambda_N\rangle = C \sum_P \varsigma^P |\lambda_{P_1}\rangle \otimes |\lambda_{P_2}\rangle \dots \otimes |\lambda_{P_N}\rangle$$

Here $\varsigma = +1$ or -1 for bosons or fermions

ς^P is (-1) or $(+1)$ for odd or even permutations ~~for fermions~~
$(+1)$ for bosons

normalization constant

$$C = \frac{1}{\sqrt{N! \prod_{\lambda=0}^{\infty} (M_\lambda!)}}$$

N - number of all particles
M_λ - occupation of each single particle state.

Example 3 particles permutations

P_1	P_2	P_3	$(-1)^P$
1	2	3	+1
1	3	2	-1
2	1	3	-1
2	3	1	+1
3	2	1	-1
3	1	2	+1

For fermions the same wave function is conveniently represented with the Slater determinant:

$$\langle x_1 x_2, \dots x_N / \lambda_1 \lambda_2 \dots \lambda_N\rangle = C \cdot \mathrm{Det}\begin{pmatrix} \psi_{\lambda_1}(x_1), & \psi_{\lambda_1}(x_2), & \dots & \psi_{\lambda_1}(x_N) \\ \psi_{\lambda_2}(x_1), & \psi_{\lambda_2}(x_2), & \dots & \psi_{\lambda_2}(x_N) \\ \vdots & & & \\ \psi_{\lambda_N}(x_1) & \dots & \dots & \psi_{\lambda_N}(x_N) \end{pmatrix}$$

These wave function are often cumbersome to deal with, in particular when the number of particles is not fixed, i.e., superposition of states with different N.

1) Any quantum state can be written as a linear superposition of some product states written in occupation representation (in a chosen single particle basis), i.e.,

$$|\psi\rangle = \sum_m \alpha_m |m\rangle \quad \text{where} \quad |m\rangle = |m_1 m_2 \ldots m_N\rangle \propto \pm |m_1\rangle \otimes |m_2\rangle \otimes \cdots |m_N\rangle$$

how many times a state is occupied

for fermions m_i can be 0 or 1

These product states are forming the many-body basis, which spans the Fock space.

2) Instead of working with 2^N (M^N bosons) many body states we would rather work with $2N$ operators.

We introduce raising/lowering ladder operators a_i^+/a_i which increase/decrease the number of particles in a given state:

$$a_i^+ |m_1 m_2, \ldots, m_i, \ldots\rangle = \sqrt{m_i+1}\, \varphi^{s_i} |m_1, m_2, \ldots, m_i+1, \ldots\rangle \qquad (2)$$

$$a_i |m_1 m_2, \ldots, m_i, \ldots\rangle = \sqrt{m_i}\, \varphi^{s_i} |m_1, m_2, \ldots, m_i-1, \ldots\rangle$$

$$\text{here} \quad s_i = \sum_{j=1}^{i-1} m_j$$

For bosons $\varphi=1$ hence sign is always positive, but we have $\sqrt{\ }$ prefactor

For fermions there is no prefactor $a_i^+|0\rangle = |1\rangle$ and $a_i^+|1\rangle = 0$ $\quad a_i|1\rangle = |0\rangle \quad a_i|0\rangle = 0$

however we have to account for the sign. The sign counts all fermions which come in Fock space before the i-th state. We could also choose the ones that come after the i-th state, but we have to be consistent once we make a choice.

- By repeated application of a_i^+ it is easy to see that:

$$|m_1 m_2, \ldots\rangle = \prod_i \frac{1}{\sqrt{m_i!}} (a_i^+)^{m_i} |0\rangle$$

No extra sign because the product is ordered and stands for: $(a_1^+)^{m_1} \cdots (a_{N-1}^+)^{m_{N-1}} (a_N^+)^{m_N} |0\rangle$

- From definition (2) it also follows that $a_i^+ a_i |m_1 \ldots m_i \ldots\rangle = m_i |m_1 \ldots m_i \ldots\rangle$

hence $a_i^+ a_i = \hat{m}_i$ is number operator.

- Note that commutation relations for operators a_i, a_i^+ take care of the sign of the wave function. The state is completely antisymmetric because

$$[a_i^+, a_j^+]_- = 0 \quad \text{and hence} \quad (a_i^+ a_j^+ + a_j^+ a_i^+)|n_1 n_2, \dots\rangle = 0$$

The fact that fermionic state can not be ocupied more than once is taken care of by the fact that $a_i^+ a_i^+ = 0$, which follows from the fact that $[a_i^+, a_i^+]_- = 0$

- What did we achieve: Instead of working with 2^N states we can work with $2N$ operators with a simple algebra.

Simple example: suppose we have 3 sites with electrons with spin

We choose the the order of single particle states:

1	2	3	4	5	6
1↑	1↓	2↑	2↓	3↑	3↓

Identify Fock space: Fock space is 2^6 large, i.e, $2^{N_{sites} \times N_{spins}}$

$|000000\rangle \equiv |0\rangle$

$|100000\rangle \equiv |\uparrow 0 0\rangle$

$|010000\rangle \equiv |\downarrow 0 0\rangle$

$|001000\rangle \equiv |0 \uparrow 0\rangle$

$\vdots$

careful with − sign

$|010001\rangle = |\downarrow 0 \downarrow\rangle = a_2^+ a_6^+ |0\rangle = -a_6^+ a_2^+ |0\rangle$

$\vdots$

$|111111\rangle \equiv |\uparrow\downarrow\ \uparrow\downarrow\ \uparrow\downarrow\rangle = \underbrace{a_1^+ a_2^+ \cdots a_6^+}_{\text{only in this order no sign}} |0\rangle$

site1 site2 site3

Instead of dealing with 2^6 states we will use 12 operators $a_1^+, \dots a_6^+, a_1, \dots a_6$

e) We need to learn how to change the single particle basis

$$|\lambda\rangle = a_\lambda^+ |0\rangle$$

We know $|\lambda\rangle$ basis is complete, hence $\sum_\lambda |\lambda\rangle\langle\lambda| = 1$

$$|\tilde\lambda\rangle = a_{\tilde\lambda}^+ |0\rangle$$

$$|\tilde\lambda\rangle = \sum_\lambda |\lambda\rangle\langle\lambda|\tilde\lambda\rangle = \sum_\lambda a_\lambda^+ |0\rangle\langle\lambda|\tilde\lambda\rangle$$

$\tilde\lambda$ can be expanded in λ complete basis

Hence $$\boxed{a_{\tilde\lambda}^+ = \sum_\lambda a_\lambda^+ \langle\lambda|\tilde\lambda\rangle}$$

example: $|\lambda\rangle = |x\rangle$

$|\tilde\lambda\rangle = |k\rangle$

$$a_k^+ = \int dx\, a^+(x) \langle x|k\rangle = \int dx\, a^+(x) \frac{1}{\sqrt{V}} e^{ikx}$$

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Repeat from previous lecture:

- From definition $a_i^+ |n_1 n_2, \ldots, n_i, \ldots\rangle = \sqrt{n_i+1}\, \varphi^{s_i} |n_1, n_2, \ldots, n_i+1, \ldots\rangle$

$a_i |n_1 n_2, \ldots, n_i, \ldots\rangle = \sqrt{n_i}\, \varphi^{s_i} |n_1, n_2, \ldots, n_i-1, \ldots\rangle$

it follows that $a_i^+ a_i |n_1 \ldots n_i \ldots\rangle = n_i |n_1 \ldots n_i \ldots\rangle$

hence $a_i^+ a_i = \hat{n}_i$ is number operator.

- By repeated application of a_i^+ it is easy to see that:

$$|n_1 n_2, \ldots\rangle = \prod_i \frac{1}{\sqrt{n_i!}} (a_i^+)^{n_i} |0\rangle$$

No extra sign because the product is ordered and stands for: $(a_1^+)^{n_1} \cdots (a_{N-1}^+)^{n_{N-1}} (a_N^+)^{n_N} |0\rangle$

- Change of basis $a_{\tilde\lambda}^+ = \sum_\lambda a_\lambda^+ \langle\lambda|\tilde\lambda\rangle$

b) <u>One body operators</u>:

examples
$$T = \sum_i \frac{p_i^2}{2m} = \int dp \, \frac{p^2}{2m} \sum_i \delta(p - p_i) = \int dp \, \frac{p^2}{2m} n_p$$
$$V = \sum_i V(x_i) = \int dx \, V(x) \sum_i \delta(x - x_i) = \int dx \, V(x) \, n(x)$$

How does the 1B operator act on a state? In diagonal representation it is simple

$$\hat{O} | n_1 n_2, \ldots n_N \rangle = \sum_\lambda \underset{\substack{\uparrow \\ \text{eigenvalue}}}{O_\lambda} n_\lambda | n_1 n_2 \ldots n_N \rangle = \sum_\lambda O_\lambda a^+_\lambda a_\lambda | n_1 n_2, \ldots n_N \rangle$$

Example: $\sum_{p_i} \frac{p^2}{2m} \cdot n_p | n_{p_1} n_{p_2} \ldots n_{p_N} \rangle$

To get general result we change the basis:

$$\hat{O} = \sum_{\lambda_1 \lambda_2 \lambda} \underset{\substack{| \\ \text{eigenvalue}}}{O_\lambda} a^+_{\lambda_1} \langle \lambda_1 | \lambda \rangle \langle \lambda | \lambda_2 \rangle a_{\lambda_2} = \sum_{\lambda_1 \lambda_2} a^+_{\lambda_1} a_{\lambda_2} \langle \lambda_1 | \hat{O} | \lambda_2 \rangle$$

because $\sum_\lambda \langle \lambda_1 | \lambda \rangle \overbrace{\langle \lambda | O | \lambda \rangle}^{O_\lambda} \langle \lambda | \lambda_2 \rangle = \langle \lambda_1 | \hat{O} | \lambda_2 \rangle$ for λ eigenbasis.

Example: $T = \int dp \, \frac{p^2}{2m} a^+_p a_p = \int dx \, a^+(x) \left(-\frac{\nabla^2}{2m} \right) a(x)$ because $\langle x | \frac{p^2}{2m} | x' \rangle = -\delta(x-x') \frac{\nabla^2}{2m}$

Reminder $\hat{p} = -i \hat{\nabla} \Rightarrow \langle x | \hat{p} | x' \rangle = \delta(x-x')(-i\nabla)$

$$\langle x | \frac{p^2}{2m} | x' \rangle = \delta(x-x') \left(-\frac{\nabla^2}{2m} \right)$$

c) Two body operator (Coulomb repulsion) in position representation

$$\underline{\hat{V}|m_1, m_2, \dots m_N\rangle} = \frac{1}{2}\sum_{i\neq j} V(\vec{r}_i - \vec{r}_j)\, \underline{|m_1 m_2 \dots m_N\rangle}$$ where $|m_1 m_2 \dots m_N\rangle = \psi^+(r_1)\psi^+(r_2)\dots\psi^+(r_N)|0\rangle$

given: $\hat{V} = \frac{1}{2}\int d\vec{r}\int d\vec{r}'\, \psi^+(\vec{r})\psi^+(\vec{r}')V(\vec{r}-\vec{r}')\psi(\vec{r}')\psi(\vec{r})$

can add s, s' by $\vec{r} \to \vec{r}, s$ and $\vec{r}' \to \vec{r}, s'$

Notice that this is not $n(\vec{r})n(\vec{r}')$: check: $\psi^+(\vec{r})\psi^+(\vec{r}')\psi(\vec{r}')\psi(\vec{r}) = -\psi^+(\vec{r})\psi^+(\vec{r}')\psi(\vec{r})\psi(\vec{r}')$

$\delta(\vec{r}-\vec{r}') - \psi(\vec{r})\psi^+(\vec{r}')$

$$= -\psi^+(\vec{r})[\delta(\vec{r}-\vec{r}') - \psi(\vec{r})\psi^+(\vec{r}')]\psi(\vec{r}')$$

$$= -\delta(\vec{r}-\vec{r}')n(\vec{r}) + n(\vec{r})n(\vec{r}')$$

proof for fermions:

$$\hat{V}|m_1 m_2 \dots m_N\rangle = \frac{1}{2}\iint d^3r\, d^3r'\, V(\vec{r}-\vec{r}')\, \underbrace{\psi^+(r)\psi^+(\vec{r}')\psi(\vec{r}')\psi(\vec{r})}\, \underbrace{\psi^+(\vec{r}_1)\psi^+(\vec{r}_2)\dots\psi^+(\vec{r}_N)|0\rangle}$$

$$\psi^+(r)\psi^+(\vec{r}')\psi(\vec{r}')\psi(\vec{r})\underbrace{\psi^+(\vec{r}_1)\psi^+(\vec{r}_2)\dots\psi^+(\vec{r}_N)|0\rangle}_{|m_1 m_2 \dots m_N\rangle}$$

$$\psi^+(r)\psi^+(\vec{r}')\psi(\vec{r}')[\delta(r-r_1) - \psi^+(\vec{r}_1)\psi(\vec{r})]\psi^+(\vec{r}_2)\dots\psi^+(\vec{r}_N)|0\rangle$$

first exchange on $\psi^+(\vec{r}_1)$ is missing in this term.

$$\psi^+(\vec{r})\psi^+(\vec{r}')\psi(\vec{r}')\Big[\sum_i \delta(\vec{r}-\vec{r}_i)(-1)^{s_i-1}\psi^+(\vec{r}_1)\dots\psi^+(\vec{r}_N) - \underbrace{\psi^+(\vec{r}_2)\dots\psi^+(\vec{r}_N)\psi(\vec{r})}_{=0}\Big]|0\rangle$$

exchange with any

ψ_i^+ is missing

for bosons the same except $(-1) \to (+1)$

$$\psi^+(\vec{r})\underbrace{\psi^+(\vec{r}')\psi(\vec{r}')}_{n(\vec{r}')}\sum_i \delta(\vec{r}-\vec{r}_i)(-1)^{s_i-1}\psi^+(\vec{r}_1)\dots\psi^+(\vec{r}_N)|0\rangle$$

will be moved together, hence no extra sign

ψ_i^+ is missing

$$\psi^+(\vec{r})\underbrace{\sum_{i\neq j}}\delta(\vec{r}-\vec{r}_i)\delta(\vec{r}'-\vec{r}_j)(-1)^{s_i-1}\psi^+(\vec{r}_1)\dots\psi^+(\vec{r}_N)|0\rangle$$

comes from the fact that ψ_i^+ was missing

ψ_i^+ is missing

$$\sum_{i\neq j}\delta(\vec{r}-\vec{r}_i)\delta(\vec{r}-\vec{r}_j)\,\psi^+(\vec{r}_1)\dots\psi^+(\vec{r}_N)$$

Conclusion: $\frac{1}{2}\iint d\vec{r}\, d\vec{r}'\, V(\vec{r}-\vec{r}')\psi^+(r)\psi^+(\vec{r}')\psi(\vec{r}')\psi(\vec{r})|m\dots\rangle = \frac{1}{2}\sum_{i\neq j}V(\vec{r}_i - \vec{r}_j)|m\dots\rangle$

which concludes the proof.

2.2. Applications of 2^{nd} quantization

Electron Ham. in 2^{nd} quantization

$$H = \sum_s \int d^3r \; a_s^+(\vec r)\left[\frac{\hat p^2}{2m} + V(\vec r)\right] a_s(\vec r) + \frac{1}{2}\underbrace{\sum_{ss'}\int d^3r\, d^3r'\, V_{ee}(\vec r-\vec r')\, a_s^+(\vec r)\, a_{s'}^+(\vec r')\, a_{s'}(\vec r')\, a_s(\vec r)}_{V_{ee}}$$

$$\frac{\hat p^2}{2m} = \left(-\frac{\nabla^2}{2m}\right)$$

a) Nearly free electrons $\quad V_{ee} << \frac{p^2}{2m}$

$$a_s^+(\vec r) = \frac{1}{\sqrt V}\sum_k e^{i\vec k\cdot\vec r} a^+_{ks}$$

$$V(\vec r) = \sum_g V_g e^{i\vec g\vec r}$$ note that for periodic $V(\vec r) \Rightarrow g \in G$ reciprocal

$$H = \sum_s \int d^3r \frac{1}{V}\sum_{kk'} e^{i(\vec k-\vec k')\vec r}\left[a^+_{ks}\frac{k^2}{2m}a_{ks} + \sum_g V_g e^{i\vec g\cdot\vec r}\right]$$ stopped here 9/20/2022

$$H = \sum_{\substack{s\\ kk'}} a^+_{ks} a_{k's}\left[\frac{k^2}{2m}\delta_{k-k'} + V_{k'-k}\right]$$ for periodic systems: $= \sum_{\substack{s\\ k,G}} a^+_{ks}\, a_{k+Gs}\left[\frac{k^2}{2m}\delta_{G=0} + V_G\right]$

Exact diagonalization of a matrix $T_{kk'} = \frac{k^2}{2m}\delta_{k-k'} + V_{k'-k}$; only k, $k+G$ mix

$$U^+ T U = E = \begin{pmatrix} \varepsilon_{k_1} & & & \\ & \varepsilon_{k_2} & & \\ & & \ddots & \\ & & & \varepsilon_{k_N}\end{pmatrix}$$

$T = U E U^+$

hence $\sum_{kk'} a_k^+ T_{kk'} a_{k'} = \sum_{kk'} a_k^+ (U E U^+)_{kk'} a_{k'} = \sum_{kk'g} a_k^+ U_{kg}\, \varepsilon_g\, (U^+)_{gk'} a_{k'} = \sum_g \alpha_g^+ \varepsilon_g \alpha_g$

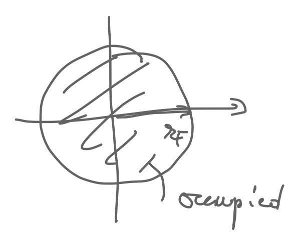
where $\boxed{\alpha_g^+ = \sum_k a_k^+ U_{kg}}$

$$H = \sum_{sg} \varepsilon_g \hat\alpha^+_{gs}\hat\alpha_{gs}$$

ground state: $|\Omega\rangle = N \prod_{\substack{\varepsilon_g < E_F\\ s}} \alpha^+_{gs}|0\rangle$

If V_g is constant then fermi surface is sphere

In general Fermi surface is complicated 2D surface in 3D space.



$\boxed{\text{Remember}}$

$$\sum_k \rightarrow V\int\frac{d^3k}{(2\pi)^3}$$

$$\alpha_g^+ = \sum_{kg} \underbrace{U_{kg}\frac{1}{\sqrt V}e^{-i\vec k\vec r}}\, a_s^+(\vec r)$$

$$\psi_g^+(\vec r) \Rightarrow \psi_g(\vec r) = \frac{1}{\sqrt V}\sum_k e^{+i\vec k\vec r} U^*_{kg} = e^{i\vec g\vec r}\frac{1}{\sqrt V}\sum_k e^{i(\vec k-\vec g)\vec r} U^*_{kg}$$

If periodic $\vec k - \vec g = \vec G$

$$\langle g_k\rangle = \frac{1}{N}\sum_k g_k = \frac{V}{N}\int\frac{d^3k}{(2\pi)^3} g(k) = V_{cell}\int\frac{d^3k}{(2\pi)^3} g(k)$$

Bloch's theorem

If Coulomb repulsion can be neglected (taken into account in a mean-field way) the solution satisfies Bloch's theorem

$$\psi_{nk}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{nk}(\vec{r}) \qquad \text{where } u_{nk}(\vec{r}+\vec{R}) = u_{nk}(\vec{r})$$

$\vec{R}$ ← lattice vector

u_{nk} is periodic

alternative form:

$$\psi_{nk}(\vec{r}+\vec{R}) = e^{i\vec{k}\vec{R}} \psi_{nk}(\vec{r})$$

Single particle potential $V(\vec{r})$ is periodic in the solid, i.e., $V(\vec{r}+\vec{R}) = V(\vec{r})$

It's fourier transform contains only reciprocal vectors, i.e., $V_{\vec{q}} = \delta_{\vec{q}\vec{G}} V_{\vec{G}}$

proof: $V_{\vec{q}} = \frac{1}{N_{cell}} \int e^{-i\vec{q}\vec{r}} V(\vec{r}) d^3r = \frac{1}{N_{cell}} \sum_{\vec{R}} \int_{V_{cell}} e^{-i\vec{q}(\vec{r}+\vec{R})} V(\vec{r}) d^3r$

$$= \frac{1}{N_{cell}} \sum_{\vec{R}} e^{-i\vec{q}\cdot\vec{R}} \underbrace{\int_{V_{cell}} e^{-i\vec{q}\vec{r}} V(\vec{r}) d^3r}_{V_q} = V_q \frac{1}{N_{cell}} \sum_{\vec{R}} e^{-i\vec{q}\cdot\vec{R}} = V_{\vec{G}} \delta_{\vec{q}=\vec{G}}$$

Note that here $V(\vec{r}) = \frac{1}{V_{cell}} \sum_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} V_{\vec{G}}$

It then follows that $H = \sum_{\vec{G}} \left(\frac{k^2}{2m_e} \delta_{G=0} + V_G \right) a_k^+ a_{k+G}$ and the matrix

$T_{kk'} = \frac{k^2}{2m} \delta_{kk'} + V_G \delta_{k-k'=G}$ mixes only momenta that differ by reciprocal vector G.

Solution must have the form $\psi_k(\vec{r}) = \sum_{\vec{G}} e^{i(\vec{k}+\vec{G})\vec{r}} u_{\vec{k},\vec{G}}$

↑ linear superposition differ by $\vec{G}$

then $\psi_k(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \underbrace{\sum_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} u_{k,\vec{G}}} \to e^{i\vec{k}\cdot\vec{r}} u_k(\vec{r})$

this must be periodic in lattice because it only has $\vec{G}$ components in Fourier expansion

Wannier functions of tight binding approximation

two simple regimes: - nearly free electrons in Bloch bands (s & p orbitals)

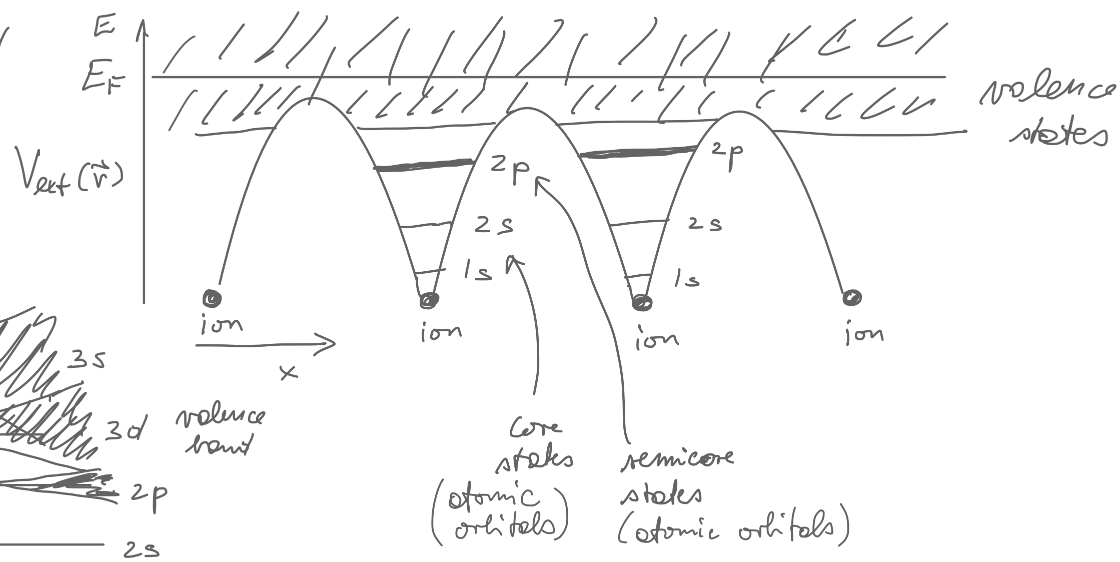
- nearly localized atomic states (for Mott insulating d orb.)

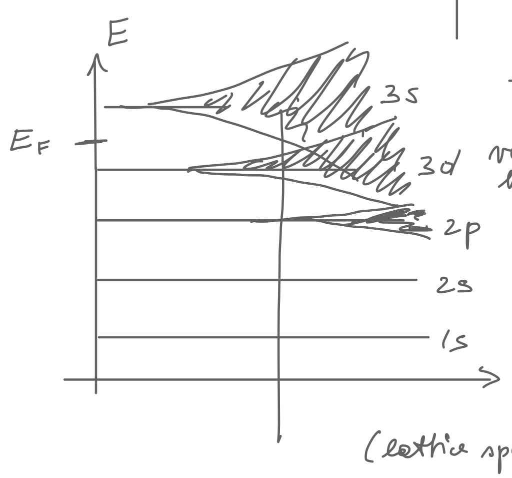
For narrow valence bands the plane waves are not a good starting point (need too many). The atomic orbitals are not a good starting point either (they are not orthogonal or complete.)

Better starting point in this situations are Wannier orbitals.

- They can be made exponentially localized provided they are made of bands with a gap in energy, and with total chern number $C=0$.

States in a solid





In this regime Wannier orbitals for 3d or 3d + 3s might be good.

Wannier orbitals

$$\boxed{\phi_n(\vec r-\vec R) = \sqrt{\frac{V_{cell}}{(2\pi)^3}}\int_{1BZ} d^3k\; e^{-i\vec k\vec R}\sum_m \underbrace{\psi_{mk}(\vec r)}_{\text{Bloch eigenvector of } H_0\psi_{mk}=\varepsilon_k\psi_{mk}}\, U_{mn}(\vec k)}$$

$U_{mn}(\vec k)$: arbitrary unitary transformation $U^+U=1$

can go back

$$\psi_{nk}(\vec r) = \sum_{\vec R\, m} e^{i\vec k\vec R}\, U^*_{nm}\,\phi_m(\vec r-\vec R)$$

$|\phi_{nR}(\vec r)| \to 0$ as $|\vec r-\vec R|$ is large

a) approach atomic orbitals in the limit $a\to\infty$ and are localized
$|\phi_n(\vec r-\vec R)|^2 \to 0$ as $|\vec r-\vec R| >> a$

b) constitute complete and orthogonal single electron basis provided by Bloch waves. (The same Hilbert space that is spanned by Bloch waves is spanned by Wannier)

$$\sum_{nk}|\psi_{nk}\rangle\langle\psi_{nk}| = \sum_{n\vec R}|\phi_n(\vec r-\vec R)\rangle\langle\phi_n(\vec r-\vec R)|$$

(just insert definition ψ_{nk} in to prove)

Proofs: a) Functional dependence

$$\phi_n(\vec r-\vec R) = \sqrt{\frac{V_{cell}}{(2\pi)^3}}\int d^3k \sum_m e^{-i\vec k\vec R}\, e^{i\vec k\cdot\vec r}\, u_m(\vec r-\vec R)\, U_{mn}(\vec k) =$$

$$\sqrt{\frac{V_{cell}}{(2\pi)^3}}\int d^3k \sum_m e^{i\vec k(\vec r-\vec R)}\, u_m(\vec r-\vec R)\, U_{mn}(\vec k)$$

depends on $\underline{\underline{\vec r-\vec R}}$

b) orthogonality

$$\int \phi_n^*(\vec r-\vec R_1)\,\phi_m(\vec r-\vec R_2)\,d^3r = \sum_{n'm'}\frac{V_{cell}}{(2\pi)^3}\iint_{1BZ} d^3k_1\, d^3k_2\; e^{i\vec k_1\vec R_1 - i\vec k_2\vec R_2}\int \underline{\psi^*_{n'k_1}(\vec r)}\, U^*_{n'n}\,\underline{\psi_{m'k_2}(\vec r)}\, U_{m'm}\, d^3r$$

we know: $\int \psi^*_{nk_1}(\vec r)\,\psi_{mk_2}(\vec r)\,d^3r = \delta_{nm}\,\delta_{k_1k_2}$ hence

$$\boxed{\int \phi_n^*(\vec r-\vec R_1)\,\phi_m(\vec r-\vec R_2)\,d^3r =}\; V_{cell}\underbrace{\int_{1BZ}\frac{d^3k}{(2\pi)^3}\, e^{i\vec k(\vec R_1-\vec R_2)}}_{\delta_{R_1-R_2}}\;\underbrace{\sum_{n'} U^*_{n'n}\,U_{n'm}}_{\delta_{nm}} = \boxed{\delta_{nm}\,\delta_{R_1-R_2}}$$

Wannier orbitals are like Fourier transform of Bloch waves, but with added flexibility of $U_{mn}(\vec k)$ that allows localization.

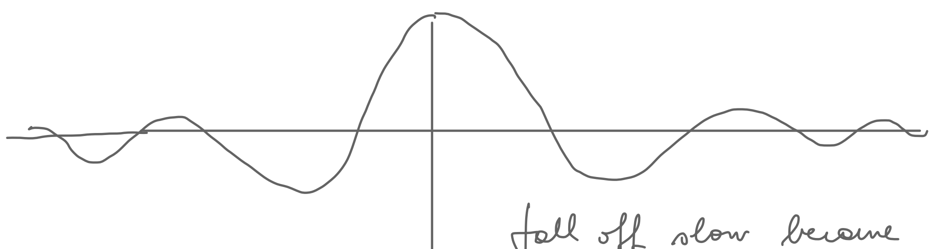
Simple exercise: In the limit of vanishing external potential, determine the Wannier orbitals for 3D square lattice

This is bad example because it does not have a gap, hence not exponentially localized. In real materials with a gap, better behaviour can be expected.

$$\psi_{nk}(\vec{r}) = \frac{1}{\sqrt{V_{cell}}} e^{i\vec{k}\vec{r}}$$

$$\phi_n(\vec{r}-\vec{R}) = \sqrt{\frac{V_{cell}}{(2\pi)^3}} \int_{1BZ} d^3k \, e^{-i\vec{k}\vec{R}+i\vec{k}\cdot\vec{r}} \frac{1}{\sqrt{V}} = \frac{a^{3/2}}{(2\pi)^{3/2}} \int_{-\pi/a}^{\pi/a} dk_x \, e^{i k_x (x-R_x)} \times \dots \times \dots$$

$$\phi_n(\vec{r}-\vec{R}) = \frac{8a^{3/2}}{(2\pi)^{3/2}} \frac{\sin\left(\pi \frac{x-R_x}{a}\right)}{(x-R_x)} \frac{\sin\left(\pi \frac{y-R_y}{a}\right)}{(y-R_y)} \frac{\sin\left(\pi \frac{z-R_z}{a}\right)}{(z-R_z)}$$

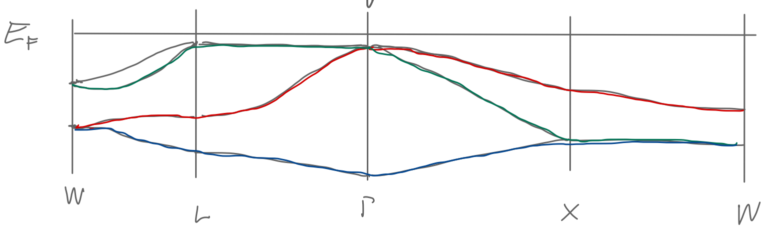


fall off slow because there is no narrow band with gap. $\varepsilon_k = \frac{k^2}{2m}$!

Why not constructing Wannier orbital by Fourier transform each band separately, i.e., set $U_{mn}(k) = \delta_{mn}$?

highly degenerate point creates kinks in $\psi_{nk}(\vec{r})$ gauge

Si bands



Suppose we sort bands across this k-path so that

$$\langle u_{nk}(\vec{r}) | u_{n'k+\Delta k}\rangle = \delta_{nn'} - O(\Delta k)$$

This means smooth gauge in momentum space, which guarantees localized Wannier functions. Any jump in k produces oscillating slow fall-off in R.

If we try to make the gauge smooth across degenerate points we come back to the same point and have different band $\Rightarrow$ We can not treat every band separately, but only the entire set of bands that overlap as a set.

Then we try to arrange the phase between neighboring k-points such that the spread of Wannier functions is minimal, i.e.,

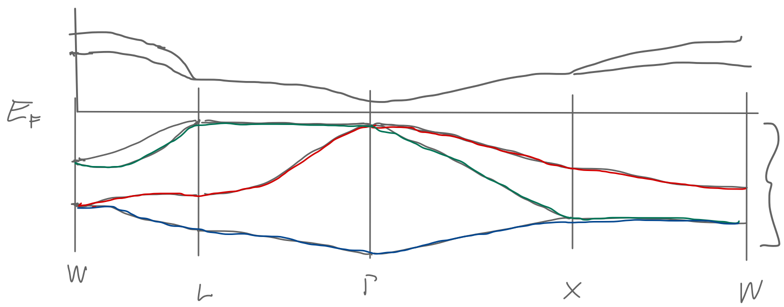
$$\Omega = \langle r^2\rangle - \langle r\rangle^2 = \min \quad \text{where} \quad \langle r^n\rangle = \int \phi_m^*(\vec{r})\, r^n\, \phi_m(\vec{r})\, d^3r$$

It turns out we need to minimize gauge dependent part (the one that depends on U)

$$\tilde{\Omega} = \sum_{n,m,\vec{R}} \Big[\underbrace{\int \phi_m^*(\vec{r}-\vec{R})\,\vec{r}\,\phi_n(\vec{r})\, d^3r}_{\frac{V_{cell}}{(2\pi)^3}\int d^3k\, e^{i\vec{k}\cdot\vec{R}} \langle u_{mk} | i\frac{\partial}{\partial k} u_{nk}\rangle \,=\, \vec{A}_{mn}\frac{V_{cell}}{(2\pi)^3}} \Big]^2 - \Big[\int |\phi_m(\vec{r})|^2\, \vec{r}\, d^3r\Big]^2$$

$\vec{A}$ is Berry connection

Finding smooth gauge across the first B.Z. is deeply connected with topology. Namely nonzero Chern number, which characterizes topological gap, causes obstruction for smooth gauge, and hence localized Wannier functions can not be found.



Assume $C \neq 0$

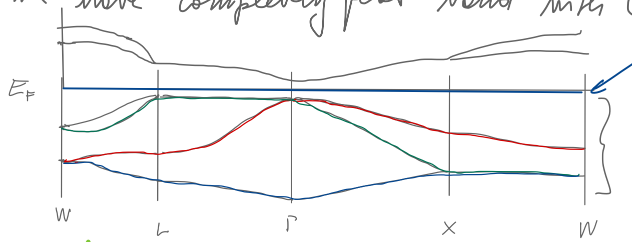
We can not make wannier out of these bands

$C = 0$

We can make Wannier here

Can say $C = f(\vec{A})$ Berry connection

If we have completely flat band with $C \neq 0$ and flatness due to toppology (not interaction)



$C \neq 0$

we could have very high $T_c \propto$

$T_c \propto g$ as opposed to $T_c \propto \Omega\, e^{-\frac{1}{g \rho_F}}$

superfluid stiffness $D \propto C$ as opposed to $D \propto e^{-\frac{1}{g \rho_F}}$

What is Chern number?

for 2D is simpler $C_1 = \frac{1}{2\pi} \oint_{2DBZ} \Omega^{12}(\vec{k})\, d^3k$ $\quad$ C chern number

$$\Omega^{\alpha\beta}(\vec{k}) = \mathrm{Tr}\left(\frac{\partial A^{\beta}}{\partial k_{\alpha}} - \frac{\partial A^{\alpha}}{\partial k_{\beta}} + [A^{\alpha}, A^{\beta}] \right) \quad \text{Berry curvature}$$

$$A^{\alpha}_{mn}(\vec{k}) = \underbrace{\int u^{*}_{mk}(\vec{r})\, i \frac{\partial}{\partial k_{\alpha}} u_{nk}(\vec{r})\, d^3r}_{\text{measures smoothness of the phase}} \quad \text{Berry connection}$$

If we have inversion symmetry, we can determine Chern number by parity check

TRIM's expressed in $\vec{b}_1, \vec{b}_2, \vec{b}_3$

$\vec{k} = 0$

$(\frac{1}{2}, 0, 0)$

$(0, \frac{1}{2}, 0)$

$(0, 0, \frac{1}{2})$

$(\frac{1}{2}, \frac{1}{2}, 0)$

$(\frac{1}{2}, 0, \frac{1}{2})$

$(0, \frac{1}{2}, \frac{1}{2})$

$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

$\hat{I}\vec{k} = -\vec{k} \sim \vec{k}$

$$\psi_{k_i}(-\vec{r}) = \underbrace{\pm}_{(-1)^{P_{k,i}}} \psi_{k_i}(\vec{r})$$

for point TRIMS $\hat{I}\vec{k} = \vec{k} + \vec{G}$

$$\prod_{\text{TRIMS}} \prod_{i} (-1)^{P_{k,i}} = \pm 1$$

if + => trivial

if − => topological

If localized Wannier functions are found, we can write tight binding Hamiltonian for the low energy bands, i.e.,

$$\boxed{H_0 = -\sum_{\substack{ij\sigma \\ mm}} t_{ij}^{mm}\, a^{+}_{mi\sigma}\, a_{mj\sigma}}$$

sites / spins

Wannier orbital type

We will show that:

$$t_{ij}^{mm} = -\langle \phi_{m_1 R_i} | H^0 | \phi_{m_2 R_j}\rangle = -FT[\, U^+(k)\, \varepsilon_k\, U(k)]$$

Creation/field operator:

$$\hat{a}_\sigma(\vec r) = \sum_{m,i} \phi_m(\vec r - \vec R_i)\, \hat{a}_{mi\sigma}$$

from continuous model to discrete model

band index, lattice site, spin

Original Hamiltonian is

$$H = \underbrace{\sum_s \int d^3r\, a_s^+(\vec r)\left[\frac{\hat{p}^2}{2m} + V(\vec r)\right] a_s(\vec r)}_{H_0} + \frac{1}{2}\sum_{ss'}\int d^3r\, d^3r'\, V_{ee}(\vec r - \vec r')\, a_s^+(\vec r)\, a_{s'}^+(\vec r')\, a_{s'}(\vec r')\, a_s(\vec r)$$

$$\frac{\hat{p}^2}{2m} = -\frac{\nabla^2}{2m}$$

$$H_0 = \sum_{\substack{m_1 m_2 \\ ij \\ \sigma}} \int d^3r\, a^+_{m_1 i\sigma}\, a_{m_2 j\sigma} \underbrace{\int d^3r\, \phi^*_{m_1}(\vec r - \vec R_i) \overbrace{\left[-\frac{\nabla^2}{2m} + V(\vec r)\right]}^{H^0} \phi_{m_2}(\vec r - \vec R_j)}_{-t_{ij}^{m_1 m_2}}$$

hence $t_{ij}^{mm} \equiv -\langle \phi_{m R_i} | H^0 | \phi_{m R_j}\rangle$

$$t_{ij}^{m_1 m_2} = -\sum_{m_1 m_2} \int d^3r \frac{V_{cell}}{(2\pi)^3} \int d^3k_1\, d^3k_2\, e^{i\vec k_1 \vec R_i}\, \psi^*_{m_1 k_1}(\vec r)\, U^*_{m_1 m_1}(k_1) \underbrace{\left[-\frac{\nabla^2}{2m} + V(\vec r)\right]}_{\varepsilon_{m_2}(k_2)} e^{-i\vec k_2 \vec R_j}\, \psi_{m_2 k_2}(\vec r)\, U_{m_2 m_2}(k_2)$$

$$\int d^3r\, \psi^*_{m_1 k_1}(\vec r)\, \psi_{m_2 k_2}(\vec r) = \delta_{m_1 m_2}\, \delta_{k_1 k_2}$$

$$t_{ij}^{m_1 m_2} = -\sum_m \frac{V_{cell}}{(2\pi)^3}\int d^3k\, e^{ik(\vec R_i - \vec R_j)} \underbrace{U^*_{m m_1}(k)\, \varepsilon_m(k)\, U_{m m_2}(k)}_{(U^+ \varepsilon_k U)_{m_1 m_2}}$$

which proves that $t_{ij}^{mm} = -FT[\, U^+(k)\, \varepsilon_k\, U(k)]$

Because $\phi(\vec r - \vec R_i)$ are localized we expect $\langle \phi_{m_1 R_i} | H_0 | \phi_{m_2 R_j}\rangle$ to fall off rapidly with $|R_i - R_j|$. Usually we consider n.n. t and next n.n t!

Next, the form of the Coulomb repulsion:

$$\hat{V} = \frac{1}{2}\sum_{ss'}\int d^3r\,d^3r'\,V_{ee}(\vec{r}-\vec{r}')\,a^+_s(\vec{r})\,a^+_{s'}(\vec{r}')\,a_{s'}(\vec{r}')\,a_s(\vec{r})$$

with $a_s(\vec{r}) = \sum_{m,i} \phi_m(\vec{r}-\vec{R}_i)\,a_{mis}$ we have

$$\hat{V} = \frac{1}{2}\sum_{\substack{ss'\\ ijlm}} U^{m_1m_2m_3m_4}_{ijlm}\; a^+_{m_1is}\,a^+_{m_2js'}\,a_{m_3ls'}\,a_{m_4ms}$$

with
$$U^{m_1m_2m_3m_4}_{ijlm} = \iint d^3r\,d^3r'\,\phi^*_{m_1}(\vec{r}-\vec{R}_i)\,\phi^*_{m_2}(\vec{r}'-\vec{R}_j)\,V_{ee}(\vec{r}-\vec{r}')\,\phi_{m_3}(\vec{r}'-\vec{R}_l)\,\phi_{m_4}(\vec{r}-\vec{R}_m)$$

$$\equiv \langle \phi_{m_1R_i}\,\phi_{m_2R_j}|\,V_{ee}\,|\phi_{m_3R_l}\,\phi_{m_4R_m}\rangle$$

The interaction in this representation tends to be short-ranged because of screening in solids, i.e., in metals V is not really $\frac{1}{r}$ but closer to $\frac{e^{-\lambda r}}{r}$.

The onsite term ($\vec{R}_i=\vec{R}_j=\vec{R}_l=\vec{R}_m$) is the largest $U^{m_1m_2m_3m_4}_{iiii}$ and is called Hubbard/Hund's interaction

- For single band we can write
$$\hat{V} = \frac{1}{2}\sum_{ss'} U_{iiii}\, a^+_{is}a^+_{is'}a_{is'}a_{is}$$
$$\frac{1}{2}\sum_{s} U_{iiii}\,\underbrace{a^+_{is}\,a^+_{i\bar{s}}\,a_{i\bar{s}}\,a_{is}}_{n_{is}\,n_{i\bar{s}}}$$
$$\hat{V} = \sum_i U_{iiii}\, n_{i\uparrow}n_{i\downarrow}$$

- For 5 d orbitals and t_{2g} shell, it can be approximately written as:

$$\hat{V} \approx (U-3J)\,\frac{\hat{N}(\hat{N}-1)}{2} - 2J\,\vec{S}^2 - \frac{1}{2}J\,\vec{L}^2 + \frac{5}{2}J\,\hat{N}$$

exact for t_{2g} d orbitals

where $\hat{N} = \sum_{ms} a^+_{ms}a_{ms}$

$$\vec{S} = \sum_{mss'} a_{ms}\,\tfrac{1}{2}\vec{\sigma}_{ss'}\,a_{ms'}$$

$$L_m = \sum_{m'm''s} i\,\varepsilon_{mm'm''}\,a^+_{m's}\,a_{m''s}$$

locally this forces 1) maximal $\vec{S}$
2) maximal $\vec{L}$ at m. $\vec{S}$

The biggest term is charging energy

$\frac{\hat{N}(\hat{N}-1)}{2}$ number of pairs

Hubbard model of Mott-Hubbard transition

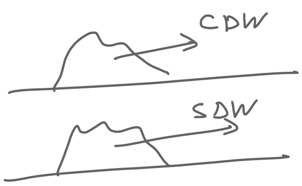
If we have a single band and only on-site interaction,

H is single band Hubbard model

$$H = -\sum_{ij} t_{ij}\, a^+_{is} a_{js} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Exact solution exists for 1D and ∞ D.

- In 1D the low energy excitations are CDW and SDW with different velocities

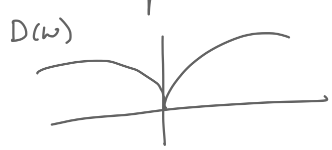


v_c

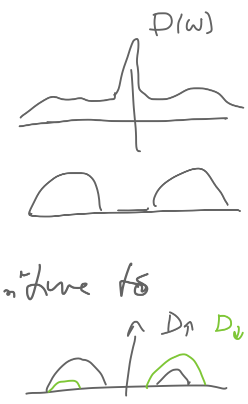
v_s

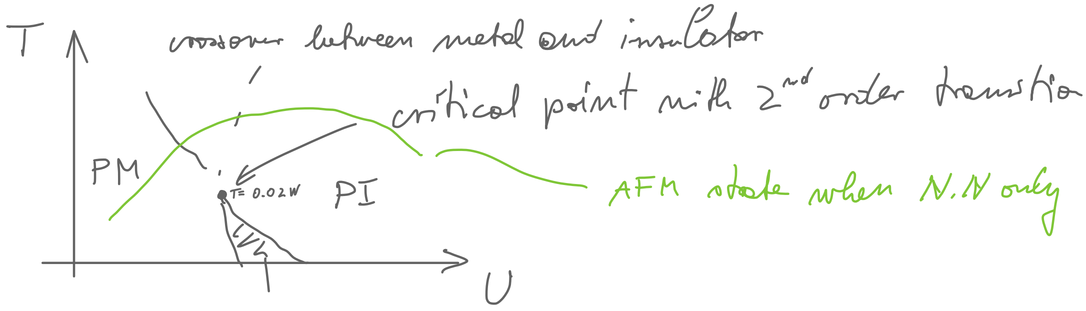
$v_c \neq v_s$ spin-charge separation

The system is always far from non-interacting Fermi gas, i.e., electron is disentangled into charge + spin wave for any $U>0$.
The spectral function has no poles that would correspond to the free electrons



- In ∞ D we have several phases
  - Fermi liquid at small U (similar to Fermi gas)
  - Mot insulator at large U (disentangled atoms)
  - Various magnetic phases at low T that are sensitive to the precise form of t_{ij}

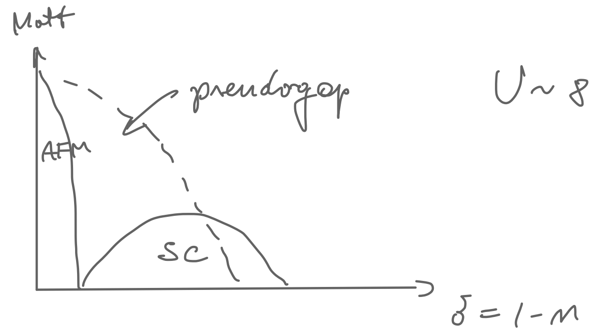




coexistence of metal and insulator
1^{st} order transition

- In 2D we do not have exact solution.

It is believed that the uniform phases roughly resemble cuprate's phase diagram. Numerical low-T studies seem to suggest that various stripe phases win at low T.



$U \sim 8t$

No consensus of pseudogap mechanism and conditions for SC.

- Is QCP at $T=0$, or first order Mott transition with very low T?
- Are there two phases at low T with different sizes of the fermi surface?
- Is SC state more stable than stripe phases? for which t, t' parameters?

Homework 1, 620 Many body

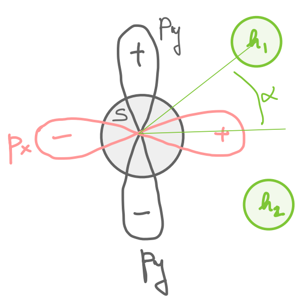
September 27, 2022

1) Using canonical transformation show that at half-filling and large interaction U the Hubbard model is approximately mapped to the Heisenberg model with the form

$$H = J \sum_{<ij>} \vec{S}_i \vec{S}_j - 1/4 \tag{1}$$

where $J = 4t^2/U$. Solution is in A&S page 63.

2) Obtain energy spectrum and the ground state wave function for water molecule in the tight-binding approximation. You can use the following tight-binding values $\varepsilon_s = -1.5$ Ry, $\varepsilon_p = -1.2$ Ry $\varepsilon_H = -1$ Ry t_s = -0.4 Ry t_p = -0.3 Ry $\alpha = 52°$



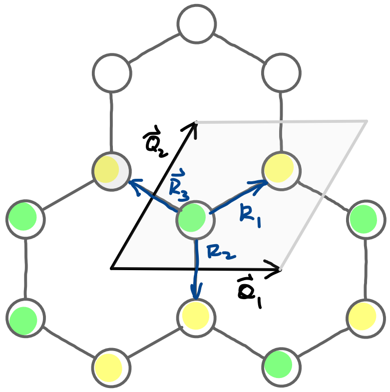
- Determine eigenvalue spectrum from tight-binding Hamiltonian
- The oxygen configuration is $2s^2\ 2p^4$ and hydrogen is $1s^1$, hence we have 8 electrons in the system. Which states are occupied in this model?
- What is the ground state wave function?

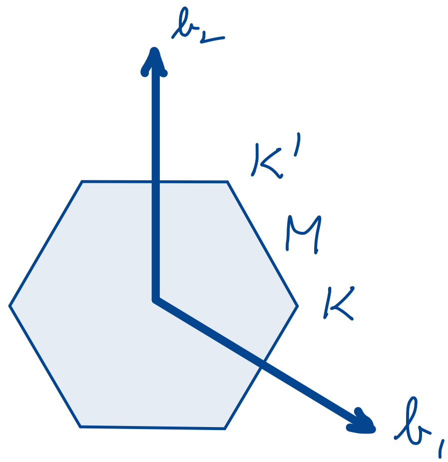
3) Obtain the band structure of graphene and plot it in the path $\Gamma - K - M - \Gamma$. The hooping integral is t.

Show that expansion around the K point in momentum space leads to the following Hamiltonian

$$H_{\mathbf{k}} = \frac{\sqrt{3}}{2} t \left(\mathbf{k} - \mathbf{K}\right) \cdot \vec{\sigma} \tag{2}$$

where $\vec{\sigma} = (\sigma^x, \sigma^y)$ and σ^α are Pauli matrices. From that argue that the energy spectrum around the K point has Dirac form.





Let's use the standard notation

$$\vec{a}_1 = a(1, 0) \tag{3}$$

$$\vec{a}_2 = a(\frac{1}{2}, \frac{\sqrt{3}}{2}) \tag{4}$$

$$\vec{b}_1 = \frac{2\pi}{a}(1, -\frac{1}{\sqrt{3}}) \tag{5}$$

$$\vec{b}_2 = \frac{2\pi}{a}(0, \frac{2}{\sqrt{3}}) \tag{6}$$

Here $r_1 = \frac{1}{3}\vec{a}_1 + \frac{1}{3}\vec{a}_2$ and $r_2 = \frac{2}{3}\vec{a}_1 + \frac{2}{3}\vec{a}_2$. The K point is at $\mathbf{K} = \frac{1}{3}\vec{b}_2 + \frac{2}{3}\vec{b}_1$ and M point is at $\vec{M} = \frac{1}{2}(\vec{b}_1 + \vec{b}_2)$.

Homework 1

1) Using canonical transformation show that at half filling and large U the Hubbard model is mapped to the Heisenberg model

$$H_{HM} = J \sum_{\langle ij \rangle} \left(S_i S_j - \tfrac{1}{4} \right)$$

$$J = \frac{4t^2}{U}$$

Solution page 63

Crucial idea is to use similarity transformation in the many body Hilbert space to transform Hamiltonian

$$\tilde{H} \rightarrow H' \equiv e^{-t\hat{O}} H e^{t\hat{O}} = H - t[O,H] + \frac{t^2}{2!}[O,[O,H]] + \cdots$$

$\hat{O}$ is Hermitian $\qquad$ O will be of the order $\frac{1}{U}$ so that $\underline{tO \ll 1}$

H' has the same many-body spectrum.

We recall: $H \equiv H_U + tH_t$ and $H_U \gg tH_t$

then:
$$H' = \underbrace{H}_{H_U + tH_t} - t[O, H_U + tH_t] + \frac{t^2}{2}[O,[O, H_U + tH_t]] + \cdots$$

$$H_U + \underbrace{tH_t - t[O,H_U]}_{=0} - t^2[O,H_t] + \frac{t^2}{2}[O,[O,H_U]] + O\left(\frac{t^2}{U}\right)$$

no term proportional to t!

We require $H_t = [O, H_U]$ this is equation for O!

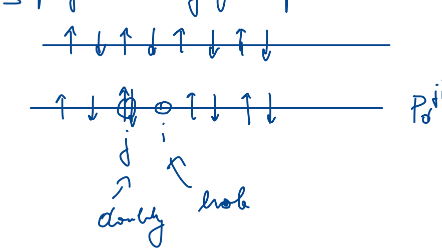
Then
$$H' = H_U - t^2[O,H_t] + \frac{t^2}{2}[O,H_t] = H_U - \frac{t^2}{2}[O,H_t] = H_U + \frac{t^2}{2}[H_t, O]$$

Here $H_t = -\sum_{\langle ij \rangle \sigma} c_{i\sigma}^+ c_{j\sigma}$ and our guess for $\hat{O} = \sum_{\langle ij \rangle} \left(P_s H_t P_d^{ji} - P_d^{ji} H_t P_s \right) \frac{1}{U}$

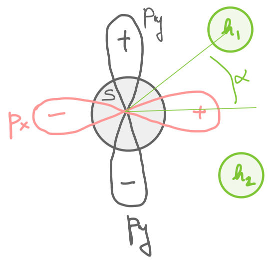
1) Prove $[O, H_U] = H_t$

2) $H_{low-energy} = P_s H' P_s = \frac{4t^2}{U} \sum_{\langle ij \rangle} \left(\vec{S}_i \vec{S}_j - \frac{1}{4} \right)$

P_s projects to singly occupied state



2) Obtain energy spectrum and ground state wave function for water molecule in tight-binding approximation



H	s	p_x	p_y	p_z	h_1^s	h_2^s
s	ε_s	0	0	0	t_s	t_s
p_x	0	ε_p	0	0	$t_p \cos\alpha$	$t_p \cos\alpha$
p_y	0	0	ε_p	0	$t_p \sin\alpha$	$-t_p \sin\alpha$
p_z	0	0	0	ε_p	0	0
h_s^1	t_s	$t_p \cos\alpha$	$t_p \sin\alpha$	0	ε_h	0
h_s^2	t_s	$t_p \cos\alpha$	$-t_p \sin\alpha$	0	0	ε_h

$\varepsilon_s = -1.5$ Ry
$\varepsilon_p = -1.2$ Ry
$\varepsilon_h = -1$ Ry
$t_s = -0.4$ Ry
$t_p = -0.3$ Ry
$\alpha = 52°$

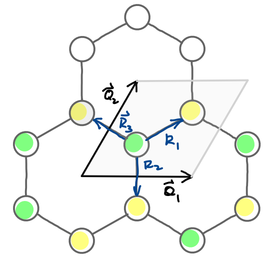
Determine eigenvalue spectrum.

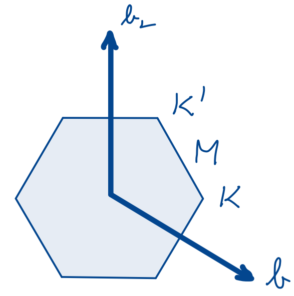
The oxygen configuration is $2s^2 2p^4$ and hydrogen $1s^1$ hence we have 8 electrons. Which states are occupied in this model?

What is the ground state wave function?

3) Obtain band structure of graphene $\mathcal{E}(\vec{k})$ and plot it in the path $\Gamma \to K \to M \to \Gamma$

orthohexagonal star





$$\vec{a}_1 = a\,(1,0)$$
$$\vec{a}_2 = a\left(\tfrac{1}{2}, \tfrac{\sqrt{3}}{2}\right)$$
$$\vec{r}_1 = \tfrac{1}{3}\vec{a}_1 + \tfrac{1}{3}\vec{a}_2$$
$$\vec{r}_2 = \tfrac{2}{3}\vec{a}_1 + \tfrac{2}{3}a_2$$

$$H = -\sum_{\langle ij\rangle} t_{ij}\left(a_i^+ b_j + b_j^+ a_i\right)$$

$$H^0 = -\sum_{\substack{\langle ij\rangle \\ k}} t_{ij}\left(e^{i\vec{k}\vec{R}_{ij}} a_k^+ b_k + e^{-i\vec{k}\vec{R}_{ij}} b_k^+ a_k\right)$$

only nearest-neighbor hopping.

How to get $\vec{b}_1, \vec{b}_2$?

$$\begin{pmatrix} \text{---}\, b_1 \,\text{---} \\ \text{---}\, b_2 \,\text{---} \\ \text{---}\, b_3 \,\text{---} \end{pmatrix}\begin{pmatrix} a_1 & a_2 & a_3 \end{pmatrix} = 2\pi\, Id$$

H_k	a_k	b_k
a_k^+	0	$f(\vec{k})$
b_k^+	$f^*(k)$	0

$$\mathcal{E}_k^2 - |f(k)|^2 = 0$$
$$\mathcal{E}_k = \pm |f(k)|$$

$$\begin{pmatrix} 1 & \frac{1}{2} & 0 \\ 0 & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}^{-1} = \begin{pmatrix} 1 & -\frac{1}{\sqrt{3}} & 0 \\ 0 & \frac{2}{\sqrt{3}} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$b_1 = \tfrac{2\pi}{a}\left(1, -\tfrac{1}{\sqrt{3}}\right)$$
$$b_2 = \tfrac{2\pi}{a}\left(0, \tfrac{2}{\sqrt{3}}\right)$$
$$\vec{k}_M = \tfrac{1}{2}\vec{b}_1 + \tfrac{1}{2}\vec{b}_2 = \tfrac{2\pi}{a}\left(\tfrac{1}{2}, \tfrac{1}{\sqrt{3}}\right)$$
$$k_K = \tfrac{1}{3}(\vec{b}_2 - \vec{b}_1) + \vec{b}_1 = \tfrac{2\pi}{a}\left(\tfrac{2}{3}, 0\right)$$

$$f(\vec{k}) = t\left(e^{i\vec{k}\vec{R}_1} + e^{i\vec{k}\vec{R}_2} + e^{i\vec{k}\cdot\vec{R}_3}\right)$$

$$\mathcal{E}_k = \pm |f(k)|^2$$

$$\vec{R}_1 = \vec{r}_2 - \vec{r}_1 = \left(\tfrac{1}{2}, \tfrac{1}{2\sqrt{3}}\right)a$$
$$\vec{R}_2 = \vec{r}_2 - \vec{r}_1 - \vec{a}_2 = \left(0, -\tfrac{1}{\sqrt{3}}\right)a$$
$$\vec{R}_3 = \vec{r}_2 - \vec{r}_1 - \vec{a}_1 = \left(-\tfrac{1}{2}, \tfrac{1}{2\sqrt{3}}\right)a$$

$$f(\vec{k}) = t\left(e^{i\frac{k_x a}{2} + i k_y a \frac{1}{2\sqrt{3}}} + e^{-i\frac{k_x a}{2} + i k_y a\frac{1}{2\sqrt{3}}} + e^{-i k_y a \frac{1}{\sqrt{3}}}\right)$$
$$f(\vec{k}) = t\left(2e^{i k_y a \frac{1}{2\sqrt{3}}}\cos\tfrac{k_x a}{2} + e^{-i k_y a\frac{1}{\sqrt{3}}}\right)$$
$$f(k) = t\left(2e^{i k_y a \frac{\sqrt{3}}{2}}\cos\tfrac{k_x a}{2} + 1\right)e^{-i k_y a \frac{1}{\sqrt{3}}}$$
$$|f(k)|^2 = t^2\left(\left(1 + 2\cos\tfrac{k_x a}{2}\cos\left(k_y a\tfrac{\sqrt{3}}{2}\right)\right)^2 + 4\cos^2\left(\tfrac{k_x a}{2}\right)\sin^2\left(k_y a\tfrac{\sqrt{3}}{2}\right)\right)$$
$$t^2\Big(1 + \underbrace{4\cos^2\tfrac{k_x a}{2}}_{2 + 2\cos k_x a} + 4\cos\tfrac{k_x a}{2}\cos\left(k_y a\tfrac{\sqrt{3}}{2}\right)\Big)$$

$$\cos^2\tfrac{\theta}{2} = \frac{1+\cos\theta}{2}$$

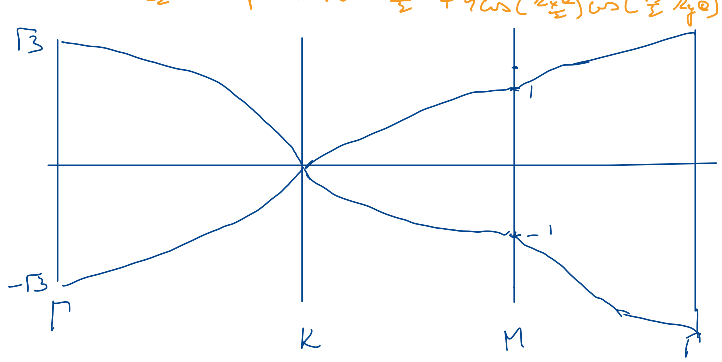
$k_x a = \pi$

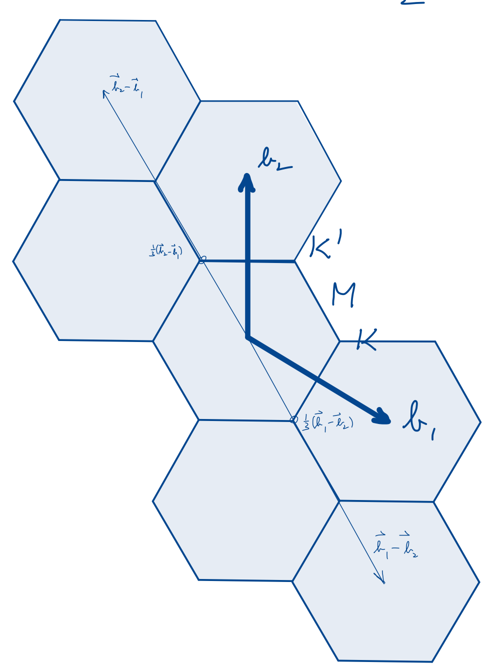
$k_y a = \frac{2\pi}{\sqrt{3}}$

$3 - 2$

Finally $\mathcal{E}_k = \pm t\sqrt{3 + \overbrace{2\cos(k_x a)}^{2\cos^2\left(\frac{k_x a}{2}\right) - 2\sin^2\left(\frac{k_x a}{2}\right)} + 4\cos\left(\tfrac{1}{2}k_x a\right)\cos\left(\tfrac{\sqrt{3}}{2}k_y a\right)}$

$$\mathcal{E}_k = \pm t\sqrt{1 + 4\cos^2\tfrac{k_x a}{2} + 4\cos\left(\tfrac{k_x a}{2}\right)\cos\left(\tfrac{\sqrt{3}}{2}k_y a\right)}$$





Show that Hamiltonian around point $\vec{K} = \frac{2\pi}{a}\left(\frac{2}{3}, 0\right)$ can be written as

$$H = \frac{\sqrt{3}}{2} t a \left(\vec{q} - \vec{k}\right)\cdot\vec{\sigma} \quad \text{where } \vec{\sigma} = (\sigma_x, \sigma_y)$$

Expand around $\vec{q} \sim \vec{K} = \frac{2\pi}{a}\left(\frac{2}{3}, 0\right)$ $\qquad \vec{g} \equiv (\vec{q} - \vec{K})a \Rightarrow \vec{q}a = \begin{pmatrix} \frac{4\pi}{3} + g_x \\ + g_y \end{pmatrix}$

We could expand ε_q, but it is easier to expand $f(q) = -t\left(2e^{iq_y a\frac{\sqrt{3}}{2}}\cos\frac{q_x a}{2} + 1\right)e^{-iq_y a\frac{1}{\sqrt{3}}}$

$$-t\left(2e^{ig_y\frac{\sqrt{3}}{2}}\cos\left(\frac{2\pi}{3} + \frac{g_x}{2}\right) + 1\right)e^{-i\frac{g_y}{\sqrt{3}}} = -t\left(2e^{ig_y\frac{\sqrt{3}}{2}}\left(-\frac{1}{2}\cos\left(\frac{g_x}{2}\right) - \frac{\sqrt{3}}{2}\sin\left(\frac{g_x}{2}\right)\right) + 1\right)e^{i\frac{g_y}{\sqrt{3}}}$$

$$\underbrace{\cos\left(\frac{2\pi}{3}\right)}_{-\frac{1}{2}}\cos\left(\frac{g_x}{2}\right) - \underbrace{\sin\left(\frac{2\pi}{3}\right)}_{\frac{\sqrt{3}}{2}}\sin\left(\frac{g_x}{2}\right)$$

$$\approx -t\left(\left(1 + \frac{\sqrt{3}}{2}ig_y\right)\left(-1 - \sqrt{3}\frac{g_x}{2}\right) + 1\right)\left(1 + i\frac{g_y}{\sqrt{3}}\right)$$

$$= -t\left(-\left(1 + \frac{\sqrt{3}}{2}ig_y\right)\left(1 + \frac{\sqrt{3}}{2}g_x\right) + 1\right)\left(1 + i\frac{g_y}{\sqrt{3}}\right)$$

$$-t\left(-\cancel{1} - \frac{\sqrt{3}}{2}(g_x + ig_y) + \cancel{1}\right) = \frac{\sqrt{3}}{2}t(g_x + ig_y)$$

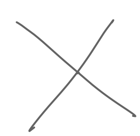
$f(q) \approx \frac{\sqrt{3}}{2}t(g_x + ig_y)$ hence

H_g	b_g	a_g
b_g^+	0	$\frac{\sqrt{3}}{2}t(g_x - ig_y)$
a_g^+	$\frac{\sqrt{3}}{2}t(g_x + ig_y)$	0

or $H_g = \frac{\sqrt{3}}{2}t\,\vec{g}\cdot\vec{\sigma}$ where $\vec{\sigma} = (\sigma^x, \sigma^y)$

$$\varepsilon_g^2 = \frac{3}{4}t^2\left(g_x^2 + g_y^2\right)$$

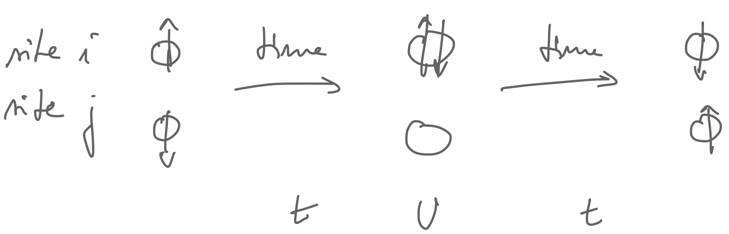
$$\varepsilon_g = \pm\frac{\sqrt{3}}{2}t|g|$$



Quantum Spin Chain & magnons (2.2.5 AS book)

Here we freeze the charge degrees of freedom and consider only the spin degrees of freedom.

We are interested in magnetic interaction between localized moments (for example in Mott insulator) The process of virtual exchange happens because of quantum tunneling even if there is a gap for charge excitation



$\rightarrow$ $J = \frac{4t^2}{U}$ according to SOPT

virtual even if gap in charge excitations

$$H = -J \sum_{\langle ij \rangle} \vec{S}_i \cdot \vec{S}_j$$

$[S_i^\alpha, S_j^\beta] = i\delta_{ij}\, \varepsilon_{\alpha\beta\gamma} S_i^\gamma$ only on the same site it does not commute

total spin $S \geq \frac{1}{2}$

$J > 0$ ferromagnet

$J < 0$ antiferromagnet

Here we will solve the problem in the limit of large spin S.

(exact solution in 1D by Bethe ansatz, in ∞ D by mean field)

How large are spin fluctuations?

$$\Delta S^\alpha \Delta S^\beta \sim |\langle [S^\alpha, S^\beta] \rangle| = \varepsilon_{\alpha\beta\gamma} |\langle S^\gamma \rangle| \lesssim S$$

$\frac{\Delta S^\alpha}{S} \frac{\Delta S^\beta}{S} \lesssim \frac{1}{S}$ Conclusion $\frac{\Delta S}{S} \propto \frac{1}{\sqrt{S}}$ so for large S are small!

$\boxed{\text{Holstein – Primakoff transformation:}}$

$$S_i^- = a_i^+ (2S - a_i^+ a_i)^{1/2}$$

here $[a_i, a_j^+] = \delta_{ij}$ are bosons

$$S_i^+ = (2S - a_i^+ a_i)^{1/2} a_i$$

$$S_i^z = S - a_i^+ a_i$$

The following identities sufficiently characterize the spin commutation relations:

$$[S^+, S^-] = 2S^z$$
$$[S^z, S^+] = S^+$$
$$[S^z, S^-] = -S^-$$

Proof: $[S^+, S^-] = [S^x + iS^y, S^x - iS^y] = -2i[S^x, S^y] = 2S^z$

$[S^z, S^+] = [S^z, S^x + iS^y] = iS^y + i(-i)S^x = S^+$

$[S^z, S^-] = [S^z, S^x - iS^y] = iS^y - i(-i)S^x = -S^-$

Holstein Primakoff satisfy these identities, hence they faithfully represent spin

Proof! $[S^+, S^-] = (2S - a^+a)^{\frac{1}{2}} a a^+ (2S - a^+a)^{\frac{1}{2}} - a^+ (2S - a^+a)^{\frac{1}{2}} (2S - a^+a)^{\frac{1}{2}} a$

$$= \underbrace{(2S-\hat{n})^{\frac{1}{2}} (1+\hat{n})(2S-\hat{n})^{\frac{1}{2}}}_{\substack{\hat{n} \text{ commutes with } f(\hat{n}) \\ (1+\hat{n})(2S-\hat{n})}} - \underbrace{a^+(2S-\hat{n})a}_{-2S\hat{n} + \underbrace{a^+\hat{n}a}_{\substack{a^+(aa^+-1)a \\ \hat{n}\hat{n}-\hat{n}}}}$$

$$= 2S + (2\cancel{S}-1)\hat{n} - \cancel{\hat{n}\hat{n}} - 2\cancel{S\hat{n}} + \cancel{\hat{n}\hat{n}} - \hat{n} = 2(S-\hat{n}) = 2S^z$$

$$[S^z, S^+] = \underbrace{\underbrace{(S - a^+a)}_{f(n)} \underbrace{(2S - a^+a)^{1/2}}_{f'(n)}}_{\text{Commute}} a - (2S - a^+a)^{1/2} a (S - a^+a) =$$

$$(2S-\hat{n})^{1/2} [(\cancel{S} - a^+a)a - a(\cancel{S} - a^+a)] = (2S-\hat{n})^{1/2} \underbrace{[a, \hat{n}]}_{=a} = S^+$$

$$-a^+aa + aa^+a$$
$$-\hat{n}a + a\hat{n}$$

When $S \gg \frac{1}{2}$ we can approximate $(2S-\hat{n})^{1/2}$ with $\sqrt{2S}$ because

$$(2S-\hat{n})^{1/2} \sim \sqrt{2S} + O\left(\frac{1}{\sqrt{S}}\right)$$

1) We start with <u>Ferromagnet</u>. We are looking for low-energy excitations magnons.

Ground state is $\quad \overset{\text{site}}{} \quad |\phi\rangle = \underset{}{\overset{1}{|S\rangle}} \otimes \overset{2}{|S\rangle} \otimes \overset{3}{|S\rangle} \cdots \overset{N}{|S\rangle}$

maximal S on each site

$$H = -\sum_{\langle ij\rangle} J_{ij}\left[S_i^z S_j^z + \tfrac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right)\right]$$

$S_i^- \approx \sqrt{2S}\, a_i^+$

$S_i^+ \approx \sqrt{2S}\, a_i$

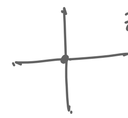
$S^z = S - \hat{n}_i$

$$H \approx -\sum_{\langle ij\rangle} J_{ij}\left[(S-\hat{n}_i)(S-\hat{n}_j) + \tfrac{1}{2}2S\left(a_i a_j^+ + a_i^+ a_j\right)\right]$$

$$-\sum_{\langle ij\rangle} J_{ij}\left[S^2 - S(\hat{n}_i + \hat{n}_j) + \hat{n}_i\hat{n}_j + S\left(a_i a_j^+ + a_i^+ a_j\right)\right]$$

non quadratic (interaction)

$$\sum_{\langle ij\rangle} J_{ij} \overset{n.n.}{=} \tfrac{1}{2} N z J$$ where z is connectivity, N is # sites



$z=4$

$$H \approx \underset{O(S^2)}{-\tfrac{1}{2}NzJS^2} + \underset{O(S)}{S\sum_{\langle ij\rangle} J_{ij}\left(a_i^+ - a_j^+\right)\left(a_i - a_j\right)} \underset{O(1)}{\cancel{-\sum_{\langle ij\rangle} J_{ij}\hat{n}_i\hat{n}_j}}$$

Fourier transform $a_q = \frac{1}{\sqrt{N}}\sum_i e^{i\vec{q}\cdot\vec{R}_i} a_i$ and $a_i = \frac{1}{\sqrt{N}}\sum_{\vec{q}\in BZ} e^{-i\vec{q}\cdot\vec{R}_i} a_{\vec{q}}$

Where $[a_q, a_{q'}^+] = \delta_{qq'}$ because of $[a_i, a_j^+] = \delta_{ij}$

$$H = -\tfrac{1}{2}NzJS^2 + S\sum_{\substack{\langle ij\rangle\\ qq'}} J_{ij}\,\frac{1}{N}\left(e^{i\vec{q}\vec{R}_i} - e^{i\vec{q}\vec{R}_j}\right)a_q^+\left(e^{-i\vec{q}'\vec{R}_i} - e^{-i\vec{q}'\vec{R}_j}\right)a_{q'}$$

$$S\sum_{qq'}\tfrac{1}{2}\sum_{R_{ij}} J_{ij}\underbrace{\frac{1}{N}\sum_i e^{i(q-q')R_i}}_{\delta_{qq'}}\left(1-e^{-iqR_{ij}}\right)\left(1-e^{iq'R_{ij}}\right)a_q^+ a_{q'}$$

$1+1-e^{iqR}-e^{-iqR} = 2(1-\cos(qR))$

actually J_{ij} takes care of n.n., hence j can run everywhere!

$$\tfrac{1}{2}S\sum_{q,\vec{R}_{ij}} J_{ij}\, 2\left(1-\cos(\vec{q}\vec{R}_{ij})\right)a_q^+ a_q$$

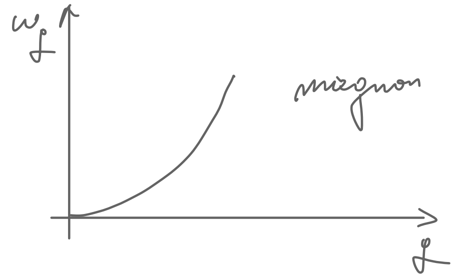
$$H = -\tfrac{1}{2}NzJS^2 + \sum_{q\in BZ}\omega_q a_q^+ a_q \quad \text{where} \quad \omega_q = S\sum_{\vec{R}_{ij}} J_{ij}\left(1-\cos(\vec{q}\cdot\vec{R}_{ij})\right)$$

1D: $\omega_q = 2SJ(1-\cos qa)$

2D square: $\omega_q = 2SJ\left[2-\cos(q_x a)-\cos(q_y a)\right]$

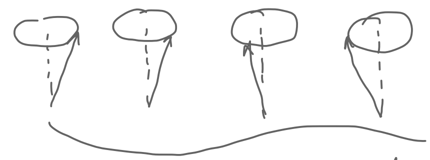
3D lattice: $\omega_q = 2SJ\left[3-\cos q_x a - \cos q_y a - \cos q_z a\right]$

Generically we expect $\omega_q(q \ll 1) \approx (SJa^2)\cdot \vec{q}^{\,2}$ using Taylor expansion of ω_q.



magnon dispersion for FM.

magnon one $a_q^+|g.s.\rangle = \frac{1}{\sqrt{N}}\sum_i e^{-i\vec{q}\vec{R}_i} \frac{S_i^-}{\sqrt{2S}}|g.s.\rangle$

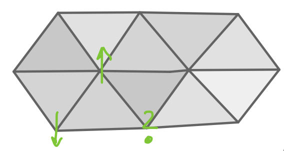


2) Antiferromagnet

Bipartite lattices can be solved with H.P. because we look at small fluctuations (magnons) from the Neél ground state.

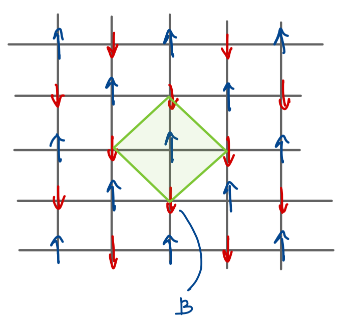
Non-bipartite lattices are frustrated and do not order. Typically have only paramagnons, i.e., diffuse scattering and no sharp excitation.

Example of non-bipartite lattice: triangular lattice



frustration on triangular lattice

On bipartite lattice we just double the size of the unit cell



new unit cell

All spins on sublattice B will be flipped $\downarrow \rightarrow \uparrow$

But this is achieved by cannonical transformation with spins rotated along x-axis.

Therefore
$$\left.\begin{aligned} S_B^x &\to S_B^x \\ S_B^y &\to -S_B^y \\ S_B^z &\to -S_B^z \end{aligned}\right\} \quad \begin{aligned} S_B^+ &\to S_B^x - iS_B^y = S_B^- \\ S_B^- &\to S_B^x + iS_B^y = S_B^+ \end{aligned}$$

Now ground state (or vacuum) is like before: $\emptyset = |S\rangle \otimes |S\rangle \otimes |S\rangle, \cdots \otimes |S\rangle$

$$H = \sum_{\langle ij\rangle} J_{ij}\left(S_i^z S_j^z + \tfrac{1}{2} S_i^+ S_j^- + \tfrac{1}{2} S_i^- S_j^+\right) = \boxed{\sum_{i\in A} \tfrac{1}{2}\sum_{j\in B}} J_{ij}\left[-S_i^z S_j^z + \tfrac{1}{2} S_i^+ S_j^+ + \tfrac{1}{2} S_i^- S_j^-\right]$$

continue:

Different choice

$$H=\sum_{\langle i,j\rangle} J_{ij}\left(S_i^z S_j^z+\frac12 S_i^+S_j^-+\frac12 S_i^-S_j^+\right)=\boxed{\sum_{i\in A}\cancel{\frac12}\sum_{j\in B}J_{ij}\left[-S_i^zS_j^z+\frac12 S_i^+S_j^++\frac12 S_i^-S_j^-\right]}$$

$$\boxed{\text{Holstein-Primakoff: }\begin{array}{ll} S^-_{i,A}\simeq\sqrt{2S}\,a_i^+ & S^-_{i,B}\simeq\sqrt{2S}\,b_i^+\\ S^+_{i,A}\simeq\sqrt{2S}\,a_i & S^+_{i,B}\simeq\sqrt{2S}\,b_i\\ S^z_A=S-\hat n_i^A & S^z_B=S-\hat n_i^B\end{array}}$$

to remind us that we have two interpenetrating sublattices

$$H=\cancel{\frac12}\sum_{\substack{i\in A\\ j\in B}}J_{ij}\Big[\underbrace{-(S-\hat n_i^A)(S-\hat n_j^B)}_{-S^2+S(n_i+n_j)-\cancel{n_in_j}}+S\,a_i^+b_j^++S\,a_ib_j\Big]$$

$$H=-\cancel{\frac12}NzJS^2+\cancel{\frac12}\sum_{\substack{i\in A\\ j\in B}}J_{ij}\,\underbrace{S\left(\hat n_i^A+\hat n_j^B+a_i^+b_j^++a_ib_j\right)}_{\text{quadratic Hamiltonian, but not usual H.O.}}$$

Can be turned in H.O. by transformation

Next $a_i=\frac{1}{\sqrt N}\sum_{q\in RBZ}e^{-i\vec q\cdot\vec R_i}a_q$ (reduced-BZ)

$b_j=\frac{1}{\sqrt N}\sum_{q\in RBZ}e^{-i\vec q'\cdot\vec R_j}b_q$

$$\Rightarrow H=-\frac{N}{\cancel{2}}zJS^2+\cancel{\frac12}\sum_{R_{ij}}J_{ij}S\Big(n_q^A+n_q^B+\frac1N\sum_{q,q'}e^{i\vec q\cdot\vec R_i+i\vec q'\cdot\vec R_j}a_q^+b_{q'}^+ +\frac1N\sum_{q,q'}e^{-i\vec q\cdot\vec R_i-i\vec q'\cdot\vec R_j}a_qb_{q'}\Big)$$

$$\underbrace{\frac1N\sum_i e^{i(\vec q+\vec q')\vec R_i}}_{\delta_{q',-q}}e^{-i\vec q'\cdot\vec R_{ij}}$$

$$H=-\frac{N}{\cancel{2}}zJS^2+\cancel{\frac12}\sum_{\substack{j\in B\\ q}}J_{ij}S\left(n_q^A+n_q^B+e^{i\vec q\cdot\vec R_{ij}}a_q^+b_{-q}^++e^{-i\vec q\cdot\vec R_{ij}}a_qb_{-q}\right)$$

Introduce structure factor: $\gamma_q=\frac12 S\sum_{R_{ij}}J_{ij}e^{i\vec q\cdot\vec R_{ij}}$ — $\vec R_{ij}$ distance to n n from one sublattice to the other

If crystal has inversion symmetry $\gamma_q=\cancel{\frac12}S\sum_\delta J_\delta\frac12\left(e^{i\vec q\cdot\vec\delta}+e^{-i\vec q\cdot\vec\delta}\right)=\cancel{\frac12}\sum_{\vec\delta}SJ_\delta\cos(\vec q\cdot\vec\delta)$

hence $\gamma_{-q}=\gamma_q$; $\gamma_0=\cancel{\frac12}SzJ$

$$H=-\frac{N}{\cancel{2}}zJS^2+\sum_q\left(\gamma_0n_q^A+\gamma_0n_q^B+\gamma_qa_q^+b_{-q}^++\gamma_{-q}a_qb_{-q}\right)$$

commute

$b\,b^+-b^+b=1$

$$H=-\frac{N}{2}zJS^2+\sum_q\gamma_0a_q^+a_q+\gamma_0\underbrace{b_{-q}^+b_{-q}}_{b_{-q}b_{-q}^+-1}+\gamma_qa_q^+b_{-q}^++\gamma_{-q}b_{-q}a_q\Big)$$

$$H=-\cancel{\frac12}NzJS^2+\sum_q\left\{\underbrace{(a_q^+,b_{-q})}_{\tilde\psi_q^+}\begin{pmatrix}\gamma_0 & \gamma_q\\ \gamma_{-q} & \gamma_0\end{pmatrix}\underbrace{\begin{pmatrix}a_q\\ b_{-q}^+\end{pmatrix}}_{\tilde\psi_q}-\gamma_0\right\}\to-\frac12NSzJ$$

$$H=-\cancel{\frac12}NzJ(S^2+S)+\psi_q^+K\psi_q$$

with $K_q\equiv\begin{pmatrix}\gamma_0 & \gamma_q\\ \gamma_q & \gamma_0\end{pmatrix}$

We will solve this H by Bogoliubov transformation

Bogoliubov transformation

2-D spinors $\psi_g = \begin{pmatrix} a_g \\ b^+_{-g} \end{pmatrix}$ $\psi^+_g = (a^+_g, b_{-g})$ with which $\hat{H} = \psi^+ K \psi + \text{const}$

We will try to solve this with linear transformation

ψ is not fermion or boson, indeed $[\psi, \psi^+] = \tau_z$

$\boxed{\phi_g = U_g \psi_g}$ with U_g is 2×2 matrix.

We need to preserve commutation relations. Since these are bosons, we have $[\psi_g, \psi^+_g] = \tau^3$

Note that for fermions $[\psi_g, \psi^+_g] = 1$ (and math is simpler).

check: $[\psi_g, \psi^+_{g'}] = \left[\begin{pmatrix} a_g \\ b^+_{-g} \end{pmatrix}, (a^+_{g'}, b_{-g'})\right] = \begin{pmatrix} [a_g, a^+_{g'}], & 0 \\ 0 & , [b^+_{-g}, b_{-g'}] \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \tau^3$

Require: $[\phi_g, \phi^+_g] = \tau^3 \Rightarrow (\tau^3)_{ij} = (U_g)_{il} [\psi_{gl}, \psi^+_{gm}] (U^+_g)_{mj} = (U_g \tau^3 U^+_g)_{ij}$

To preserve commutation relations we thus require: $\boxed{U_g \tau_3 U^+_g = \tau_3}$ For bosons U is not unitary!

We defined before $\phi_g = U_g \psi_g \Rightarrow \psi_g = U^{-1}_g \phi_g$

$\psi^+_g = \phi^+_g (U^{-1}_g)^+$

we want

We are diagonalizing $\hat{H} = \psi^+_g K \psi_g = \phi^+_g (U^{-1})^+ K U^{-1} \phi_g = \phi^+_g \underbrace{\begin{pmatrix} \omega^{(1)}_g & 0 \\ 0 & \omega^{(2)}_g \end{pmatrix}}_{\tilde{K}} \phi_g$

Need to diagonalize $(U^{-1})^+ K U^{-1} \equiv \tilde{K} \in$ diagonal

not similarity transformation like $\tilde{K} = T^{-1} K T$

because $\tau_3 = U \tau_3 U^+ \Rightarrow 1 = \tau_3 U \tau_3 U^+ \Rightarrow (U^+)^{-1} = \tau_3 U \tau_3$

Hence we diagonalize $\tilde{K} = \tau_3 U \tau_3 K U^{-1}$

or equivalently $\tau_3 \tilde{K} = \begin{pmatrix} \omega^{(1)}_g & 0 \\ 0 & -\omega^{(2)}_g \end{pmatrix} = U (\tau_3 K) U^{-1}$

Yes, now it is similarity transformation!

Hence eigenvalues/eigenvectors of $\tau_3 K$ are simply related to eigenvalues of $\tilde{K}$

Recall our original problem $K = \begin{pmatrix} \aleph_0, & \aleph_g \\ \aleph_g, & \aleph_0 \end{pmatrix}$ and $\tau_3 K = \begin{pmatrix} \aleph_0 & , \aleph_g \\ -\aleph_g & , -\aleph_0 \end{pmatrix}$

Eigenvalues: $\text{Det} \begin{pmatrix} \aleph_0 - \lambda_g, & \aleph_g \\ -\aleph_g & , -\aleph_0 - \lambda_g \end{pmatrix} = 0$

$-(\aleph_0 - \lambda_g)(\aleph_0 + \lambda_g) + \aleph_g^2$

$\aleph_0^2 - \lambda_g^2 = \aleph_g^2 \Rightarrow \lambda_g = \pm\sqrt{\aleph_0^2 - \aleph_g^2}$

$\omega_g \equiv \sqrt{\aleph_0^2 - \aleph_g^2}$

here $\aleph_g = \frac{1}{2} S J \sum_{\vec{\delta}} \cos \vec{g}\cdot\vec{\delta}$

Hence $U \tau_3 K U^{-1} = \begin{pmatrix} \omega_g & , 0 \\ 0 & , -\omega_g \end{pmatrix}$

$\tilde{K} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} \omega_g & , 0 \\ 0 & , -\omega_g \end{pmatrix} = \begin{pmatrix} \omega_g, & 0 \\ 0, & \omega_g \end{pmatrix}$

What is ω_q in real systems

$$\gamma_{\vec{q}} = \cancel{\tfrac{1}{2}} SJ \sum_{\vec{\delta}} \cos \vec{q}\cdot\vec{\delta} \qquad \text{and} \qquad \omega_q = \sqrt{\gamma_0^2 - \gamma_q^2}$$

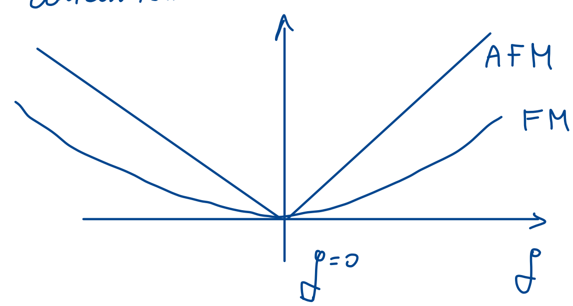
1D:
$$\gamma_q = 2SJ \cos qa$$
$$\omega_q = 2SJ\sqrt{1-\cos^2 qa} = 2SJ|\sin qa|$$

generic small $\vec{q}$:
$$\gamma_q \approx \cancel{\tfrac{1}{2}} SJ \sum_{\delta} 1 - \tfrac{1}{2}(\vec{q}\cdot\vec{\delta})^2 = \gamma_0\Big(1 - \frac{1}{z}\sum_{\delta}(\vec{q}\cdot\vec{\delta})^2\Big)$$
$$\omega_q^2 = \gamma_0^2 - \gamma_q^2 = \gamma_0^2 - \gamma_0^2\Big(1 - \frac{1}{z}\sum_{\delta}(\vec{q}\cdot\vec{\delta})^2\Big)^2 \approx \frac{2\gamma_0^2}{z}\sum_{\vec{\delta}}(\vec{q}\cdot\vec{\delta})^2$$
$$\omega_q = \frac{\gamma_0}{\sqrt{z/2}}\sqrt{\sum_{\vec{\delta}}(\vec{q}\cdot\vec{\delta})^2}$$

2D square: $\dfrac{\gamma_0}{\sqrt{2}}\sqrt{q_x^2+q_y^2} = \dfrac{\gamma_0}{\sqrt{2}}|\vec{q}|$

3D square: $\dfrac{\gamma_0}{\sqrt{3}}\sqrt{q_x^2+q_y^2+q_z^2} = \dfrac{\gamma_0}{\sqrt{3}}|\vec{q}|$

conclusion



- valid even for $S=\frac{1}{2}$, and very good for $S=\frac{3}{2}, \frac{5}{2}, \ldots$
- at integer spins 1, 2, 3 the Ising anisotropy tends to open up the gap

What is a magnon?

Eigenvectors?

$$\mathcal{U} \quad \tau_3 \cdot K \quad \cdot \mathcal{U}^{-1} = \tau_3 \tilde{K}$$

hence $\tau_3 K \mathcal{U}^{-1} = \mathcal{U}^{-1}\tau_3 \tilde{K} = \tau_3 \tilde{K}\mathcal{U}^{-1}$ because $\tau_3 \tilde{K}$ is diagonal

equivalently: $$\left(\tau_3 K - \begin{pmatrix}\omega_q & 0 \\ 0 & -\omega_q\end{pmatrix}\right)\mathcal{U}^{-1} = 0$$

$$\begin{pmatrix} N_0 \mp \omega_q , & N_q \\ -N_q , & -(N_0 \mp \omega_q)\end{pmatrix}\begin{pmatrix} u_\pm \\ -u_\mp \end{pmatrix} = 0$$

Check: $$(N_0 \mp \omega_q)\sqrt{\frac{N_0 \pm \omega_q}{2\omega_q}} - N_q\sqrt{\frac{N_0 \mp \omega_q}{2\omega_q}} = 0$$

$$\sqrt{\frac{N_0 \mp \omega_q}{2\omega_q}}\left(\sqrt{\underbrace{N_0^2 - \omega_q^2}_{N_q^2}} - N_q\right) = 0 \quad \checkmark$$

since $\omega_q^2 = N_0^2 - N_q^2$

$$u_+ = \sqrt{\frac{N_0 + \omega_q}{2\omega_q}} \qquad \text{so that} \quad \mathcal{U}^{-1} = \begin{pmatrix} u_+ & -u_- \\ -u_- & u_+ \end{pmatrix}$$

$$u_- = \sqrt{\frac{N_0 - \omega_q}{2\omega_q}} \qquad \mathcal{U} = \begin{pmatrix} u_+ & u_- \\ u_- & u_+ \end{pmatrix}$$

Requirement for commutation relations $\underline{u_+^2 - u_-^2 = 1}$

Check: $$\frac{N_0 + \omega_q}{2\omega_q} - \left(\frac{N_0 - \omega_q}{2\omega_q}\right) = 1 \quad \checkmark$$

$$H = \psi^\dagger K \psi$$

$$H = \phi^\dagger \tilde{K} \phi = \sum_q (\alpha_q^\dagger, \beta_{-q})\begin{pmatrix}\omega_q & 0 \\ 0 & \omega_q\end{pmatrix}\begin{pmatrix}\alpha_q \\ \beta_{-q}^\dagger\end{pmatrix} = \sum_q \alpha_q^\dagger \alpha_q \, \omega_q + \beta_{-q}^\dagger \beta_{-q}\omega_q + \omega_q$$

$$\phi_q = \mathcal{U}\psi_q \Rightarrow \begin{pmatrix}\alpha_q \\ \beta_{-q}^\dagger\end{pmatrix} = \begin{pmatrix} u_+ , & u_- \\ u_- , & u_+\end{pmatrix}\begin{pmatrix} a_q \\ b_{-q}^\dagger\end{pmatrix} \quad \text{or} \quad \alpha_q^\dagger = \sqrt{\frac{N_0 + \omega_q}{2\omega_q}}\, a_q^\dagger + \sqrt{\frac{N_0 - \omega_q}{2\omega_q}}\, b_{-q}$$

coherence factors

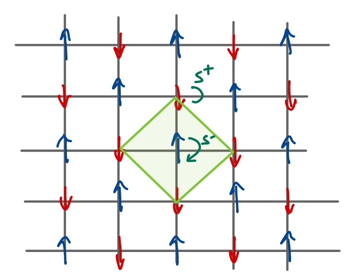
$\frac{1}{\sqrt{2S}} S_A^-$ $\qquad$ $\frac{1}{\sqrt{2S}} S_B^+$

close to $q \to 0$ $\omega_q \propto |q| \ll N_0$

then $u_+ = u_- \approx \frac{c}{\sqrt{|q|}}$

equal amount of a & $b^\dagger$

S^+ on sublattice A and S^- on sublattice B propagating in opposite directions.



Homework: Su-Schrieffer-Heeger model on page 86
The Kondo problem page 91

Construction of the path integral (Chpt 3)

This chapter is about single particle dynamics, expressed in terms of Feynman path integral.

Next chapter is generalization to many body problem using functional field integral

Particle starts at position q_i (coordinate) and ends at q_f.
What is probability $P(q_i \to q_f)$ allowing all Q.M. allowed transitions

Schrödinger Eq: $\boxed{i\hbar \frac{\partial}{\partial t}|\Psi(t)\rangle = H|\Psi(t)\rangle}$, which can be formally solved as

$$\boxed{|\Psi(t')\rangle = \underbrace{e^{-\frac{i}{\hbar}H(t'-t)}\,\Theta(t'-t)}_{U(t'-t)}\,|\Psi(t)\rangle}$$

$U(t'-t)$ is time evolution operator

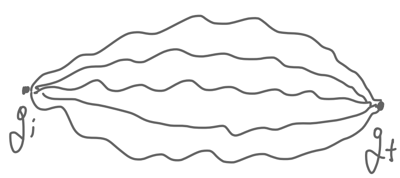
Note $\Theta(t) = \begin{cases} 1 & t \geq 0 \\ 0 & t < 0 \end{cases}$ introduced for causal response

$\langle q_f|$ / Sch. Eq.

$$\langle q_f|\Psi(t_f)\rangle = \langle q_f| e^{-\frac{i}{\hbar}H(t_f-t_i)}\,\Theta(t_f-t_i)\,|\Psi(t_i)\rangle$$

$$\int dq_i\, |q_i\rangle\langle q_i| = 1$$

$$\langle q_f|\Psi(t_f)\rangle = \Psi(q_f, t_f) = \int dq_i \underbrace{\langle q_f| e^{-\frac{i}{\hbar}H(t_f-t_i)}\,\Theta(t_f-t_i)|q_i\rangle}_{U(q_f t_f, q_i t_i)} \underbrace{\langle q_i|\Psi(t_i)\rangle}_{\Psi(q_i, t_i)}$$ because $\int dq\, |q\rangle\langle q| = 1$



time evolution for the wavefunction

$$P(q_i \to q_f) = |U(q_f t_f, q_i t_i)|^2$$ probability that the system goes from $\Psi(q_i t_i)$ to $\Psi(q_f t_f)$

Let's make many small steps rather than one large step: $\boxed{\text{Trotter-Suzuki}}$ decomposition

$$U(q_f t_f, q_i t_i) = \langle q_f| e^{-\frac{i}{\hbar}H\Delta t}\, e^{-\frac{i}{\hbar}H\Delta t} \cdots e^{-\frac{i}{\hbar}H\Delta t}|q_i\rangle$$ with $\Delta t \cdot N = t$ and $N \to \infty$

Crucial point $e^{-\frac{i}{\hbar}H\Delta t} = e^{-\frac{i}{\hbar}V\Delta t}\, e^{-\frac{i}{\hbar}T\Delta t} + O(\Delta t^2)$ where $H = V + T$

Because $e^A e^B = e^{A+B}\, e^{\frac{1}{2}[A,B] + \frac{1}{12}[A,[A,B]] + \cdots}$ Baker-Campel-Hausdorff formula
we will neglect terms of of $(\Delta t)^2$, so that it will look like T and V commute.

$$U(q_f t_f, q_i t_i) = \langle q_f| e^{-\frac{i}{\hbar}T\Delta t}\, e^{-\frac{i}{\hbar}V\Delta t}\, e^{-\frac{i}{\hbar}T\Delta t}\, e^{-\frac{i}{\hbar}V\Delta t} \qquad e^{-\frac{i}{\hbar}T\Delta t}\, e^{-\frac{i}{\hbar}V\Delta t} |q_i\rangle$$

$$\iint dq_N dp_N |q_N\rangle\langle q_N|p_N\rangle\langle p_N| \qquad \iint dq_{N-1} dp_{N-1} |q_{N-1}\rangle\langle q_{N-1}|p_{N-1}\rangle\langle p_{N-1}| \qquad \iint dq_1 dp_1 |q_1\rangle\langle q_1|p_1\rangle\langle p_1| \qquad \int dq_0 |q_0\rangle\langle q_0|$$

$$U(q_f t_f, q_i t_i) = \iint \cdots \int \delta_{q_f=q_N}\, \delta_{q_i=q_0} \langle q_N|p_N\rangle\langle p_N| e^{-\frac{i}{\hbar}T(p_N)\Delta t}\, e^{-\frac{i}{\hbar}V(q_{N-1})\Delta t} |q_{N-1}\rangle\langle q_{N-1}|p_{N-1}\rangle \cdots \langle q_1|p_1\rangle\langle p_1| e^{-\frac{i}{\hbar}T(p_1)\Delta t}\, e^{-\frac{i}{\hbar}V(q_0)\Delta t} |p_0\rangle$$

Note that $\boxed{f(\hat{p})|p\rangle = \underset{\text{eigenvalue}}{f(p)}|p\rangle}$ and similar for $f(\hat{q})$

Also note $\langle q_i|p_j\rangle = \frac{1}{\sqrt{2\pi}} e^{\frac{i}{\hbar} q_i p_j}$ plane wave in x-representation

$$U(q_f t_f, q_i t_i) = \int dq_0 \prod_{i=1}^{N} \iint dq_i dp_i \langle q_i|p_i\rangle\langle p_i| e^{-\frac{i}{\hbar}T(p_i)\Delta t - \frac{i}{\hbar}V(q_{i-1})\Delta t} |q_{i-1}\rangle\, \delta_{q_i=q_0}\, \delta_{q_f=q_N}$$

$$= \int dq_0 \left(\prod_{i=1}^{N} \iint dq_i \frac{dp_i}{2\pi} \right) \delta_{q_i=q_0}\, \delta_{q_f=q_N}\, e^{\sum_{i=1}^{N} \left(\frac{i}{\hbar} q_i p_i - \frac{i}{\hbar} p_i q_{i-1} - \frac{i}{\hbar} T(p_i)\Delta t - \frac{i}{\hbar} V(q_{i-1})\Delta t \right)}$$

$$\sum_{i=1}^{N} \frac{i}{\hbar} \Delta t \left(\frac{q_i - q_{i-1}}{\Delta t} p_i - T(p_i) - V(q_{i-1}) \right) \longrightarrow \frac{i}{\hbar} \int_{t_i}^{t_f} dt \left[\dot{q} p - T(p) - V(q) \right]$$

Finally

$$U(q_f t_f, q_i t_i) = \int \mathcal{D}[q,p]\, e^{\frac{i}{\hbar} \int_{t_i}^{t_f} dt\, \underbrace{[\dot{q} p - H(p,q)]}_{L}} \quad \text{where} \quad \int \mathcal{D}[q,p] \equiv \int_{\substack{q_f = q_N \\ q_i = q_0}} \prod_{i=1}^{N} dq_i \frac{dp_i}{2\pi}$$

We just derived: $\boxed{\langle q_f | U | q_i\rangle = \int \mathcal{D}[q,p]\, e^{\frac{i}{\hbar} S} \quad \text{with} \quad S = \int_{t_i}^{t_f} dt \left[\dot{q} p - H(p,q) \right]}$

Example: $H(p,q) = \frac{p^2}{2m} + V(q)$

$$U(q_f t_f, q_i t_i) = \delta_{q_i=q_0}\, \delta_{q_f=q_N} \int \prod_{i=1}^{N} dq_i \frac{dp_i}{2\pi}\, e^{\frac{i}{\hbar} \Delta t \sum_{i=1}^{N} \left[\frac{\Delta q_i}{\Delta t} p_i - \frac{p_i^2}{2m} - V(q_{i-1}) \right]}$$

Gaussian Integrals

Real: $\displaystyle\int_{-\infty}^{\infty} dx\, e^{-\frac{a}{2}x^2} = \sqrt{\frac{2\pi}{a}}$; $Re\, a>0$

Note: a can be a complex number, but $Re(a)>0$!

$$\int_{-\infty}^{\infty} dx\, e^{-\frac{a}{2}x^2+bx} = \sqrt{\frac{2\pi}{a}}\, e^{\frac{b^2}{2a}} \;;\; Re\, a>0$$

$$-\frac{a}{2}\left(x-\frac{b}{a}\right)^2+\frac{b^2}{2a}$$

Complex:

$$\int d(z,z^+)\, e^{-z^+ w z} = \int dx\,dy\, e^{-(x-iy)w(x+iy)} = \int dx\,dy\, e^{-(x^2+y^2)w} = \frac{\pi}{w} \;;\; Re\, w>0$$

z complex variable

$z^+ = z^*$

$$\boxed{\int d(z,z^+)\, e^{-z^+wz+u^+z+z^+v}} = \underbrace{\int d(z,z^+)\, e^{-(z-\frac{u}{w^+})^+w(z-\frac{v}{w})}}\, e^{\frac{u^+v}{w}} = \boxed{\frac{\pi}{w}\, e^{\frac{u^+v}{w}} \;;\; Re\, w>0}$$

$$\int dx\,dy\, e^{-(x-iy-\frac{u^+}{w})w(x+iy-\frac{v}{w})} = \int d\tilde{x}\,d\tilde{y}\, e^{-(\tilde{x}-i\tilde{y})w(\tilde{x}+i\tilde{y})} = \frac{\pi}{w}$$

$$\left.\begin{aligned} x-iy-\frac{u^+}{w} &= \tilde{x}-i\tilde{y} \\ x+iy-\frac{v}{w} &= \tilde{x}+i\tilde{y}\end{aligned}\right\} \quad \begin{aligned}\tilde{x} &= x-\frac{1}{2}\frac{u^++v}{w} \\ \tilde{y} &= y+\frac{1}{2}i\frac{v-u^+}{w}\end{aligned}$$

Higher dimensions:

generic matrix that can be diagonalized $\quad A=O^+DO$

Real: $$\int d\vec{v}\, e^{-\frac{1}{2}\vec{v}^+A\vec{v}} = \int d\vec{v}\, e^{-\frac{1}{2}(O\vec{v})^+ D\, O\vec{v}} = \int d\vec{\tilde{v}}\, e^{-\frac{1}{2}\vec{\tilde{v}}^+D\vec{\tilde{v}}} = \prod_i\sqrt{\frac{2\pi}{D_i}} = \frac{(2\pi)^{N/2}}{(Det\,A)^{1/2}}$$

$OO^+=1$

$\vec{v}$ is real vector;

A is real positive definite symmetric matrix ; It is sufficient if symmetric part is positive definite.

diagonalizing A: $OAO^T = D$; $\quad O\vec{v} = \vec{\tilde{v}}$; $d\vec{v} = d\vec{\tilde{v}}$ because $Det\,O=1$

$$\boxed{\int d\vec{v}\, e^{-\frac{1}{2}\vec{v}^+A\vec{v}+\vec{j}\cdot\vec{v}}} = \int d\vec{v}\, e^{-\frac{1}{2}(\vec{v}-A^{-1}\vec{j})^+A(\vec{v}-A^{-1}\vec{j})+\frac{1}{2}\vec{j}A^{-1}\vec{j}} = \boxed{\frac{(2\pi)^{N/2}}{(Det\,A)^{1/2}}\, e^{\frac{1}{2}\vec{j}A^{-1}\vec{j}}} \;;\; A \text{ symmetric}$$

Important identity for perturbation theory

$$\frac{\partial}{\partial j_n}\frac{\partial}{\partial j_m}\left.\int d\vec{v}\, e^{-\frac{1}{2}\vec{v}^+A\vec{v}+\vec{j}\cdot\vec{v}}\right|_{j=0} = \frac{\partial}{\partial j_n}\frac{\partial}{\partial j_m}\frac{(2\pi)^{N/2}}{(Det\,A)^{1/2}}\left. e^{\frac{1}{2}\vec{j}A^{-1}\vec{j}}\right|_{j=0}$$

$$\boxed{\int d\vec{v}\, e^{-\frac{1}{2}\vec{v}^+A\vec{v}}\, v_n v_m = \frac{(2\pi)^{N/2}}{(Det\,A)^{1/2}}\,\frac{1}{2}\left((A^{-1})_{nm}+(A^{-1})_{mn}\right)}$$

If we define the following: $\frac{(\mathrm{Det} A)^{1/2}}{(2\pi)^{N/2}} \int d\vec{v}\, e^{-\frac{1}{2}\vec{v}^{+} A \vec{v}}\, O \equiv \langle O \rangle$ then we can write

$$\boxed{\langle v_n v_m \rangle = (A^{-1})_{nm}}$$ for symmetric A.

We could also prove: $\langle v_{m_1} v_{m_2} v_{m_3} v_{m_4} \rangle = \underbrace{(A^{-1})_{m_1 m_2}(A^{-1})_{m_3 m_4} + (A^{-1})_{m_1 m_3}(A^{-1})_{m_2 m_4} + (A^{-1})_{m_1 m_4}(A^{-1})_{m_2 m_3}}_{\text{all combinations}}$

This can be used to prove Wicks theorem

Can be generalized to any number of pair-products.

stopped 10/11/2022

Complex multi-D case

$$\int d(v^+, v)\, e^{-\vec{v}^{+} A \vec{v}} = \pi^N \mathrm{Det}(A^{-1}) \qquad \text{here} \quad d(v^+, v) = \prod_i dv_i'\, dv_i''$$

A has to have a positive definite hermitian part: $A = \underbrace{\tfrac{1}{2}(A + A^{+})}_{\substack{\text{hermitian}\\ \text{part should be}\\ \text{positive definite}}} + \tfrac{1}{2}(A - A^{+})$

Easy to prove for A positive definite hermitian matrix.

$$\boxed{\int d(v^+, v)\, e^{-\vec{v}^{+} A \vec{v} + \vec{w}^{+}\vec{v} + \vec{v}^{+}\vec{w}'} = \pi^N \mathrm{Det}(A^{-1})\, e^{\vec{w}^{+} A^{-1} \vec{w}'}}$$

Finally the identity:

by taking derivative with r.t. w, w'

$$\boxed{\langle v_{i_1}^{+} v_{i_2}^{+} \cdots v_{i_m}^{+} v_{j_1} v_{j_2} \cdots v_{j_m} \rangle = \sum_{\substack{P \\ \text{All permutations}}} (A^{-1})_{j_1 i_{P_1}} (A^{-1})_{j_2 i_{P_2}} \cdots (A^{-1})_{j_m i_{P_m}}}$$

where $\langle \cdots \rangle = \frac{1}{\pi^N} \mathrm{Det}(A) \int d(v^+, v)\, e^{-v^+ A v}$

Proof for 1st order: $\langle v_i^{+} v_j \rangle = (A^{-1})_{ji}$

$$\frac{\partial^2}{\partial j_i^{+} \partial j_i} \int d(v^+, v)\, e^{-v^+ A v + j^+ v + v^+ j} = \int d(v^+, v)\, e^{-v^+ A v}\, v_i^{+} v_j$$

$$\overset{\shortparallel}{\frac{\partial^2}{\partial j_i^{+} \partial j_i}} \frac{\pi^N}{\mathrm{Det} A}\, e^{j^+ A^{-1} j} = \frac{\pi^N}{\mathrm{Det} A} (A^{-1})_{ji}$$

Back to our example $U(q_f t_f, q_i t_i) = \delta_{q_i=q_0}\,\delta_{q_f=q_N} \displaystyle\int \prod_{i=1}^{N} dq_i \frac{dp_i}{2\pi}\, e^{\frac{i}{\hbar}\Delta t \sum_{i=1}^{N}\left[\frac{\Delta q_i}{\Delta t}p_i - \frac{p_i^2}{2m} - V(q_{i-1})\right]}$

Integral over p:

Needs regularization
$A = \left(\frac{i}{\hbar}\frac{\Delta t}{m} + \delta\right) I$
with $\delta \to 0 \Rightarrow$ gaussian integral applies

$\longrightarrow$ $\left.\begin{aligned} A &= \frac{2i}{\hbar}\frac{\Delta t}{2m}\cdot I \\ j &= \frac{i}{\hbar}\Delta t \frac{\Delta q}{\Delta t} \end{aligned}\right\}$ $j A^{-1} j = \frac{i}{\hbar}\Delta t \left(\frac{\Delta q}{\Delta t}\right)^2 m \Rightarrow \frac{i}{\hbar}\Delta t\, m \dot{q}^2$

We use:

$$\int d\vec{v}\, e^{-\frac{1}{2}\vec{v}^{T} A \vec{v} + \vec{j}\cdot\vec{v}} = \frac{(2\pi)^{N/2}}{(\mathrm{Det}\, A)^{1/2}}\, e^{\frac{1}{2}\vec{j} A^{-1}\vec{j}}$$

Finally $$\prod_{i=1}^{N}\int \frac{dp_i}{2\pi}\, e^{\frac{i}{\hbar}\Delta t \sum_{i=1}^{N}\left(\frac{\Delta q_i}{\Delta t}p_i - \frac{p_i^2}{2m}\right)} = \frac{(2\pi)^{N/2}}{(2\pi)^N}\frac{1}{\underbrace{\left(\frac{i}{\hbar}\frac{\Delta t}{m}\right)^{N/2}}_{\mathrm{Det}}}\, e^{\frac{1}{2}\frac{i}{\hbar}\Delta t\, m \dot{q}^2}$$

$$U(q_f t_f, q_i t_i) = \delta_{q_i=q_0}\,\delta_{q_f=q_N}\frac{1}{\left(2\pi\frac{i}{\hbar}\frac{\Delta t}{m}\right)^{N/2}}\cdot \int \prod_{i=1}^{N} dq_i\, e^{\frac{i}{\hbar}\Delta t \sum_{i=1}^{N}\left[\frac{1}{2}m\dot{q}_i^2 - V(q_{i-1})\right]}$$

We can hence also write

$$U(q_f t_f, q_i t_i) = \int \mathcal{D}[q]\, e^{\frac{i}{\hbar}\int_{t_i}^{t_f} dt\, \mathcal{L}[q,\dot{q}]} \qquad \text{where } \mathcal{D}[q] = \left(\frac{\hbar m}{2\pi i \Delta t}\right)^{N/2}\delta_{q_i=q_0}\,\delta_{q_f=q_N}\prod_{n} dq_n$$

Free particle can be computed in closed form because $\dot{q} = \text{const} = \frac{q_f - q_i}{t_f - t_i}$

$$U(q_f t_f, q_i t_i) = \frac{1}{\left(2\pi\frac{i}{\hbar}\frac{\Delta t}{m}\right)^{N/2}}\cdot \int \prod_{i=1}^{N} dq_i\, \delta_{q_i=q_0}\,\delta_{q_f=q_N}\, e^{\frac{i}{\hbar}\int_{t_i}^{t_f}\frac{1}{2}m\dot{q}^2 dt} = \text{const.}\; e^{\frac{i}{\hbar}\frac{1}{2}m\frac{(q_f-q_i)^2}{t_f-t_i}}$$

and $P(q_f, q_i) = |U|^2 = 1$

Skip

Semiclassical approximation requires $\delta S = 0$, i.e., the system goes through path where Feynman integral contribution is largest because the exponent has saddle point

$$\langle q_f | U | q_i \rangle = \int D[q,p]\, e^{\frac{i}{\hbar} S} \approx e^{\frac{i}{\hbar} S_{classical}} + \dots$$

With definition $S = \int_{t_i}^{t_f} dt\,[\dot{q}p - H(p,q)]$ then $\delta S = 0$ requires

$$\delta S = \int dt \left\{ [\delta \dot{q}\, p + \dot{q}\,\delta p - \frac{\partial H}{\partial p}\delta p - \frac{\partial H}{\partial q}\delta q \right]$$

by parts $\displaystyle \int dt \left\{ \delta q \left[-\dot{p} - \frac{\partial H}{\partial q} \right] + \delta p \left[\dot{q} - \frac{\partial H}{\partial p} \right] \right\} = 0$

hence classical EOM: $\dot{q} = \frac{\partial H}{\partial p}$ and $\dot{p} = -\frac{\partial H}{\partial q}$

Next step: Fluctuations around the saddle point

$q = q_{classical} + r(t)$ where $r(t)$ is small

We can expand the action $S[\{q_{classical} + r\}] = S_{classical} + \frac{1}{2}\iint dt'dt'' \frac{\delta^2 S}{\delta q(t')\,\delta q(t'')} r(t')r(t'')$

example: $\mathcal{L} = \frac{m\dot{q}^2}{2} - V(q) \Rightarrow S[\{q+r\}] = \int dt\,[\frac{1}{2}m(\dot{q}+\dot{r})^2 - V(q+r)] =$

$$\int dt\,[\tfrac{1}{2}m\dot{q}^2 + \underline{m\dot{q}\dot{r}} + \tfrac{1}{2}m\dot{r}^2 - V(q) - \underline{\frac{\partial V}{\partial q} r} - \frac{1}{2}\frac{\partial^2 V}{\partial q^2} r^2 + \dots]$$

vanishes because Lagrange Eq. are satisfied

$S[\{q+r\}] \approx S_{class}[q] + \int dt\,[\frac{1}{2}m\dot{r}^2 - \frac{1}{2}\frac{\partial^2 V}{\partial q^2} r^2]$

by parts $-\frac{1}{2}m r\ddot{r}$

$= S_{class}[q] + \int dt\,[-\frac{1}{2} r (m\ddot{r} + \frac{\partial^2 V}{\partial q^2} r)]$

$= S_{class}[q] - \frac{1}{2}\int dt\, r(t)\,[m\frac{\partial^2}{\partial t^2} + \frac{\partial^2 V}{\partial q^2}]\, r(t)$

$$\langle q_f | U | q_i \rangle = \sum_{\substack{\text{all classical}\\ \text{solutions}}} e^{\frac{i}{\hbar} S^j_{classical}} \underbrace{\int D[r]\, e^{-\frac{i}{2\hbar}\int dt\, r(t)\,[m\frac{\partial^2}{\partial t^2} + \frac{\partial^2 V}{\partial q^2}]\, r(t)}}_{\text{Gaussian integral, which can be evaluated exactly...}}$$

Functional field integral   Chpt 4. A&S

1) In Feynman path integral formalism we were dealing with a single particle characterized by path $q(t)$.

In functional field integral formalism we deal with a field like $\phi(x,t)$ defined in $(d+1)$ dimensional space

2) In Feynman path integral we formulated integral on eigenstates of T and V operators, namely p and q.

In many body problem of 2nd quantized operators we want to work in the $\boxed{\text{eigenbasis of the operator } a}$, which is called $\boxed{\text{coherent states}}$.

Coherent states for bosons

The coherent states are
$$\boxed{|\phi\rangle \equiv e^{\sum_i a_i^+ \phi_i} |0\rangle}$$

bosonic creation operator   complex number   vacuum

We will prove: $\boxed{a_i|\phi\rangle = \phi_i|\phi\rangle}$ hence $|\phi\rangle$ is eigenvector and ϕ_i eigenvalue of operator a_i

complex number

proof:
$$a_i|\phi\rangle = a_i e^{\sum_j \phi_j a_j^+}|0\rangle = e^{\sum_{j\neq i}\phi_j a_j^+} a_i e^{\phi_i a_i^+}|0\rangle .$$ We need $a e^{\phi a^+}|0\rangle$ to continue.

a_j for $j\neq i$ commute with a_i and each other

What is $a e^{\phi a^+}|0\rangle$?

Define $a e^{\phi a^+} \equiv X$

multiply with $e^{-\phi a^+}$ on both sides:

$$\underbrace{e^{-\phi a^+} a e^{\phi a^+}}_{a-\phi[a^+,a]+\frac{\phi^2}{2}[a^+,[a^+,a]]+\dots} = e^{-\phi a^+}X \quad ; \text{ because } e^{-\phi a^+} a e^{\phi a^+} = a+\phi \Rightarrow e^{-\phi a^+}X = a+\phi \Rightarrow \underbrace{e^{\phi a^+} e^{-\phi a^+}}_{=1} X = e^{\phi a^+}(a+\phi)$$

hence $X = e^{\phi a^+}(a+\phi)$

Check: $\left(1-\phi a^+ + \frac{1}{2!}\phi^2(a^+)^2 - \frac{1}{3!}\phi^3(a^+)^3 + \dots\right) a \left(1+\phi a^+ + \frac{1}{2!}\phi^2(a^+)^2 + \frac{1}{3!}\phi^3(a^+)^3 + \dots\right)$

$$a + \phi(-a^+a + a a^+) + \frac{1}{2!}\phi^2\underbrace{\left((a^+)^2 a + a(a^+)^2 - 2a^+ a a^+\right)}_{\substack{[a^+,[a^+,a]] = \\ a^+(a^+a - aa^+) - (a^+a - aa^+)a^+}} + \dots = a+\phi$$

Now we answer what is $\underbrace{a\, e^{\phi a^+}}_{\overset{\shortparallel}{X}}|0\rangle = e^{\phi a^+}(a+\phi)|0\rangle = e^{\phi a^+}\phi|0\rangle$

Finally:

$$a_i|\phi\rangle = e^{\sum_{j\neq i}\phi_j a_j^+}\, a_i\, e^{\phi_i a_i^+}|0\rangle = \phi_i\, e^{\sum_j \phi_j a_j}|0\rangle = \phi_i|\phi\rangle$$

which concludes the proof.

Important properties of coherent states

1) $a_i|\phi\rangle = \phi_i|\phi\rangle$

2) $\langle\phi|a_i^+ = \langle\phi|\phi_i^* \equiv \langle\phi|\bar{\phi}$

3) $a_i^+|\phi\rangle = \frac{\partial}{\partial\phi_i}|\phi\rangle$

proof: $a_i^+ e^{\sum_j a_j^+\phi_j}|0\rangle = e^{\sum_{j\neq i} a_j^+\phi_j}\underbrace{a_i^+ e^{a_i^+\phi_i}}|0\rangle$

$\frac{\partial}{\partial\phi_i}(e^{a_i^+\phi_i})|0\rangle = \frac{\partial}{\partial\phi_i}(e^{a_i^+\phi_i + \sum_{j\neq i} a_j^+\phi_j}|\phi\rangle)$

4) $\langle\vartheta|\phi\rangle = e^{\sum_i \bar{\vartheta}_i\phi_i}$

$\langle\phi|\vartheta\rangle = e^{\sum_i \bar{\phi}_i\vartheta_i}$

proof: $\langle\vartheta| = \langle 0|e^{\sum_j \bar{\vartheta}_j a_j}$

$\langle\vartheta|\phi\rangle = \langle 0|e^{\sum_j \bar{\vartheta}_j a_j}|\phi\rangle = \langle 0|e^{\sum_j \bar{\vartheta}_j\phi_j}|\phi\rangle = e^{\sum_j \bar{\vartheta}_j\phi_j}\underbrace{\langle 0|\phi\rangle}_{\overset{\shortparallel}{1}}$

a is eigenoperator

$\langle 0|e^{\phi a^+}|0\rangle = \langle 0|1+\phi a^+ + \frac{1}{2}\phi(a^+)^2\cdots|0\rangle$
$\quad 1 \quad 0 \quad 0$

5)

$$\int\prod_i \frac{d\bar{\phi}_i\, d\phi_i}{\pi}\, e^{-\sum_i\bar{\phi}_i\phi_i}|\phi\rangle\langle\phi| = I$$

Here $d\bar{\phi}_i\, d\phi_i = d\,\mathrm{Re}\,\phi_i\, d\,\mathrm{Im}\,\phi_i$; Note, we also write $\int\prod_i\frac{d\bar{\phi}_i\, d\phi_i}{\pi} \equiv \int d(\phi_i^+\phi_i)$

We use Schur lemma: If all a_i and a_i^+ commute with a certain operator, then the operator is a constant.

Discussion: Any operator can be expressed in terms of a_i and a_i^+ and complex numbers.

If operator commutes with all a_i and a_i^+, it does not contain any operator a_i or a_i^+, hence it must be a constant.

Proof that identity commutes with all a_i :

$$a_i \int d(\phi^+,\phi)\, e^{-\sum_\ell \bar\phi_\ell \phi_\ell} |\phi\rangle\langle\phi| = \int d(\phi^+,\phi)\, \underbrace{\phi_i\, e^{-\sum_\ell \bar\phi_\ell \phi_\ell}}_{\left(-\frac{\partial}{\partial\bar\phi_i} e^{-\sum_\ell \bar\phi_\ell \phi_\ell}\right)} |\phi\rangle\langle\phi|$$

$$= \int d(\phi^+,\phi) \left(-\frac{\partial}{\partial\bar\phi_i} e^{-\sum_\ell \bar\phi_\ell \phi_\ell} |\phi\rangle\right)\langle\phi| \underset{\text{by parts}}{=} \int d(\phi^+,\phi)\, e^{-\sum_\ell \bar\phi_\ell \phi_\ell} |\phi\rangle \underbrace{\frac{\partial}{\partial\bar\phi_i}(\langle\phi|)}_{\langle\phi|a_i} =$$

Crucial point ϕ is periodic

$\left.\begin{array}{l}\phi(-\infty)=\phi(\infty)\\ \phi(0)=\phi(\beta)\end{array}\right\}$ bosons

$$= \int d(\phi^+,\phi)\, e^{-\sum_\ell \bar\phi_\ell \phi_\ell} |\phi\rangle\langle\phi| a_i$$

we used the fact: $a_i^+|\phi\rangle = \frac{\partial}{\partial\phi_i}|\phi\rangle$

hence conjugate : $\langle\phi|a_i = \frac{\partial}{\partial\bar\phi_i}\langle\phi|$

Similarly we can prove $I\cdot a_i^+ = a_i^+ I$, hence I commutes with all operators, and it must be a constant.

For the constant, we know $\langle 0|C|0\rangle = C$, hence we should show that $\langle 0|I|0\rangle = 1$. Proof:

$$\langle 0| \int d(\phi^+,\phi)\cdot e^{-\sum_\ell \bar\phi_\ell \phi_\ell} |\phi\rangle \underbrace{\langle\phi|0\rangle}_{=1} = \int d(\phi^+,\phi)\, e^{-\sum_\ell \bar\phi_\ell \phi_\ell} =$$

$$= \prod_j \left(\int \frac{d\bar\phi_j\, d\phi_j}{\pi} e^{-\bar\phi_j \phi_j} \right) = 1$$

Note that $\int \prod_j \frac{d\bar\phi_j\, d\phi_j}{\pi} |\phi\rangle\langle\phi| \neq 1$, i.e., we need the extra exponent in between.

This is because $|\phi\rangle\langle\phi|$ form an overcomplete basis.

Less essential properties of coherent states:

1) The Heissenberg uncertainty achieves its minimum in a coherent state, i.e., $\Delta x \Delta p = \frac{\hbar}{2}$.

Heissenberg uncertainty on fluctuations of variables A, B

$$\Delta A \, \Delta B \geq \frac{1}{2} |\langle [A,B] \rangle|$$

$$\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$$

Coherent states satisfy the minimum uncertainty relation.

To prove: $\langle \phi | (a + a^+) | \phi \rangle = \phi + \phi^*$

$$\langle \phi | a^+ = \langle \phi | \phi^*$$

$$a a^+ - a^+ a = 1$$

$$\langle \phi | a - a^+ | \phi \rangle = \phi - \phi^*$$

$$\langle \phi | (a + a^+)^2 | \phi \rangle = \langle \phi | \underbrace{a^2}_{\phi^2} + \underbrace{a a^+}_{1 + a^+ a = 1 + \phi^* \phi} + \underbrace{a^+ a}_{\phi^* \phi} + \underbrace{(a^+)^2}_{(\phi^*)^2} | \phi \rangle = \phi^2 + 2\phi\phi^* + (\phi^*)^2 + 1 = (\phi + \phi^*)^2 + 1$$

$$\langle \phi | (a - a^+)^2 | \phi \rangle = \langle \phi | a^2 - a a^+ - a^+ a + (a^+)^2 | \phi \rangle = (\phi - \phi^*)^2 - 1$$

$$\phi^2 - 1 - a^+ a$$

$$x = \sqrt{\frac{\hbar}{2m\omega}} (a + a^+)$$

$$p = i \sqrt{\frac{\hbar m \omega}{2}} (a^+ - a)$$

$$\langle x^2 \rangle - \langle x \rangle^2 = \frac{\hbar}{2m\omega} \langle \phi | (a + a^+)^2 | \phi \rangle - \frac{\hbar}{2m\omega} (\langle \phi | a + a^+ | \phi \rangle)^2 = \frac{\hbar}{2m\omega} \left((\phi + \phi^*)^2 + 1 - (\phi + \phi^*)^2 \right) = \frac{\hbar}{2m\omega}$$

$$\langle p^2 \rangle - \langle p \rangle^2 = -\frac{\hbar m \omega}{2} \langle \phi | (a^+ - a)^2 | \phi \rangle + \frac{\hbar m \omega}{2} (\langle \phi | a^+ - a | \phi \rangle)^2 = -\frac{\hbar m \omega}{2} \left((\phi^* - \phi)^2 - 1 - (\phi^* - \phi)^2 \right) = \frac{\hbar m \omega}{2}$$

$$\Delta x \cdot \Delta p = \sqrt{\frac{\hbar}{2m\omega} \frac{\hbar m \omega}{2}} = \frac{\hbar}{2}$$

2) They have time evolution like a classical oscilator and are the closest state to classical harmonic oscilator

⋮

Coherent states for fermions

stopped 10/13/2022

We are looking for state that satisfies: $a_i|\eta\rangle = \eta_i|\eta\rangle$

annihilation operator, state, eigenvalue

The problem is that a's anticommute:

$a_i a_j = -a_j a_i$ hence $\underline{\eta_i \eta_j = -\eta_j \eta_i}$

not true for complex numbers

How to solve the conundrum?

Mathematicians invented $\boxed{\text{grassmann numbers}}$.

Properties of Grassmann numbers:

1) $\eta_i, \eta_j \in \mathcal{A}$ $\in$ means grassmann

to be on the safe side (I do not think we need that. I can not prove anticommutation rule with that!)

then $\cancel{c_0} + c_1^i \eta_i + c_2^j \eta_j \in \mathcal{A}$ where $c_0, c_1^i, c_2^j \in \mathbb{C}$

complex numbers

but $c_1 = 0$ $c_2 = 0$ is not allowed

We can multiply grass. with complex numbers and sum them up.

2) The product of grassmann numbers is

a) $\boxed{\text{associative} \quad (\eta_1 \eta_2)\eta_3 = \eta_1(\eta_2 \eta_3)}$

b) $\boxed{\text{anticommutative} \quad \eta_1 \eta_2 = -\eta_2 \eta_1}$

for any pair of η_1 and η_2 we have $[\eta_1, \eta_2]_- = 0$

no delta function!

c) $\eta^2 = 0$

because $\eta \cdot \eta = -\eta\eta \Rightarrow \eta^2 = 0$

d) three number $\eta_1 \eta_2 \eta_3 = \eta_3 \eta_1 \eta_2$ behave like fermions, $\boxed{\text{but no } \delta \text{ function}}$.

They behave similar to fermions, but it is much simpler to manipulate, because we do not need to keep track of extra term arising from δ functions

3) We will extensively use functions of grassmann numbers:

$$\boxed{f(\eta_1, \eta_2, \dots \eta_n) = \sum_{m=0}^{\infty} \sum_{i_1, i_2, \dots i_m} \frac{1}{m!} \frac{\partial^m f\,(\eta=0)}{\partial\eta_{i_1}\partial\eta_{i_2}\cdots\partial\eta_{i_m}} \eta_{i_m}\eta_{i_{m-1}} \cdots \eta_{i_1}}$$ ← the order matters!

example: $e^{-(\eta_1+\eta_2)}$ $= 1 - (\eta_1+\eta_2) - \frac{1}{2!}(\underbrace{\eta_1^2}_{=0} + \underbrace{\eta_1\eta_2 + \eta_2\eta_1}_{=0} + \underbrace{\eta_2^2}_{=0}) + \frac{1}{3!}(\underbrace{\eta_1^3}_{=0} + \underbrace{\eta_1\eta_2\eta_3 + \dots}_{=0} \quad)$

$= 1 - \eta_1 - \eta_2$

1D function $f(\eta) = \underline{f(0) + f'(0)\eta} + \underbrace{\tfrac{1}{2} f''(0)\underbrace{\eta^2}_{=0} + \dots}_{=0}$

4) Differentiation

We define $\boxed{\frac{\partial}{\partial\eta_i}\eta_j \equiv \delta_{ij}}\,\left(-\eta_j\frac{\partial}{\partial\eta_i}\right)$

differentiation is $\boxed{\text{anticommutative}}$

$$\frac{\partial}{\partial\eta_i}\eta_j = -\eta_j\frac{\partial}{\partial\eta_i}$$

example: $\frac{\partial}{\partial\eta_2}(\eta_1\eta_2) = -\frac{\partial}{\partial\eta_2}(\eta_2\eta_1) = -\eta_1$

$= \eta_1\left(-\frac{\partial}{\partial\eta_2}\right)\eta_2 = -\eta_1$

5) Integration

We define $\int d\eta_i\, \eta_i \equiv 1$ and $\int d\eta_i \equiv 0$

From definition it follows that integration and differentiation is the same operation:

$$\int d\eta\, f(\eta) = \int d\eta\,[f(0) + f'(0)\eta] = f'(0)$$

$$\frac{\partial}{\partial\eta}(f(\eta)) = \frac{\partial}{\partial\eta}(f(0) + f'(0)\eta) = f'(0)$$

6) In physics, we need to mix grassmann variables with fermion operators $\eta_i a_j$

We define: $\boxed{[\eta_i, a_j]_- = 0}$

7) Fermionic coherent states are:

$$\boxed{|\eta\rangle = e^{-\sum_i \eta_i a_i^+}|0\rangle = e^{\sum_i a_i^+\eta_i}|0\rangle}$$

note the minus sign compared to bosons

here it looks like bosons

Proof:

$$a_i|\eta\rangle = a_i\, e^{-\sum_j \eta_j a_j^+}|0\rangle = e^{-\sum_{j\neq 0}\eta_j a_j^+}\, a_i\, e^{a_i^+\eta_i}$$

$$\underbrace{\underbrace{1+a_i^+\eta_i}+\tfrac{1}{2!}(a_i^+\eta_i)^2+\dots}$$

$$(a_i^+\eta_i)^2 = -(a_i^+)^2\eta_i^2 = 0$$

$$(a_i + a_i a_i^+\eta_i)|0\rangle = \eta_i|0\rangle$$

$$= \eta_i(1-\eta_i a_i^+)|0\rangle$$

$$= \eta_i\, e^{-\eta_i a_i^+}|0\rangle$$

hence: $a_i|\eta\rangle = e^{-\sum_{j\neq 0}\eta_j a_j^+}\eta_i\, e^{-\eta_i a_i^+} = \eta_i|\eta\rangle$

More on properties of coherent states:

1) $a_i|\eta\rangle = \eta_i|\eta\rangle$

grassmann

2) $\langle\eta|a_i^+ = \langle\eta|\eta_i^+$

Here η^+ is new grassmann number. (Like taking ϕ and ϕ^* as independent variables instead of $\mathrm{Re}\,\phi$ and $\mathrm{Im}\,\phi$)

Because $\langle\eta| = \langle 0|e^{-\sum_i a_i\eta_i^+}$

3) $a_i^+|\eta\rangle = -\frac{\partial}{\partial\eta_i}|\eta\rangle$ (for bosons it is $a_i^+|\phi\rangle = \frac{\partial}{\partial\phi_i}|\phi\rangle$ hence generic $a_i^+|\eta\rangle = \varsigma\frac{\partial}{\partial\eta_i}|\eta\rangle$)

4) $\langle\varphi|\eta\rangle = e^{\sum_i\varphi_i^+\eta_i}$

Proof: $\langle 0|e^{\sum_i\varphi_i^+ a_i}|\eta\rangle = \langle 0|e^{\sum_i\varphi_i^+\eta_i}|\eta\rangle = e^{\sum_i\varphi_i^+\eta_i}\underbrace{\langle 0|\eta\rangle}_{1}$

η eigenstate of $a_i \to \eta_i$

$$\langle 0|e^{-\sum_i\eta_i a_i^+}|0\rangle = \langle 0|1|0\rangle + \underbrace{\dots}_{0}$$

5) $\int\prod_i d\eta_i^+ d\eta_i\; e^{-\sum_j\eta_j^+\eta_j}|\eta\rangle\langle\eta| = I$

(for bosons $\int\prod_i\frac{d\phi_i^+ d\phi_i}{\pi}\, e^{-\sum_i\phi_i^+\phi_i}|\phi\rangle\langle\phi| = I$ hence generic $\int d(\phi^+,\phi)\, e^{-\sum_i\phi_i^+\phi_i}|\phi\rangle\langle\phi| = I$)

We could use $\boxed{\int\prod_i d\eta_i^+ d\eta_i \equiv \int d(\eta^+,\eta)}$

Proof: identical to bosons

$$a_i I = \int d(\eta^+,\eta)\, e^{-\sum_e \eta_e^+\eta_e}\, \eta_i |\eta\rangle\langle\eta| = \int \prod_j d\eta_j^+ d\eta_j \left(-\frac{\partial}{\partial\eta_i^+}\, e^{-\sum_e \eta_e^+\eta_e}\, |\eta\rangle\right)\langle\eta| =$$

$$\underset{\text{by parts}}{=} \int \prod_j d\eta_j^+ d\eta_j\, e^{-\sum_e \eta_e^+\eta_e}\, |\eta\rangle\left(\frac{\partial}{\partial\eta_i^+}\langle\eta|\right) \underset{\substack{\downarrow \\ \text{see below}}}{=} \int \prod_j d\eta_j^+ d\eta_j\, e^{-\sum_e \eta_e^+\eta_e}\, |\eta\rangle\langle\eta|\, a_i = I\, a_i$$

$$\frac{\partial}{\partial\eta^+}\langle\eta| = \frac{\partial}{\partial\eta_i^+}\langle 0| e^{\sum_j \eta_j^+ a_j} = \langle 0|\frac{\partial}{\partial\eta_i^+} e^{\sum_j \eta_j^+ a_j} = \langle 0| e^{\sum_{j\neq i}\eta_j^+ a_j}\, \underbrace{\frac{\partial}{\partial\eta_i^+} e^{\eta_i^+ a_i}}_{\underbrace{\frac{\partial}{\partial\eta_i^+}(1+\eta_i^+ a_i)}_{a_i}}$$

$$|\eta\rangle = e^{-\sum_i \eta_i a_i^+}|0\rangle$$
$$\langle\eta| = \langle 0| e^{-\sum_i a_i \eta_i^+}$$

$$a_i\, e^{\eta_i^+ a_i} = a_i(1+\eta_i^+ a_i), \quad a_i a_i = 0$$

$$= \langle 0| e^{\sum_j \eta_j^+ a_j}\, a_i = \langle\eta| a_i$$

From Schur lemma it follows $I = \text{const.}$

The correct constant:
$$\langle 0|I|0\rangle = \int\prod_j d\eta_j^+ d\eta_j\, e^{-\sum_e \eta_e^+\eta_e}\, \underset{1}{\langle 0|\eta\rangle}\underset{1}{\langle\eta|0\rangle}$$
$$= \prod_j\left(\int d\eta_j^+ d\eta_j\,(1-\eta_j^+\eta_j)\right) = \prod_j 1 = 1$$
$$0 + 1 = 1$$

Alternative (useful) proof:

Let's limit ourselves to one component. The generalization is simple.

$$\int d\eta^+ d\eta\, e^{-\eta^+\eta}\, |\eta\rangle\langle\eta| = I$$

where $|\eta\rangle = e^{-\eta a^+}|0\rangle$

$\langle\eta| = \langle 0| e^{-a\eta^+}$

Then $\langle 0|I|0\rangle = 1$ as proven above

$\langle 1|I|1\rangle = 1$ because $\int d\eta^+ d\eta\, e^{-\eta^+\eta}\langle 1|\eta\rangle\langle\eta|1\rangle = \int d\eta^+ d\eta\, \underset{(1+\eta\eta^+)}{e^{-\eta^+\eta}}\, \eta\eta^+ = 1$

$$\langle 1|\eta\rangle = \langle 1|(1+a^+\eta)|0\rangle = \langle 1|a^+|0\rangle\eta = \eta$$

careful: $\langle 1|-\eta a^+|0\rangle = \langle 1|-\eta|1\rangle \neq -\eta$, $\simeq \eta$

can not pull η out from state $|1\rangle$ without − sign!!

Similarly $\langle 1|I|0\rangle = 0$

$\langle 0|I|1\rangle = 0$ hence this is identity.

Gaussian integrals for fermions

stopped 10/18/2022

1) $\int d\eta^+ d\eta \; e^{-\eta^+ a \eta} = a$ $\qquad$ (proof: $\int d\eta^+ d\eta \,(1+\underbrace{\eta a \eta^+}) = a$

notice the order!

2) $\int \prod_i d\eta_i^+ d\eta_i \; e^{-\sum_{ij} \eta_i^+ A_{ij} \eta_j} \equiv \boxed{\int d(\eta^+,\eta)\, e^{-\vec\eta^+ A \vec\eta} = Det(A)}$

A Hermitian : $A = U^+ D U$ where $D = diag(D_i)$

$$\int \prod_i d\eta_i^+ d\eta_i \; e^{-\vec\eta^+ U^+ D U \vec\eta} = \int \underbrace{\prod_i d\varphi_i^+ d\varphi_i}_{Det U \cdot Det U^+ = I} e^{-\sum_j \varphi_j^+ \varphi_j D_j} = \int d\varphi_1^+ d\varphi_1 \cdots d\varphi_N^+ d\varphi_N \,(1+\varphi_1\varphi_1^+ D_1)(1+\varphi_2\varphi_2^+ D_2)\cdots(1+\varphi_N\varphi_N^+ D_N)$$

$$= D_1 \cdot D_2 \cdots D_N = Det(A)$$

pairs jump, no extra minus sign

$U\vec\eta = \vec\varphi$ i.e., $\sum_j U_{ij}\eta_j = \varphi_i$

$\vec\eta^+ U^+ = \vec\varphi^+$ i.e., $\sum_j \eta_j^+ U^*_{ij} = \varphi_i^+$

Valid for non-Hermitian matrices. Proof for 2×2:

$$e^{-\eta_1^+\eta_1 A_{11} - \eta_1^+\eta_2 A_{12} - \eta_2^+\eta_1 A_{21} - \eta_2^+\eta_2 A_{22}}$$

example 2×2: $\iiiint d\eta_1^+ d\eta_1 d\eta_2^+ d\eta_2 \Big[(1 - \underbrace{\eta_1^+\eta_1 A_{11} - \eta_1^+\eta_2 A_{12} \cdots}_{\text{will give } 0} + \frac{1}{2}\big(\underbrace{\eta_1^+ A_{11}\eta_1 + \eta_2^+ A_{22}\eta_2}_{} + \underbrace{\eta_1^+ A_{12}\eta_2 + \eta_2^+ A_{21}\eta_1}_{}\big)^2 + \dots\Big]$

$\frac{1}{2}\big(\eta_1^+ A_{11}\eta_1 \eta_2^+ A_{22}\eta_2 + \eta_2^+ A_{22}\eta_2 \eta_1^+ A_{11}\eta_1\big) = \eta_2\eta_2^+\eta_1\eta_1^+ A_{11}A_{22}$

$\frac{1}{2}\big(\eta_1^+ A_{12}\eta_2 \eta_2^+ A_{21}\eta_1 + \eta_2^+ A_{21}\eta_1 \eta_1^+ A_{12}\eta_2\big) = -\eta_2\eta_2^+\eta_1\eta_1^+ A_{12}A_{21}$

+ other terms vanish after integration

$$\iiiint d\eta_1^+ d\eta_1 d\eta_2^+ d\eta_2 \; \eta_2\eta_2^+\eta_1\eta_1^+ (A_{11}A_{22} - A_{12}A_{21}) = Det(A)$$

We can prove similarly that the above formula is valid for arbitrary A. It does not need be Hermitian.

3) $\int d(\eta^+,\eta)\, e^{-\vec\eta^+ A \vec\eta + \vec w^+ \cdot \vec\eta + \vec\eta^+ \cdot \vec w'} = e^{\vec w^+ A^{-1} \vec w'} \, \underline{Det(A)}$ $\qquad$ for bosons $\dfrac{e^{\vec w^+ A^{-1}\vec w'}}{Det(A)}$

Proof: $\eta^+ A \vec\eta - \vec w^+ \cdot \vec\eta - \vec\eta^+ \cdot \vec w' = \underbrace{(\vec\eta^+ - \vec w^+ A^{-1})\, A\, (\vec\eta - A^{-1}\vec w')}_{\eta^+ A \eta - \vec w^+ \vec\eta - \vec\eta^+ \vec w' + \vec w^+ A^{-1} \vec w'} - \vec w^+ A^{-1} \vec w'$

$$\int d(\eta^+,\eta)\, e^{-(\vec\eta^+ - \vec w^+ A^{-1}) A (\eta - A^{-1}\vec w') + \vec w^+ A^{-1} \vec w'} = \int \prod_i d\varphi_i^+ d\varphi_i \, e^{-\vec\varphi^+ A \vec\varphi} \cdot e^{\vec w^+ A^{-1} \vec w'} = Det A \times e^{\vec w^+ A^{-1} \vec w'}$$

$\vec\eta^+ - \vec w^+ A^{-1} = \vec\varphi^+$

$\vec\eta - A^{-1}\vec w' = \vec\varphi$

note $[\vec\varphi^+ A \vec\varphi, \vec w^+ A^{-1} \vec w'] = 0$

because always in pairs.

non-trivial step!

5) $$\langle \eta_{i_1} \eta_{i_2} \cdots \eta_{i_N} \eta^+_{j_N} \cdots \eta^+_{j_2} \eta^+_{j_1} \rangle = \sum_P \underline{(-1)^P} (A^{-1})_{i_1 j_{P_1}} (A^{-1})_{i_2 j_{P_2}} \cdots (A^{-1})_{i_N j_{P_N}}$$

where $$\langle O \rangle = \frac{1}{\underline{\text{Det}\,A}} \int e^{-\vec{\eta}^+ A \vec{\eta}}\, O$$

different from bosons!

Proof of the lowest order :

$$\int d(\eta^+, \eta)\, \underbrace{e^{-\vec{\eta}^+ A \vec{\eta} + \vec{w}^+ \vec{\eta} + \vec{\eta}^+ \vec{w}}}_{\text{expand left}} = \underbrace{e^{\vec{w}^+ A^{-1} \vec{w}}\, \text{Det}(A)}_{\text{expand right}}$$

$$\frac{1}{\text{Det}A} \int \prod_\ell d\eta_\ell^+ d\eta_\ell\; e^{-\vec{\eta}^+ A \vec{\eta}} \Big(1 + \underbrace{\vec{w}^+ \vec{\eta} + \vec{\eta}^+ \vec{w}}_{\text{only one } \eta \Rightarrow \text{vanishes}} + \tfrac{1}{2}(\vec{w}^+ \vec{\eta} + \vec{\eta}^+ \vec{w})^2 + \cdots \Big) = 1 + \vec{w}^+ A^{-1} \vec{w} + \cancel{\tfrac{1}{2}(\vec{w}^+ A^{-1} \vec{w})^2 + \cdots}$$

first order: $$\int \prod_\ell d\eta_\ell^+ d\eta_\ell\; e^{-\vec{\eta}^+ A \vec{\eta}}\, \eta_i = 0$$

$$\int \prod_\ell d\eta_\ell^+ d\eta_\ell \left(1 - \vec{\eta}^+ A \vec{\eta} + \tfrac{1}{2}(\vec{\eta}^+ A \vec{\eta})^2 + \cdots\right) \eta_i$$

will never have a pair
odd number of η's $\Rightarrow$ vanishes

second order:

$$1 + \frac{1}{\text{Det}A} \int \prod_\ell d\eta_\ell^+ d\eta_\ell\; e^{-\vec{\eta}^+ A \vec{\eta}}\, \tfrac{1}{2}(\vec{w}^+ \vec{\eta} + \vec{\eta}^+ \vec{w})^2 = 1 + \vec{w}^+ A^{-1} \vec{w} + O(w^2)$$

$$\underbrace{\tfrac{1}{2}(w_i^+ \eta_i \eta_j^+ w_j + \eta_j^+ w_j w_i^+ \eta_i)}_{\eta_i \eta_j^+ w_i^+ w_j} + \cdots$$

$$\underset{\text{left side}}{w_i^+ w_j \langle \eta_i \eta_j^+ \rangle} = \underset{\text{right side}}{w_i^+ (A^{-1})_{ij} w_j} \Rightarrow \langle \eta_i \eta_j^+ \rangle = (A^{-1})_{ij}$$

To prove higher order we need to expand to the appropriate order.

Field integral for the partition function

We want to evaluate $Z = Tr(e^{-\beta(H-\mu N)})$ or equivalently $Z = \sum_m \langle m | I \, e^{-\beta(\hat{H}-\mu \hat{N})} | m \rangle$

Reminder: coherent states $|\psi\rangle = e^{\sum_i a_i^+ \psi_i} |0\rangle$ valid for both bosons and fermions

ψ_i are either complex numbers or grassmann numbers.

$$I = \int d(\psi^+, \psi) \, e^{-\sum_i \psi_i^+ \psi_i} |\psi\rangle\langle\psi| \quad \text{valid for both fermion \& bosons}$$

$$Z = \sum_m \int d(\psi^+, \psi) \, e^{-\sum_i \psi_i^+ \psi_i} \langle m|\psi\rangle\langle\psi| e^{-\beta(\hat{H}-\mu\hat{N})} |m\rangle$$

passing $\langle m|$ through Grassmann variables can give − sign, but here a pair of Grassmanns → safe!

we want to eliminate $\sum_m |m\rangle\langle m|$ which is also 1.

$$Z = \int d(\psi^+, \psi) \, e^{-\sum_i \psi_i^+ \psi_i} \langle \pm\psi | e^{-\beta(\hat{H}-\mu\hat{N})} \sum_m |m\rangle\langle m|\psi\rangle$$

for fermions − ⇒ the origin of antiperiodic boundary condition for fermions!

H is fully symmetric (it always transforms like a number A_{ij}) hence we can forget it here.

why −? $\langle m|\psi\rangle\langle\psi|m\rangle = \langle -\psi|m\rangle\langle m|\psi\rangle$ for fermions

Proof! We will prove that $\sum_m \langle m|\psi\rangle\langle\psi|m\rangle = \prod_i (1 + \psi_i \psi_i^+)$ while

$\sum_m \langle\psi|m\rangle\langle m|\psi\rangle = \prod_i (1 - \psi_i \psi_i^+)$

hence we need to flip sign on one ψ!

Start with: $\sum_m \langle m| e^{\sum_i a_i^+ \psi_i} |0\rangle\langle 0| e^{\sum_i \psi_i^+ a_i} |m\rangle$

$\langle m| = \langle m_1 m_2 \dots m_N|$, $m_i = 0$ or 1

Concentrate on single state here (because $a^+\psi$ behaves like boson for all other states and commutes)

$$\sum_{m_i} \langle m_i | e^{a_i^+ \psi_i} |0\rangle\langle 0| e^{\psi_i^+ a_i} |m_i\rangle =$$

$$= \underbrace{\langle 0| e^{a_i^+ \psi_i} |0\rangle}_{=1} \underbrace{\langle 0| e^{\psi_i^+ a_i} |0\rangle}_{=1} + \langle 1| e^{a_i^+ \psi_i} |0\rangle\langle 0| e^{\psi_i^+ a_i} |1\rangle$$

$$= 1 + \langle 1 | 1 + a_i^+ \psi_i |0\rangle\langle 0| 1 + \psi_i^+ a_i |1\rangle = 1 + \psi_i \psi_i^+$$

$\langle 0|\psi_i|0\rangle\langle 0|\psi_i^+|0\rangle$

Next $\sum_{m_i} \langle \psi | m_i \rangle \langle m_i | \psi \rangle = \sum_{m_i} \langle 0 | e^{\psi_i^+ \varrho_i} | m_i \rangle \langle m_i | e^{\varrho_i^+ \psi_i} | 0 \rangle =$

$$\underbrace{\langle 0 | e^{\psi_i^+ \varrho_i} | 0 \rangle}_{1} \underbrace{\langle 0 | e^{\varrho_i^+ \psi_i} | 0 \rangle}_{1} + \langle 0 | e^{\psi_i^+ \varrho_i} | 1 \rangle \langle 1 | e^{\varrho_i^+ \psi_i} | 0 \rangle$$

$$\langle 0 | \psi_i^+ \underbrace{\varrho_i | 1 \rangle}_{|0\rangle} \underbrace{\langle 1 | \varrho_i^+}_{\langle 0|} \psi_i | 0 \rangle$$

$$\langle 0 | \psi_i^+ | 0 \rangle \langle 0 | \psi_i | 0 \rangle$$

$$= 1 + \psi_i^+ \psi_i$$

$$= \underline{\underline{1 - \psi_i \psi_i^+}}$$

Why can we concentrate on single state?

$$\langle m_1 m_2 \cdots m_N | e^{\sum_i \varrho_i^+ \psi_i} | 0 \rangle = \langle m_1 m_2 \cdots m_N | \prod_i e^{\varrho_i^+ \psi_i} | 0 \rangle = \langle m_1 | \otimes \langle m_2 | \otimes \cdots \langle m_N | e^{\varrho_1^+ \psi_1} e^{\varrho_2^+ \psi_2} \cdots | 0 \rangle =$$

because $[\varrho_i^+ \psi_i, \varrho_j^+ \psi_j] = 0$ for $i \neq j$

$\varrho_i^+ \psi_i$ commutes, hence we have

$$= \prod_i \left(\langle m_i | e^{\varrho_i^+ \psi_i} \right) | 0 \rangle$$

Back to partition function

$$\boxed{Z = \int d(\psi_0^+, \psi_0)\, e^{-\sum_i \psi_{i0}^+ \psi_{i0}} \langle \xi \psi_0 | e^{-\beta(\hat{H} - \mu \hat{N})} | \psi_0 \rangle}$$

where $\xi = \pm 1$ for fermions/bosons

$\xi \psi(0) = \psi(\beta)$ we will have antiperiodic boundary conditions for fermions and periodic for bosons

these ψ have certain time like $t=0$. Later we will introduce them for every time slice.

Next Trotter-Suzuki $\beta = \Delta\tau \cdot N$ and $N \to \infty$

$$Z = \int d(\psi_0^+, \psi_0)\, e^{-\sum_i \psi_{i0}^+ \psi_{i0}} \langle \xi \psi_0 | e^{-\Delta\tau(H-\mu N)}\, I_{N-1}\, e^{-\Delta\tau(H-\mu N)} \cdots\ I_1 e^{-\Delta\tau(H-\mu N)} | \psi_0 \rangle$$

$$I_{N-1} = \int d(\psi_{N-1}^+, \psi_{N-1})\, e^{-\sum_i \psi_{N-1 i}^+ \psi_{N-1 i}} |\psi_{N-1}\rangle\langle \psi_{N-1}| \qquad I_1 = \int d(\psi_1^+, \psi_1)\, e^{-\sum_i \psi_{1i}^+ \psi_{1i}} |\psi_1\rangle\langle\psi_1|$$

$$Z = \int d(\psi_0^+, \psi_0) \cdots d(\psi_{N-1}^+, \psi_{N-1})\, e^{-\sum_i (\psi_{i0}^+ \psi_{i0} + \cdots + \psi_{N-1 i}^+ \psi_{N-1 i})} \times$$

time slice

$$\times \langle \underbrace{\xi \psi_0}_{\psi_N = \psi(t=\beta)} | e^{-\Delta\tau(H - \mu\hat{N})} | \psi_{N-1} \rangle \langle \psi_{N-1} | e^{-\Delta\tau(H-\mu N)} | \psi_{N-2} \rangle \cdots \langle \psi_1 | e^{-\Delta\tau(H-\mu N)} | \psi_0 \rangle$$

$$\boxed{Z = \int \prod_t d(\psi_t^+, \psi_t)\, e^{-\sum_{i,t=0}^{N-1} \psi_{it}^+ \psi_{it}} \times \prod_{t=0}^{N-1} \langle \psi_{t+1} | e^{-\Delta\tau(\hat{H} - \mu\hat{N})} | \psi_t \rangle}$$

$\psi_N = \xi\psi(t=0) = \psi(t=\beta)$
$\psi_0 = \psi(t=0)$

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We need: $\langle \psi_{t+1} | e^{-\Delta\tau(H-\mu N)} | \psi_t \rangle$? We require H has the "normal order" form

$$H = \sum_{ij} h_{ij}\, a_i^+ a_j + \sum_{ijem} V_{ijem}\, a_i^+ a_j^+ a_e a_m$$

Then $\langle \psi_{t+1} | e^{-\Delta\tau(H-\mu N)} | \psi_t \rangle = \langle \psi_{t+1} | e^{-\Delta\tau(H[\psi_{t+1}^+, \psi_t] - \mu N[\psi_{t+1}^+, \psi_t])} | \psi_t \rangle$

coherent states are eigenstates of ψ operator, hence acting on the left or right give numbers!

where $H[\psi_{t+1}^+, \psi_t] = \sum_{ij} h_{ij} \psi_{t+1 i}^+ \psi_{tj} + \sum_{ijem} V_{ijem}\, \psi_{t+1 i}^+ \psi_{t+1 j}^+ \psi_{te} \psi_{tm} \to h_{ij} \psi^+(\tau)\psi(\tau) + V_{ijem} \psi_i^+(\tau)\psi_j^+(\tau)\psi_e(\tau)\psi_m(\tau)$

Then $\langle \psi_{t+1} | e^{-\Delta\tau(H-\mu N)} | \psi_t \rangle = e^{-\Delta\tau(H[\psi_{t+1}^+, \psi_t] - \mu N[\psi_{t+1}^+, \psi_t])} \langle \psi_{t+1} | \psi_t \rangle = e^{-\Delta\tau(H[\psi_{t+1}^+, \psi_t] - \mu N[\psi_{t+1}^+, \psi_t])} \times e^{\sum_{i,t} \psi_{it+1}^+ \psi_{it}}$

from properties of coherent states!

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$$Z = \int \prod_{t=0}^{N-1} d(\psi_t^+, \psi_t)\; e^{-\sum_{i,t=0}^{N-1} \psi_{it}^+ \psi_{it}} \times \prod_{t=0}^{N-1} \langle \psi_{t+1} | e^{-\Delta\tau(\hat{H}-\mu\hat{N})} | \psi_t \rangle$$

$\psi_N = \zeta\psi(t=0) = \psi(t=\beta)$

$\psi_0 = \psi(t=0)$

Finally put together

$$Z = \int \prod_{t=0}^{N-1} d(\psi_t^+, \psi_t)\; e^{-\sum_{t=0}^{N-1} \Delta\tau (H[\psi_{t+1}^+, \psi_t] - \mu N[\psi_{t+1}^+, \psi_t]) + \sum_{i,t=0}^{N-1} \psi_{it+1}^+ \psi_{it} - \psi_{it}^+ \psi_{it}}$$

$\psi_N = \psi(\beta)$

$\psi_0 = \psi(0)$

exponent: $-\sum_{t=0}^{N-1} \Delta\tau \left(H[\psi_{t+1}^+, \psi_t] - \mu N[\psi_{t+1}^+, \psi_t] - \sum_{i,t=0}^{N-1} \frac{(\psi_{it+1}^+ - \psi_{it}^+)}{\Delta\tau} \psi_{it} \right)$

$\lim N \to \infty$: $-\int_0^\beta d\tau \left[H[\psi^+(\tau), \psi(\tau)] - \mu N(\tau) - \underbrace{\left(\frac{\partial \psi^+}{\partial\tau}\right)\psi(\tau)}_{\text{by parts}} \right]$

$$\int_0^\beta d\tau \frac{\partial\psi^+}{\partial\tau}\psi(\tau) = \underbrace{\psi^+\psi\Big|_0^\beta}_{\psi^+(\beta)\psi(\beta) - \psi^+(0)\psi(0) = 0} - \int_0^\beta \psi^+ \frac{\partial}{\partial\tau}\psi = -\int_0^\beta \psi^+ \frac{\partial}{\partial\tau}\psi$$

exponent: $-\int_0^\beta d\tau \left[H[\psi^+(\tau), \psi(\tau)] - \mu N(\tau) + \psi^+(\tau)\frac{\partial}{\partial\tau}\psi(\tau) \right]$

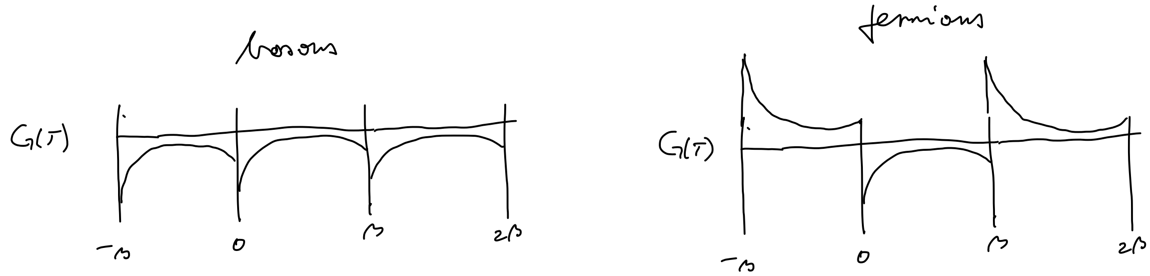
define: $\prod_{t=0}^{N-1} d(\psi_{ti}^+, \psi_{ti}) = \mathcal{D}[\psi^+, \psi]$

Finally:

$$Z = \int \mathcal{D}[\psi^+, \psi]\; e^{-\int_0^\beta d\tau \left(\sum_i \psi_i^+(\tau)\left(\frac{\partial}{\partial\tau} - \mu\right)\psi_i(\tau) + H[\psi^+(\tau), \psi(\tau)] \right)}$$

all ψ ψ^+ are time dependent!

We had to define that $\psi(\tau)$ is periodic / antiperiodic for bosons / fermions



(Anti) Periodic field $\Rightarrow$ Fourier transform is discrete:

$$\psi(\tau) = \frac{1}{\sqrt{\beta}} \sum_m \psi_m \, e^{-i\omega_m \tau} \qquad \underbrace{\psi_m}_{\psi_{\omega_m}} = \frac{1}{\sqrt{\beta}} \int_0^\beta \psi(\tau)\, e^{i\omega_m \tau} d\tau$$

Matsubara frequencies: $\omega_m = \begin{cases} 2\pi m/\beta & \text{for bosons} \\ (2m+1)\pi/\beta & \text{for fermions} \end{cases}$

Check $\psi(\tau+\beta) = \frac{1}{\sqrt{\beta}} \sum_m \psi_m \, e^{-i\omega_m \tau} \underbrace{e^{-i\omega_m \beta}}_{\xi = \pm 1} = \xi \psi(\tau)$ as expected.

Non-interacting electrons

$$Z = \int \mathcal{D}[\psi^+ \psi]\, e^{-\int_0^\beta d\tau \int \psi^+(\vec{r},\tau)\left[\frac{\partial}{\partial\tau} - \mu - \frac{\nabla^2}{2m}\right]\psi(\vec{r},\tau)\, d^3\vec{r}}$$

Double Fourier transform: $\psi(\vec{r},\tau) = \frac{1}{\sqrt{V}}\frac{1}{\sqrt{\beta}}\sum_{\vec{p},\, i\omega_n} \psi_{(\vec{p},\, i\omega_n)}\, e^{i(\vec{p}\cdot\vec{r} - \omega_n \tau)}$

on the lattice $\vec{p} \in$ I.B.Z.

transformation unitary, hence $\int \mathcal{D}[\psi^+(\vec{r},\tau)\psi] = \int \mathcal{D}[\psi^+_{p\omega}\psi_{p\omega}]$

exponent: $\int_0^\beta d\tau \int d^3\vec{r}\, \frac{1}{V\beta}\sum_{\substack{p_1 p_2 \\ n_1 n_2}} \psi^+_{(\vec{p}_1\omega_{n_1})}\, e^{-i(\vec{p}_1\vec{r} - \omega_{n_1}\tau)}\left[\frac{\partial}{\partial\tau} - \mu - \frac{\nabla^2}{2m}\right] e^{i(\vec{p}_2\cdot\vec{r} - \omega_{n_2}\tau)}\psi_{(p_2,\omega_{n_2})}$

$$\sum_{\substack{p_1 p_2 \\ n_1 n_2}} \psi^+_{(\vec{p}_1,\omega_{n_1})}\psi_{(\vec{p}_2,\omega_{n_2})}\left[-i\omega_{n_2} - \mu + \frac{\vec{p}_2^{\,2}}{2m}\right] \underbrace{\frac{1}{V}\int d^3r\, e^{i(\vec{p}_2 - \vec{p}_1)\vec{r}}}_{\delta_{\vec{p}_1 = \vec{p}_2}}\ \underbrace{\frac{1}{\beta}\int_0^\beta e^{i(\omega_{n_1} - \omega_{n_2})\tau}\, d\tau}_{\delta_{n_1 = n_2}}$$

exponent: $-\sum_{\vec{p},n} \psi^+_{(\vec{p},\omega_n)}\psi_{(\vec{p},\omega_n)}\left[i\omega_n + \mu - \frac{\vec{p}^{\,2}}{2m}\right]$

$$Z = \int \mathcal{D}[\psi^+_{\vec{p}n}, \psi_{\vec{p}n}]\, e^{\sum_{pn} \psi^+_{\vec{p}n}\psi_{\vec{p}n}\left[i\omega_n + \mu - \frac{\vec{p}^{\,2}}{2m}\right]} = \prod_{\vec{p}n}\left(\int d(\psi^+_{\vec{p}n}, \psi_{\vec{p}n})\, e^{-\psi^+_{\vec{p}n}\psi_{\vec{p}n}(\varepsilon_{\vec{p}} - i\omega_n)}\right)$$

each p, n independent contribution

$\varepsilon_p = \frac{p^2}{2m} - \mu$

$$= \prod_{\vec{p}n}(\varepsilon_{\vec{p}} - i\omega_n)^{-\xi} \cdot \begin{Bmatrix} 1 & \text{fermions} \\ \cancel{\pi^N}\ 1 & \text{bosons} \end{Bmatrix}$$

becomes definition!

fermions: $\int \prod_\ell d\eta^+_\ell d\eta_\ell\, e^{-\vec{\eta}\cdot A\cdot\vec{\eta}} = \mathrm{Det}(A)$

bosons: $\int \prod_\ell d\left(\frac{z^+_\ell, z_\ell}{\pi}\right) e^{-\vec{z}^+ A \vec{z}} = \frac{1}{\mathrm{Det}(A)}$

$$Z = e^{-\beta F} \Rightarrow F = -T\ln Z = \xi T \sum_{\vec{p}n} \ln(\varepsilon_{\vec{p}} - i\omega_n)$$

Matsubara summation

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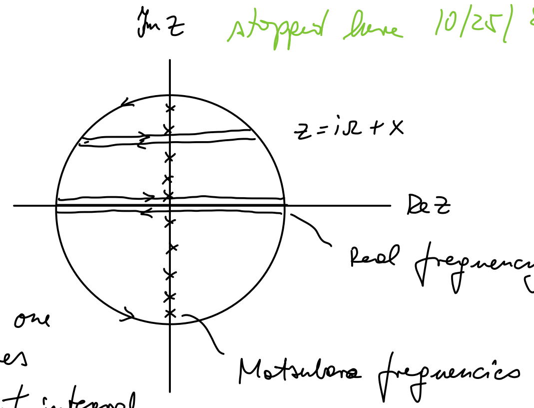
$$S = T\sum_{i\omega_m} g(i\omega_m) = \oint \frac{dz}{2\pi i} \left\{ \begin{array}{c} -f(z) \\ f(-z) \\ M(z) \\ -M(-z) \end{array} \right\} g(z)$$

contour which avoids all singularities or branch-cuts of $g(z)$, but contains all Matsubara frequencies

choose the one that gives convergent integral



Proof by Residue theorem! $\oint dz\, h(z) g(z) = 2\pi i \sum_{i\omega_m} \underbrace{\mathrm{Res}(h, i\omega_m) \cdot g(i\omega_m)}_{\text{only } h \text{ has residuums, while } g \text{ is analytical.}}$

Residue of $f(z) = \frac{1}{e^{\beta z}+1}$ at $z = i\omega_m = \frac{(2m+1)\pi}{\beta}$

$f(z)$: $f(i\omega_m + x) = \frac{1}{e^{(2m+1)\pi + \beta x}+1} = \frac{1}{-e^{\beta x}+1} = \frac{1}{-1-\beta x+1} = -\frac{1}{\beta}\cdot\frac{1}{x} \Rightarrow \mathrm{Res}(f, \omega_m) = -\frac{1}{\beta}$

$f(-z)$: $f(-i\omega_m - x) = \frac{1}{e^{-(2m+1)\pi - \beta x}+1} = \frac{1}{-e^{-\beta x}+1} = \frac{1}{-1+\beta x+1} = \frac{1}{\beta}\cdot\frac{1}{x} \Rightarrow \mathrm{Res}(f, \omega_m) = \frac{1}{\beta}$

Residue of $M(z) = \frac{1}{e^{\beta z}-1}$ at $z = i\omega_m = \frac{2m\pi}{\beta}$

$M(z)$: $M(i\omega_m + x) = \frac{1}{e^{2m\pi + \beta x}-1} = \frac{1}{\beta \cdot x}$

$M(-z)$: $M(-i\omega_m - x) = \frac{1}{e^{2m\pi - \beta x}-1} = -\frac{1}{\beta x}$

Conclusion

$$\oint dz\, f(z) g(z) = 2\pi i \sum_{\omega_m} \left(-\frac{1}{\beta}\right) g(i\omega_m)$$

$$\oint dz\, f(-z) g(z) = 2\pi i \sum_{\omega_m} \left(\frac{1}{\beta}\right) g(i\omega_m)$$

$$\oint dz\, M(z) g(z) = 2\pi i \sum_{\omega_m} \frac{1}{\beta} g(i\omega_m)$$

$$\oint dz\, M(-z) g(z) = 2\pi i \sum_{\omega_m} \left(-\frac{1}{\beta}\right) g(i\omega_m)$$

contour such that $g(z)$ is analytical!

Back to free energy

$$F = \xi T \sum_{\vec{p}\,n} \ln(\varepsilon_{\vec{p}} - i\omega_n) = \oint \frac{dz}{2\pi i} \begin{Bmatrix} f(z) \\ M(z) \end{Bmatrix} \ln(\xi_p - z)\, e^{z\cdot\delta}$$

$z \to \infty \quad f(z), M(z) \to e^{-\beta z} \to 0$ converges

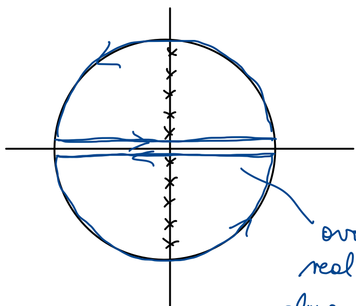
$z \to -\infty \quad f(z), M(z) \to 1, -1$

$\ln(\xi_p - z) \to \ln(z)$ diverges!

$f(z) \ln(\xi_p - z)\, e^{z\delta} \to \ln(|z|)\, e^{-|z|\delta}$ converges!

We could use $\begin{Bmatrix} -f(-z) \\ -M(-z) \end{Bmatrix} e^{-z\delta}$ also converges

Contour



$\ln(\xi_p - z)$ has branch-cut on the real axis

actually poles at $z = \xi_p$, but p can be continuous...

avoid real axis

always works for fermions, because the first Matsubara point is at $\pi \cdot T$

$$F \equiv \sum_p F_p$$

$z = x + i\eta\,;\ \eta \ll 1 \qquad z = x - i\delta \qquad z = Re^{i\phi}\,;\ R \gg 1$

$$F_p = \int_{-\infty}^{\infty} \frac{dx}{2\pi i} f(x) \ln(\xi_p - x - i\eta)\, e^{x\delta} + \int_{\infty}^{-\infty} \frac{dx}{2\pi i} f(x) \ln(\xi_p - x + i\eta)\, e^{x\delta} +$$

should vanish because $f(z)\, e^{z\delta} \ln(-z) \to 0$

$$= \int_{-\infty}^{\infty} \frac{dx}{2\pi i} f(x) \left[\ln(\xi_p - x - i\eta) - \ln(\xi_p - x + i\eta)\right] e^{x\delta}$$

It converges now even for $\delta = 0$, hence we can safely set it to zero.

$$\underset{\text{by parts}}{=} -\int_{-\infty}^{\infty} \frac{dx}{2\pi i} \left(\xi \frac{1}{\beta} \ln(1 - \xi e^{-\beta x})\right) \left(\frac{-1}{\xi_p - x - i\eta} - \frac{-1}{\xi_p - x + i\eta}\right)$$

$$\underline{f(x) = -\frac{d}{dx} \frac{1}{\beta} \ln(1 + e^{-\beta x})} \qquad \text{for bosons: } \underline{M(x) = \frac{d}{dx} \frac{1}{\beta} \ln(1 - e^{-\beta x})}$$

$$F_p = \xi \int_{-\infty}^{\infty} \frac{dx}{2\pi i} \frac{1}{\beta} \ln(1 - \xi e^{-\beta x}) \Big(\underbrace{\frac{1}{\xi_p - x - i\eta}}_{P\frac{1}{\xi_p - x} + i\pi\delta(\xi_p - x)} - \underbrace{\frac{1}{\xi_p - x + i\eta}}_{P\frac{1}{\xi_p - x} - i\pi\delta(\xi_p - x)} \Big) = \xi \int_{-\infty}^{\infty} \frac{dx}{2\pi i} \frac{1}{\beta} \ln(1 - \xi e^{-\beta x})\, 2i\pi\delta(\xi_p - x) = \xi T \ln(1 - \xi e^{-\beta \xi_p})$$

Finally: $F = -\sum_p T \ln(1 + e^{-\beta\xi_p})$

for bosons $F = \sum_p T \ln(1 - e^{-\beta\xi_p})$

Homework 2, 620 Many body

October 13, 2022

1) Problem 4.5.5 in A&S: Using the frequency summation technique compute the following correlation functions:

$$\chi^s(\mathbf{q}, i\Omega) = -\frac{1}{\beta}\sum_{\mathbf{p}, i\omega_n} G^0(\mathbf{p}, i\omega_n)G^0(-\mathbf{p}+\mathbf{q}, -i\omega_n + i\Omega) \tag{1}$$

$$\chi^c(\mathbf{q}, i\Omega) = -\frac{1}{\beta}\sum_{\mathbf{p}, i\omega_n} G^0(\mathbf{p}, i\omega_n)G^0(\mathbf{p}+\mathbf{q}, i\omega_n + i\Omega) \tag{2}$$

where

$$G^0(\mathbf{q}, i\omega_n) = \frac{1}{i\omega_n - \varepsilon_p} \tag{3}$$

and $i\Omega$, $i\omega_n$ are bosonic, fermionic Matsubara frequencies, respectively.

2) Problem 4.5.6 in A&S: Pauli paramagnetic susceptibility occurs due to the coupling of the magnetic field to the spin of the conduction electrons. The corresponding Hamiltonian is:

$$H = H^0[c^\dagger, c] - \mu_0\vec{B}\sum_{\mathbf{k},s,s'} c^\dagger_{\mathbf{k},s}\vec{\sigma}_{s,s'}c_{\mathbf{k},s'} \tag{4}$$

where H^0 is the non-interacting electron Hamiltonian with dispersion ε_k.

Calculate the free energy of the system (in the presence of the magnetic field) and show that the magnetic susceptibility ($\chi = \partial^2 F/\partial B^2$ at $B = 0$) at low temperature is $\frac{\mu_0}{2}\rho(E_F)$, where $\rho(E_F)$ is the density of electronic states at the Fermi level.

3) Problem 4.5.7 in A& S: Electron-phonon coupling.

In the first few lectures we showed how we can obtain the phonon dispersion in a material. The quantum solution in terms of independent harmonic oscillators has the usual form

$$H_{ph} = \sum_{\mathbf{q},\nu} \omega_{\mathbf{q},\nu}\, a^\dagger_{\mathbf{q},\nu}a_{\mathbf{q},\nu} \tag{5}$$

where $\mathbf{q}$ is momentum in the 1BZ, and ν is a phonon branch. The Fourier transform of the oscillation amplitude is

$$u^\nu_{\mathbf{q},\alpha,j} = \frac{1}{\sqrt{N}}\sum_{\mathbf{R}_n} u^\nu_{n,\alpha,j}e^{-i\mathbf{q}\mathbf{R}_n} \tag{6}$$

Here α is the Wickoff position in the unit cell, j is x, y, z and $\mathbf{R}_n$ is the lattice vector to unit cell at $\mathbf{R}_n = n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$, and N is the number of unit cells in the solid.

The solution of the Quantum Harmonic Oscilator (QHO) gives the relation between operators $a_{\mathbf{q},p}$ and the position operator, which is in this case given by

$$u^{\nu}_{\mathbf{q},\alpha,j} = \frac{1}{\sqrt{2M_\alpha \omega_{\mathbf{q},\nu}}} \varepsilon^{\nu}_{\alpha,j}(\mathbf{q})(a_{\mathbf{q},\nu} + a^{\dagger}_{-\mathbf{q},\nu}) \tag{7}$$

Here $\varepsilon^{\nu}_{\alpha,j}(\mathbf{q})$ (or $\vec{\varepsilon}^{\nu}_{\alpha}(\mathbf{q})$) is the phonon polarization, and M_α is the ionic mas at Wickoff position α.

When solving the phonon problem, we wrote the following equation

$$[H_e + \sum_{i,j} V_{e-i}(\mathbf{r}_j - \mathbf{R}_i) + \sum_{i \neq j} V_{i-i}(\mathbf{R}_i - \mathbf{R}_j)]\, |\psi_{electron}\rangle = E_{electron}[\{\mathbf{R}\}]\, |\psi_{electron}\rangle \tag{8}$$

which gives the solution of the electron problem in the static lattice approximation (Born-Oppenheimer), where $\mathbf{R}_i$ are lattice vectors of ions, H_e is the electron Hamiltonian, and V_{e-i} and V_{i-i} are electron-ion and ion-ion Coulomb repulsions, respectively.

Due to ionic vibrations, the displacement of ions creates an additional term in the Hamiltonian, which according to the above equation, should be proportional to

$$H_{e-i} = \int d^3r \sum_{n,\alpha} [V_{e-i}(\mathbf{r} - \mathbf{R}_{n\alpha} - \vec{u}_{n\alpha}) - V_{e-i}(\mathbf{r} - \mathbf{R}_{n\alpha})]\rho_{electron}(\mathbf{r}) \tag{9}$$

where $\mathbf{R}_{n\alpha}$ is position of an ion at Wickoff position α and unit cell n.

– Using above equations, shows that for small phonon-displacement u, the electron-phonon coupling should have the form

$$H_{e-i} = \sum_{\alpha,j,\mathbf{q},\nu,\sigma,i_1,i_2,\mathbf{k}} c^{\dagger}_{i_1,\mathbf{k}+\mathbf{q},\sigma} c_{i_2,\mathbf{k},\sigma} (a_{\mathbf{q},\nu} + a^{\dagger}_{-\mathbf{q},\nu}) \frac{g^{\mathbf{k},\mathbf{q}}_{i_1,i_2,\alpha,\nu}}{\sqrt{2M_\alpha \omega_{\mathbf{q},\nu}}} \tag{10}$$

where the electron field operator is expanded in Bloch basis

$$\psi_\sigma(\mathbf{r}) = \sum_{\mathbf{k},i} \psi_{\mathbf{k},i}(\mathbf{r}) c_{\mathbf{k},i,\sigma} \tag{11}$$

and the matrix elements g are given by

$$g^{\mathbf{k},\mathbf{q}}_{i_1,i_2,\alpha,\nu} = \frac{1}{\sqrt{N}} \sum_j \varepsilon^{\nu}_{\alpha,j}(\mathbf{q})\, \langle \psi_{\mathbf{k}+\mathbf{q},i_1} | \sum_n e^{i\mathbf{q}\mathbf{R}_n} \frac{\partial V_{e-i}(\mathbf{r} - \mathbf{R}_{n\alpha})}{\partial R_{n\alpha,j}} |\psi_{\mathbf{k},i_2}\rangle \tag{12}$$

Explain why the above integration $\langle \psi_{\mathbf{k}+\mathbf{q},i_1} | ... | \psi_{\mathbf{k},i_2}\rangle$ can be carried over a single unit cell, rather than the entire solid.

– Now use the following approximations to simplify the above Hamiltonian

* We have only one type of atom in the unit cell, i.e., $M_\alpha = M$.
* We consider only one Bloch band, i.e., $c_{i_1\mathbf{k}} = c_\mathbf{k}$ in our model.
* We consider the longitudinal phonon with $\omega_{\mathbf{q},\nu} = \omega_\mathbf{q}$ and approximate form

$$g^{\mathbf{k},\mathbf{q}}_{i_1,i_2,\alpha,\nu} \approx \delta_{i_1,i_2}\, iq_\nu\, \gamma. \tag{13}$$

Show that H_{e-i} is

$$H_{e-i} = \gamma \sum_{\nu,\mathbf{q},\sigma,\mathbf{k}} c^\dagger_{\mathbf{k}+\mathbf{q},\sigma} c_{\mathbf{k},\sigma} (a_{\mathbf{q},\nu} + a^\dagger_{-\mathbf{q},\nu}) \frac{iq_\nu}{\sqrt{2M\omega_\mathbf{q}}} \tag{14}$$

– Introduce Grassmann field $\psi_{\mathbf{q}\sigma}$ for the coherent states of the electrons $c_{\mathbf{k}\sigma}$ and complex fields $\Phi_{\mathbf{q},j}$ for phonon operators $a_{\mathbf{q},j}$, and show that the action of the electron-phonon problem has the form

$$S = \int_0^\beta d\tau \sum_{\mathbf{k},\sigma} \psi^\dagger_{\mathbf{k}\sigma} (+\partial_\tau + \varepsilon_\mathbf{k}) \psi_{\mathbf{k}\sigma} + \int_0^\beta d\tau \sum_{\mathbf{q},\nu} \Phi^\dagger_{\mathbf{q},\nu} (+\partial_\tau + \omega_\mathbf{q}) \Phi_{\mathbf{q},\nu} \tag{15}$$

$$+\gamma \int_0^\beta \sum_{\nu,\mathbf{q},\sigma,\mathbf{k}} \psi^\dagger_{\mathbf{k}+\mathbf{q},\sigma} \psi_{\mathbf{k},\sigma} (\Phi_{\mathbf{q},\nu} + \Phi^\dagger_{-\mathbf{q},\nu}) \frac{iq_\nu}{\sqrt{2M\omega_\mathbf{q}}} \tag{16}$$

– Introduce fields in Matsubara space ($\psi_{\mathbf{k}\sigma}(\tau) \to \psi_{\mathbf{k}\sigma,n}$ and $\Phi_{\mathbf{q},\nu}(\tau) \to \Phi_{\mathbf{q},\nu,m}$) to transform the action S to the diagonal form. Next, use the functional field integral technique to integrate out the phonon fields, and obtain the effective electron action of the form

$$S_{eff} = \sum_{\mathbf{k},\sigma,n} \psi^\dagger_{\mathbf{k}\sigma} (-i\omega_n + \varepsilon_\mathbf{k}) \psi_{\mathbf{k}\sigma} - \frac{\gamma^2}{2M} \sum_{\mathbf{q},m,\mathbf{k},\mathbf{k}'\sigma,\sigma'} \frac{q^2}{\omega_\mathbf{q}^2 + \Omega_m^2} \psi^\dagger_{\mathbf{k}+\mathbf{q},\sigma} \psi^\dagger_{\mathbf{k}'-\mathbf{q},\sigma'} \psi_{\mathbf{k}'\sigma'} \psi_{\mathbf{k}\sigma}. \tag{17}$$

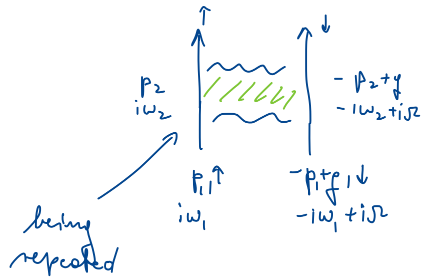
Notice that at small frequency $\Omega_m \to 0$ this interaction is attractive, which is the necessary condition for the conventional superconductivity to occur.

Explain why ions with small mass (like hydrides with Hydrogen) could achieve high-Tc with conventional superconductivity. Somewhat counterintuitive is the requirement that the phonon frequency should be large (and not small), as naively suggested by the dimensional analysis. Comment why you think high phonon frequency might still be beneficial to superconductivity?

Homework

1) Frequency summation A&S p. 185

- Cooper instability requires the following particle-particle susceptibility

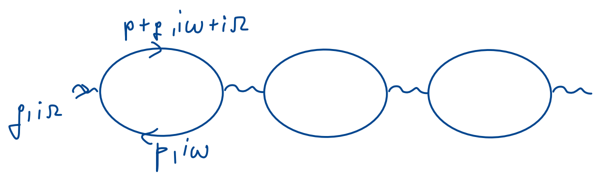


$$\chi(q, i\Omega) = -\frac{1}{\beta}\sum_{\substack{i\omega_m \\ \vec{p}}} \mathcal{G}^0(\vec{p}, i\omega_m)\,\underbrace{\mathcal{G}^0(-\vec{p}+\vec{q}, -i\omega_m}_{\text{fermionic}}+\underbrace{i\Omega}_{\text{bosonic}})$$

Use frequency summation to evaluate Matsubara sum.

Here $\mathcal{G}^0(\vec{p}, i\omega_m) = \dfrac{1}{i\omega_m - \varepsilon_p}$

- Density-density response function (dielectric function) requires the following expression (polarization)



$$\chi(q, i\Omega) = -\frac{1}{\beta}\sum_{\substack{i\omega_m \\ \vec{p}}} \mathcal{G}^0(\vec{p}, i\omega_m)\,\mathcal{G}^0(\vec{p}+\vec{q}, i\omega_m+i\Omega)$$

2) Pauli paramagnetism A&S 186

$$H = H_0 - \mu_0 \vec{B}\cdot\vec{S} = H_0[c^+c] - \mu_0 B_z \tfrac{1}{2}(\hat{n}_\uparrow - \hat{n}_\downarrow)$$

Calculate free energy $F(B)$ and show that susceptibility is:

$$\chi = \frac{\delta^2 F}{\delta B^2} \xrightarrow{T=0} \frac{\mu_0^2}{2}\rho(E_F)$$

$$\chi^s(q,i\Omega) = -\frac{1}{\beta}\sum_{p,i\omega} \mathcal{G}^0_p(i\omega_m)\,\mathcal{G}^0_{-p+q}(-i\omega_n+i\Omega)$$

$$= -\frac{1}{\beta}\sum_{p,i\omega} \frac{1}{i\omega_m-\varepsilon_p}\;\frac{1}{-i\omega_m+i\Omega-\varepsilon_{q-p}}$$

$$= -\frac{1}{\beta}\sum_{p,i\omega}\left(\frac{1}{i\omega_m-\varepsilon_p}+\frac{1}{-i\omega_m+i\Omega-\varepsilon_{q-p}}\right)\frac{1}{i\Omega-\varepsilon_{q-p}-\varepsilon_p}$$

$$= -\sum_p\left(f(\varepsilon_p)-f(-\varepsilon_{q-p}+i\Omega)\right)\frac{1}{i\Omega-\varepsilon_{q-p}-\varepsilon_p} = \sum_p \frac{-f(\varepsilon_p)+f(-\varepsilon_{q-p})}{i\Omega-\varepsilon_p-\varepsilon_{q-p}} = \sum_p \frac{1-f(\varepsilon_{q-p})-f(\varepsilon_p)}{i\Omega-\varepsilon_p-\varepsilon_{q-p}}$$

$$\chi^c(q,i\Omega) = -\frac{1}{\beta}\sum_{p,i\omega_m} \mathcal{G}^0_p(i\omega_m)\,\mathcal{G}^0_{p+q}(i\omega_m+i\Omega)$$

$$= -\frac{1}{\beta}\sum_{p,i\omega_m} \frac{1}{i\omega_m-\varepsilon_p}\;\frac{1}{i\omega_m+i\Omega-\varepsilon_{p+q}} = -\frac{1}{\beta}\sum_{p,i\omega_m}\left(\frac{1}{i\omega_m-\varepsilon_p}-\frac{1}{i\omega_m+i\Omega-\varepsilon_{p+q}}\right)\frac{1}{i\Omega+\varepsilon_p-\varepsilon_{p+q}}$$

$$= -\sum_p \frac{f(\varepsilon_p)-f(\varepsilon_{p+q})}{i\Omega+\varepsilon_p-\varepsilon_{p+q}}$$

Electron- phonon coupling

$$H_{ph} = \sum_{\vec{q}\nu} \omega_{\vec{q}\nu}\, a^+_{\vec{q}\nu}\, a_{\vec{q}\nu}$$

$$u^{\nu}_{\vec{q}\alpha j} = \frac{1}{\sqrt{N}} \sum_{\vec{R}_m} u^{\nu}_{m\alpha j}\, e^{-i\vec{q}\cdot\vec{R}_m}$$

Wickoff   x, y, z

$\vec{R}_m = m_1\vec{a}_1 + m_2\vec{a}_2 + m_3\vec{a}_3$

$\vec{q} = \frac{m_1}{N_1}\vec{b}_1 + \frac{m_2}{N_2}\vec{b}_2 + \frac{m_2}{N_3}\vec{b}_3$: 1BZ

$$u^{\nu}_{\vec{q}\alpha j} = \frac{1}{\sqrt{2M_\alpha \omega_{\vec{q}\nu}}}\, \varepsilon^{\nu}_{\alpha j}(\vec{q})\left(a_{\vec{q}\nu} + a^+_{-\vec{q}\nu}\right)$$ from $\hat{x}$ of Q.H.O

polarization
unit vector in direction of vibration

From this it follows $\boxed{u^{\nu}_{m\alpha j} = \frac{1}{\sqrt{N}} \sum_{\vec{q}} e^{i\vec{q}\cdot\vec{R}_m} \frac{1}{\sqrt{2M_\alpha \omega_{\vec{q}\nu}}}\, \varepsilon^{\nu}_{\alpha j}(\vec{q})\left(a_{\vec{q}\nu} + a^+_{-\vec{q}\nu}\right)}$

$$H_{e-i} = \int d^3r \sum_{m,\alpha} \left[V_{e-i}(\vec{r}-\vec{R}_{m\alpha}-\vec{u}_{m\alpha}) - V_{e-i}(\vec{r}-\vec{R}_{m\alpha})\right] \rho_{electron}(\vec{r})$$

$$H_{e-i} = \int d^3r \sum_{m,\alpha,j,\nu} \left(\frac{\partial V_{e-i}(\vec{r}-\vec{R}_{m\alpha})}{\partial R_{m\alpha j}}\right) u^{\nu}_{m\alpha j} \cdot \sum_{z} \psi^+_z(\vec{r})\,\psi_z(\vec{r})$$

use $\psi_z(\vec{r}) = \sum_{z,i} \psi_{z_i}(\vec{r})\, c_{z i_z}$
number   operator

$$H_{e-i} = \sum_{m,\alpha,j,\nu} \int d^3r \underbrace{\left(\frac{\partial V_{e-i}(\vec{r}-\vec{R}_{m\alpha})}{\partial R_{m\alpha j}}\right)}_{2} \underbrace{\frac{1}{\sqrt{N}}}_{5} \sum_{\vec{q}} \underbrace{e^{i\vec{q}\cdot\vec{R}_m}}_{3} \underbrace{\frac{1}{\sqrt{2M_\alpha\omega_{\vec{q}\nu}}}}_{1} \underbrace{\varepsilon^{\nu}_{\alpha j}(\vec{q})}_{6} \underbrace{\left(a_{\vec{q}\nu} + a^+_{-\vec{q}\nu}\right)}_{4} \sum_{z z_1 z_2 i_1 i_2} \underbrace{\psi^+_{z_1 i_1}(\vec{r})}_{1} \underbrace{\psi_{z_2 i_2}(\vec{r})}_{4} \underbrace{c^+_{z_1 i_1 z}}_{2} \underbrace{c_{z_2 i_2 z}}_{3}$$

$$\int d^3r\, \psi^+_{z_1 i_1}(\vec{r}) \sum_m \left(\frac{\partial V_{e-i}(\vec{r}-\vec{R}_{m\alpha})}{\partial R_{m\alpha j}}\right) e^{i\vec{q}\vec{R}_m} \psi_{z_2 i_2}(\vec{r}) = \int d^3r \sum_m e^{i(z_2-z_1)\vec{r} + i\vec{q}\vec{R}_m} u^*_{z_1 i_1}(\vec{r}) \frac{\partial V_{e-i}(\vec{r}-\vec{R}_{m\alpha})}{\partial R_{m\alpha j}} u_{z_2 i_2}(\vec{r})$$

$\psi_{z i}(\vec{r}) = u_{z i}(\vec{r})\, e^{i\vec{z}\vec{r}}$
periodic

$\vec{r} = \vec{R}_m + \vec{r}_1$ ← within one unit cell
can be split

$$\int d^3r_1 \underbrace{\sum_m e^{i(\vec{z}_2-\vec{z}_1+\vec{q})\vec{R}_m}}_{\delta(z_1 = z_2+q)} {}^{+\, i(\vec{z}_2-\vec{z}_1)\vec{r}_1}\, u^*_{z_1 i_1}(\vec{r}_1) \frac{\partial V_{ei}(\vec{r}_1-\vec{R}_{m\alpha})}{\partial R_{m\alpha j}} u_{z_2 i_2}(\vec{r}_1)$$

forces → $\delta(z_1 = z_2+q)$

$$\langle \psi_{z+q\, i_1} | \sum_m e^{i\vec{q}\cdot\vec{R}_m} \frac{\partial V_{e-i}(\vec{r}-\vec{R}_{m\alpha})}{\partial R_{m\alpha j}} | \psi_{z i_2}\rangle = \int_{1 U.C.} d^3r \underbrace{\sum_m e^{-i\vec{q}(\vec{r}-\vec{R}_m)} u^*_{z+q\, i_1}(\vec{r}) \frac{\partial V_{ei}(\vec{r}-\vec{R}_{m\alpha})}{\partial R_{m\alpha j}} u_{z i_2}(\vec{r})}$$

this function is periodic in 1U.C.
$\vec{r} \to \vec{r}+R$ and $\vec{R}_m \to \vec{R}_m + \vec{R}$

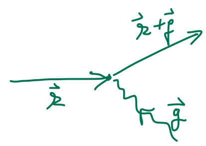
$$H_{e-i} = \sum_{\substack{\alpha\nu \\ \vec{q}\,\sigma k_1 k_2 i_1 i_2}} \frac{1}{\sqrt{2M_\alpha \omega_{q\nu}}}\, c^+_{k+q, i_1 \sigma}\, c_{k i_2 \sigma} \left(a_{q\nu} + a^+_{-q\nu}\right) \underbrace{\frac{1}{\sqrt{N}} \sum_j \varepsilon^\nu_{\alpha j}(\vec q) \langle \psi_{k+q\, i_1} | \sum_m e^{i\vec q\cdot \vec R_m} \frac{\partial V_{e-i}(\vec r - \vec R_{m\alpha})}{\partial R_{m\alpha j}} | \psi_{k i_2}\rangle}_{g^{\vec k,\vec q}_{i_1 i_2 \alpha\nu}}$$

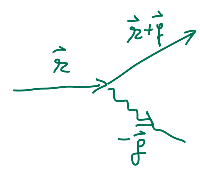
$$H_{e-i} = \sum_{\substack{\alpha\nu \\ \vec{q}\,\sigma k_1 k_2 i_1 i_2}} \frac{1}{\sqrt{2M_\alpha \omega_{q\nu}}}\, c^+_{k+q, i_1 \sigma}\, c_{k i_2 \sigma} \left(a_{q\nu} + a^+_{-q\nu}\right) g^{\vec k,\vec q}_{i_1 i_2 \alpha\nu}$$

Simplifications: $$H_{e-i} = \sum_{\nu\, k, \vec q, \sigma} \frac{i q_\nu N}{\sqrt{2M\omega_q}}\, c^+_{k+q\sigma} c_{k\sigma} \left(a_{q\nu} + a^+_{-q\nu}\right)$$

Note $N \propto \frac{1}{\sqrt{N}}$

check





$$Z = \int \mathcal{D}[\psi^+,\psi]\,\mathcal{D}(\phi^+\phi)\, e^{-S[\psi,\phi]}$$

$$S[\psi,\phi] = \int_0^\beta d\tau \sum_{\vec q j} \phi^+_{qj}\left(+\frac{\partial}{\partial\tau} + \omega_{qj}\right)\phi_{qj} + \int_0^\beta d\tau \sum_{k\sigma} \psi^+_{k\sigma}\left(+\frac{\partial}{\partial \tau} + \varepsilon_k\right)\psi_{k\sigma} + \int_0^\beta d\tau \sum_{\vec k \vec q j \sigma} \frac{N i q_j}{\sqrt{2M\omega_q}}\, \psi^+_{k+q}\psi_k \left(\phi_{qj} + \phi^+_{-qj}\right)$$

F.T.: $$\phi_{qj}(\tau) = \frac{1}{\sqrt\beta}\sum_m \phi_{qjm}\, e^{-i\Omega_m \tau}$$
$$\psi_{qj}(\tau) = \frac{1}{\sqrt\beta}\sum_m \psi_{qjm}\, e^{-i\omega_m \tau}$$

$$S[\psi,\phi] = \sum_{\vec q j m} \phi^+_{qjm}(-i\Omega_m + \omega_{qj})\phi_{qjm} + \sum_{k\sigma m} \psi^+_{k\sigma m}(-i\omega_m + \varepsilon_k)\psi_{k\sigma m} + \sum_{\substack{kqj\sigma \\ mn}} \frac{N i q_j}{\sqrt{2M\omega_q}} \frac{1}{\sqrt\beta}\, \psi^+_{k+q\, m+n}\psi_{kn}\left(\phi_{qjm} + \phi^+_{-qj-m}\right)$$

Integrate out bosons: $(\omega_q - i\Omega_m) = A_{qjm}\, I$; $M_{qm} \equiv \sum_{k,n} \psi^+_{k+q, m+n}\psi_{kn}$

$r_{qj} = \frac{i q_j N}{\sqrt{2M\omega_q \beta}}$

$$\prod_{qjm}\int d(\phi^+_{qjm},\phi_{qjm})\, e^{-\phi^+_{qjm}(\omega_{qj} - i\Omega_m)\phi_{qjm} - \phi^+_{-qj-m}\underbrace{M_{-q-m} r_{-qj}}_{w} - \phi_{qjm}\underbrace{\hat M_{qm} r_{qj}}_{w^+}}$$

$$\prod_{qjm}\left[\frac{1}{(\omega_{qj} - i\Omega_m)}\cdot e^{M_{qjm} r_{qj} \frac{1}{\omega_{qj} - i\Omega_m} r_{qj} M_{-q-m}}\right] = \prod_{qjm}\frac{1}{(\omega_{qj}-i\Omega_m)}\, e^{\sum_{qjm}\frac{r_{qj} r_{-qj}}{\omega_{qj} - i\Omega_m}\hat M_{-q-m}\hat M_{qm}}$$

$$\boxed{\text{remind: } \int d(\phi^+,\phi)\, e^{-\vec\phi^+ A\vec\phi + \vec w^+\vec\phi + \vec\phi^+\vec w'} = \frac{1}{\mathrm{Det}(A)}\, e^{\vec w^+ A^{-1}\vec w'}}$$

$$Z = \left[\prod_{qjm}\frac{1}{(\omega_{qj} - i\Omega_m)}\right]\int \mathcal{D}[\psi^+\psi]\, e^{-S_{el} + \sum_{qjm}\frac{r_{qj} r_{-qj}}{\omega_{qj} - i\Omega_m}\hat M_{-q-m}\hat M_{qm}}$$

$$S_{eff.}[\psi^+,\psi] = \sum_{k\sigma m}\psi^+_{k\sigma m}(-i\omega_m + \varepsilon_k)\psi_{k\sigma m} - \frac{1}{\beta}\sum_{kqm}\frac{N^2 \sum_j q_j^2}{2M\omega_q\, (\omega_q - i\Omega_m)}\, \psi^+_{k+q, m+n}\psi_{kn}\psi^+_{k'-q, m'-m}\psi_{k'm'}$$

symmetric with respect to $\Omega_m \to -\Omega_m$

$$S_{eff.}[\psi^+,\psi] = \sum_{k2} \psi^+_{k2}(-i\omega_n + \varepsilon_k)\psi_{k2} - \sum_{q m} \frac{\lambda^2 \sum_j g_j^2}{2M\omega_q \underbrace{(\omega_q - i\Omega_m)}} \hat{n}_{q m}\hat{n}_{-q,-m}$$

$$\frac{1}{2}\left(\frac{1}{\omega_q - i\Omega_m} + \frac{1}{\omega_q + i\Omega_m}\right) = \frac{\omega_q}{\omega_q^2 + \Omega_m^2}$$

because of longitudinal choice

$$S_{eff.}[\psi^+,\psi] = \sum_{k2} \psi^+_{k2}(-i\omega_n + \varepsilon_k)\psi_{k2} - \sum_{q m} \frac{\lambda^2}{2M} \frac{g^2}{\omega_q^2 + \Omega_m^2} \hat{n}_{q m}\hat{n}_{-q,-m}$$

small M better, because interaction stronger

real axis: $\frac{g^2}{\omega_q^2 - \Omega^2}$ $\Rightarrow$ negative up to ω_q

hence large ω_q better

On real axis $\quad \frac{1}{\omega_q^2 - (i\Omega_m)^2} \to \frac{1}{\omega_q^2 - \Omega^2}$ hence sign change at $\Omega \approx \omega_q$.

Perturbation theory (5 and 7 in A&S)

stopped 10/27/2022

- Existed before functional field integral
- Well covered in Mahan's book, which does not use functional integrals

We write $S = S_0 + \Delta S$

S_0: here quadratic (can be developed for any solvable S_0, but Feynman diagrams are way more complicated then)

ΔS: any type of interaction typically $\chi^+\chi^+\psi\psi$ but it may also contain $\chi^+\psi$ or $\chi^+\psi(\phi+\phi^+)$ ...

Chpt 7 in A&S

To proceed we need to introduce the lowest possible correlation function, i.e., the single particle Green's function

physical observable $\quad G^{\text{retarded}}_{ij}(t-t') = -i\Theta(t-t')\langle [a_i(t), a^+_j(t')]_{-\xi}\rangle$ $\quad$ + for fermions, − for bosons

t is here real time

ij can be momentum + spin $(\vec{p}, s)$ or position and spin $(\vec{r}, s)$

imaginary time $\tau = it$ $\quad G_{ij}(\tau-\tau') = -\langle T_\tau\, a_i(\tau)\, a^+_j(\tau')\rangle$ $\quad$ in imaginary time T_τ replaces commutator.

But what is $a_i(t)$? We are used to fields being t-dependent. What about operators?

It is defined in Heissenberg representation.

Schroedinger representation: $i\frac{\partial}{\partial t}|\psi\rangle = H|\psi\rangle \Rightarrow |\psi(t)\rangle = e^{-iHt}\Theta(t)\,|\psi(0)\rangle$ (real time)

Heissenberg representation: $|\psi\rangle$ is not time dependent, but operators are.

Operators evolve as: $\boxed{O(t) = e^{iHt}\,O\,e^{-iHt}}$

hence $\boxed{\frac{\partial O(t)}{\partial t} = e^{iHt}\, i[H,O]\, e^{-iHt} = i[H, O(t)]}$

The two representation are equivalent, because they give the same physical response function:

Schroedinger: $\underbrace{\langle\psi_1(t)|\,O\,|\psi_2(t)\rangle}_{\langle\psi_1(0)|e^{iHt}Oe^{-iHt}|\psi_2(0)\rangle}$

Heissenberg: $\langle\psi_1|e^{iHt}\,O\,e^{-iHt}|\psi_2\rangle$, with $\langle\psi_1| = \langle\psi_1(0)|$ and $|\psi_2\rangle = |\psi_2(0)\rangle$

There is a third representation, interaction (Dirac) representation:

$$|\psi_I(t)\rangle \equiv e^{iH_0 t}\,|\psi_s(t)\rangle = e^{iH_0 t}\,e^{-iHt}\,Q(t)\,|\psi(0)\rangle$$

$$O_I(t) \equiv e^{iH_0 t}\,O\,e^{-iH_0 t}$$

hence both $|\psi_I(t)\rangle$ and $O_I(t)$ are time dependent, but O_I has trivial time dependence.

It also gives the same observabels:

$$\langle\psi_I(t)|\,O_I(t)\,|\psi_I(t)\rangle = \langle\psi_s(t)|\,\underbrace{e^{-iH_0 t}\,e^{iH_0 t}}_{=1}\,O\,\underbrace{e^{-iH_0 t}\,e^{iH_0 t}}_{=1}\,|\psi_s(t)\rangle$$

We will not use this representation.

Heisenberg representation is most useful for us, because it is easy to translate to functional integral: $Q(t) \leftrightarrow \psi(t)$.

How are quantities calculated in Heisenberg representation?

$Z = \mathrm{Tr}(e^{-\beta H})$ Here $\boxed{H}$ might be $\boxed{\hat{H} - \mu\hat{N}}$ for grand potential

We introduce $H(\tau) = \sum_{ij} h_{ij}\, Q_i^{+}\cancel{(\tau)}\, Q_j\cancel{(\tau)} + \sum_{ijkl} V_{ijkl}\, Q_i^{+}\cancel{(\tau)}\, Q_j^{+}\cancel{(\tau)}\, Q_k\cancel{(\tau)}\, Q_l\cancel{(\tau)} - \sum_i \underline{j_i^{+}(\tau)}\, Q_i\cancel{(\tau)} + Q_i^{+}\cancel{(\tau)}\, \underline{j_i(\tau)}$

here H does not need $H(\tau)$ because $H(\tau) = e^{H\tau}\, H(0)\, e^{-H\tau} = H(0)$

$$\boxed{Z = \mathrm{Tr}\left(T_\tau\, e^{-\int_0^\beta d\tau\, H(\tau)}\right)}$$

If $H(\tau) = H(0)$ this is the same as $\mathrm{Tr}(e^{-\beta H})$

(If H is t-independent, we did not do anything because $\int_0^\beta d\tau\, H(\tau) = \beta H$

But this formula is valid even for time dependent H with source fields $j^{+}Q + Q^{+}j$

Define time ordering operator: $T_\tau\, Q_1(\tau_1)\, Q_2(\tau_2) = \begin{cases} \tau_1 \geq \tau_2: & Q_1(\tau_1)\, Q_2(\tau_2) \\ \tau_1 < \tau_2: & \xi\, Q_2(\tau_2)\, Q(\tau_1) \end{cases}$

always orders all operators in time

For example the correlation functions in imaginary time are derived by

$$\boxed{G_{i_1 i_2}(\tau_1-\tau_2) = -\frac{\partial^2 \ln Z}{\partial j_{i_2}(\tau_2)\, \partial j^+_{i_1}(\tau_1)}\Bigg|_{j=0}} = -\frac{1}{Z}\frac{\partial^2}{\partial j_{i_2}(\tau_2)\, \partial j^+_{i_1}(\tau_1)} \mathrm{Tr}\left(T_\tau\, e^{-\int_0^\beta d\tau \left(H - \sum_\ell j^+_\ell(\tau) Q_\ell(\tau) + Q^+_\ell(\tau) j_\ell(\tau)\right)}\right)\Bigg|_{j=0}$$

$$= -\frac{1}{Z}\mathrm{Tr}\left(T_\tau\, e^{-\int_0^\beta d\tau H} Q_{i_1}(\tau_1)\, Q^+_{i_2}(\tau_2)\right)$$

$$\equiv -\langle T_\tau\, Q_{i_1}(\tau_1)\, Q^+_{i_2}(\tau_2)\rangle$$

Why do we need time ordering?

assume $\tau_1 > \tau_2$

$$G_{i_1 i_2}(\tau_1-\tau_2) = -\langle T_\tau\, Q_{i_1}(\tau_1)\, Q^+_{i_2}(\tau_2)\rangle = -\frac{1}{Z}\mathrm{Tr}\left(e^{-\beta H} e^{H\tau_1} Q_{i_1} e^{-H\tau_1} e^{H\tau_2} Q^+_{i_2} e^{-H\tau_2}\right)$$

Definition of Heisenberg operators

H here is t-independent

$$= -\frac{1}{Z}\mathrm{Tr}\left(e^{-\int_{\tau_1}^{\beta} H d\tau} Q_{i_1}\, e^{-\int_{\tau_2}^{\tau_1} H d\tau} Q^+_{i_2}\, e^{-\int_0^{\tau_2} H d\tau}\right)$$

$$\equiv -\frac{1}{Z}\mathrm{Tr}\left(T_\tau\, e^{-\int_0^\beta H d\tau} Q_{i_1}(\tau_1)\, Q^+_{i_2}(\tau_2)\right)$$

$$\boxed{\chi_{i_1 i_2 i_3 i_4}(\tau_1-\tau_2) = \frac{\partial^4 \ln Z}{\partial j^+_{i_4}(\tau_2)\, \partial j_{i_3}(\tau_2)\, \partial j^+_{i_2}(\tau_1)\, \partial j_{i_1}(\tau_1)}\Bigg|_{j=0}}$$

$$\chi_{i_1 i_2 i_3 i_4}(\tau_1-\tau_2) = \frac{\partial^4 \ln \mathrm{Tr}\left(e^{-\int_0^\tau d\tau \left[H - \sum_i j^+_i(\tau) Q_i(\tau) + Q^+_i(\tau) j_i(\tau)\right]}\right)}{\partial j^+_{i_4}(\tau_2)\, \partial j_{i_3}(\tau_2)\, \partial j^+_{i_2}(\tau_1)\, \partial j_{i_1}(\tau_1)}\Bigg|_{j=0}$$

$$\chi_{i_1 i_2 i_3 i_4}(\tau_1-\tau_2) = \langle T_\tau\, Q^+_{i_1}(\tau_1) Q_{i_2}(\tau_1) Q^+_{i_3}(\tau_2) Q_{i_4}(\tau_2)\rangle - \langle T_\tau Q^+_{i_1} Q_{i_2}\rangle\langle T_\tau Q^+_{i_3} Q_{i_4}\rangle$$
$$- \langle T_\tau Q^+_{i_1}(\tau_1) Q_{i_4}(\tau_2)\rangle\langle T_\tau Q_{i_2}(\tau_1) Q^+_{i_3}(\tau_2)\rangle$$

We will use this knowledge to derive the same correlation functions in functional field integral representation.

Stopped 11/3/2022

$$\boxed{G_{i_1 i_2}(\tau_1-\tau_2) = -\frac{\partial^2 \ln Z}{\partial j_{i_2}(\tau_2)\,\partial j^+_{i_1}(\tau_1)}\Bigg|_{j=0}} = -\frac{1}{Z}\frac{\partial^2}{\partial j_{i_2}(\tau_2)\,\partial j^+_{i_1}(\tau_1)}\mathrm{Tr}\left(T_\tau\, e^{-\int_0^\beta d\tau\left(H-\sum_\ell j^+_\ell(\tau)Q_\ell(\tau)+Q^+_\ell(\tau)j_\ell(\tau)\right)}\right)\Bigg|_{j=0}$$

$$+\underbrace{\frac{1}{Z}\frac{\partial Z}{\partial j_{i_2}(\tau_2)}\frac{1}{Z}\frac{\partial Z}{\partial j^+_{i_1}(\tau_1)}}_{\langle Q^+_{i_2}\rangle\langle Q_{i_1}\rangle}\Bigg|_{j=0}$$

vanishes

here $\frac{1}{Z}\frac{\partial Z}{\partial j_{i_2}(\tau_2)} = \langle Q^+_{i_2}\rangle$

$$= -\langle T_\tau Q_{i_1}(\tau_1)\, Q^+_{i_2}(\tau_2)\rangle$$

$$\chi_{i_1 i_2 i_3 i_4}(\tau_1-\tau_2) = \frac{\partial^4 \ln \mathrm{Tr}\left(e^{-\int_0^\tau d\tau\left[H-\sum_i j^+_i(\tau)Q_i(\tau)+Q^+_i(\tau)j_i(\tau)\right]}\right)}{\partial j^+_{i_4}(\tau_2)\,\partial j_{i_3}(\tau_2)\,\partial j^+_{i_2}(\tau_1)\,\partial j_{i_1}(\tau_1)}\Bigg|_{j=0}$$

$$= \langle Q^+_{i_1}(\tau_1)Q_{i_2}(\tau_1)Q^+_{i_3}(\tau_2)Q_{i_4}(\tau_2)\rangle - \langle Q^+_{i_1}(\tau_1)Q_{i_2}(\tau_1)\rangle\langle Q^+_{i_3}(\tau_2)Q_{i_4}(\tau_2)\rangle$$

$$-\langle Q^+_{i_1}(\tau_1)Q_{i_4}(\tau_2)\rangle\,\underbrace{\langle Q_{i_2}(\tau_1)Q^+_{i_3}(\tau_2)\rangle}_{=(-1)\langle Q^+_{i_3}(\tau_2)Q_{i_2}(\tau_1)\rangle}$$

connected correlation function

$$= \langle Q^+_{i_1}(\tau_1)Q_{i_2}(\tau_1)Q^+_{i_3}(\tau_2)Q_{i_4}(\tau_2)\rangle - G_{i_2 i_1}(0^-)\,G_{i_4 i_3}(0^-) + G_{i_1 i_4}(\tau_2-\tau_1)\,G_{i_2 i_3}(\tau_1-\tau_2)$$

Back to Functional Integral and correlation functions

(AGS page 379 just argues that since equal time correlation functions $\langle O \rangle$ can be obtained by derivative, the time dependent should work also. We will prove it)

In Heisenberg representation

$$G_{i_1 i_2}(\tau_1-\tau_2) = -\left.\frac{\partial^2 \ln Z}{\partial j_{i_2}(\tau_2)\, j^+_{i_1}(\tau_1)}\right|_{j=0} = \qquad \text{with } H \to H_0 - \sum_i j_i^+(\tau)\, Q_i(\tau) + Q_i^+(\tau)\, j_i(\tau)$$

Crucial point: To get Functional Integral for Z we replace $Q_i(\tau) \to \psi_i(\tau)$ and use

$$S = \int_0^\beta \Big(\sum_i \psi_i^+ \big(\tfrac{\partial}{\partial\tau} - \mu\big)\psi_i - H[\psi]\Big)\, d\tau$$

$$G_{i_1 i_2}(\tau_1-\tau_2) = -\left.\frac{\partial^2}{\partial j_{i_2}(\tau_2)\, j^+_{i_1}(\tau_1)}\right|_{j=0} \ln \int D[\psi^+\psi]\, e^{-\int_0^\beta d\tau \left(\sum_i \psi_i^+(\tau)\left(\frac{\partial}{\partial\tau}-\mu\right)\psi_i(\tau) + H_0 - \sum_i j_i^+(\tau)\psi_i(\tau) + \psi_i^+(\tau) j_i(\tau)\right)}$$

$$= -\underbrace{\frac{\int D[\psi^+,\psi]\, e^{-S}\, \psi_{i_1}(\tau_1)\, \psi^+_{i_2}(\tau_2)}{\int D[\psi^+,\psi]\, e^{-S}}}_{\text{In functional field integral}} \equiv -\langle \psi_{i_1}(\tau_1)\, \psi^+_{i_2}(\tau_2)\rangle = -\underbrace{\langle T_\tau\, Q_{i_1}(\tau_1)\, Q^+_{i_2}(\tau_2)\rangle}_{\text{we derived before in Heisenberg picture}}$$

In functional field integral we do not need explicit time ordering because functional integral is time ordered

no need for T_τ!

here $\langle O \rangle = \dfrac{\int D[\psi^+\psi]\, e^{-S}\, O}{\int D[\psi^+\psi]\, e^{-S}}$

It is generally true:

$$\langle T_\tau Q_{i_1}(\tau_1)\, Q^+_{i_2}(\tau_2)\, Q_{i_3}(\tau_3)\, Q^+_{i_4}(\tau_4)\rangle = \frac{1}{Z}\int D[\psi^+,\psi]\, e^{-S}\, \psi_{i_1}(\tau_1)\, \psi^+_{i_2}(\tau_2)\, \psi_{i_3}(\tau_3)\, \psi^+_{i_4}(\tau_4)$$

any time dependent average of operators

replace operators with corresponding fields

Back to $\boxed{\text{Green's function:}}$ (in Heissenberg representation)

Real time physical green's function

$$\boxed{G^{retarded}_{pp'}(t-t') = -i\Theta(t-t')\langle [a_p(t), a^+_{p'}(t')]_{-\varsigma}\rangle}$$

We will use Lehman representation to establish connection between retarded (physical) G.F. and imaginary time G.F.

$$G^{retarded}_{pp'}(t-t') = -i\Theta(t-t')\frac{1}{Z}\sum_n \langle n|e^{-\beta H}\left[e^{iHt} a_p e^{-iH(t-t')} a^+_{p'} e^{-iHt'} - \varsigma e^{iHt'} a^+_{p'} e^{-iH(t'-t)} a_p e^{-iHt}\right]|n\rangle$$

complete set of many body states

$\sum_m |m\rangle\langle m|$ $\qquad$ $\sum_m |m\rangle\langle m|$

$$= -i\Theta(t-t')\frac{1}{Z}\sum_{n,m}\Big[e^{-\beta E_n + i(E_n - E_m)(t-t')} \underbrace{-\varsigma e^{-\beta E_m + i(E_n-E_m)(t-t')}}_{\text{switch } n\leftrightarrow m}\Big]\langle n|a_p|m\rangle\langle m|a^+_{p'}|n\rangle$$

$$= -i\Theta(t-t')\frac{1}{Z}\sum_{n,m}\left(e^{-\beta E_n} - \varsigma e^{-\beta E_m}\right) e^{i(E_n - E_m)(t-t')}\langle n|a_p|m\rangle\langle m|a^+_{p'}|n\rangle$$

In Real frequency $\quad G^{retarded}_{pp'}(\omega) = \int_{-\infty}^{\infty} d(t-t')\, e^{i\omega(t-t')} G^{ret}_{pp'}(t-t')$

$$G^{ret}_{pp'}(\omega) = -i\frac{1}{Z}\sum_{n,m}\left(e^{-\beta E_n} - \varsigma e^{-\beta E_m}\right)\langle n|a_p|m\rangle\langle m|a^+_{p'}|n\rangle \underbrace{\int_0^\infty e^{i(\omega + E_n - E_m)\Delta t - \delta\Delta t}\, d\Delta t}_{\frac{0-1}{i(\omega + E_n - E_m + i\delta)}}$$

has to be $-\delta\Delta t$ to converge!

$$\boxed{G^{ret}_{pp'}(\omega) = \frac{1}{Z}\sum_{n,m}\frac{\left(e^{-\beta E_n} - \varsigma e^{-\beta E_m}\right)}{(\omega + E_n - E_m + i\delta)}\langle n|a_p|m\rangle\langle m|a^+_{p'}|n\rangle}$$

Lehman representation

+ retarded
− advanced

Example $p = p' = \vec{k}$ momentum and fermions:

$$G^{ret}_{k}(\omega) = \frac{1}{Z}\sum_{nm} \frac{e^{-\beta E_n} + e^{-\beta E_m}}{\omega + E_n - E_m + i\delta} |\langle n | O_k | m \rangle|^2$$

Spectral function $\boxed{A_k(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\, G^{ret}_k(\omega)}$ measured in ARPES

more generally $A_{pp'}(\omega) = \frac{1}{2\pi i}\left[G_{pp'}(\omega+i\delta) - \overset{G^{+}(\omega+i\delta)}{\overset{\shortparallel}{G_{p'p}}}(\omega - i\delta)\right]$ positive definite matrix

We know $\frac{1}{\omega - \Omega + i\delta} = P\frac{1}{\omega-\Omega} - i\pi\delta(\omega-\Omega)$ if $\Omega \in \mathbb{R}$

$\frac{1}{\omega - \Omega - i\delta} = P\frac{1}{\omega-\Omega} + i\pi\delta(\omega-\Omega)$

$$\boxed{A_k(\omega) = \sum_{nm} \frac{\left(e^{-\beta E_n} + e^{-\beta E_m}\right)}{Z} |\langle n|O_k|m\rangle|^2 \delta(\omega + E_n - E_m) \geq 0}$$

$$\boxed{\int A_k(\omega)\, d\omega =} \sum_{nm} \frac{\left(e^{-\beta E_n} + e^{-\beta E_m}\right)}{Z} |\langle n|O_k|m\rangle|^2 = \frac{1}{Z}\sum_{nm} \langle n| e^{-\beta E_n} O_k |m\rangle\langle m| O_k^{+} |n\rangle + \langle n| O_k |m\rangle\langle m| e^{-\beta E_m} O_k^{+} |n\rangle$$

$$= \sum_n \frac{1}{Z} \mathrm{Tr}\left(e^{-\beta H}\underbrace{(O_k O_k^{+} + O_k^{+} O_k)}_{=1}\right) = \boxed{1}$$

$$\boxed{G^{ret}_k(\omega) = \int \frac{A_k(x)\, dx}{\omega - x + i\delta} \quad \text{Kramers-Kronig relation } \checkmark}$$

proof:

$$\int \frac{A_k(x)\,dx}{\omega - x + i\delta} = \int dx \frac{1}{\omega - x + i\delta} \sum_{nm} \frac{\left(e^{-\beta E_n} + e^{-\beta E_m}\right)}{Z} |\langle n|O_k|m\rangle|^2 \delta(x + E_n - E_m)$$

$$= \sum_{nm} \frac{\left(e^{-\beta E_n} + e^{-\beta E_m}\right)}{Z} |\langle n|O_k|m\rangle|^2 \frac{1}{\omega - E_m + E_n + i\delta} \quad \checkmark$$

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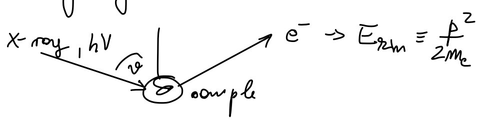
stopped 11/3/2022

$A_k(\omega)$ is measured directly by ARPES:



$\frac{p^2}{2m_e} = E_{kin} = h\nu - \phi - \varepsilon_k$

outgoing free electron; energy of photon; work function; binding energy of electron

$h\nu$ ~ 6eV ... 200eV

$\phi \sim 4eV$ work function

ε_k we want to determine

$k_\parallel$ crystal momentum to be determined

Momentum of photon is negligible hence:

$p_\parallel = k_\parallel$

$\sqrt{2m_e \underset{\text{measure}}{E_{kin}}}\,\sin\vartheta = \underset{\text{get}}{k_\parallel}$ → get ε_k

Want $\varepsilon_k(k)$

$$\frac{1}{\omega - \Omega + i\delta} = P\frac{1}{\omega - \Omega} - i\pi\,\delta(\omega - \Omega)$$

$$\int_{-\infty}^{\infty}\frac{d\omega}{\omega-\Omega+i\delta} = P\int_{-\infty}^{\infty}\frac{d\omega}{\omega-\Omega} - i\pi$$

$$\|$$

$$\lim_{\varepsilon\to 0}\underbrace{\int_{-\infty}^{\Omega-\varepsilon}\frac{d\omega}{\omega-\Omega+i\delta} + \int_{\Omega+\varepsilon}^{\infty}\frac{d\omega}{\omega-\Omega+i\delta}}_{\displaystyle \| \; P\int\frac{d\omega}{\omega-\Omega+i\delta}} + \underbrace{\int_{-\varepsilon}^{\varepsilon}\frac{dx}{x+i\delta}}_{\displaystyle \ln(\varepsilon+i\delta)-\ln(-\varepsilon+i\delta) = -i\pi}$$

Non-interacting system

$$\langle n | c_k | m \rangle$$

$$\quad E_n \qquad\qquad E_m$$

$$\boxed{A_k(\omega) = \sum_{nm} \frac{\left(e^{-\beta E_n} + e^{-\beta E_m}\right)}{Z} |\langle n | c_k | m\rangle|^2 \delta(\omega + E_n - E_m)}$$

$$E_n = E_m - \varepsilon_k \Rightarrow E_m - E_n = \varepsilon_k$$

$$A_k(\omega) = \underbrace{\sum_{nm} \frac{\left(e^{-\beta E_n} + e^{-\beta E_m}\right)}{Z} |\langle n | c_k | m\rangle|^2}_{\text{like } \int A_k(\omega)\, d\omega = 1} \delta(\omega - \varepsilon_k)$$

$$= \delta(\omega - \varepsilon_k) \cdot 1$$

Then: $G^{ret}_k(\omega) = \dfrac{1}{\omega - \varepsilon_k + i\delta}$ from K.K. $G^{ret}_k(\omega) = \displaystyle\int \frac{A_k(x)\, dx}{\omega - x + i\delta}$

Interacting system

$$|\Omega\rangle = \underbrace{c_k^{+} |n\rangle}$$

Not eigenstate $|m\rangle$ ⇒ after some time we have a superposition of eigenstates

$$\underbrace{\langle n | c_k(t)}_{\langle \Omega(t)|} \underbrace{c_k^{+}(0) | n\rangle}_{|\Omega(0)\rangle} \sim e^{-\frac{t}{\tau}} \Rightarrow G \sim \frac{1}{\omega + i/\tau}$$

↑ overlap decays wit time

↖ self energy

In the Fermi liquid picture:

$$G_k(\omega) = \frac{Z_k}{\omega + \mu - \frac{k^2}{2m^*} + i\delta} + G_k^{incoh}(\omega) \sim \frac{Z_k}{\omega + \mu - \varepsilon_k \frac{m}{m^*} + i\delta} + G_k^{incoh}(\omega)$$

$$A_k(\omega) = Z_k\, \delta\left(\omega + \mu - \varepsilon_k \frac{m}{m^*}\right) + A_k^{incoh}(\omega)$$

↑ quasiparticle renormalization amplitude

Imaginary time Green's function $\tau = it$

It is easier to manipulate and calculate. To get real time response use Wick's rotation $G_{\tau}(i\omega) \to G_{\tau}(\omega + i\delta)$

$$G_{i_1 i_2}(\tau_1 - \tau_2) = -\left.\frac{\partial^2 \ln Z}{\partial j_{i_2}(\tau_2)\, j^{+}_{i_1}(\tau_1)}\right|_{j=0} \equiv -\langle T_\tau\, Q_{i_1}(\tau_1)\, Q^{+}_{i_2}(\tau_2)\rangle$$

no commutator instead time ordering

$$-\langle T_\tau\, Q_{i_1}(\tau_1 - \tau_2)\, Q^{+}_{i_2}(0)\rangle$$

Is equivalent to $G_{i_1 i_2}(\tau) = -\Theta(\tau)\langle Q_{i_1}(\tau) Q^{+}_{i_2}(0)\rangle - \varsigma\, \Theta(-\tau)\langle Q^{+}_{i_2}(0)\, Q_{i_1}(\tau)\rangle$

We use Lehman representation to establish relationship between $G_{i_1 i_2}(\tau)$ and $G^{ret}_{i_1 i_2}(t)$

$$\boxed{G_{pp'}(\tau) = -\langle T_\tau\, O_p(\tau)\, O_{p'}(0)\rangle}$$ hence

$$G_{pp'}(\tau) = -\Theta(\tau)\frac{1}{Z}\sum_m \langle m| e^{-\beta H} e^{H\tau} O_p \underset{I}{\uparrow} e^{-H\tau} O_{p'}^{+}|m\rangle$$
$$-\zeta\,\Theta(-\tau)\frac{1}{Z}\sum_m \langle m| e^{-\beta H} O_{p'}^{+} \underset{I}{\uparrow} e^{H\tau} O_p\, e^{-H\tau}|m\rangle$$

$$G_{pp'}(\tau) = -\Theta(\tau)\frac{1}{Z}\sum_{m,m}\langle m|O_p|m\rangle\langle m|O_{p'}^{+}|m\rangle\, e^{-\beta E_m + (E_m - E_m)\tau}$$
$$-\zeta\,\Theta(-\tau)\frac{1}{Z}\sum_{m,m}\langle m|O_{p'}^{+}|m\rangle\langle m|O_p|m\rangle\, e^{-\beta E_m + (E_m - E_m)\tau}$$

$$G_{pp'}(i\omega_m) = \int_0^\beta e^{i\omega_m\tau} G_{pp'}(\tau)\, d\tau \quad \text{and} \quad G_{pp'}(\tau) = \frac{1}{\beta}\sum_{i\omega_m} e^{-i\omega_m\tau} G_{pp'}(i\omega_m)$$

Matsubara frequencies, because we know it must satisfy (anti)periodicity.

$$G_{pp'}(i\omega_z) = -\frac{1}{Z}\sum_{m,m}\langle m|O_p|m\rangle\langle m|O_{p'}^{+}|m\rangle \int_0^\beta e^{(E_m - E_m)\tau + i\omega_z\tau}\left(e^{-\beta E_m}\Theta(\tau) + \zeta\, \underline{e^{-\beta E_m}\Theta(-\tau)}\right)d\tau$$

does not contribute

$$\underbrace{\frac{e^{\beta(i\omega_z + E_m - E_m)} - 1}{i\omega_z + E_m - E_m}\, e^{-\beta E_m}}_{\dfrac{\zeta e^{-\beta E_m} - e^{-\beta E_m}}{i\omega_z + E_m - E_m}}$$

$$e^{\beta i\omega_z} = \zeta = \begin{cases} -1 & \text{fermions} \\ +1 & \text{bosons}\end{cases}$$

$$\boxed{G_{pp'}(i\omega_z) = \frac{1}{Z}\sum_{m,m}\langle m|O_p|m\rangle\langle m|O_{p'}^{+}|m\rangle\, \frac{e^{-\beta E_m} - \zeta e^{-\beta E_m}}{i\omega_z + E_m - E_m}}$$

compare with

$$\boxed{G^{ret}_{pp'}(\omega) = \frac{1}{Z}\sum_{m,m}\frac{\left(e^{-\beta E_m} - \zeta e^{-\beta E_m}\right)}{(\omega + E_m - E_m + i\delta)}\langle m|O_p|m\rangle\langle m|O_{p'}^{+}|m\rangle}$$

only need to replace $G_z(i\omega) \to G_z(\omega + i\delta)$

This is not entirely trivial when $G_z(i\omega_m)$

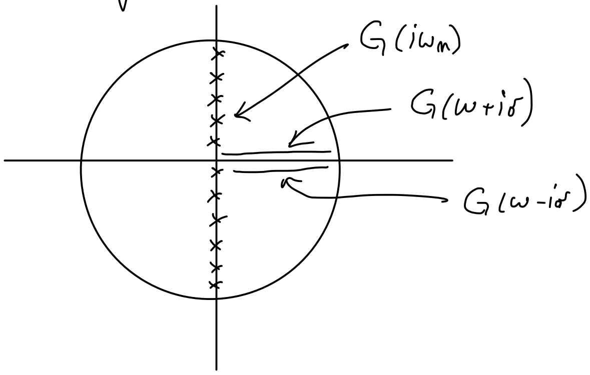
- is known with finite precision (Pade, maxent)
- is known analytically but not in an analytic form

example: $$\frac{e^{\beta i\omega_m}}{i\omega_m - \varepsilon_z} \neq \frac{e^{\beta(\omega + i\delta)}}{\omega - \varepsilon_z + i\delta} \quad \text{at } \omega \to \infty \text{ diverges, hence non-analytic}$$

$$\parallel$$

$$\frac{\zeta}{i\omega_m - \varepsilon_z} = \frac{\zeta}{\omega - \varepsilon_z + i\delta} \quad \text{is analytic} \checkmark$$

Generalize the Green's function into entire complex plane



$$G(z) = \int \frac{A(x)}{z - x + i\delta}\, dx \quad \text{where} \quad A(x) = -\frac{1}{2\pi i}\left[G(x+i\delta) - G^{+}(x-i\delta)\right]$$

What can be computed from the Green's function?

1) partial / total density $G_p(\tau \to 0^-) = \langle c_p^{+} c_p \rangle = n_p$ here $p = (\vec{p}, s)$ (momentum, spin)

2) kinetic energy $T = \langle \sum_p \varepsilon_p c_p^{+} c_p \rangle = \sum_p \varepsilon_p G_p(\tau \to 0^-)$

3) current density : $\vec{j} = \frac{i}{2m}\left[(\vec{\nabla} a^{+}(\vec{r}, \tau))\, a(\vec{r}, \tau) - a^{+}(\vec{r}, \tau)(\nabla a(\vec{r}, \tau)) \right]$

$$\vec{j} = \frac{i}{2m} \lim_{\vec{r} \to \vec{r}\,'} \left(\vec{\nabla}_{\vec{r}} - \vec{\nabla}_{\vec{r}\,'} \right) \langle a^{+}(\vec{r}, \tau)\, a(\vec{r}\,', \tau) \rangle$$

$$G(\vec{r}\,', \vec{r}, \tau \to 0^-)$$

$$\vec{j} = \frac{i}{2m} \lim_{\vec{r} \to \vec{r}\,'} \left(\vec{\nabla}_{\vec{r}} - \vec{\nabla}_{\vec{r}\,'} \right) G(\vec{r}\,', \vec{r}, \tau \to 0^-)$$ need to be calculated with electric field turned on.

4) total energy $\sum_k a_k^{+} [\hat{H}_0, a_k] = -H_0$ because H_0 is of quadratic form

$\sum_k a_k^{+} [\hat{V}, a_k] = -2V$ when $\hat{V}$ is of quartic form

(can be given for homework)

Let's consider: $\left(\frac{\partial}{\partial\tau} - \varepsilon_p + \mu\right) G_p(\tau\to 0^-) = \langle a_p^\dagger(0) \frac{\partial}{\partial\tau} a_p(\tau)\rangle - (\varepsilon_p-\mu)\, n_p$

$\frac{\partial}{\partial\tau} a_p(\tau) = [H, a_p(\tau)]$ because $a_p(\tau) = e^{H\tau} a_p e^{-H\tau}$

$$= \langle a_p^\dagger [H, a_p]\rangle - (\varepsilon_p-\mu)\, n_p$$

Hence $\sum_p \left(\frac{\partial}{\partial\tau} - \varepsilon_p+\mu\right) G_p(\tau\to0^-) = \sum_p \underbrace{\langle a_p^\dagger[H_0,a_p]\rangle}_{-\langle H_0\rangle} + \underbrace{\sum_p\langle a_p^\dagger[V,a_p]\rangle}_{-\langle 2V\rangle} - \underbrace{\sum_p(\varepsilon_p-\mu)\, n_p}_{-\langle H_0\rangle}$

$$= -2E_{tot}$$

Hence $E_{tot} = -\frac12\sum_p\left(\frac{\partial}{\partial\tau} - \varepsilon_p+\mu\right)G_p(\tau\to0^-)$ or

$$G_p(\tau) = \frac1\beta \sum_{i\omega} e^{-i\omega_m\tau} G_p(i\omega_m)$$

$$E_{tot} = \frac{T}{2}\sum_{p,\omega_m}(i\omega_m+\varepsilon_p-\mu)\,G_p(i\omega_m)$$

not well converging because $G_p(i\omega)\to \frac{1}{i\omega}$ and $i\omega\cdot G(i\omega)\to 1$

$$G_p(i\omega_m) = \frac{1}{i\omega_m+\mu-\varepsilon_p-\Sigma_p(i\omega_m)}$$

$$E_{tot} = \frac T2 \sum_{p,\omega_m} \frac{i\omega_m+\mu-\varepsilon_p-\Sigma_p(i\omega_m) - 2\mu+2\varepsilon_p+\Sigma_p(i\omega_m)}{i\omega_m+\mu-\varepsilon_p-\Sigma_p(i\omega)} = \frac T2\sum_{p,i\omega_m}\left(1 + [\Sigma_p(i\omega)+2(\varepsilon_p-\mu)]\,G_p(i\omega_m)\right)$$

$$T\sum_m 1\cdot e^{i\omega_m\cdot\delta} = -\oint\frac{dz}{2\pi i} f(z)\, e^{z\delta} = 0$$

$$E_{tot} = T\sum_{p,i\omega_m}\left[\varepsilon_p-\mu+\frac12\Sigma_p(i\omega_m)\right]G_p(i\omega) \equiv Tr\left(\left(H_0-\mu+\frac12\Sigma\right)G\right)$$

hence $\langle V\rangle = \frac12 Tr(\Sigma G)$ and $T = Tr(H_0 G)$

Back to $\boxed{\text{Perturbation Theory}}$ (following Negele - Orland)

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First for single particle G, which is easier:

$$G_{i_1 i_2}(\tau_1,\tau_2) = -\frac{1}{Z}\int D[\psi^+,\psi]\, e^{-S_0-\Delta S}\, \psi_{i_1}(\tau_1)\psi^+_{i_2}(\tau_2)$$

$$= -\frac{1}{Z}\sum_{m=0}^{\infty}\int D[\psi^+,\psi]\, e^{-S_0}\, \frac{(-\Delta S)^m}{m!}\psi_{i_1}(\tau_1)\psi^+_{i_2}(\tau_2) \equiv -\frac{Z_0}{Z}\sum_{m=0}^{\infty}\left\langle \frac{(\Delta S)^m}{m!}\psi_{i_1}(\tau_1)\psi^+_{i_2}(\tau_2)\right\rangle_0$$

here $S_0 = \int_0^\beta d\tau \sum_i \psi_i^+(\tau)\left(\frac{\partial}{\partial\tau} - \mu + \varepsilon_{ij}\right)\psi_j(\tau)$ is quadratic.

in momentum it is diagonal ε_k

and $Z_0 = \int D[\psi^+,\psi]\, e^{-S_0}$

and $\langle O\rangle = \int D[\psi^+,\psi]\, e^{-S_0}\, O$

We derived before the identity

$$\langle \psi_{i_1}\psi_{i_2}\cdots\psi_{i_N}\psi^+_{j_N}\cdots\psi^+_{j_2}\psi^+_{j_1}\rangle_0 = \sum_P (\zeta)^P (A^{-1})_{i_1 j_{P_1}}\cdots(A^{-1})_{i_N j_{P_N}} \qquad (1)$$

where $\langle O\rangle = (\mathrm{Det}\,A)^{\zeta}\int e^{-\sum_{ij}\psi_i^+ A_{ij}\psi_j}\, O$

Here $A = \left(\frac{\partial}{\partial\tau} - \mu + \varepsilon_{ij}\right) \leftarrow$ matrix in $(\tau,i)\,(\tau',j)$

$$A_{(\tau i,\tau' j)} = \delta(\tau-\tau')\left(\frac{\partial}{\partial\tau'} - \mu + \varepsilon_{ij}\right) \equiv -\left[G^0(\tau i,\tau' j)\right]^{-1}$$

so that $(A^{-1})_{(\tau i,\tau' j)} = -G^0(\tau i,\tau' j) = -G^0_{ij}(\tau-\tau')$

which is called $\boxed{\text{Wick's theorem}}$. The "recipy" is to express $(\Delta S)^m$ in expansion, and use Eq (1) to evaluate term by term.

- Note that: $\langle \psi_{i_1}\psi^+_{j_1}\rangle_0 = (A^{-1})_{i_1 j_1}$ hence we can also write

$$\langle \psi_{i_1}\psi_{i_2}\cdots\psi_{i_N}\psi^+_{j_N}\cdots\psi^+_{j_2}\psi^+_{j_1}\rangle_0 = \sum_P (\zeta)^P \langle \psi_{i_1}\psi^+_{j_{P_1}}\rangle_0 \langle \psi_{i_2}\psi^+_{j_{P_2}}\rangle_0 \cdots \langle \psi_{i_N}\psi^+_{j_{P_N}}\rangle_0$$

Wick's theorem requires all possible contractions of the average.
Note that this is only valid for quadratic S_0!

- Note: any correlation function can be expanded in the same way

$$\langle X(\tau_1\tau_2 .. \tau_2)\rangle = \frac{Z_0}{Z}\sum_{m=0}^{\infty}\left\langle \frac{(-\Delta S)^m}{m!} X(\tau_1\tau_2,\ldots\tau_2)\right\rangle_0$$

To prove $A = -[G^0]^{-1}$

Fourier transform of: $S_0 = \int_0^\beta d\tau \sum_{i,j} \psi_i^+(\tau)\left(\frac{\partial}{\partial\tau} - \mu + \varepsilon_{ij}\right)\psi_j(\tau)$; $\psi_i(\tau) = \frac{1}{\sqrt{\beta}}\sum_{\omega_n}\psi_i(\omega_n)\, e^{-i\omega_n\tau}$

$$S_0 = \sum_n \psi_i^+(\omega_n)\underbrace{(-1)(i\omega_n + \mu - \varepsilon_{ij})}_{-G_{ij}^{0\,-1}(i\omega_n)}\psi_j(\omega_n)$$

back to time

then $$S_0 = \int_0^\beta d\tau\, d\tau' \sum_{ij}\psi_i^+(\tau)\left[-G^0\right]^{-1}_{(i\tau,j\tau')}\psi_j(\tau')$$

matrix in i,j and τ,τ'

$$[G^0]^{-1}_{(i\tau,j\tau')} = [G^0_{ij}(\tau,\tau')]^{-1} = \delta(\tau-\tau')\left[-\frac{\partial}{\partial\tau'} + \mu - \varepsilon_{ij}\right]$$

Normally we should also expand denominator Z i.e.,

$$Z = \sum_{n=0}^{\infty}\int D[\psi^+\psi]\, e^{\int_0^\beta \psi^+[G^0]^{-1}\psi}\,\frac{(-\Delta S)^n}{n!} = \frac{Z_0}{Z}\sum_{n=0}^{\infty}\left\langle\frac{(-\Delta S)^n}{n!}\right\rangle_0$$

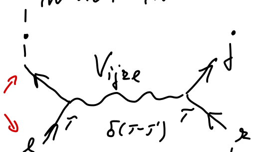
We will show that "linked cluster theorem" allows us to expand only nominator and sum instead "the connected" Feynman diagrams.

Finally, we need to specify the form of the interaction, for example

$$\Delta S = \int_0^\beta d\tau \sum_{ijkl} \frac{1}{2} V_{ijkl}\, \psi^+_i(\tau)\psi^+_j(\tau)\psi_k(\tau)\psi_l(\tau)$$

which we choose to draw like

i,l have the same spin



Fourier →

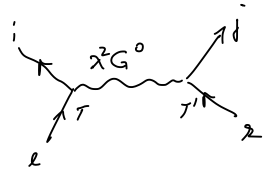
where $V_{ijkl} = \langle \phi^*_i(\vec r)\, \phi^*_j(\vec r')\, | V_c(\vec r - \vec r')|\, \phi_k(\vec r')\, \phi_l(\vec r)\rangle$

this is instantaneous interaction

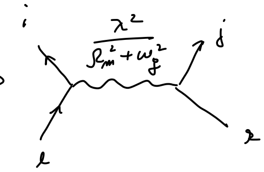
we can also handle retarded interaction

the phonon interaction is dynamic, and has the form

$$\Delta S = \int_0^\beta d\tau\, \psi^+_i(\tau)\psi_l(\tau)\, \frac{1}{2}\lambda^2 G^0_{ph}(\tau-\tau')\, \psi^+_j(\tau')\psi_k(\tau') \quad {}_{ijkl}$$



Fourier →



Let's evaluate a few terms!

$$G_{i_1 i_2}(\tau_1-\tau_2) = -\frac{Z_0}{Z}\sum_{m=0}^{\infty} \left\langle \frac{(-\Delta S)^m}{m!}\, \psi_{i_1}(\tau_1)\, \psi^+_{i_2}(\tau_2)\right\rangle_0$$

0) order $G_{i_1 i_2}(\tau_1-\tau_2) = \frac{Z_0}{Z} G^0_{i_1 i_2}(\tau_1-\tau_2)$ $\quad \tau_2\, i_2 \longrightarrow i_1\, \tau_1$

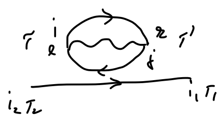
straight line with arrow stands for G^0

1) order

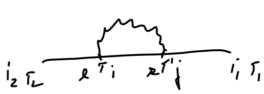
$$G_{i_1 i_2}(\tau_1-\tau_2) = +\frac{Z_0}{Z}\sum_{ijkl}\frac{1}{2}V_{ijkl}\int_0^\beta d\tau\, \langle \psi^+_i(\tau)\psi^+_j(\tau')\psi_k(\tau')\psi_l(\tau)\psi_{i_1}(\tau_1)\psi^+_{i_2}(\tau_2)\rangle_0$$

$$-\langle \psi^+_i(\tau)\psi^+_j(\tau')\psi^+_{i_2}(\tau_2)\psi_k(\tau')\psi_l(\tau)\psi_{i_1}(\tau_1)\rangle_0$$

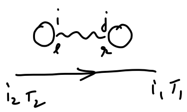
3! terms



1) $\langle \psi^+_i(\tau)\psi_k(\tau')\rangle_0 \langle \psi^+_j(\tau')\psi_l(\tau)\rangle_0 \langle \psi^+_{i_2}(\tau_2)\psi_{i_1}(\tau_1)\rangle_0 = G^0_{ki}(\tau'-\tau)\, G^0_{lj}(\tau-\tau')\, G^0_{i_1 i_2}(\tau_1-\tau_2)$

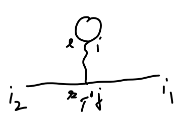


2) $-\langle \psi^+_i(\tau)\psi_k(\tau')\rangle_0 \langle \psi^+_j(\tau')\psi_{i_1}(\tau_1)\rangle_0 \langle \psi^+_{i_2}(\tau_2)\psi_l(\tau)\rangle_0 = -G^0_{ki}(\tau'-\tau)\, G^0_{i_1 j}(\tau_1-\tau')\, G^0_{l i_2}(\tau-\tau_2)$

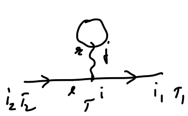


3) $-\langle \psi^+_i(\tau)\psi_l(\tau)\rangle_0 \langle \psi^+_j(\tau')\psi_k(\tau')\rangle_0 \langle \psi^+_{i_2}(\tau_2)\psi_{i_1}(\tau_1)\rangle_0 = -G^0_{li}(\tau=0^-)\, G^0_{kj}(\tau=0^-)\, G^0_{i_1 i_2}(\tau_1-\tau_2)$

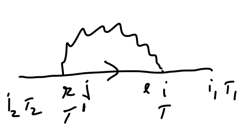
requires 0^- because of correct order of $\psi^+\psi$



4) $\langle \psi^+_i(\tau)\psi_l(\tau)\rangle_0 \langle \psi^+_j(\tau')\psi_{i_1}(\tau_1)\rangle_0 \langle \psi^+_{i_2}(\tau_2)\psi_k(\tau')\rangle_0 = G^0_{li}(\tau=0^-)\, G^0_{i_1 j}(\tau_1-\tau')\, G^0_{k i_2}(\tau'-\tau_2)$



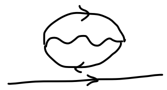
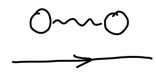
5) $\langle \psi^+_i(\tau)\psi_{i_1}(\tau_1)\rangle_0 \langle \psi^+_j(\tau')\psi_k(\tau')\rangle_0 \langle \psi^+_{i_2}(\tau_2)\psi_l(\tau)\rangle_0 = G^0_{i_1 i}(\tau_1-\tau)\, G^0_{kj}(\tau=0^-)\, G^0_{l i_2}(\tau-\tau_2)$

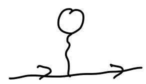


6) $-\langle \psi^+_i(\tau)\psi_{i_1}(\tau_1)\rangle_0 \langle \psi^+_j(\tau')\psi_l(\tau)\rangle_0 \langle \psi^+_{i_2}(\tau_2)\psi_k(\tau')\rangle_0 = -G^0_{i_1 i}(\tau_1-\tau)\, G^0_{lj}(\tau-\tau')\, G^0_{k i_2}(\tau'-\tau_2)$

Stopped Nov 10, 2022

Two types of diagrams:

Disconnected  

Connected  

This works at any order:

n vertices inside

Connected: 

m vertices disconnected

Disconnected:  at least two pieces

m<n vertices inside

Linked Cluster Theorem! The disconnected diagrams exactly cancel the denominator $\frac{Z^0}{Z}$.

Therefore it can be written $G_{i_1 i_2}(\tau_1-\tau_2) = \sum_{m=0}^{\infty} \left\langle \frac{(-\Delta S)^m}{m!} \psi_{i_1}(\tau_1)\psi^+_{i_2}(\tau_2)\right\rangle_0^{connected}$

Proof:

$$G_{i_1 i_2}(\tau_1-\tau_2) = -\frac{Z_0}{Z}\sum_{n=0}^{\infty}\frac{1}{n!}\sum_{m=0}^{n}\langle(-\Delta S)^m \psi_{i_1}(\tau_1)\psi^+_{i_2}(\tau_2)\rangle_0 \langle(-\Delta S)^{n-m}\rangle_0 \binom{n}{m}$$

number of ways to distribute (ΔS) vertices between $(\Delta S)^m$ and $(\Delta S)^{n-m}$

$$\frac{1}{n!}\ \frac{n!}{(n-m)!\,m!}$$

$$G_{i_1 i_2}(\tau_1-\tau_2) = -\frac{Z_0}{Z}\sum_{n,m}\langle(-\Delta S)^m \psi_{i_1}(\tau_1)\psi^+_{i_2}(\tau_2)\rangle_0^{con}\frac{1}{m!}\cdot\langle(-\Delta S)^{n-m}\rangle\frac{1}{(n-m)!} \qquad *$$

$$= -\frac{Z_0}{Z}\sum_{m}\left\langle\frac{(-\Delta S)^m}{m!}\psi_{i_1}(\tau_1)\psi^+_{i_2}(\tau_2)\right\rangle^{con}\times\sum_{k=0}^{\infty}\langle(-\Delta S)^k\rangle\frac{1}{k!}$$

But $\frac{Z}{Z_0} = \sum_{k=0}^{\infty}\left\langle\frac{(-\Delta S)^k}{k!}\right\rangle$ hence

$$\boxed{G_{i_1 i_2}(\tau_1-\tau_2) = \sum_{m}\left\langle\frac{(-\Delta S)^m}{m!}\psi_{i_1}(\tau_1)\psi^+_{i_2}(\tau_2)\right\rangle_0^{connected}}$$

$$* \quad \sum_{n=0}^{\infty} \sum_{m=0}^{n} \langle (-\Delta S)^m O \rangle \frac{1}{m!} \langle (-\Delta S)^{n-m} \rangle \frac{1}{(n-m)!}$$

For $m=0$:
$$\sum_{n=0}^{\infty} \frac{\langle (-\Delta S^n) \rangle}{n!} = \frac{Z}{Z_0}$$

For $m=1$:
$$\frac{\langle (-\Delta S) O \rangle}{1!} \sum_{n=1} \frac{\langle (-\Delta S)^{n-1} \rangle}{(n-1)!} = \frac{\langle (-\Delta S) O \rangle}{1!} \frac{Z}{Z_0}$$

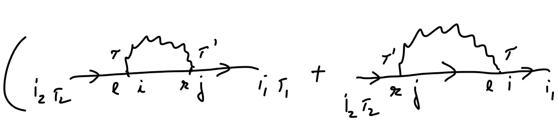
For any m :
$$\frac{\langle (-\Delta S)^m O \rangle}{m!} \sum_{n=m}^{\infty} \frac{\langle (-\Delta S)^{n-m} \rangle}{(n-m)!} = \frac{\langle (-\Delta S)^m O \rangle}{m!} \frac{Z}{Z_0}$$

Topologically equivalent diagrams and symmetry factors

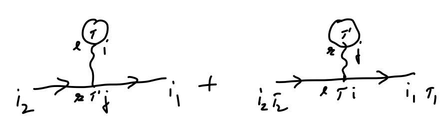
Symmetry of the Interaction vertices

At the lowest order we got two Hartree & two Fock diagrams because there are two ways to name vertices

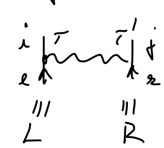
$(\ell, i) \leftrightarrow (r, j)$
$\quad \tau \qquad\quad \tau'$

$\frac{1}{2} V_{ij r\ell} \times \Big($  $\Big)$

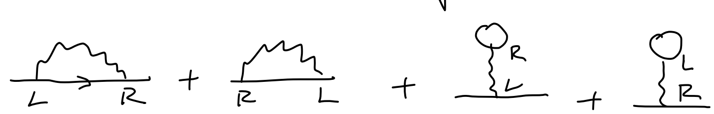
which is exactly canceled by $\frac{1}{2}$ in definition of V.

$\frac{1}{2} V_{ij r\ell} \times \Big($  $\Big)$

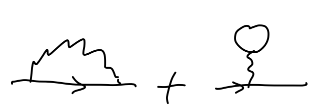
This works at any order and $\left(\frac{1}{2} V_{ijr\ell}\right)^n$ and 2^n ways of rearranging indices in interaction.

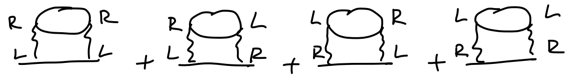
(Negele - Orland defines labeled & unlabeled diagrams. In labeled diagrams we label left - right part for each interaction 
Alternatively we assign direction for bosonic propagator $\quad L \quad R$)

If we consider labeled diagrams we have two copies of diagrams



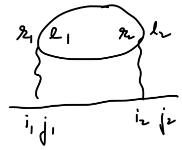
but if we consider unlabeled, we have only one copy!



At order 2 we have  2^2 labeled diagrams for each unlabeled diagram.

Conclusion from interaction at order n: $\left(\frac{1}{2}\right)^n (V_{ijkl})^n$ is exactly canceled by 2^n labeled copies of the same unlabeled diagram.

In addition, at order n we have extra $n!$ ways to rearrange indices between different interactions, i.e.,



can exchange $(i_1 j_1 k_1 l_1) \leftrightarrow (i_2 j_2 k_2 l_2)$ and gives the same graph.

This $n!$ different arrangement can be used to simplify the equation

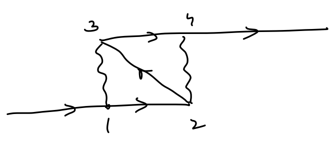
$$G_{i_1 i_2}(\tau_1-\tau_2) = -\sum_{n=0}^{\infty} \left\langle \frac{(-\Delta S)^n}{n!} \psi_{i_1}(\tau_1)\psi^+_{i_2}(\tau_2)\right\rangle_0^{\text{connected, labeled}}$$

$$G_{i_1 i_2}(\tau_1-\tau_2) = -\sum_{n=0}^{\infty} \frac{1}{2^n\, n!} \left\langle \left(\int_0^\beta d\tau\, d\tau' \sum_{ijkl} V_{ijkl}\, \psi^+_i(\tau)\psi^+_j(\tau')\psi_k(\tau')\psi_l(\tau)\right)^n \psi_{i_1}(\tau_1)\psi^+_{i_2}(\tau_2)\right\rangle_0^{\text{connected, labeled}}$$

$$G_{i_1 i_2}(\tau_1-\tau_2) = -\sum_{n=0}^{\infty} \left\langle \left(\int_0^\beta d\tau\, d\tau' \sum_{ijkl} V_{ijkl}\, \psi^+_i(\tau)\psi^+_j(\tau')\psi_k(\tau')\psi_l(\tau)\right)^n \psi_{i_1}(\tau_1)\psi^+_{i_2}(\tau_2)\right\rangle_0^{\text{connected, unlabeled}}$$

sometimes we also write connected – topologically different

What are topologically different diagrams?



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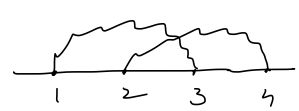
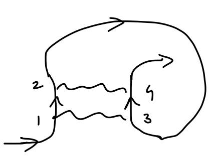


the same diagram



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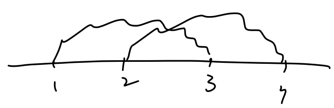

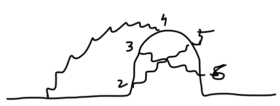

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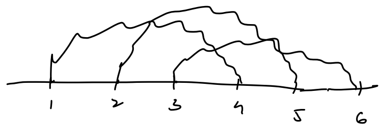
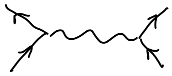
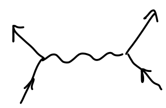


Rules for Feynman diagrams for G:

Draw all topologically distinct connected diagrams composed of n vertices  and directed lines $\nearrow$.

[Two diagrams are topologically distinct if they cannot be deformed so as to coincide completely including the direction of the arrows on electron propagators]

For each topologically distinct diagram evaluate contributions as follows

- Assign time/frequency and momentum/site/orbital labels
- For each vertex assign factor $V_{\underbrace{ij}_{out}\underbrace{kl}_{in}}$  and for each line

$$\text{line} \begin{cases} G_{ij}(\tau_{end} - \tau_{start}) & \overset{}{\underset{j\ \tau_{start}}{\longrightarrow}}\ i\ \tau_{end} \\ G_{ij}(i\omega_n) & j \underset{i\omega_n}{\longrightarrow} i \end{cases}$$

conserve frequency in each vertex

- Sum over all internal indices and

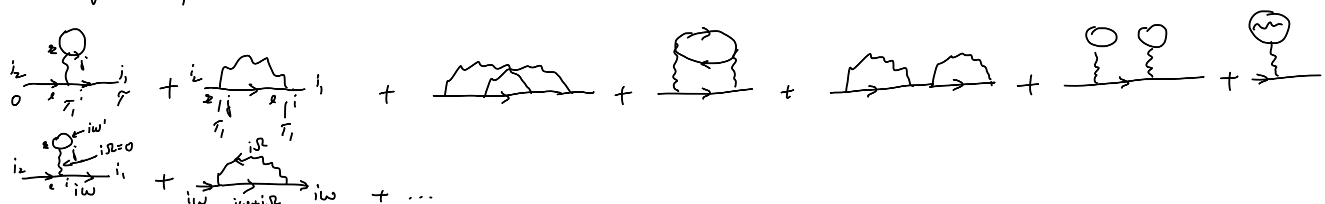
$$\begin{cases} \text{Integrate over all time } [0, \beta]. \\ \text{Sum over all internal Matsubara frequencies} \end{cases}$$

- Multiply the result by $\begin{cases} (-1)^n \xi^{n_L}, & \text{in time} \\ \dfrac{(-1)^n}{\beta^n} \xi^{n_L} & \text{in frequency} \end{cases}$

where n_L is the number of closed fermionic loops

Stopped Nov 15/2022

Check for first two order:



$$G^{(1)}_{i_1 i_2}(\tau) = \sum_{ijkl} (-1)^2 \int_0^\beta d\tau_1 V_{ijkl} G^0_{i_1 i}(\tau-\tau_1) G^0_{l i_2}(\tau_1) G^0_{kj}(0^-) + (-1)\int_0^\beta d\tau_1 V_{ijkl} G^0_{i_1 i}(\tau-\tau_1) G_{k i_2}(\tau_1) G^0_{lj}(0^-) + \cdots$$

$$G^{(1)}_{i_1 i_2}(i\omega) = \sum_{ijkl} \frac{(-1)^2}{\beta} \sum_{i\omega'} V_{ijkl} G^0_{i_1 i}(i\omega) G^0_{l i_2}(i\omega) G^0_{kj}(i\omega') + \frac{(-1)}{\beta}\sum_{i\Omega} V_{ijkl} G^0_{i_1 i}(i\omega) G^0_{k i_2}(i\omega) G^0_{lj}(i\omega + i\Omega) + \cdots$$

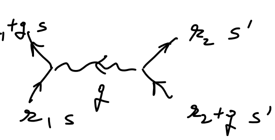
Simplifications of perturbative series for G

1) Transform to conserved indices: momentum and frequency

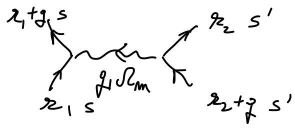
$$G^0_{kk'}(i\omega_m) = -\delta_{kk'}\int_0^\beta \langle T_\tau\, a_k(\tau)\, a_k^+(0)\rangle e^{i\omega_m\tau}$$ hence $\xrightarrow{k,\,\omega_m}$

Coulomb interaction in momentum space $V_q = \frac{8\pi}{q^2+\lambda}$ corresponds to $V(\vec r-\vec r') = \frac{2\, e^{-\sqrt{\lambda} r}}{|\vec r-\vec r'|}$

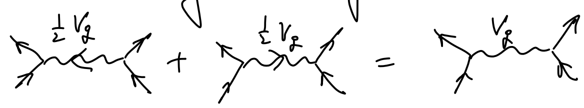
hence we can write $\hat V = \frac{1}{2}\sum_{k_1 k_2 s s'} \psi^+_{k_1+q\, s}\, \psi^+_{k_2 s'}\, \psi_{k_2+q\, s'}\, \psi_{k_1, s}\, V_q$ and



when retarded

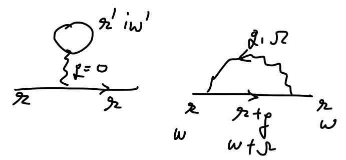


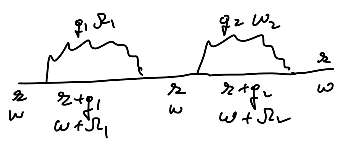
Note: $\frac{1}{2}$ from V_{ijkl} was eliminated by considering unlabeled diagrams. Here similar rule applies. We have



consider only one contribution.

Example:





$$G_k(i\omega) = \frac{(-1)^2}{\beta}\sum_{i\omega' k'} G^0_{k'}(i\omega')\, V_{q=0}\, [G^0_k(i\omega)]^2 + \frac{(-1)}{\beta}\sum_{\substack{i\Omega\\ q}} G^0_{k+q}(i\omega+i\Omega)\, V_q\, [G^0_k(i\omega)]^2 +$$
$$\left[\frac{(-1)}{\beta}\sum_{\substack{i\Omega\\ q}} G^0_{k+q}(i\omega+i\Omega)\, V_q\right]^2 [G^0_k(i\omega)]^3$$

2) Dyson Equation

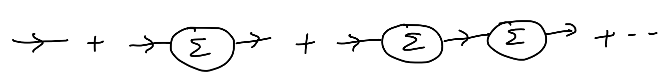
Diagrams like  are better handled by geometric sum, and the resulting quantity Σ is usually better converging than G.

We write $G = (G^{0^{-1}} - \Sigma)^{-1} = G^0 + G^0\Sigma G^0 + G^0\Sigma G^0 \Sigma G^0 + \cdots$

zeroth order term

$[G_k(i\omega)]^2$ legs are removed

takes care of all single particle reducible diagrams.

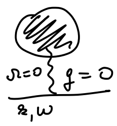
In general $G =$ 

hence Σ should be one particle irreducible: does not fall into two pieces by cutting a single particle line

Modification of rules for self-energy (as compared to G):

- Draw all topologically distinct connected single particle irreducible diagrams.
- Cut legs from the diagram.
- All tadpole diagrams contribute a constant, and can be eliminated by redefining (properly recalculating) the chemical potential / single particle potential.

Tadpole:

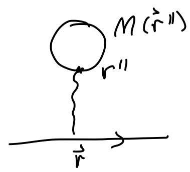


because $\Sigma_k(i\omega_n) = V_{q=0}\cdot$ constant
independent of k and ω_n

is like μ in $G = (i\omega + \mu - \varepsilon_k - \Sigma_k(\omega))^{-1}$

all constants absorbed in redefining μ.

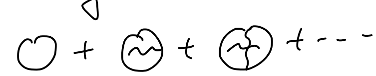
In general tadpole is the Hartree potential



$$\Sigma(\vec r,\vec r') = \delta(\vec r-\vec r')\cdot\int V_c(\vec r-\vec r'')\, n(\vec r'')\, d^3r''$$

It starts with $\Sigma(\vec r,\vec r') = \delta(\vec r-\vec r')\int V_c(\vec r-\vec r'')\, n^0(\vec r'')\, d^3r''$

and then n^0 is replaced by more sophisticated approximation for density



We usually remove these diagrams from perturbation, and just self-consistently evaluate density n and Hartree potential for this density.

Hence perturbation on Hartree state is very convenient, which can drop tadpoles.

Expansion for free energy

We wrote $\frac{Z}{Z_0} = \sum_{n=0}^{\infty} \frac{\langle (-\Delta S)^n \rangle_0^{all}}{n!}$ and use it to cancel all disconnected diagrams. But we did not develop rules to evaluate Z.

Rules are similar, but their is a complication for high symmetry diagrams.

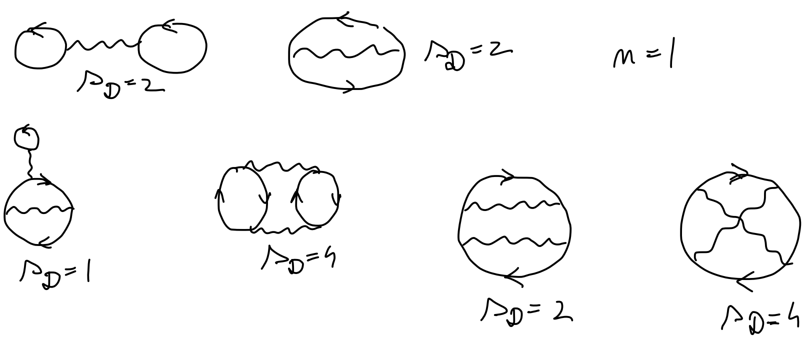
We can derive "linked cluster theorem" for thermodynamic potential, which states

$$\frac{Z}{Z_0} = \sum_{n=0}^{\infty} \frac{\langle (-\Delta S)^n \rangle_0^{all}}{n!} = \exp\left(\sum_{n=0}^{\infty} \frac{\langle (-\Delta S)^n \rangle_0^{\text{connected-topologically distinct}}}{s_D} \right)$$

Here s_D is a symmetry factor for a given diagram, and is an integer that enumerates how many copies of the same diagram we obtain when exchanging indices on all interactions.

There are $2^n \cdot n!$ possible exchanges of indices, and most generate topologically distinct diagrams, while some don't. When there are external legs (like perturbation for G) $s_D = 1$, but considering vacuum-to-vacuum diagrams $s_D \geq 1$.

Examples:



Proof through functional derivative

$$Z = \sum_{n=0}^{\infty} \int \mathcal{D}[\psi^+\psi]\, e^{\int_0^\beta \psi^+_{i}(\tau) [G^0]^{-1}_{i\tau, j\tau'} \psi_j(\tau')} \frac{(-\Delta S)^n}{n!}$$

$$\frac{\delta \ln Z}{\delta [G^0]^{-1}_{(i\tau, j\tau')}} = \frac{1}{Z} \sum_{n=0}^{\infty} \int \mathcal{D}[\psi^+\psi]\, e^{\int_0^\beta \psi^+_{i}(\tau) [G^0]^{-1}_{i\tau, j\tau'} \psi_j(\tau')} \frac{(-\Delta S)^n}{n!} \psi^+_i(\tau) \psi_j(\tau') = G_{ji}(\tau'-\tau)$$

$$G^T = \frac{\delta \ln Z}{\delta [G^0]^{-1}} = \frac{\delta G^0}{\delta [G^0]^{-1}} \frac{\delta \ln Z}{\delta G^0}$$

Note: $G^0[G^0]^{-1} = 1$

$$\delta G^0 [G^0]^{-1} + G^0 \delta [G^0]^{-1} = 0$$

$$\delta G^0 = - G^0 [\delta G^0]^{-1} G^0$$

$$G^T = \frac{\delta \ln Z}{\delta [G^0]^{-1}} = - G^0 \frac{\delta \ln Z}{\delta G^0} G^0$$

$$G^T = -\left[G^0 \frac{\delta \ln Z}{\delta G^0} G^0\right]$$

Functional derivative $\frac{\delta \ln Z}{\delta G^0}$ is a simple cutting of G^0 propagator in expansion for $\ln Z$.

Note : $Z^0 = \mathrm{Det}[-G_0^{-1}]$

$$\ln Z_0 = \ln \mathrm{Det}[-G_0^{-1}] = -\mathrm{Tr}\ln(-G_0)$$

$$\left(\frac{\delta \ln Z_0}{\delta G_0}\right)^T = G_0^{-1}$$

hence at order 0: $G^{(0)T} = -(G_0 G_0^{-1} G_0) = -G_0$

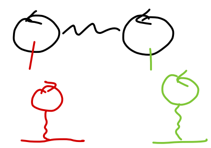
$G^{(0)}(\beta-\tau) = G_0(\tau)$

$$G_{ij}(\tau) = -\langle T_\tau Q_i(\tau) Q_j^+(0)\rangle = \begin{cases} 0<\tau<\beta & -\langle Q_i(\tau) Q_j^+(0)\rangle \\ -\beta<0<\tau & \langle Q_j^+(0) Q_i(\tau)\rangle \end{cases}$$

We know that each topologically distinct diagram should appear only once in expansion of G.

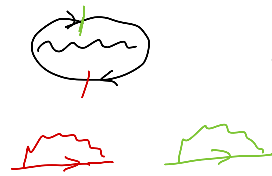
If $\frac{\delta \ln Z}{\delta G^0}$ produces multiple copies of the same diagram, it must have symmetry factor $S_D > 1$.

Example:

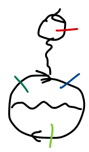


same diagram

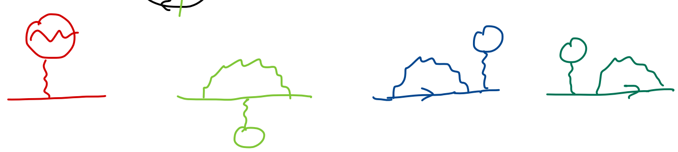
hence $S_D = 2$

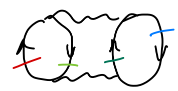


again $S_D = 2$

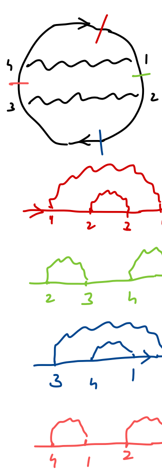


$S_D = 1$

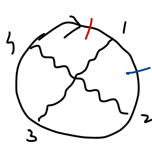




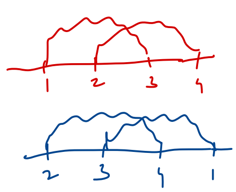
$S_D = 4$



$S_D = 2$



$S_D = 4$

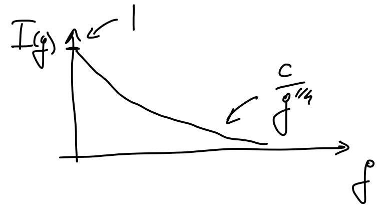


Convergence of perturbative series - how to make it convergent

Harmonic oscillator "like" $S=\int_0^\beta \left[\bar\phi_\tau(\partial_\tau + \omega_f)\phi_\tau + \frac{1}{4} g\, \phi_\tau^4\right] d\tau \Rightarrow S = (\omega_f - i\omega_n)|\phi_{f\omega_n}|^2 + \frac{1}{4} g\, |\phi_{f\omega_n}|^4$

Atland & Simons warning of perturbative expansion

$$I(g)=\int \frac{d\phi}{\sqrt{2\pi}}\, e^{-\frac{1}{2}x^2-\frac{1}{4}g x^4} = \frac{e^{\frac{1}{8g}}}{2\sqrt{\pi g}}\, \text{BesselK}\left[\frac{1}{4}, \frac{1}{8g}\right]$$



$$I(g)=\int\frac{dx}{\sqrt{2\pi}}\, e^{-\frac{1}{2}x^2-\frac{g}{\cancel{4}}x^4} = \int \frac{dx}{\sqrt{2\pi}}\, e^{-\frac{1}{2}x^2}\sum_{m=0}^\infty \frac{(-\frac{g}{\cancel{4}})^m}{m!}\, x^{4m} = \sum_{m=0}^\infty \frac{(-\frac{g}{\cancel{4}})^m}{m!}\,\frac{(4m)!}{2^{2m}(2m)!}$$

$$\boxed{\text{Stirling: } z! \sim \sqrt{2\pi}\, z^{z+\frac{1}{2}} e^{-z}}$$

$$\approx \sum_{m=0}^\infty \left(\frac{4m}{e}\right)^m \frac{1}{\sqrt{\pi m}}(-g)^m \approx \sum_{m=0}^\infty \left(-\frac{4gm}{e}\right)^m\frac{1}{\sqrt{\pi m}}$$

$$\int \frac{dx}{\sqrt{2\pi}}\, e^{-\frac{1}{2}x^2} x^{4m} = \frac{(4m)!}{2^{2m}(2m)!} \approx \left(\frac{4m}{e}\right)^{2m}\sqrt{2}$$

even for very small g the expansion diverges at sufficiently large m. If g is large, perturbation fails instantly! *

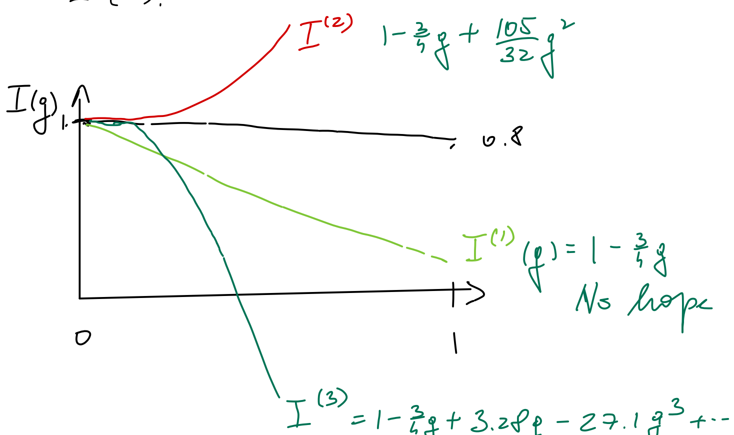
$\frac{4gm_c}{e}>1$

$m_c > \frac{e}{4g}$

Example $g=1 \Rightarrow m_c \approx 1$

Note: $(4m-1)!! = (4m-1)(4m-3)\cdots 1$

$$\left(\frac{(4m)!}{2^{2m}(2m)!} = \frac{4m(4m-1)(4m-2)(4m-3)(4m-4)\cdots}{2\cdot 2m \quad 2(2m-1) \quad 2(2m-2)\cdots} = (4m-1)(4m-3)\cdots\right.$$



No hope for large g!

* Fundamental issue: - g changes the frequency of oscillation.

- Overlap between oscillator with frequency 1 and renormalized frequency with perturbation is vanishing.

Trick by Kleinert and Feynman:

$$I^{exact}(g) = \int \frac{dq}{\sqrt{2\pi}}\, e^{-\frac{1}{2}x^2 - \frac{1}{4} g x^4} = \frac{e^{\frac{1}{8g}}}{2\sqrt{\pi g}}\ \text{BesselK}\left[\tfrac{1}{4}, \tfrac{1}{8g}\right]$$

$$I(g,\Omega) = \int \frac{dq}{\sqrt{2\pi}}\, e^{-\frac{1}{2}\Omega^2 x^2 - \varphi\left(\frac{1}{4} g x^4 - \underbrace{\frac{1}{2}(\Omega^2-1)x^2}_{\text{counter term}}\right)}$$

$$= \Big|_{\varphi=1} \int \frac{dq}{\sqrt{2\pi}}\, e^{-\frac{1}{2}\Omega^2 x^2} \sum_{n=0}^{\infty} \frac{(-\varphi)^n}{n!}\left(\frac{1}{4} g x^4 - \frac{1}{2}(\Omega^2-1)x^2\right)^n$$

0) Introduce variational parameter Ω

1) Expand in φ and not g

2) At each order optimize $I(g,\Omega)$ with principle of minimal sensitivity, i.e.,

$$\frac{d I(g,\Omega)}{d\Omega} = 0 \Rightarrow \Omega_n \text{ at order } n$$

3) $I_1(\Omega_1, g)$, $I_2(\Omega_2, g)$, $\dots$ $I_n(\Omega_n, g)$ will likely converge.

$\Omega x = y$

$$I(g,\Omega) = \int \frac{dy}{\sqrt{2\pi}}\, e^{-\frac{1}{2}y^2} \sum_{n=0}^{\infty} \frac{1}{\Omega^{2n+1}} \frac{(-\varphi)^n}{n!}\left(\frac{1}{4}\frac{g}{\Omega^2} y^4 - \frac{1}{2}(\Omega^2-1) y^2\right)^n = \sum_{n=0}^{\infty} \frac{1}{\Omega^{2n+1}} \frac{(-\varphi)^n}{n!} \sum_{m=0}^{n} \binom{n}{m}\left(\frac{g}{4\Omega^2}\right)^m \left[-\frac{1}{2}(\Omega^2-1)\right]^{n-m} \int \frac{dy}{\sqrt{2\pi}}\, e^{-\frac{1}{2}y^2}\, y^{\overbrace{4m+2n-2m}^{2m+2n}}$$

$$= \sum_{n=0}^{\infty} \frac{\varphi^n}{\Omega^{2n+1}} \frac{(-1)^n}{\cancel{n!}} \sum_{m=0}^{n} \cancel{\binom{n}{m}} \left(\frac{g}{4\Omega^2}\right)^m \left[-\frac{1}{2}(\Omega^2-1)\right]^{n-m} \frac{(2(m+n))!}{2^{m+n}(m+n)!}\, \frac{\cancel{n!}}{(n-m)!\,m!} = \sum_{n=0}^{\infty}\sum_{m=0}^{n} \frac{(-1)^m}{2^{2n}} \left(\frac{g}{4}\right)^m \frac{(\Omega^2-1)^{n-m}}{\Omega^{2(m+n)+1}}\, \frac{(2(m+n))!}{(m+n)!\,(n-m)!\,m!}$$

$I^0(g,\Omega) = \frac{1}{\Omega}$ no optimum

$$I^1(g,\Omega) = \frac{1}{\Omega} + \frac{1}{2\Omega^3}\left(-\frac{3}{2}\frac{g}{\Omega^2} + \Omega^2 - 1\right) = -\frac{3}{4}\frac{g}{\Omega^5} - \frac{1}{2\Omega^3} + \frac{3}{2}\frac{1}{\Omega} \Rightarrow \frac{dI^1}{d\Omega} = +\frac{15}{4}\frac{g}{\Omega^6} + \frac{3}{2}\frac{1}{\Omega^4} - \frac{3}{2}\frac{1}{\Omega^2} = 0$$

$$\Omega^4 - \Omega^2 - \frac{5}{2}g = 0$$

$$\Omega_0^2 = \frac{1}{2}\left(1 \pm \sqrt{1+10g}\right)$$

$$\Omega^4 = \Omega^2 + \frac{5}{2}g$$

$$I^1(g,\Omega^0) = \frac{1}{2\Omega^5}\left(-\frac{3}{2}g - \Omega^2 + 3\Omega^4\right) = \frac{1}{2\Omega^5}\left(-\frac{3}{2}g - \Omega^2 + 3\left(\Omega^2 + \frac{5}{2}g\right)\right)$$

$$= \frac{1}{2\Omega^5}\left[-\frac{3}{2}g + 2\Omega^2 + \frac{15}{2}g\right] = \frac{(3g+\Omega^2)}{\Omega^5} = \frac{\left(3g + \frac{1}{2} + \frac{1}{2}\sqrt{1+10g}\right)}{\left[\frac{1}{2}\left(1+\sqrt{1+10g}\right)\right]^{5/2}}$$

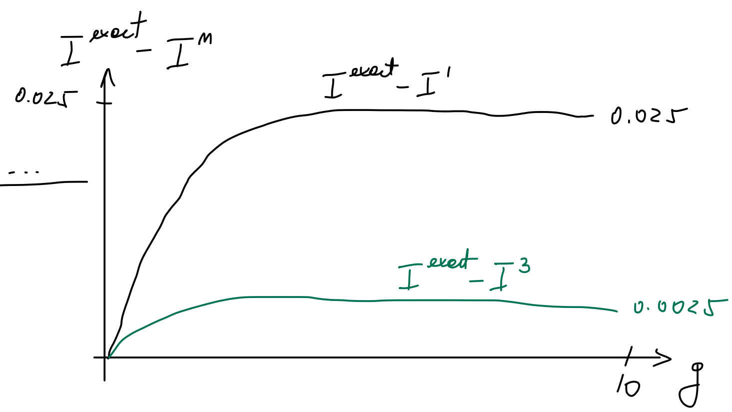
$$I^1(g\to\infty, \Omega^0) \approx \frac{3g}{\left(\frac{\sqrt{10}}{2}\right)^{5/2}}\, g^{-1/4} \approx 0.954\, g^{-1/4}$$

$$I^{exact}(g\to\infty) = 1.023\, g^{-1/4}$$

$I^2(g,\Omega)$ no optimum

$$I^3(g,\Omega) = \frac{1}{\Omega} + \frac{1}{2\Omega^3}\left(-\frac{3}{2}\frac{g}{\Omega^2} + \Omega^2 - 1\right) + \frac{-3465 g^3 + \dots}{128\,\Omega^{13}}$$

$$I^3(g, \Omega_{optimized}) \approx 1.011\, g^{-1/4}$$



Comparison of perturbation with functional integral

$$Z(g) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, e^{-\frac{1}{2}x^2 - \frac{1}{4}gx^4} = \sum_{n=0}^{\infty} Z_n g^n = \sum_{n=0}^{\infty}\int_{-\infty}^{\infty}\frac{dx}{\sqrt{2\pi}} e^{-\frac{1}{2}x^2}\frac{(-1)^n}{n!}\left(\frac{gx^4}{4}\right)^n \Rightarrow Z_n = \left(\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-\frac{1}{2}x^2} x^{4n}\right)\frac{(-1)^n}{4^n\, n!}$$

Evaluating Z_n by functional integral technique:

change of variable: $x = \sqrt{k}\, y$

$$Z_k = \frac{(-1)^k}{4^k k!}\int_{-\infty}^{\infty} e^{-\frac{1}{2}x^2} x^{4k}\frac{dx}{\sqrt{2\pi}} = \frac{(-1)^k}{4^k k!} k^{2k+\frac{1}{2}}\int_{-\infty}^{\infty}\frac{dy}{\sqrt{2\pi}} e^{-\frac{1}{2}ky^2} y^{4k}$$

$$= \frac{(-1)^k}{4^k k!} e^{2k\ln k}\sqrt{k}\int\frac{dy}{\sqrt{2\pi}} e^{-k\underbrace{\left(\frac{1}{2}y^2 - 2\ln y^2\right)}}$$

$$A(y) = \frac{y^2}{2} - 2\ln y^2$$

Using gaussian integral for stationarity:

stationary condition: $\frac{\partial A}{\partial y} = y - \frac{4}{y} = 0$ or $y = \pm 2$

fluctuations around: $\frac{\partial^2 A}{\partial y^2} = 1 + \frac{4}{y^2} = 2$

$$A \approx A(\pm 2) + \frac{1}{2}\frac{\partial^2 A}{\partial y^2}(y\mp 2)^2 = 2(1-\ln 4) + \frac{1}{2}2(y\mp 2)^2$$

Then
$$Z_k \sim \frac{(-1)^k}{4^k k!} e^{2k\ln k}\sqrt{k}\int_{-\infty}^{\infty}\frac{dy}{\sqrt{2\pi}} e^{-k[2(1-\ln 4) + (y\mp 2)^2]}$$

$$= \frac{(-1)^k}{4^k k!} e^{2k\ln k}\sqrt{k}\, e^{-2k(1-\ln 4)}\frac{1}{\sqrt{2k}}\cdot 2$$

$$= \frac{(-1)^k}{k!}\frac{e^{2k(\ln k - 1 + \ln 4)}}{2^{2k}}\sqrt{2}$$

$$= \frac{(-1)^k}{k!}\left(\frac{2k}{e}\right)^{2k}\sqrt{2} \approx \frac{(-1)^k}{\sqrt{2\pi}}\left(\frac{e}{k}\right)^k\frac{\sqrt{2}}{\sqrt{k}}\left(\frac{2k}{e}\right)^{2k} =$$

$$= (-1)^k\left(\frac{4k}{e}\right)^k\frac{1}{\sqrt{\pi k}}$$

finally
$$Z(g) = \sum_{n=0}^{\infty}\left(-\frac{4gn}{e}\right)^n\frac{1}{\sqrt{\pi n}}$$

which is the same as before doing straightforward expansion,

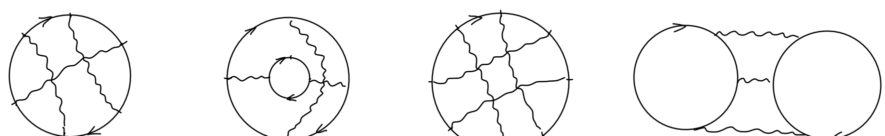
Homework 3, 620 Many body

November 17, 2022

1) Draw all connected topologically distinct (unlabeled) Feynman diagrams for the self-energy up to the second order with expansion on the Hartree state. Exclude tadpoles, which are accounted for by expanding on the Hartree state with redefined single particle potential.

   Assume that the system is translationally invariant, use momentum and frequency basis to write complete expression for the value of these diagrams. Use the Coulomb interaction v_q and single-particle propagator $G^0_{\mathbf{k}}(i\omega_n)$ in your expressions.

2) Calculate the symmetry factors for the following Feynman diagrams, which contribute to $logZ$ expansion.



3) The Uniform Electron Gas is translationally invariant homogeneous system of interacting electrons, which is kept in-place by uniformly distributed positive background charge. The action for the model is

$$S[\psi] = \sum_{\mathbf{k},\sigma} \int_0^\beta d\tau \; \psi^\dagger_{\mathbf{k}\sigma}(\tau)(\frac{\partial}{\partial\tau} - \mu + \varepsilon_k)\psi_{\mathbf{k}\sigma}(\tau)$$
$$+\frac{1}{2V} \sum_{\sigma,\sigma'\mathbf{k},\mathbf{k}',\mathbf{q}\neq 0} v_{\mathbf{q}} \int_0^\beta d\tau \; \psi^\dagger_{\mathbf{k}+\mathbf{q},\sigma}(\tau)\psi^\dagger_{\mathbf{k}'-\mathbf{q},\sigma'}(\tau)\psi_{\mathbf{k}',\sigma'}(\tau)\psi_{\mathbf{k},\sigma}(\tau) \tag{1}$$

   Here $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$ and $v_q = \frac{e_0^2}{\varepsilon_0 q^2}$ is the Coulomb repulsion. The uniform density n_0 is equal to the number of electrons per unit volume, i.e., $n_0 = N_e/V$ for charge neutrality. The density n_0 is usually expressed in terms of distance parameter r_s, which is the typical radius between two electrons, and is defined by $1/n^0 = 4\pi r_s^3/3$. Furthermore, the Coulomb repulsion and the single-particle energy can be conveniently expressed in Rydberg units (13.6 eV$= \hbar^2/(2ma_0^2)$, a_0 Bohr radius), in which $v_q = 8\pi/q^2$ and $\varepsilon_{\mathbf{k}} = k^2$, and all momentums are measured in $1/a_0$.

   – Show that the Fermi momentum $k_F = (9\pi/4)^{1/3}/r_s$, where $E_F = k_F^2$ in these units.

– Show that the kinetic energy per density is $E_{kin}/(Vn_0) = \varepsilon_{kin} = \frac{3}{5}k_F^2$ or $\varepsilon_{kin} = 2.2099/r_s^2$.

– Calculate the exchange (Fock) self-energy diagram and show it has the form

$$\Sigma^x_{\mathbf{k}} = -\frac{2k_F}{\pi} S\left(\frac{k}{k_F}\right) \tag{2}$$

where

$$S(x) = 1 + \frac{1-y^2}{2y} \log\left|\frac{1+y}{1-y}\right| \tag{3}$$

Note that $S(x)$ can be obtained by the following integral

$$S(x) = \frac{1}{x}\int_0^1 du\, u \log\left|\frac{u+x}{u-x}\right| \tag{4}$$

– Derive the expression for the effective mass of the system, which is defined in the following way

$$G_{\mathbf{k}\approx k_F}(\omega \approx 0) = \frac{Z_k}{\omega - \frac{k^2-k_F^2}{2m^*}} \tag{5}$$

Start from the definition of the Green's function $G_{\mathbf{k}}(\omega) = 1/(\omega + \mu - \varepsilon_{\mathbf{k}} - \Sigma_{\mathbf{k}}(\omega))$ and Taylor's expression of the self-energy

$$\Sigma_{\mathbf{k}\approx k_F}(\omega \approx 0) = \Sigma_{k_F}(0) + \frac{\partial \Sigma_{k_F}(0)}{\partial \omega}\omega + \frac{\partial \Sigma_{k_F}(0)}{\partial k}(k - k_F) \tag{6}$$

and define $Z_k^{-1} = 1 - \frac{\partial \Sigma_{k_F}(0)}{\partial \omega}$ and take into account the validity of the Luttinger's theorem (the volume of the Fermi surface can not change by interaction). Show that under these assumptions, the effective mass of the quasiparticle is

$$\frac{m}{m^*} = Z_k \left(1 + \frac{m}{k_F}\frac{\partial \Sigma_{k_F}(0)}{\partial k}\right) \tag{7}$$

– Use the exchange self-energy and show that within Hartee-Fock approximation the effective mass is vanishing. Is there any quasiparticle left at the Fermi level in this theory? What does that mean for the stability of the metal in this approximation? What is the cause of (possible) instability?

stopped 11/22/2022

– What is the form of the spectral function $A_k(\omega)$ near $k = k_F$ and $\omega = 0$?

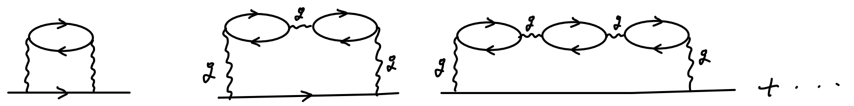
– Calculate the contribution to the total energy of the exchange self-energy, which is defined by

$$\Delta E_{tot} = \frac{T}{2}\sum_{\mathbf{k},\sigma,i\omega_n} G_{\mathbf{k}}(i\omega_n)\Sigma_{\mathbf{k}}(i\omega_n) \tag{8}$$

Show that $\Delta E_{tot}/(n_0 V) = -0.91633/r_s$ is Rydberg units.

Note that the correction to the kinetic energy, which goes as $1/r_s^2$ is large when r_s is large, i.e., when the density is small (dilute limit).

- Evaluate the higher order correction for self-energy of the RPA form, which is composed of the following Feynman diagrams

$\Sigma_k(i\omega) =$ 

Show that the self-energy can be evaluated to

$$\Sigma_{\mathbf{k}}(i\omega_n) = -\frac{1}{\beta} \sum_{\mathbf{q}, i\Omega_m} v_q^2 G^0_{\mathbf{k}+\mathbf{q}}(i\omega_n + i\Omega_m) \frac{P_q(i\Omega_m)}{1 - v_q P_q(i\Omega_m)} \tag{9}$$

where

$$P_q(i\Omega_m) = \frac{1}{\beta} \sum_{i\omega_n, \mathbf{k}, s} G^0_{\mathbf{k}}(i\omega_n) G^0_{\mathbf{k}+\mathbf{q}}(i\omega_n + i\Omega_m) \tag{10}$$

- Show that the Polarization function $P_q(i\Omega_m)$ on the real axis ($i\Omega_m \to \Omega + i\delta$) takes the following form

$$P_q(\Omega + i\delta) = -\frac{k_F}{4\pi^2} \left(\mathcal{P}\left(\frac{\Omega}{k_F^2} + i\delta, \frac{q}{k_F} \right) + \mathcal{P}\left(-\frac{\Omega}{k_F^2} - i\delta, \frac{q}{k_F} \right) \right) \tag{11}$$

where

$$\mathcal{P}(x, y) = \frac{1}{2} - \left[\frac{(x + y^2)^2 - 4y^2}{8y^3} \right] \left[\log\left(x + y^2 + 2y\right) - \log\left(x + y^2 - 2y\right) \right] \tag{12}$$

- RPA contribution to the total energy is again

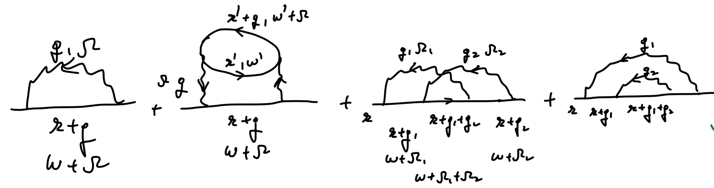
$$\Delta E_{tot} = \frac{T}{2} \sum_{\mathbf{k}, s, i\omega_n} G^0_{\mathbf{k}}(i\omega_n) \Sigma_{\mathbf{k}}(i\omega_n) \tag{13}$$

Show that within this RPA approximation the total energy takes the form

$$\Delta E_{tot} = -\frac{V}{2} \int \frac{d^3\mathbf{q}}{(2\pi)^3} \int \frac{d\Omega}{\pi} n(\Omega) \mathrm{Im} \left\{ \frac{v_q^2 P_q(\Omega + i\delta)^2}{1 - v_q P_q(\Omega + i\delta)} \right\} \tag{14}$$

The analytic expression for this total energy contribution can not expressed in a closed form, however, an asymptotic expression for small r_s has the form $\Delta E_{tot}/n_0 \approx -0.142 + 0.0622 \log(r_s)$, which signals that the total energy is not an analytic function of r_s or density, hence perturbation theory in powers of v_q is bound to fail. Analytic solution of this problem is still not available, and only numerical estimates by QMC can be found in literature. Note that this total energy density is at the heart of the Density Functional Theory.

Homework: Draw all diagrams for self-energy (excluding tad-poles) up to the second order and write expression in momentum frequency space.

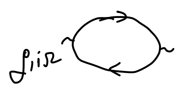
order: $\Sigma_k(i\omega) =$ 

non - skeleton

exchange or Fock — a — b — c

$$\Sigma^x_k(i\omega) = \frac{(-1)}{\beta}\sum_{i\Omega,\,q} V_q\, G^0_{k+q}(i\omega+i\Omega) = -\sum_q V_q\, n^0_{k+q} \quad \text{i.e., static}$$

$$\Sigma^{(2a)}_k(i\omega) = \frac{(-1)^2}{\beta^2}(-1)\sum_{\substack{q,k',s'\\ \omega',\Omega}} V_q^2\, G^0_{k'}(i\omega')\,G^0_{k'}(i\omega'+i\Omega)\, G_{k+q}(i\omega+i\Omega) \Rightarrow \frac{-1}{\beta}\sum_{q,i\Omega} V_q^2\, P^0_q(i\Omega)\, G_{k+q}(i\omega+i\Omega)$$

Define polarization $P^0_q(i\Omega) \equiv$ 

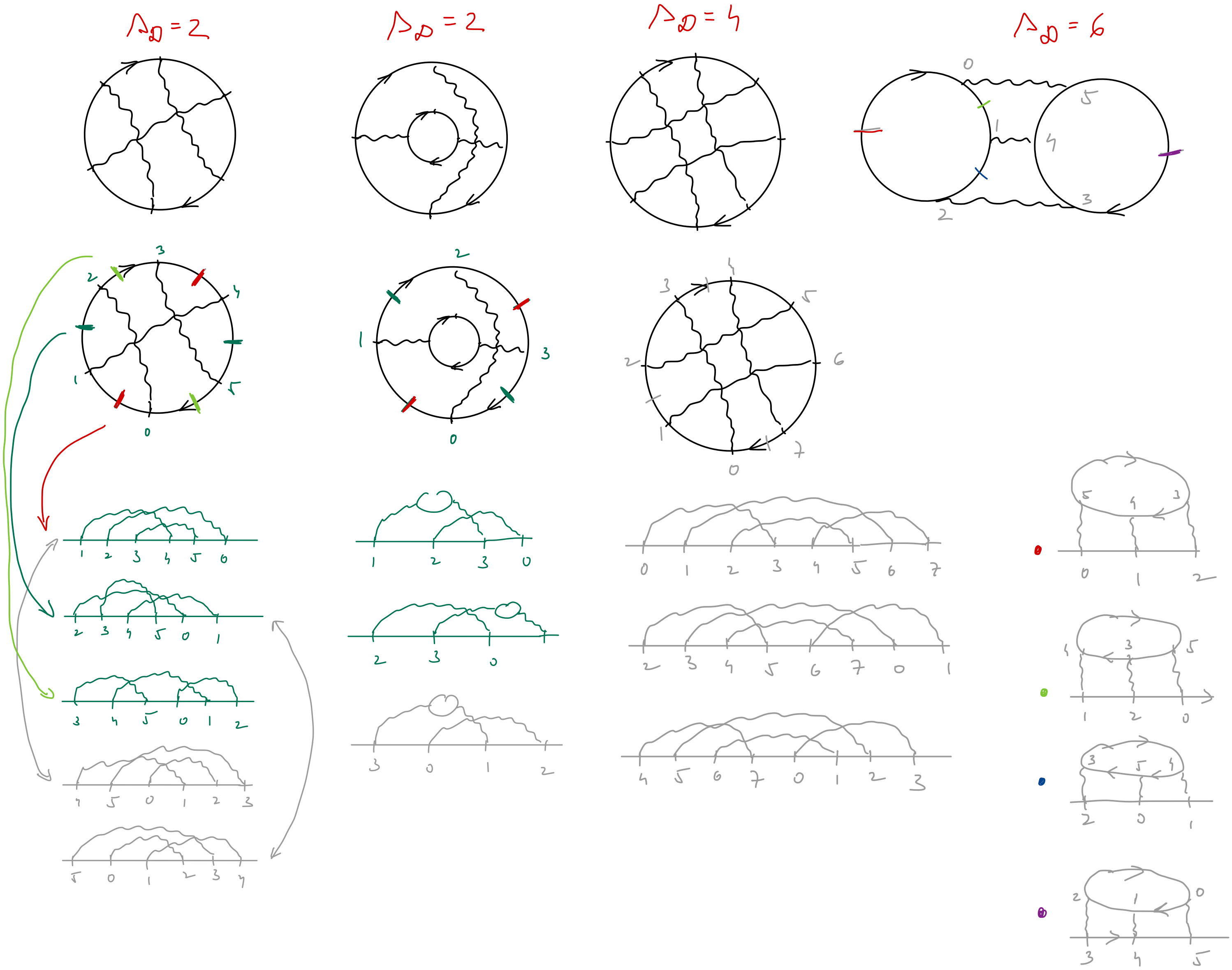
$= \frac{1}{\beta}\sum_{k',\omega',s'} G^0_{k'}(i\omega)\, G^0_{k'+q}(i\omega+i\Omega)$

$$\Sigma^{(2b)}_k(i\omega) = \frac{(-1)^2}{\beta^2}\sum_{\substack{q_1\, q_2\\ \Omega_1,\Omega_2}} G^0_{k+q_1}(i\omega+i\Omega_1)\, G^0_{k+q_2}(i\omega+i\Omega_2)\, G^0_{k+q_1+q_2}(i\omega+i\Omega_1+i\Omega_2)\, V_{q_1} V_{q_2}$$

$$\Sigma^{(2c)}_k(i\omega) = \frac{(-1)^2}{\beta^2}\sum_{\substack{q_1\, q_2\\ \Omega_1,\Omega_2}} \left[G^0_{k+q_1}(i\omega+i\Omega_1)\right]^2 \underbrace{G^0_{k+q_1+q_2}(i\omega+i\Omega_1+i\Omega_2)}_{n^0_{k+q_1+q_2}} V_{q_1} V_{q_2}$$

Homework: Calculate the symmetry factor of the following diagram:

Draw the diagram for G that are generated by $\frac{\delta \ln Z}{\delta G^0}$.



Homework 3 on UEG

Fermi momentum: $n = \frac{3}{4\pi r_s^3} = \frac{1}{V} N_e = 2 \int \frac{d^3k}{(2\pi)^3} n_k = 2 \int_0^{k_F} \frac{dk\, 4\pi k^2}{8\pi^3} = \frac{1}{\pi^2}\frac{k_F^3}{3} \Rightarrow k_F^3 = \frac{3\pi^2 \cdot 3}{4\pi}\frac{1}{r_s^3}$

$\uparrow$ spin

and $k_F = \left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{r_s}$

$E_F = \frac{\hbar^2 k_F^2}{2m} = \underbrace{\left(\frac{\hbar^2}{2m a_0^2}\right)}_{1Ry}\left(\frac{k_F}{a_0}\right)^2 \Rightarrow \frac{E_F}{1Ry} = \tilde{k}_F^2$

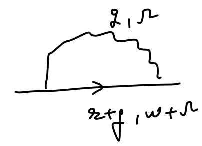
$$E_{kin} = \sum_{k s} n_k \frac{\hbar^2 k^2}{2m} = 1Ry \times \underset{\text{spin}}{\overset{\uparrow}{2}}\, V \int \frac{d^3k}{(2\pi)^3} k^2 f(\varepsilon_k)$$

$$\frac{E_{kin}}{1Ry} = V \frac{2\, 4\pi}{8\pi^3}\int_0^{k_F} dk\, k^2 k^2 = \frac{V}{\pi^2}\frac{k_F^5}{5} = \left(\frac{V}{\pi^2}\frac{k_F^3}{3}\right)\left(\frac{3}{5}k_F^2\right) = V n_0 \frac{3}{5} k_F^2 \Rightarrow \frac{E_{kin}}{V n_0} = \underbrace{\frac{3}{5}\left(\frac{9\pi}{4}\right)^{2/3}}\frac{1}{r_s^2}$$

Note:

$$\boxed{\frac{1}{V}\sum_q = \int \frac{d^3q}{(2\pi)^3}}$$

– Calculate the exchange contribution to self energy



$$\Sigma_k^x = \frac{(-1)}{\beta V}\sum_{q, i\Omega} v_q G^0_{k+q}(i\omega + i\Omega) = -\frac{1}{V}\sum_q v_q n_{k+q} = -\int \frac{d^3q}{(2\pi)^3} n_q v_{q-k} = -\int \frac{d^3q}{(2\pi)^3} f(\varepsilon_q)\frac{8\pi}{|\vec{q}-\vec{k}|^2}$$

$T=0 \rightarrow$

$$= -\int_0^{k_F} dq \frac{2\pi q^2}{(2\pi)^3}\int_{-1}^{1} d(\cos\vartheta)\frac{8\pi}{q^2+k^2-2kq\cos\vartheta} = \frac{2}{\pi}\int_0^{k_F} dq\, q^2 \int_{-1}^{1}\frac{dx}{q^2+k^2-2kqx} = \frac{2}{\pi}\int_0 dq\, q^2 \frac{1}{2kq}\ln(q^2+k^2-2kqx)\Big|_1^{-1} = \frac{2}{\pi}\frac{1}{2k}\int_0^{k_F} dq\, q \ln\left(\frac{(q+k)^2}{(q-k)^2}\right)$$

$$= -\frac{2}{\pi k}\int_0^{k_F} dq\, q \ln\left|\frac{q+k}{q-k}\right| = -\frac{2}{\pi}\frac{k_F}{y}\int_0^1 du\, u \ln\left|\frac{u+y}{u-y}\right|$$

$$\frac{q}{k_F} = u;\quad \frac{k}{k_F} = y$$

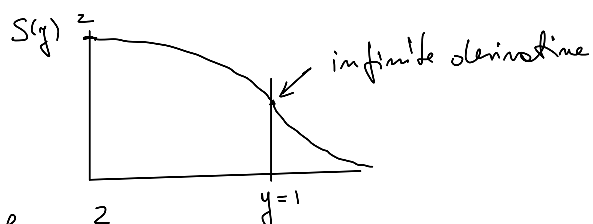
$$S(y) \equiv \frac{1}{y}\int_0^1 du\, u \ln\left|\frac{u+y}{u-y}\right|$$

$$S(y) = 1 + \frac{1-y^2}{2y}\ln\left|\frac{1+y}{1-y}\right|$$

stopped $\Rightarrow$

$$\frac{k}{k_F} = y$$

$$\Sigma_k^x = -\frac{2k_F}{\pi} S\left(\frac{k}{k_F}\right)$$



What is effective mass of electron within HF theory?

$$G_k(\omega) = \frac{1}{\omega + \mu - \frac{k^2}{2m} - \Sigma_k(\omega)} \qquad \Sigma_k(\omega) \approx \Sigma_{k_F}(\omega=0) + \frac{\partial \Sigma_{k_F}}{\partial \omega}\omega + \frac{\partial \Sigma_{k_F}}{\partial k}(k-k_F)$$

$$\approx \frac{1}{\underbrace{\omega\left(1-\frac{\partial\Sigma_{k_F}}{\partial\omega}\right)}_{Z_k^{-1}} + \underbrace{\mu - \frac{k_F^2}{2m}}_{\tilde{\mu}} - \underbrace{\frac{k^2-k_F^2}{2m}}_{\substack{\| \\ (k-k_F)\frac{k_F}{m}}} - \Sigma^0_{k_F} - \frac{\partial\Sigma_{k_F}}{\partial k}(k-k_F)} = \frac{1}{\frac{\omega}{Z_k} + \tilde{\mu} - \Sigma^0_{k_F} - (k-k_F)\left[\frac{k_F}{m} + \frac{\partial\Sigma_{k_F}(0)}{\partial k}\right]}$$

$\tilde{\mu} = \Sigma^0_{k_F}$ — Luttinger's theorem

$$Z_k \equiv \frac{1}{1-\frac{\partial\Sigma_k}{\partial\omega}}$$

$$\approx \frac{Z_k}{\omega - \frac{(k-k_F)k_F}{m} Z_k\left[1 + \frac{m}{k_F}\frac{\partial\Sigma_{k_F}(0)}{\partial k}\right]}$$

$$G_k(\omega) \approx \frac{Z_k}{\omega - \frac{(k-k_F)k_F}{m^*}} \approx \frac{Z_k}{\omega - \frac{k^2-k_F^2}{2m^*}}$$

$$\frac{m}{m^*} \equiv Z_k\left[1 + \frac{m}{k_F}\frac{\partial\Sigma_{k_F}(0)}{\partial k}\right]$$

For HF: $\frac{m^*}{m} = \frac{1}{1+\frac{m}{k_F}\frac{d\Sigma_{k_F}}{dk}}$ $\qquad \frac{d\Sigma_{k_F}}{dk} = -\frac{2}{\pi}S'(1) = \infty$

$\frac{m^*}{m} = 0$ which means infinite bandwidth $\rightarrow$ metal unstable

$$\varepsilon_k = \frac{\hbar^2 k^2}{2m} = \left(\frac{\hbar^2}{2m a_0^2}\right) a_0^2 k^2 = 1Ry\,(a_0 k)^2$$

What is the spectral function near the fermi level?

$$A_k(\omega) = -\frac{1}{\pi}\operatorname{Im} G_k(\omega) = -\frac{1}{\pi}\operatorname{Im}\left(\frac{1}{\omega - (k-k_F)2k_F\left[1-\frac{1}{2k_F}\frac{2}{\pi}S'(1)\right]+i\delta}\right) \rightarrow 0$$ near $k\sim k_F$ and $\omega = 0$

Total energy: We proved before that $E_{tot} = T\sum_{p,\omega_m}\left[\varepsilon_p - \cancel{\mu} + \frac{1}{2}\Sigma_p(i\omega_m)\right]G_p(i\omega)$

For Σ^x we have $\Delta E_{tot} = \frac{1}{2}\frac{1}{\beta}\sum_{i\omega}\Sigma^x_k G_k(i\omega) = \sum_k \frac{1}{2}\Sigma^x_k n_k$

$$\Delta E_{tot} = \sum_{k,s}\left(\cancel{a_0^2 k^2} - \frac{1}{2}\frac{2k_F a_0}{\pi}S\left(\frac{k}{k_F}\right)\right)n_k = \underset{\uparrow\ \text{spin}}{2}V\int_0^{k_F}\frac{d^3k}{(2\pi)^3}\left(\cancel{a_0^2k^2} - \frac{k_F a_0}{\pi}S\left(\frac{k}{k_F}\right)\right) = \frac{V}{\pi^2}\int_0^{k_F}dk\,k^2\left(\cancel{a_0^2k^2} - \frac{k_F a_0}{\pi}S\left(\frac{k}{k_F}\right)\right)$$

$$\Delta E_{tot} = \frac{V}{\pi^2}\left[\cancel{\frac{k_F^5 a_0^2}{5}} - \frac{k_F^4 a_0}{\pi}\int_0^1 dx\,x^2 S(x)\right] = \underbrace{\frac{V}{\pi^2}\frac{k_F^3}{3}}_{=(Vn^0)}\left[\underbrace{\cancel{\frac{3}{5}(a_0k_F)^2}}_{\uparrow\ \cancel{\frac{3}{5}\left(\frac{9\pi}{4}\right)^{2/3}}\frac{1}{r_s^2}} - \frac{3k_F}{\pi}\underbrace{\int_0^1 dx\,x^2 S(x)}_{\frac{1}{2}}\right]$$

$$\frac{3}{2\pi}\left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{r_s}$$

Note: $\int_0^1 dx\,x^2 S(x) = \frac{1}{2}$

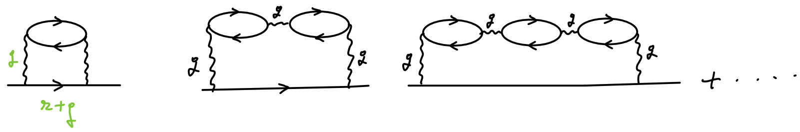
$$\frac{E_{tot}}{Ry\cdot V n_0} = \frac{3}{5}\cdot\left(\frac{9\pi}{4}\right)^{2/3}\frac{1}{r_s^2} - \frac{3}{2\pi}\left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{r_s} = \frac{2.2099}{r_s^2} - \underline{\underline{\frac{0{,}91633}{r_s}}}$$

Note also: $n \equiv \frac{3}{4\pi a_0^3 r_s^3} = 2\int\frac{d^3k}{(2\pi)^3}n_k = 2\int_0^{k_F}\frac{dk\,4\pi k^2}{8\pi^3} = \frac{1}{\pi^2}\frac{k_F^3}{3}$ hence $k_F = \left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{a_0 r_s}$

we know $\frac{\hbar^2}{2m a_0^2} = 1Ry = 13.6\,eV$ hence $\varepsilon_k = \frac{\hbar^2 k^2}{2m}$ in Ry is $\varepsilon_k = 1Ry\cdot a_0^2 k^2$

Evaluate Feynman diagrams of the form! David Pines and Bohm

$\Sigma_k(i\omega) =$



RPA

$$\Sigma_k(i\omega) = -\frac{1}{\beta}\sum_{q,i\Omega} \frac{V_q^2}{V}\, G^0_{k+q}(i\omega+i\Omega)\left[P_q(i\Omega) + V_q P_q^2(i\Omega) + \cdots\right] = -\frac{1}{\beta V}\sum_{q,i\Omega} V_q^2\, G^0_{k+q}(i\omega+i\Omega)\,\frac{P_q(i\Omega)}{1 - V_q P_q(i\Omega)}$$

one more order, but also one more loop, hence +1

where: $P_q(i\Omega) = \frac{1}{\beta V}\sum_{i\omega,k,s} G^0_k(i\omega)\, G^0_{k+q}(i\omega+i\Omega)$

$$P_q(i\Omega) = \frac{1}{\beta V}\sum_{k,s,i\omega} \frac{1}{i\omega-\varepsilon_k}\,\frac{1}{i\omega+i\Omega-\varepsilon_{k+q}} = \frac{1}{\beta V}\sum_{k,s,i\omega}\left(\frac{1}{i\omega-\varepsilon_k} - \frac{1}{i\omega+i\Omega-\varepsilon_{k+q}}\right)\frac{1}{i\Omega+\varepsilon_k-\varepsilon_{k+q}}$$

$$= \frac{1}{V}\sum_{k,s}\frac{f(\varepsilon_k)-f(\varepsilon_{k+q})}{i\Omega+\varepsilon_k-\varepsilon_{k+q}}$$

$$P_q(\Omega+i\delta) = 2\int\frac{d^3k}{(2\pi)^3}\,\frac{f(\varepsilon_k)-f(\varepsilon_{k+q})}{\Omega+\varepsilon_k-\varepsilon_{k+q}+i\delta} = 2\int\frac{d^3k}{(2\pi)^3}\left[\frac{f(\varepsilon_k)}{\Omega+\varepsilon_k-\varepsilon_{k+q}+i\delta} - \frac{f(\varepsilon_k)}{\Omega+\varepsilon_{k-q}-\varepsilon_k+i\delta}\right]$$

$$P_q(\Omega+i\delta) = \frac{2\cdot 2\pi}{8\pi^3}\int_0^{k_F} dk\, k^2\int_{-1}^{1}dx\left[\frac{1}{\Omega+k^2-(k^2+q^2+2kqx)+i\delta} - \frac{1}{\Omega+(k^2+q^2-2kqx)-k^2+i\delta}\right]$$

$$P_q(\Omega+i\delta) = \frac{1}{2\pi^2}\int_0^{k_F} dk\, k^2\int_{-1}^{1}dx\left[\frac{1}{\Omega-q^2-2kqx+i\delta} - \frac{1}{\Omega+q^2-2kqx+i\delta}\right]$$

$$P_q(\Omega+i\delta) = \frac{1}{2\pi^2}\int_0^{k_F} dk\, k^2\left[-\frac{1}{2kq}\ln(\Omega-q^2-2kqx+i\delta) + \frac{1}{2kq}\ln(\Omega+q^2-2kqx+i\delta)\right]_{-1}^{1}$$

$$P_q(\Omega+i\delta) = \frac{1}{4\pi^2 q}\int_0^{k_F} dk\, k\left[\ln\left(\frac{\Omega-q^2+2kq+i\delta}{\Omega-q^2-2kq+i\delta}\right) + \ln\left(\frac{\Omega+q^2-2kq+i\delta}{\Omega+q^2+2kq+i\delta}\right)\right]$$

$\frac{\Omega}{k_F^2} \equiv x \qquad \frac{q}{k_F} = y \qquad \frac{k}{k_F} = u$

$$P\left(y=\frac{q}{k_F},\, x=\frac{\Omega+i\delta}{k_F^2}\right) = \frac{k_F}{4\pi^2}\,\frac{1}{y}\int_0^1 du\, u\left[\ln\left(\frac{-x+y^2-2yu}{-x+y^2+2yu}\right) + \ln\left(\frac{x+y^2-2yu}{x+y^2+2yu}\right)\right]$$

$$-\frac{1}{y}\int_0^1 du\, u\,\ln\left(\frac{x+y^2-2yu}{x+y^2+2yu}\right) = \frac{x+y^2}{2y^2} - \frac{(x+y^2)^2-4y^2}{8y^3}\left[\ln(x+y^2+2y) - \ln(x+y^2-2y)\right]$$

$$= \frac{x}{2y^2} + \frac{1}{2} - \frac{(x+y^2)^2-4y^2}{8y^3}\left[\ln(x+y^2+2y) - \ln(x+y^2-2y)\right]$$

$$= \frac{x}{2y^2} + \mathcal{P}(x,y)$$

$$\mathcal{P}(x,y) \equiv \frac{1}{2} - \left[\frac{(x+y^2)^2-4y^2}{8y^3}\right]\left[\ln(x+y^2+2y) - \ln(x+y^2-2y)\right]$$

$$P\left(y=\frac{q}{k_F},\, x=\frac{\Omega+i\delta}{k_F^2}\right) = -\frac{k_F}{4\pi^2}\left[\mathcal{P}\left(-\frac{\Omega+i\delta}{k_F^2},\, \frac{q}{k_F}\right) + \mathcal{P}\left(\frac{\Omega+i\delta}{k_F^2},\, \frac{q}{k_F}\right)\right]$$

Note $\displaystyle\int_0^{k_F} dk\, k \left[\ln(a+bk) - \ln(a-bk)\right] = \frac{a}{b} k_F + \frac{a^2 - k_F^2 b^2}{2b^2}\left[\ln(a - k_F b) - \ln(a + k_F b)\right]$

hence $a = \Omega - q^2$, $b = 2q$ $\qquad$ $a = \Omega + q^2$, $b = -2q$

$$P_q(\Omega+i\delta) = \frac{1}{4\pi^2 q}\left[\frac{\Omega - q^2}{2q} k_F + \frac{(\Omega-q^2)^2 - 4q^2k_F^2}{8q^2}\ln\left(\frac{\Omega - q^2 - 2k_F q}{\Omega - q^2 + 2k_F q}\right) + \frac{\Omega + q^2}{-2q}k_F + \frac{(\Omega+q^2)^2 - 4q^2k_F^2}{8q^2}\ln\left(\frac{\Omega+q^2+2k_F q}{\Omega+q^2-2k_F q}\right)\right]$$

$$P_q(\Omega+i\delta) = \frac{1}{4\pi^2 q}\left[-q k_F + \frac{(\Omega-q^2)^2 - 4q^2k_F^2}{8q^2}\ln\left(\frac{\Omega - q^2 - 2k_F q}{\Omega - q^2 + 2k_F q}\right) + \frac{(\Omega+q^2)^2 - 4q^2k_F^2}{8q^2}\ln\left(\frac{\Omega+q^2+2k_F q}{\Omega+q^2-2k_F q}\right)\right]$$

$$P_q(\Omega+i\delta) = -\frac{k_F}{4\pi^2}\left[1 - \frac{(\Omega-q^2)^2 - 4q^2k_F^2}{8q^3k_F}\ln\left(\frac{\Omega - q^2 - 2k_F q}{\Omega - q^2 + 2k_F q}\right) - \frac{(\Omega+q^2)^2 - 4q^2k_F^2}{8q^3k_F}\ln\left(\frac{\Omega+q^2+2k_F q}{\Omega+q^2-2k_F q}\right)\right]$$

$$P_q(\Omega+i\delta) = -\frac{k_F}{4\pi^2}\left[1 - \frac{1}{8k_F q}\left\{\left[\frac{(\Omega-q^2)^2}{q^2} - 4k_F^2\right]\ln\left(\frac{\Omega - q^2 - 2k_F q}{\Omega - q^2 + 2k_F q}\right) + \left[\frac{(\Omega+q^2)^2}{q^2} - 4k_F^2\right]\ln\left(\frac{\Omega+q^2+2k_F q}{\Omega+q^2-2k_F q}\right)\right\}\right]$$

$$P_q(\Omega+i\delta) = -\frac{k_F}{4\pi^2}\left[1 - \frac{1}{8k_F q}\left\{\left[\frac{(\Omega-q^2)^2}{q^2} - 4k_F^2\right]\ln\left(\frac{\Omega - q^2 - 2k_F q}{\Omega - q^2 + 2k_F q}\right) + \left[\frac{(\Omega+q^2)^2}{q^2} - 4k_F^2\right]\ln\left(\frac{\Omega+q^2+2k_F q}{\Omega+q^2-2k_F q}\right)\right\}\right]$$

$$\Delta E_{tot} = \frac{I}{2} \sum_{k, i\omega, s} G^0_{ks}(i\omega) \Sigma_{ks}(i\omega)$$

Note G^0 rather than G!

Recall: $$\Sigma_k(i\omega) = -\frac{1}{\beta V} \sum_{q, i\Omega} v_q^2 \, G^0_{k+q}(i\omega + i\Omega) \frac{P_q(i\Omega)}{1 - v_q P_q(i\Omega)}$$

Hence $$\Delta E_{tot} = -\frac{1}{2V\beta^2} \sum_{k, q, i\omega, i\Omega, s} G^0_{ks}(i\omega) G^0_{k+q}(i\omega + i\Omega) v_q^2 \frac{P_q(i\Omega)}{1 - v_q P_q(i\Omega)} \; ; \quad \text{but } P_q(i\Omega) = \frac{1}{\beta V} \sum_{i\omega, k, s} G^0_k(i\omega) G^0_{k+q}(i\omega + i\Omega)$$

$$\Delta E_{tot} = -\frac{1}{2\beta} \sum_{q\, i\Omega} v_q^2 \frac{P_q^2(i\Omega)}{1 - v_q P_q(i\Omega)}$$

$$= -\frac{1}{2} \sum_q \oint \frac{dz}{2\pi i} n(z) \left[\frac{v_q^2 P_q^2(z)}{1 - v_q P_q(z)} \right]$$

$$= -\frac{1}{2} \sum_q \int \frac{dx}{\pi} n(x) \, \mathrm{Im} \left\{ \frac{v_q^2 P_q^2(x)}{1 - v_q P_q(x)} \right]$$

$$\boxed{\Delta E_{tot} = -\frac{V}{2} \int \frac{d^3q}{(2\pi)^3} \int \frac{dx}{\pi} n(x) \, \mathrm{Im} \left\{ \frac{v_q^2 P_q^2(x)}{1 - v_q P_q(x)} \right]}$$

$$P_q(\Omega + i\delta) \equiv -\frac{k_F}{4\pi^2} \left[\mathcal{P}\left(\frac{\Omega}{k_F^2} + i\delta, \frac{q}{k_F}\right) + \mathcal{P}\left(-\frac{\Omega}{k_F^2} - i\delta, \frac{q}{k_F}\right) \right]$$

$$\mathcal{P}(x, y) \equiv \frac{1}{2} - \left[\frac{(x + y^2)^2 - 4y^2}{8y^3} \right] \left[\ln(x + y^2 + 2y) - \ln(x + y^2 - 2y) \right]$$

$$= -\frac{V}{2} \int_0^\infty \frac{dq \, 4\pi q^2}{8\pi^3} \int_{-\infty}^{\infty} \frac{d\Omega}{\pi} n(\Omega) \, \mathrm{Im} \left\{ \frac{v_q P_q(\Omega + i\delta)}{1 - v_q P_q(\Omega + i\delta)} - v_q P_q(\Omega + i\delta) \right]$$

$$v_q P_q(\Omega) = \frac{8\pi}{q^2} \left(-\frac{k_F}{4\pi^2} \right) \left[\mathcal{P}\left(\frac{\Omega}{k_F^2} + i\delta, \frac{q}{k_F}\right) + \mathcal{P}\left(-\frac{\Omega}{k_F^2} - i\delta, \frac{q}{k_F}\right) \right]$$

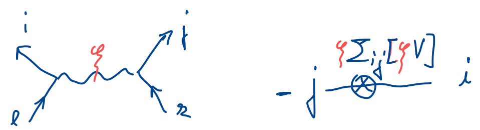
$$= -\frac{2}{\pi} \frac{k_F}{q^2} \left[\mathcal{P}\left(\frac{\Omega}{k_F^2} + i\delta, \frac{q}{k_F}\right) + \mathcal{P}\left(-\frac{\Omega}{k_F^2} - i\delta, \frac{q}{k_F}\right) \right]$$

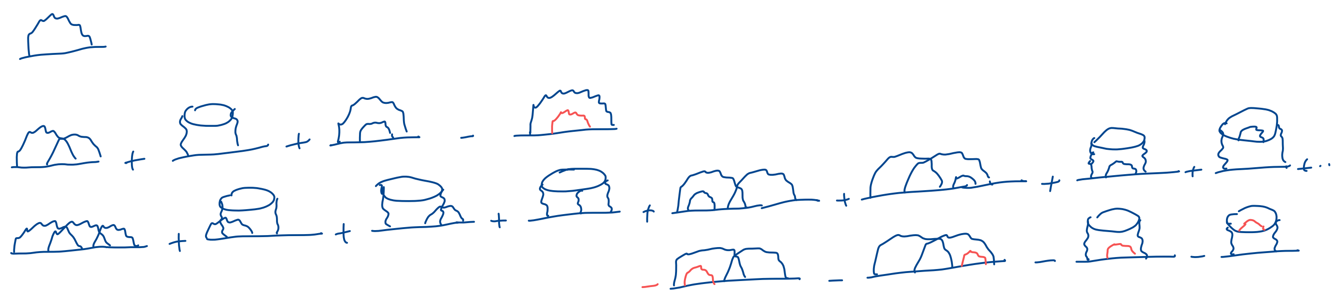
Bold Expansion (Skip)

$$G_{i_1 i_2}(\tau_1-\tau_2)\sum_{m=0}^{\infty}\int \mathcal{D}[\psi^+\psi]\, e^{\int_0^\beta \psi^+[G^0]^{-1}\psi - \Delta S(V)} \qquad \psi_{i_1}(\tau_1)\psi^+_{i_2}(\tau_2)$$

$$=\sum_{m=0}^{\infty}\int \mathcal{D}[\psi^+\psi]\, e^{\int_0^\beta \psi^+([G^0]^{-1}-\Sigma)\psi - \int_0^\beta d\tau\left(\xi \frac{1}{2} V_{ij\ell\ell}\psi_i^+\psi_j^+\psi_\ell\psi_\ell - \xi\Sigma_{ij}[\xi V]\psi_i^+\psi_j\right)} \psi_{i_1}(\tau_1)\psi^+_{i_2}(\tau_2)$$

$$=\sum_{m=0}^{\infty}\frac{(-1)^m}{m!}\left\langle\left(\int_0^\beta d\tau d\tau' \frac{1}{2}\xi V_{ij\ell\ell}\psi_i^+\psi_j^+\psi_\ell\psi_\ell - \xi\Sigma_{ij}[\xi V]\psi_i^+\psi_j\right)^m \psi_{i_1}(\tau_1)\psi^+_{i_2}(\tau_2)\right\rangle_{ss}^{\text{connected}}$$





$$Z=\int \mathcal{D}[\psi^+\psi]\, e^{\int\psi^+[[G^0]^{-1}-\Sigma]\psi - \int(\xi\Delta\mathcal{L} - \xi\Sigma[\xi V]\psi^+\psi)d\tau}$$

$$=\sum_{m=0}^{\infty}\int \mathcal{D}[\psi^+\psi]\, e^{\int\psi^+[G^{-1}]\psi}\frac{(-1)^m}{m!}\left[\int(\xi\Delta\mathcal{L} - \xi\Sigma[\xi V]\psi^+\psi)d\tau\right]^m = \exp\left(\sum_{m=0}^{\infty}\frac{(-1)^m}{m!}\frac{1}{\Delta_{\mathcal{D}}}\left\langle\left[\int(\xi\Delta\mathcal{L} - \xi\Sigma[\xi V]\psi^+\psi)d\tau\right]^m\right\rangle_{\text{connected, topologically distinct}}\right)$$

$$\ln Z = \ln Z^{(0)} + \sum_{m=1,\alpha}^{\infty}\mathcal{D}_{m\alpha}[G,\Delta\mathcal{L},\Sigma]$$

$$\ln Z = \mathrm{Tr}\ln G + \sum_{m=1,\alpha}^{\infty}\Phi_{m\alpha}^{\text{skeleton}}\times(1-\Delta_\alpha)$$

where Δ_α is symmetry factor, such that $\dfrac{\delta\Phi_{m\alpha}}{\delta G}=\Sigma_{m\alpha}$

hence $\sum_{m\alpha}\Phi_{m\alpha}^{\text{skeleton}}(1-\Delta_\alpha) = \Phi^{\text{skeleton}} - \mathrm{Tr}(\Sigma G)$

$$\langle m\rangle = \sum_{m=0}^{\infty}\int \mathcal{D}[\psi^+\psi]\, e^{\int_0^\beta\psi^+[G_0^{-1}-\Sigma]\psi}\frac{(-1)^m}{m!}(\Delta S - \psi^+\Sigma\psi)^m\, m$$

$$=\langle \Delta S - \psi^+\Sigma\psi\rangle_{ss}$$

$$\frac{1}{\beta}\left(\mathrm{Tr}(\Delta G) - \mathrm{Tr}(\Sigma_p G_p)\right)$$

Homogeneous electron gas : Plasma theory of interacting electrons

We have interacting electrons in a uniform positive background with charge $n_0 = \frac{N_e}{V}$ where N_e is number of electrons and V is volume.

This background charge keeps overall charge neutrality and ensures electron density n_0 to be uniform in space.

$$v_c(\vec{r}-\vec{r}') = \frac{2}{|\vec{r}-\vec{r}'|} \quad (\text{In Ry units}) \quad \text{then} \quad v_q = \frac{8\pi}{q^2}$$

$$S[\psi] = \int_0^\beta d\tau \sum_s \int d^3r\, \psi^+_s(\vec{r},\tau)\left(\frac{\partial}{\partial\tau} - \mu - \frac{\nabla^2}{2m}\right)\psi_s(\vec{r},\tau) + \int_0^\beta d\tau \sum_{ss'} \int d^3r\, d^3r'\, \frac{1}{2} \psi^+_s(\vec{r})\, \psi^+_{s'}(\vec{r}')\, \psi_{s'}(\vec{r}')\, \psi_s(\vec{r})\, v_c(\vec{r}-\vec{r}')$$

$$- \int_0^\beta d\tau \int d^3r\, d^3r'\, \psi^+_s(\vec{r},\tau)\psi_s(\vec{r},\tau)\, n_0(\vec{r}')\, v_c(\vec{r}-\vec{r}')$$

$$+ \int_0^\beta d\tau \int d^3r\, d^3r'\, \frac{1}{2} n_0(\vec{r})\, n_0(\vec{r}')\, v_c(\vec{r}-\vec{r}')$$

$$\psi_s(\vec{r}) = \frac{1}{\sqrt{V}} \sum_k e^{i\vec{k}\cdot\vec{r}}\, \psi_{ks}(\tau)$$

$$v_c(\vec{r}) = \frac{1}{V}\sum_q v_q\, e^{i\vec{q}\cdot\vec{r}} = \int \frac{d^3q}{(2\pi)^3} v_q\, e^{i\vec{q}\cdot\vec{r}}$$

; note $\sum_q \to V\int \frac{d^3q}{(2\pi)^3}$ hence $\frac{2}{r} \to \frac{8\pi}{q^2}$

$$S[\psi] = \int_0^\beta d\tau \sum_{k,s} \psi^+_{ks}(\tau)\left(\frac{\partial}{\partial\tau} - \mu + \frac{k^2}{2m}\right)\psi_{ks}(\tau) + \int_0^\beta d\tau \sum_{\substack{ss' \\ kk'q}} \frac{1}{2V} v_q\, \psi^+_{k+q s}\, \psi^+_{k'-q s'}\, \psi_{k's'}\, \psi_{ks}$$

$$- \int_0^\beta d\tau \underbrace{\sum_{\substack{s \\ kq}} \psi^+_{k+q s}\psi_{ks}\, n_0}_{-N_e v_{q=0} n_0}\, \underbrace{v_q \frac{1}{V}\underbrace{\int d^3r'\, e^{i\vec{q}\cdot\vec{r}'}}_{\delta_{q=0}}}_{v_c(\vec{r}-\vec{r}')} + \underbrace{\int_0^\beta d\tau\, \frac{1}{2} n_0^2\, \frac{1}{V}\sum_q v_q \underbrace{\int e^{i\vec{q}\cdot(\vec{r}-\vec{r}')} d^3r\, d^3r'}_{\delta_{q=0}\cdot V^2}}_{+\frac{1}{2}(n_0 V)^2 \frac{1}{V} v_{q=0}}$$

$$n_0 = \frac{N_e}{V}$$

at $q=0$: $\frac{1}{2V} v_{q=0} N_e^2$

Conclusion : the three term exactly cancel : we are left with

$$S[\psi] = \int_0^\beta d\tau \sum_{k,s} \psi^+_{ks}(\tau)\left(\frac{\partial}{\partial\tau} - \mu - \frac{k^2}{2m}\right)\psi_{ks}(\tau) + \int_0^\beta d\tau \sum_{\substack{ss' \\ kk' \\ q\neq 0}} \frac{1}{2V} v_q\, \psi^+_{k+q s}\, \psi^+_{k'-q s'}\, \psi_{k's'}\, \psi_{ks}$$

We did perturbative calculation for the homework. Here we will use Functional integral to accomplish the same!

For the second homework we derived the effective electron-electron interaction from electron phonon coupling. Here we want to accomplish the opposite. Given electron-electron interaction, we want to rewrite it in terms of electron-boson interaction. This is accomplished by Hubbard-Stratonovich transformation.

We start by identity $I = \int D[\phi^+\phi]\, e^{-\frac{1}{2}\sum_q \int_0^\beta d\tau\, \phi^+_q(\tau) V_q^{-1} \phi_q(\tau)} =$

contains prefactor $D[\phi^+\phi] = \frac{\prod_q d(\phi_q, \phi_q)}{\pi^N Det(V_q)}$

We will use $\phi(\vec r,\tau) \in R$, hence $\phi^+_q = \phi_{-q}$

Next, shift variable $\phi_q \to \phi_q + i V_q \rho_q$ (note, we need i for repulsive interaction!)

$$\phi^+_q = \phi_{-q} \to \phi_{-q} + i V_{-q} \rho_{-q}$$

$$I = \int D[\phi^+\phi]\, e^{-\frac{1}{2\beta}\sum_{q\,\Omega_m} (\phi^+_{qm} + i\rho_{-q,-m} V_{-q}) V_q^{-1} (\phi_{qm} + i V_q \rho_{qm})}$$

$$-\frac{1}{2\beta}\left[\phi^+_{qm} V_q^{-1} \phi_{qm} + i\rho_{-q,-m}\phi_{qm} + i\phi^+_{qm}\rho_{qm} - V_q \rho_{-q,-m}\rho_{qm}\right]$$

$$e^{-\frac{1}{2\beta}\sum_{q\Omega_m} V_q \rho_{qm}\rho_{-q,-m}} = \int D[\phi^+,\phi]\, e^{-\frac{1}{2\beta}\sum_{qm}\left[\phi^+_{qm} V_q^{-1}\phi_{qm} + \underbrace{i\rho_{qm}\phi_{-q,-m} + i\rho_{qm}\phi^+_{qm}}_{2i\rho_{qm}\phi_{-q,-m}}\right]}$$

to exclude $q=0$, we set $\phi_{q=0}=0$!

here we need $q \neq 0$

Here $\rho_{qm} = \int_0^\beta \sum_{k\sigma} \psi^+_{k+q\,\sigma}(\tau)\, \psi_{k\sigma}(\tau)\, e^{-i\Omega_m\tau}\, d\tau$

Hence $\frac{1}{2\beta}\sum_{i\Omega_m} \rho_{qm}\rho_{-q,-m} = \frac{1}{2\beta}\sum_{\substack{i\Omega_m\\ k\sigma\\ k'\sigma'}} \iint_0^\beta \psi^+_{k+q\sigma}(\tau)\psi_{k\sigma}(\tau)\psi^+_{k'-q\sigma'}(\tau')\psi_{k'\sigma'}(\tau')\, e^{-i\Omega_m\tau + i\Omega_m\tau'}\, d\tau\, d\tau'$

$$\frac{1}{\beta}\sum_{i\Omega_m} e^{i\Omega_m(\tau-\tau')} = \delta(\tau-\tau')$$

$$= \frac{1}{2}\int_0^\beta d\tau \sum_{\substack{kk'\\ \sigma\sigma'}} \psi^+_{k+q\sigma}(\tau)\psi_{k\sigma}(\tau)\psi^+_{k'-q\sigma'}(\tau)\psi_{k'\sigma'}(\tau)$$

$$Z = \int \mathcal{D}[\psi^\dagger\psi]\, e^{-\int_0^\beta d\tau \sum_{k,\sigma} \psi^\dagger_{k\sigma}(\tau)(\partial_\tau - \mu + \varepsilon_k)\psi_{k\sigma}(\tau) \;-\; \int_0^\beta d\tau \sum_{q\neq 0} \frac{1}{2} V_q\, \rho_q(\tau)\rho_{-q}(\tau)}$$

$$= \int \mathcal{D}[\psi^\dagger\psi] \int \mathcal{D}[\phi^\dagger\phi]\, e^{-\frac{1}{\beta}\sum_{k,\sigma,m} \psi^\dagger_{k\sigma m}(-i\omega_m - \mu + \varepsilon_k)\psi_{k\sigma m} - \frac{1}{2\beta}\sum_{qm}\left[\phi^\dagger_{qm} V_q^{-1}\phi_{qm} + 2i\,\rho_{qm}\,\phi_{-q,-m}\right]}$$

to set $q\neq 0$ we will assume $\phi_{q=0} = 0$

$$S_{eff} = \frac{1}{\beta}\sum_{k\sigma m} \psi^\dagger_{k\sigma m}\left(-i\omega_m - \mu + \varepsilon_k\right)\psi_{k\sigma m} + \frac{1}{\beta}\sum_{q\, m}\left(\frac{1}{2}\phi_{-q,-m} V_q^{-1}\phi_{qm} + i\,\phi_{q,m}\,\rho_{-q,-m}\right)$$

$$\rho_{qm} = \int_0^\beta \sum_{k\,\sigma} \psi^\dagger_{k+q\,\sigma}(\tau)\,\psi_{k\sigma}(\tau)\, e^{-i\Omega_m\tau}\, d\tau \qquad \psi_k(\tau) = \frac{1}{\sqrt{\beta}}\sum_{i\omega_m} e^{-i\omega_m\tau}\psi_{km}$$

$$\rho_{qm} = \sum_{\substack{k\sigma\\ m\, m'}} \psi^\dagger_{k+q,\sigma,m+m'}\,\psi_{k,\sigma,m}\,\underbrace{\frac{1}{\beta}\int_0^\beta e^{+i(\omega_m+\Omega_m)\tau - i\omega_m\tau - i\Omega_m\tau}\, d\tau}_{1}$$

$$S_{eff} = \frac{1}{\beta}\sum_{\substack{k\sigma m\\ m',q}} \psi^\dagger_{k-q,\sigma,m-m'}\left((-i\omega_m - \mu + \varepsilon_k)\,\delta_{\Omega_m, q=0} + i\,\phi_{qm}\right)\psi_{k\sigma m} + \frac{1}{\beta}\sum_{q\, m}\left(\frac{1}{2}\phi_{-q,-m} V_q^{-1}\phi_{qm}\right)$$

Now we have only quadratic terms for fermions. We can integrate fermions out.

We have interaction mediated by bosons, instead of direct Coulomb.

Note:
- $i\phi_q$ is because V_q is repulsive
- bosons have no dynamical term $\phi^\dagger_q\left(\frac{\partial}{\partial\tau} + \omega_q\right)\phi_q$ hence interaction is static.

- Is Hubbard-Stratonovich decoupling of interaction unique? No.

There are three decouplings:

- density-density channel
- Cooper channel
- Fock-exchange channel

$$\hat{V} = \sum_{\substack{k k' \\ \sigma, q}} \frac{1}{2} \psi^+_{k+q\sigma} \psi^+_{k'-q\sigma'} v_q \psi_{k'\sigma'} \psi_{k\sigma}$$

Δ^+ $\quad$ ρ_q $\quad$ ρ^x

$$\rho_q = \sum_{k,\sigma} \psi^+_{k+q\sigma} \psi_{k\sigma}$$

$$\Delta_{k+k'} = \sum_{\sigma\sigma'} \psi_{k'\sigma'} \psi_{k\sigma} \, g^{\sigma\sigma'}_{kk'}$$

needed for SC. $\qquad$ singlet / triplet channel

- Why is H.S. useful? We want to find better saddle point approximations.

The saddle poin approximation in original fermion only formulation is the Hartree Fock approximation.

Namely:
$$\frac{\delta S}{\delta \psi^+_{(r,\tau)}} = 0 = \left(\frac{\partial}{\partial\tau} - \mu - \frac{\hbar^2\nabla^2}{2m}\right)\psi_\sigma(\vec{r},\tau) + \underbrace{\int d^3r' \sum_{\sigma'} \psi^+_{\sigma'}(\vec{r}') v(\vec{r}-\vec{r}') \psi_{\sigma'}(\vec{r}') \psi_\sigma(\vec{r})}_{\text{mean field}}$$

$$\int d^3r' \, v_c(\vec{r}-\vec{r}') \psi_\sigma(\vec{r}) \langle \psi^+_{\sigma'}(\vec{r}') \psi_{\sigma'}(\vec{r}')\rangle$$
$$- \int d^3r' \, v_c(\vec{r}-\vec{r}') \psi_{\sigma'}(\vec{r}') \langle \psi^+_{\sigma'}(\vec{r}') \psi_\sigma(\vec{r})\rangle$$

hence
$$\left(\left(\frac{\partial}{\partial\tau} - \mu - \frac{\hbar^2\nabla^2}{2m} + v_H(\vec{r})\right)\delta(\vec{r}-\vec{r}') - v_x(\vec{r}',\vec{r})\right)\psi_\sigma(\vec{r}',\tau) = 0$$

where
$$\left.\begin{aligned} v_H(\vec{r}) &= \int d^3r' \, v_c(\vec{r}-\vec{r}') \, n(\vec{r}') \\ v_x(\vec{r}',\vec{r}) &= v_c(\vec{r}-\vec{r}') \, n(\vec{r}',\vec{r}) \end{aligned}\right\} \text{Hartree-Fock}$$

By changing the variables to electron – boson interaction we will generate different saddle point approximation.

The steps we need to take:

1) Integrate out fermions
2) Consider saddle point in bosonic variables
3) Check fluctuations around the saddle point

$$S_{eff} = \frac{1}{\beta}\sum_{\substack{k\sigma n\\ m, q}} \psi^+_{k-q,\sigma, n-m} \left((-i\omega_n - \mu + \varepsilon_k)\delta_{\Omega_m, q=0} + i\,\phi_{qm}\right)\psi_{k\sigma n} + \frac{1}{\beta}\sum_{q\,m}\left(\frac{1}{2}\phi_{-q,-m} V_q^{-1}\phi_{qm}\right)$$

$$Z = \int D[\phi^+\phi]\int D[\psi^+\psi]\, e^{-\frac{1}{\beta}\sum_{qm}\frac{1}{2}\phi^+_{qm}V_q^{-1}\phi_{qm} + \frac{1}{\beta}\sum_{\substack{k\sigma n\\ m q}}\psi^+_{k-q,\sigma,n-m}\left((i\omega_n+\mu-\varepsilon_k)\delta_{q\Omega_m=0} - i\,\phi_{qm}\right)\psi_{k\sigma n}}$$

$$\text{Define } \left[\mathcal{G}_0^{-1}[\phi]\right]_{p_1 n_1, p_2 n_2} = \left(i\omega_{n_2} + \mu - \varepsilon_{p_2}\right)\delta_{p_1=p_2}\delta_{n_1=n_2} - i\,\phi_{p_2-p_1, n_2-n_1}$$

$$Z = \int D[\phi^+\phi]\, e^{-\frac{1}{\beta}\sum_{qm}\frac{1}{2}\phi^+_{qm}V_q^{-1}\phi_{qm}}\, Det(-\mathcal{G}_0^{-1}) = \int D[\phi^+\phi]\, e^{-\frac{1}{\beta}\sum_{qm}\frac{1}{2}\phi^+_{qm}V_q^{-1}\phi_{qm} + \ln Det(-\mathcal{G}_0^{-1})}$$

$\ln Det\, A = Tr \ln A$ because in eigenbasis $\ln Det\, A = \ln\left(\prod_{\lambda_i} \ln\lambda_i\right) = \sum_{\lambda_i}\ln\lambda_i$

$$Z = \int D[\phi^+\phi]\, e^{-\frac{1}{\beta}\sum_{qm}\frac{1}{2}\phi^+_{qm}V_q^{-1}\phi_{qm} + Tr\ln(-\mathcal{G}_0^{-1}[\phi])}$$

and $\boxed{S_{eff}[\phi] = \frac{1}{\beta}\sum_{qm}\frac{1}{2}\phi^+_{qm}V_q^{-1}\phi_{qm} - Tr\ln(-\mathcal{G}_0^{-1}[\phi])}$

stopped 12/1/2022

Up to here this is exact. Now we start making approximations.

This is highly non linear problem in bosonic ϕ variables.

2) Saddle point: $\frac{\delta S_{eff}[\phi]}{\delta \phi_{\rho m}} = 0 = V_\rho^{-1}\phi^+_{\rho m} - \frac{\delta}{\delta \phi_{\rho m}} \mathrm{Tr}\ln(-\mathcal{G}^{-1}[\phi])$

$$V_\rho^{-1}\phi^+_{\rho m} - \mathrm{Tr}\left(\mathcal{G}\frac{\delta \mathcal{G}^{-1}}{\delta \phi_{\rho m}}\right)$$

$$[\mathcal{G}_\sigma^{-1}[\phi]]_{p_1 m_1, p_2 m_2} = (i\omega_{m_2} + \mu - \varepsilon_{p_2})\delta_{p_1=p_2}\delta_{m_1=m_2} - i\phi_{p_2-p_1, m_2-m_1}$$

$$\frac{\delta \mathcal{G}^{-1}}{\delta \phi_{\rho m}} = -i\,\delta_{p_2-p_1=\rho}\,\delta_{m_2-m_1=m}$$

$$\mathrm{Tr}\left(\mathcal{G}_\sigma \frac{\delta \mathcal{G}_\sigma^{-1}}{\delta \phi_{\rho m}}\right) = \sum_{\substack{m_1 m_2 \\ p_1 p_2 \\ \sigma}} \mathcal{G}_{p_1 m_1; p_2 m_2}\,\delta_{m_1-m_2=m}\,\delta_{p_1-p_2=\rho}\,(-i)$$

Saddle point Eq:
$$\underbrace{V_\rho^{-1}}_{\frac{\rho^2}{8\pi}}\phi^+_{\rho m} = -i\sum_{m_1, p_1, \sigma} \mathcal{G}_{p_1 m_1; p_1-\rho, m_1-m}$$

Guess solution:

For $\rho \neq 0$ $\phi_\rho = 0$ is a solution because $\mathcal{G}[\phi=0] = \mathcal{G}^0$ which we know is translationally invariant, hence $\delta_{p_2=p_1}$ and vanishes at finite ρ.

The point $\rho=0$ is excluded from the model, because uniform background.

3) Fluctuations around saddle point:

Define $G^0 = i\omega_m + \mu - \varepsilon_p$ hence $[\mathcal{G}_\sigma^{-1}]_{p_1 m_1, p_2 m_2} = (G^0)^{-1}\cdot I - i\phi_{p_2-p_1, m_2-m_1}$

Define $\bar{\phi}_{p_1 m_1, p_2 m_2} = \phi_{p_2-p_1, m_2-m_1}$ $\qquad = (G^0)^{-1} I - i\bar{\phi}$

$$S_{eff}[\phi] = \frac{1}{\beta}\sum_{\rho m}\frac{1}{2}\phi^+_{\rho m}V_\rho^{-1}\phi_{\rho m} - \mathrm{Tr}\ln\left(-(G^0)^{-1}(I - iG^0\bar{\phi})\right)$$

$$S_{eff}[\phi] = \frac{1}{\beta}\sum_{\rho m}\frac{1}{2}\phi^+_{\rho m}V_\rho^{-1}\phi_{\rho m} + \underbrace{\mathrm{Tr}\ln(-G^0)}_{S^0} - \mathrm{Tr}\ln(1 - iG^0\bar{\phi}) \quad ; \ln(1-x) = -x - \frac{1}{2}x^2 + \dots$$

$$S_{eff}[\phi] = S^0 + \frac{1}{\beta}\sum_{\rho m}\frac{1}{2}\phi^+_{\rho m}V_\rho^{-1}\phi_{\rho m} + \mathrm{Tr}\Big(\underbrace{iG^0\bar{\phi}}_{\to 0} + \frac{i^2}{2}G^0\bar{\phi}G^0\bar{\phi} + \frac{i^3}{3}(G^0\phi)^3 + \frac{i^4}{4}(G^0\phi)^4 + \dots\Big)$$

G^0 requires $\rho=0$, and $\phi_{\rho=0}=0$

$$S_{eff}[\phi] = S^0 + \frac{1}{\beta}\sum_{\rho m}\frac{1}{2}\phi^+_{\rho m}V_\rho^{-1}\phi_{\rho m} - \frac{1}{2}\mathrm{Tr}(G^0\bar{\phi}G^0\bar{\phi}) \quad -\frac{i}{3}\mathrm{Tr}((G^0\phi)^3) + \frac{1}{4}\mathrm{Tr}((G^0\phi)^4)$$

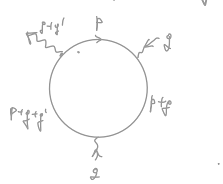
$$S_{eff}[\phi] = S^0 + \frac{1}{\beta}\sum_{q m} \frac{1}{2}\phi^+_{qm} V_q^{-1}\phi_{qm} - \frac{1}{2}\mathrm{Tr}\left(G^0\Phi G^0\Phi\right) - \frac{1}{3}\mathrm{Tr}\left((G^0\phi)^3\right) + \frac{1}{4}\mathrm{Tr}\left((G^0\phi)^4\right)$$

$$-\frac{1}{2}\frac{1}{\beta^2}\sum_{\substack{pp'\sigma\\ mm'}} G^0_{pm,pm}\Phi_{p'-p,m'-m} G^0_{p'm',p'm'}\Phi_{p-p',m-m'}$$

part of Tr when in imaginary frequency

$p-p'=q \quad m-m'=m$

$$S_{eff}[\phi] = S^0 + \frac{1}{\beta}\sum_{qm}\frac{1}{2}\phi_{-q,-m}\phi_{qm}\left[V_q^{-1} - \frac{1}{\beta}\sum_{p,m,\sigma} G^0_p(i\omega_m)G^0_{p-q}(i\omega_m - i\Omega_m)\right] - \frac{1}{3}\frac{1}{\beta^3}\sum G^0_p G^0_{p+q} G^0_{p+q+q'}\phi_q\phi_{q'}\phi_{-q-q'}$$



Define: $P_q(i\Omega) \equiv \frac{1}{\beta}\sum_{p,m,\sigma} G^0_p(i\omega_m)G^0_{p-q}(i\omega_m - i\Omega_m)$

Then

$$S_{eff}[\phi] = S^0 + \frac{1}{\beta}\sum_{qm}\frac{1}{2}\phi_{-q,-m}\phi_{qm}\underbrace{V_q^{-1}\left[1 - V_q P_q(i\Omega)\right]}$$

This is screened coulomb interaction

$$W_q^{-1} \equiv V_q^{-1}\left[1 - V_q P_q(i\Omega)\right]$$
$$= \frac{q^2}{8\pi}\left[1 - \frac{8\pi}{q^2}P_q(i\Omega)\right]$$

We define $\frac{V_q}{\varepsilon_q} = W_q$, i.e., is the screened repulsion, hence $\varepsilon_q = 1 - V_q P_q(i\Omega)$ so that electromagnetic response in a medium is screened $D_{q\omega} = \varepsilon_{q\omega}E_{q\omega}$

$$Z = \int D[\phi^+\phi]\, e^{-S_{eff}[\phi]} = Z_0\left(\mathrm{Det}\left[V_q^{-1} - P_q(i\Omega)\right]\right)^{-\frac{1}{2}}$$ bosonic and real ϕ

$$\ln Z = \ln Z_0 - \frac{1}{2}\ln \mathrm{Det}\left(V_q^{-1} - P_q(i\Omega)\right) = \ln Z_0 - \frac{1}{2}\mathrm{Tr}\ln\left(V_q^{-1} - P_q(i\Omega)\right)$$

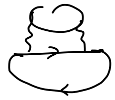
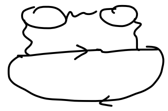
$$-\frac{1}{2}\sum_{\substack{i\Omega\\ q}}\Big(\underbrace{\ln V_q^{-1}}_{\to 0} + \ln\left(1 - V_q P_q(i\Omega)\right)\Big)$$

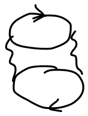
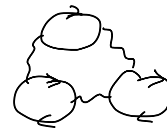
$$\ln Z = \ln Z_0 - \frac{1}{2}\sum_{q, i\Omega}\ln\left(1 - V_q P_q(i\Omega)\right)$$

$$-\beta F = -\beta F_0 - \frac{1}{2}\sum_{\substack{i\Omega\\ q}}\ln\left(1 - V_q P_q(i\Omega)\right)$$

$$F = F_0 + \frac{T}{2}\sum_{i\Omega, q}\ln\left(1 - V_q P_q(i\Omega)\right)$$

To make connection with perturbative RPA results from the homework we note that the interaction energy we used was

$$E_{pot} = \frac{1}{2} Tr(\Sigma G^0) = \frac{1}{2}\Big[$$  $+$  $+$  $+ \cdots \Big]$

$$= \frac{1}{2}\Big[$$  $+$  $+$  $+ \cdots \Big]$

How to get F from E?

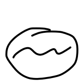
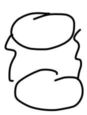
We know that $Z = Tr(e^{-\beta H}) = Tr(e^{-\beta(H_0+V)})$

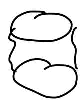
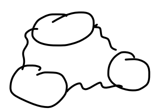
We multiply each interaction by coupling constant λ and take derivative with respect to λ, i.e.,

$$\frac{\delta}{\delta\lambda}\ln Z_\lambda = \frac{\delta}{\delta\lambda}\ln Tr\left(e^{-\beta(H_0+\lambda V)}\right) = \frac{1}{Z_\lambda} Tr\left(e^{-\beta H}(-\beta V)\right) = -\frac{\beta}{\lambda}\frac{Tr(e^{-\beta H}\lambda V)}{Z_\lambda}$$

$$e^{-\beta F} = \ln Z$$

$$\frac{\delta F}{\delta\lambda} = -\frac{1}{\beta}\frac{\delta \ln Z_\lambda}{\delta\lambda} = \frac{1}{\lambda}\langle E_{pot}(\lambda)\rangle \quad \text{then} \quad F = F^0 + \int_0^1 \frac{d\lambda}{\lambda}\langle E_{pot}\rangle$$

Hence $F - F^0 = \frac{1}{2}\int_0^1 \frac{d\lambda}{\lambda}\Big[\lambda$  $+ \lambda^2$  $+ \lambda^3$  $+ \cdots\Big]$

$= \frac{1}{2}\Big[$  $+ \frac{1}{2}$  $+ \frac{1}{3}$  $+ \cdots\Big]$

Hence $F - F^0 = -\frac{T}{2}\sum_{f,i\Omega_m} V_f P_f(i\Omega) + \frac{1}{2}[V_f P_f(i\Omega)]^2 + \frac{1}{3}[V_f P_f(i\Omega)]^3 + \cdots = \frac{T}{2}\sum_{f,i\Omega_m}\ln(1 - V_f P_f(i\Omega_m))$

$$-\frac{1}{2}\Big[X + \frac{1}{2}X^2 + \frac{1}{3}X^3 + \frac{1}{4}X^4 + \cdots\Big] = \frac{1}{2}\ln(1-X)$$

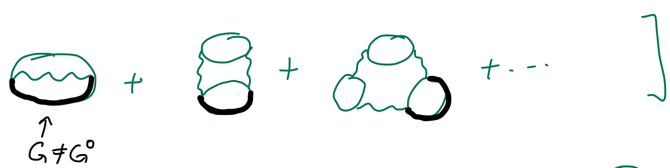
hence identical result for free energy and hence the same G and dielectric response.

Skip this in class, but just for your information.

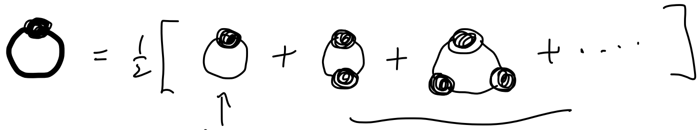
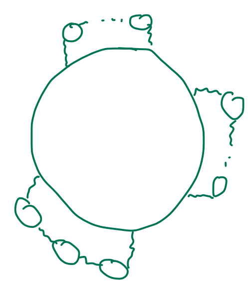
This is actually approximation on top of RPA approximation, and would not work if we were to systematically improve on the self-energy.

$E_{pot} = \frac{1}{2} Tr(\Sigma \cdot G)$ hence

this is G and not G^0 as we used for homework and in plasma theory

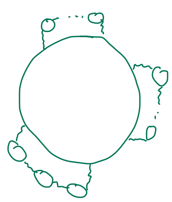
$E_{pot} = \frac{1}{2}\Big[$  $\Big]$

Define $\Sigma =$ 

$E_{pot} = \frac{1}{2}$  $= \frac{1}{2}$ 

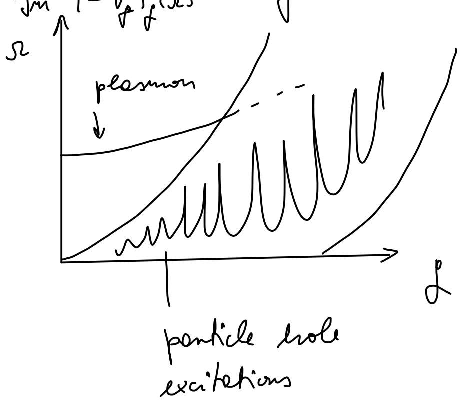
this was used before

these were neglected

$\Omega - \Omega_0 = \frac{1}{2}\int_0^1 \frac{d\lambda}{\lambda}$  $= -\frac{1}{\beta}\sum_{n=0}^{\infty}\left\langle \frac{(-\Delta S)^n}{n!} \right\rangle_0$ connected-topologically distinct and single particle reducible

Conclusion: Saddle point approximation on Hubbard-Stratonovich field, which couples to the density, gives RPA approximation.

$$\mathrm{Im}\,\frac{P_q(\Omega)}{1-V_q P_q(\Omega)} = \chi_q(\Omega) \quad \text{– charge or spin susceptibility}$$



plasmon satisfies $V_q P_q = 1$ and $\varepsilon_q = 1 - V_q P_q = 0$

and $W_q \to \infty$

$$P_q(\Omega+i\delta) \equiv -\frac{k_F}{4\pi^2}\left[\mathcal{P}\left(\frac{\Omega}{k_F^2}+i\delta,\frac{q}{k_F}\right)+\mathcal{P}\left(-\frac{\Omega}{k_F^2}-i\delta,\frac{q}{k_F}\right)\right] \qquad \frac{\Omega}{k_F^2}\equiv x \text{ and } \frac{q}{k_F}=y$$

$$\mathcal{P}(x,y) \equiv \frac{1}{2} - \left[\frac{(x+y^2)^2-4y^2}{8y^3}\right]\left[\ln(x+y^2+2y)-\ln(x+y^2-2y)\right] \; ; \qquad \varepsilon = 1 - V_q P_q$$

$$\lim_{q\to 0} \mathrm{Re}\, P_q$$

$y \to 0$ with $x \gg y$

$$\mathcal{P} \approx \underbrace{-\frac{x}{2y^2}+\frac{4}{3x}}_{\text{odd in } \Omega} - \frac{4(5x-4)}{15x^3}y^2$$

$$-\frac{4}{3}\frac{y^2}{x^2} \quad \text{even in } \Omega$$

$$\lim_{\substack{q\to 0\\ \Omega \text{ finite}}} P_q = -\frac{k_F \cdot 2}{4\pi^2}(-1)\frac{4}{3}\frac{q^2}{k_F^2}\frac{k_F^4}{\Omega^2} = +\frac{2k_F^3}{3\pi^2}\frac{q^2}{\Omega^2}$$

hence
$$\lim_{q\to 0} V_q P_q = \frac{8\pi}{q^2}\frac{q^2}{\Omega^2}\left(\frac{2}{3}\frac{k_F^3}{\pi^2}\right) = \frac{16}{3\pi}\frac{k_F^3}{\Omega^2} = \frac{16\pi}{\Omega^2}\underbrace{\left(\frac{k_F^3}{3\pi^2}\right)}_{= n_0}$$

hence $V_q P_q = 1$ when $\Omega_p^2 = 16\pi n_0$ long lived oscilations plasma frequency.

plasma frequency^2 proportional to density.

Electron phonon interaction in metals & superconductivity

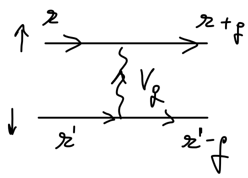
Recall homework problem $\quad H_{e-i} = N \sum_{q,\nu} \frac{i\, q_\nu}{\sqrt{2 M \omega_q}} \left(\phi_{q\nu} + \phi^+_{-q\nu}\right) \rho_q$

When phonons are integrated out, we get

$$S_{eff.}[\psi^+,\psi] = \sum_{k2} \psi^+_{k2}(-i\omega_n + \varepsilon_k)\psi_{k2} - \sum_{kqm} \frac{N^2}{2M} \frac{q^2}{\omega_q^2 + \Omega_m^2} \hat{M}_{q^m} \hat{M}_{-q,-m}$$

Historic introduction to SC

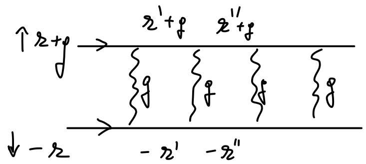
Cooper instability



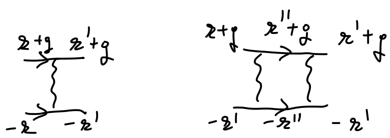
$$\psi^+_{k+q\uparrow}\psi^+_{k'-q\downarrow}\psi_{k'\downarrow}\psi_{k\uparrow} V_q \; ; \; V_q = \begin{cases} -g \; ; & \frac{|k^2-k_F^2|}{2m} < \omega_D \\ 0 & \text{otherwise} \end{cases}$$

Coulomb interaction, but only between $\uparrow$ and $\downarrow$ electron

If $V_q < 0$, Cooper noticed that something dramatic occurs, i.e., metal is unstable. Consider the ladder diagrams



the interaction is approximated with a constant for simplicity. The constant is negative



$$\Gamma = g - g\left(-\tfrac{1}{\beta}\right) \underbrace{\sum_{\substack{i\omega''_m \\ k''}} \mathcal{G}_{-k''}(-i\omega''_m)\, \mathcal{G}_{k''+q}(i\omega_{m''} + i\Omega)}_{B(i\Omega)} + (gB)^2 + \cdots = \frac{g}{1 - gB}$$

$$B_q(i\Omega) = \frac{1}{\beta} \sum_{\substack{i\omega''_m \\ k''}} \mathcal{G}_{-k''}(-i\omega''_m)\, \mathcal{G}_{k''+q}(i\omega_{m''} + i\Omega)$$

Note: ladders have opposite sign as bubbles (because no new fermionic loop) but here $g<0$, so the overall sign seems the same as in RPA. But $B_q(\Omega)$ is very different from $P_q(i\Omega)$

From HW II jump to *

$$B_q(i\Omega) = \frac{1}{\beta}\sum_{\substack{i\omega''_m\\ k''}} \mathcal{G}_{-k''}(-i\omega''_m)\,\mathcal{G}_{k''+q}(i\omega_{m''}+i\Omega) = \frac{1}{\beta}\sum_{\substack{i\omega\\ k}} \frac{1}{-i\omega_m-\xi_{-k}}\,\frac{1}{i\omega_m+i\Omega-\xi_{k+q}} =$$

$$= \frac{1}{\beta}\sum_{\substack{i\omega\\ k}} \left(\frac{1}{-i\omega_m-\xi_{-k}} + \frac{1}{i\omega_m+i\Omega-\xi_{k+q}}\right)\frac{1}{i\Omega-\xi_{k+q}-\xi_{-k}} = \sum_k \frac{f(\xi_{k+q}) - \overbrace{f(-\xi_{-k})}^{=\,1-f(\xi_{-k})}}{i\Omega-\xi_{k+q}-\xi_{-k}}$$

$$B_q(i\Omega) = -\sum_k \frac{1-f(\xi_{-k})-f(\xi_{k+q})}{i\Omega-\xi_{k+q}-\xi_{-k}} \quad *$$

Let's assume inversion symmetry $\xi_{-k}=\xi_k$

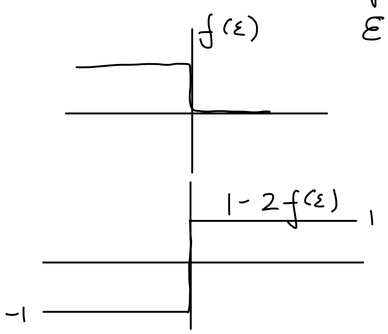
$$B_{q\to 0}(i\Omega) = -\sum_k \frac{1-2f(\xi_k)}{i\Omega-2\xi_k} = -\int d\varepsilon\, D(\varepsilon)\,\frac{1-2f(\varepsilon)}{i\Omega-2\varepsilon}$$

Here we introduce density of states, i.e.,

$$D(\varepsilon) = \sum_k \delta(\varepsilon-\varepsilon_k)$$

$$B_{q\to 0}(i\Omega\to 0) = \int d\varepsilon\, D(\varepsilon)\,\frac{\overbrace{1-2f(\varepsilon)}^{th\left(\frac{\beta\varepsilon}{2}\right)}}{2\varepsilon} \approx D(0)\,\frac{1}{2}\int_{-L}^{L}\frac{d\varepsilon}{|\varepsilon|} \to \infty$$

↑ largest around $\varepsilon\sim 0$ $\qquad \varepsilon=0$ or $k=k_F$



Better approximation

$$B_{q=0}(\Omega=0) \approx D(0)\int_T^{\omega_D}\frac{d\varepsilon}{\varepsilon} = D(0)\ln\frac{\omega_D}{T}$$

when $\varepsilon<T$ f is not step function

ω_D is the energy up to which interaction is attractive.

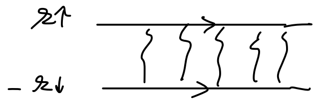
Finally $\qquad \Gamma = \dfrac{g}{1-g D_0 \ln\frac{\omega_D}{T}}$

Note the sign is such that there is a pole in Γ at T_c

In RPA $\qquad W = \dfrac{V_0}{1-V_q P_q}$ but $P_{q\sim 0}(\Omega\sim 0) < 0$ hence no instability

only at $\Omega \gg q$ $P_q>0$ and we get plasmon.

Conclusion: We have special temperature $1 = gD_0 \ln \frac{\omega_D}{T_c}$ and $T_c = \omega_D e^{-\frac{1}{gD_0}}$ at which effective interaction between electrons is diverging!



interaction infinitely strong at T_c!

Since we expect a phase transition, we can not continue perturbation accross the boundary. We need to set up perturbation around a different mean field state, which is BCS mean field state. The lowest order perturbation gives Migdel-Eliashberg Eq, which are state of the art Eq. for conventional superconductors. But first we need new mean field state.

BCS Theory as a mean field theory

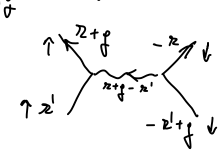
We consider only the part of the interaction which gives rise to diverging interaction (for simplicity), repulsion g, w independent, i.e., static and local.

$$\frac{1}{2} c^\dagger_{k+q\,s}\, c^\dagger_{-k\,s'}\, c_{-k'+q\,s'}\, c_{k's}$$

$$H = \sum_k \varepsilon_k c^\dagger_{ks} c_{ks} - \frac{1}{V}\sum_{k,k',q} g_{kk'}\, c^\dagger_{k+\cancel{q}\uparrow}\, c^\dagger_{-k\downarrow}\, c_{-k'+\cancel{q}\downarrow}\, c_{k'\uparrow}$$

we take only $q=0$

$$g_{kk'} = \begin{cases} g & \left|\frac{k^2-k'^2}{2m}\right| < \omega_D \\ 0 & \text{otherwise} \end{cases}$$



slightly different but equivalent choice of momenta

Consider mean field decoupling of interaction

$$c^\dagger_{k+\cancel{q}\,s}\, c^\dagger_{-k\,\bar{s}}\, c_{-k'+\cancel{q}\,\bar{s}}\, c_{k's} \to c^\dagger_{k+\cancel{q}\,s}\, c^\dagger_{-k\,\bar{s}} \langle c_{-k'+\cancel{q}\,\bar{s}}\, c_{k's}\rangle + \langle c^\dagger_{k+\cancel{q}\,s}\, c^\dagger_{-k\,\bar{s}}\rangle c_{-k'+\cancel{q}\,\bar{s}}\, c_{k's}$$

If we decomple interaction in particle-hole channel we get Hartree Fock.
This decoupling in particle-particle channel usually vanishes. However we are not considering normal state.

Let's consider many body ground state wave function $|\Omega\rangle$, for which we have nonzero expectation value

$$\Delta = \frac{g}{V}\sum_k \langle\Omega|\, C_{-k\downarrow} C_{k\uparrow}\,|\Omega\rangle \quad \text{and consequently}$$

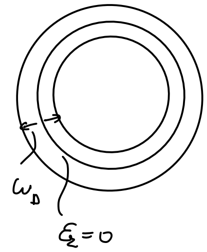
$$\Delta^+ = \frac{g}{V}\sum_k \langle\Omega|\, C^+_{k\uparrow} C^+_{-k\downarrow}\,|\Omega\rangle$$

For now this is purely mathematical consideration. Not clear if it is stable.

Δ plays the role of the order parameter, which clearly vanishes in normal state, and if nonzero below T_c gives new ground state.

BCS Hamiltonian only keeps $q=0$ part of the interaction, which is relevant in the equilibrium and g being nonzero only in the interval $-\omega_D < \varepsilon_k < \omega_D$ where $\varepsilon_k = \frac{k^2}{2m} - \frac{k_F^2}{2m}$

$$H = \sum_k \varepsilon_k C^+_{ks} C_{ks} - \frac{g}{V}\sum_{\substack{k,k'\\ s}} C^+_{k\uparrow} C^+_{-k\downarrow} C_{-k'\downarrow} C_{k'\uparrow}$$



then $$H^{MF} = \sum_k \varepsilon_k C^+_{ks} C_{ks} - \sum_k \Delta^+ C_{-k\downarrow} C_{k\uparrow} + C^+_{k\uparrow} C^+_{-k\downarrow}\Delta$$

$$= \sum_k \underbrace{(C^+_{k\uparrow}, C_{-k\downarrow})}\begin{pmatrix} \varepsilon_k & -\Delta \\ -\Delta^+ & -\varepsilon_{-k}\end{pmatrix}\begin{pmatrix} C_{k\uparrow} \\ C^+_{-k\downarrow}\end{pmatrix} + \varepsilon_{-k}$$

Bogoliubov Hamiltonian has a form of quadratic Hamiltonian, hence solvable

$$H^{MF} = \sum_k \Psi_k^+ H_k \Psi_k + \text{const.} \;;$$

What are commutation relations of Ψ_k?

$$[\Psi_k, \Psi_k^+]_+ = \left[\begin{pmatrix} C_{k\uparrow} \\ C^+_{-k\downarrow}\end{pmatrix}, (C^+_{k\uparrow}, C_{-k\downarrow})\right]_+ = \begin{pmatrix} [C_{k\uparrow}, C^+_{k\uparrow}]_+ & [C_{k\uparrow}, C_{-k\downarrow}]_+ \\ [C^+_{-k\downarrow}, C^+_{k\uparrow}]_+ & [C^+_{-k\downarrow}, C_{-k\downarrow}]_+ \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1\end{pmatrix}$$

hence Ψ_k behave like normal fermionic operators.

Diagonalization $\phi_q = U_q \Psi_q$ with $U_q U_q^+ = 1$, hence unitary transformation

Compare that with bosonic problem for magnons in AFM: $\boxed{\phi_q = \mathcal{U}_q \psi_q}$ $\boxed{\mathcal{U}_q \tau_3 \mathcal{U}_q^+ = \tau_3}$

for fermions $\boxed{\phi_q = \mathcal{U}_q \psi_q}$ $\boxed{\mathcal{U}_q \mathcal{U}_q^+ = 1}$

$$H^{MF} = \sum_k \psi_k^+ H_k \psi_k = \sum_k \phi_k^+ \underbrace{\mathcal{U}_k H_k \mathcal{U}_k^+}\phi_k$$

$$\mathrm{Det}\begin{pmatrix} \varepsilon_k - \lambda_k, & -\Delta \\ -\Delta^+, & -\varepsilon_{-k}-\lambda_k \end{pmatrix} = 0 \qquad -(\varepsilon_k - \lambda_k)(\varepsilon_{-k}+\lambda_k) - |\Delta|^2 = 0$$

$$\lambda_k^2 - \varepsilon_k^2 - |\Delta|^2 = 0$$

$$\lambda_k = \pm\sqrt{\varepsilon_k^2 + |\Delta|^2}$$

Eigenvectors $\mathcal{U}_k = \begin{pmatrix} \cos\vartheta_k, & \sin\vartheta_k \\ \sin\vartheta_k, & -\cos\vartheta_k \end{pmatrix}$ so that $\begin{pmatrix} \phi_{k\uparrow} \\ \phi^+_{-k\downarrow} \end{pmatrix} = \begin{pmatrix} \cos\vartheta_k, & \sin\vartheta_k \\ \sin\vartheta_k, & -\cos\vartheta_k \end{pmatrix}\begin{pmatrix} c_{k\uparrow} \\ c^+_{-k\downarrow} \end{pmatrix}$

To determine ϑ_k, we note $\mathcal{U}_k H_k \mathcal{U}_k^+ = \begin{pmatrix} \lambda_k & 0 \\ 0 & -\lambda_k \end{pmatrix}$ with $\lambda_k = \sqrt{\varepsilon_k^2 + |\Delta|^2}$

then $H_k = \mathcal{U}_k^+ \begin{pmatrix} \lambda_k & 0 \\ 0 & -\lambda_k \end{pmatrix} \mathcal{U}_k$

$$\begin{pmatrix} c, & s \\ s, & -c \end{pmatrix}\begin{pmatrix} \lambda & 0 \\ 0 & -\lambda \end{pmatrix}\begin{pmatrix} c, & s \\ s, & -c \end{pmatrix} = \begin{pmatrix} \varepsilon, & -\Delta \\ -\Delta, & -\varepsilon \end{pmatrix}$$

$$\begin{pmatrix} (c^2 - s^2)\lambda, & 2cs\cdot\lambda \\ 2cs\cdot\lambda, & -(c^2-s^2)\lambda \end{pmatrix} = \begin{pmatrix} \varepsilon, & -\Delta \\ -\Delta, & -\varepsilon \end{pmatrix}$$ hence $\cos^2\vartheta_k - \sin^2\vartheta_k = \boxed{\dfrac{\varepsilon_k}{\sqrt{\varepsilon_k^2 + \Delta^2}} = \cos 2\vartheta_k}$

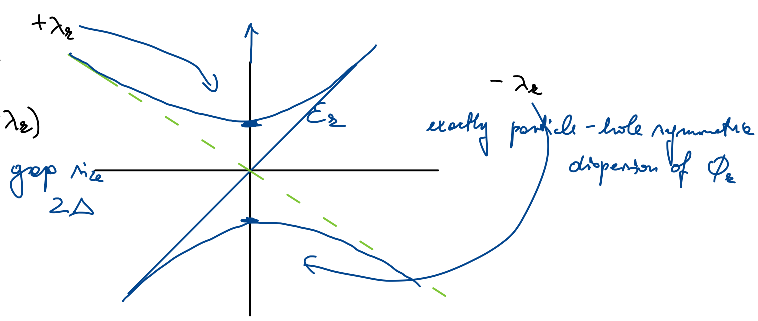
$2\cos\vartheta_k \sin\vartheta_k = \boxed{-\dfrac{\Delta}{\sqrt{\varepsilon_k^2 + \Delta^2}} = \sin 2\vartheta_k}$

Solution $H^{MF} = \sum_k (\phi^+_{k\uparrow}, \phi_{-k\downarrow})\begin{pmatrix} \lambda_k & 0 \\ 0 & -\lambda_k \end{pmatrix}\begin{pmatrix} \phi_{k\uparrow} \\ \phi^+_{-k\downarrow} \end{pmatrix} + \varepsilon_{-k}$

$$H^{MF} = \sum_k \lambda_k (\phi^+_{k\uparrow}\phi_{k\uparrow} - \phi_{-k\downarrow}\phi^+_{-k\downarrow}) + \varepsilon_k$$

$$H^{MF} = \sum_k \lambda_k (\phi^+_{k\uparrow}\phi_{k\uparrow} + \phi^+_{-k\downarrow}\phi_{-k\downarrow}) + (\varepsilon_k - \lambda_k)$$

$$H^{MF} = \sum_{ks} \lambda_k \phi^+_{ks}\phi_{ks} + \sum_k (\varepsilon_k - \lambda_k)$$



The ground state of H^{MF} hamiltonian is the vacuum state of ϕ_k operators, such that $\phi_{ki}|\Omega\rangle = 0$ for any k, and hence $H^{MF}|\Omega\rangle = 0$

and $\phi^+_{ki}|\Omega\rangle$ creates excitations out of vacuum state.

The vacuum state hence is $|\Omega\rangle = \prod_k \phi_{k\uparrow}\phi_{-k\downarrow}\underbrace{|\text{normal state g.s.}\rangle}_{\prod_{k<k_F} c^+_{k\downarrow}\, c^+_{k\uparrow}\,|0\rangle \,\equiv\, |ngs\rangle}$

$$\begin{pmatrix}\phi_{k\uparrow}\\ \phi^+_{-k\downarrow}\end{pmatrix} = \begin{pmatrix}\cos\vartheta_k & \sin\vartheta_k\\ \sin\vartheta_k & -\cos\vartheta_k\end{pmatrix}\begin{pmatrix}c_{k\uparrow}\\ c^+_{-k\downarrow}\end{pmatrix} = \begin{pmatrix}\cos\vartheta_k\, c_{k\uparrow} + \sin\vartheta_k\, c^+_{-k\downarrow}\\ \sin\vartheta_k\, c_{k\uparrow} - \cos\vartheta_k\, c^+_{-k\downarrow}\end{pmatrix}$$

$$\phi_{-k\downarrow} = \sin\vartheta_k\, c^+_{k\uparrow} - \cos\vartheta_k\, c_{-k\downarrow}$$

$$|\Omega\rangle = \prod_k \phi_{-k\downarrow}\phi_{k\uparrow}|ngs\rangle = \prod_k(\sin\vartheta_k\, c^+_{k\uparrow} - \cos\vartheta_k\, c_{-k\downarrow})(\cos\vartheta_k\, c_{k\uparrow} + \sin\vartheta_k\, c^+_{-k\downarrow})|ngs\rangle$$

$$|\Omega\rangle = \prod_k\left(-\cos^2\vartheta_k\, c_{-k\downarrow}c_{k\uparrow} + \sin^2\vartheta_k\, c^+_{k\uparrow}c^+_{-k\downarrow} + \cos\vartheta_k\sin\vartheta_k\left(c^+_{k\uparrow}c_{k\uparrow} + c^+_{-k\downarrow}c_{-k\downarrow} - 1\right)\right)|ngs\rangle$$

$$|\Omega_{BCS}\rangle = \prod_{|k|>k_F}(\cos\vartheta_k - \sin\vartheta_k\, c^+_{k\uparrow}c^+_{-k\downarrow}) \times \prod_{|k|<k_F}(\sin\vartheta_k + \cos\vartheta_k\, c_{-k\downarrow}c_{k\uparrow})\,|ngs\rangle$$

Consequently the ground state energy is

$$H|\Omega_{BCS}\rangle = \sum_k \lambda_k \phi^+_{ks}\underbrace{\phi_{ks}\prod_{k'}\phi_{k'\uparrow}\phi_{-k'\downarrow}|ngs\rangle}_{=0} + \sum_k(\varepsilon_k - \lambda_k)|\Omega_{BCS}\rangle$$

$$E_0 = \langle\Omega_{BCS}|H|\Omega_{BCS}\rangle = \sum_k \varepsilon_k - \sqrt{\varepsilon_k^2+\Delta^2} < 0$$

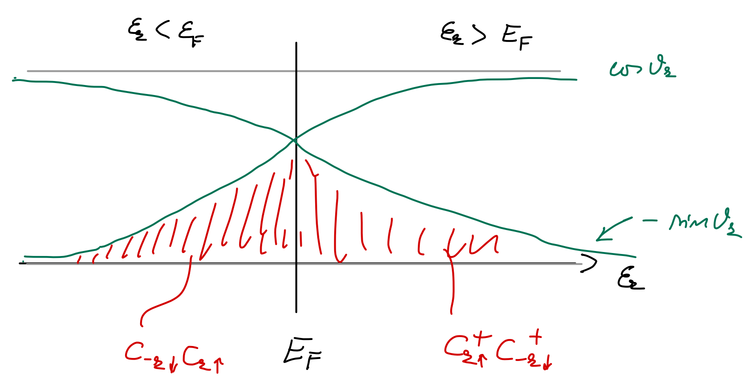
this state is lower in energy than normal state

Where are the cooper pairs?

$$|\Omega_{BCS}\rangle = \prod_{|k|>k_F}(\cos\vartheta_k - \sin\vartheta_k\, c^+_{k\uparrow}c^+_{-k\downarrow}) \times \prod_{|k|<k_F}(\sin\vartheta_k + \cos\vartheta_k\, c_{-k\downarrow}c_{k\uparrow})\,|ngs\rangle$$

$$\cos\vartheta_k = \sqrt{\frac{1}{2}\left(1+\frac{\varepsilon_k}{\sqrt{\varepsilon_k^2+\Delta^2}}\right)}$$

$$\sin\vartheta_k = -\sqrt{\frac{1}{2}\left(1-\frac{\varepsilon_k}{\sqrt{\varepsilon_k^2+\Delta^2}}\right)}$$



There are no cooper pairs far from E_F, because distinction between CP and electrons far from E_F are non-existent. Only near E_F the distinction is visible and leads to gap opening.

stopped Dec 8/2022

We started with mean field ansatz $\Delta = \frac{g}{V}\sum_q \langle\Omega| C_{-q\downarrow} C_{q\uparrow}|\Omega\rangle$ 1

which we now need to verify is stable.

We derived before $\begin{pmatrix}\phi_{q\uparrow}\\ \phi^+_{-q\downarrow}\end{pmatrix} = \begin{pmatrix}\cos\vartheta_q C_{q\uparrow} + \sin\vartheta_q C^+_{-q\downarrow}\\ \sin\vartheta_q C_{q\uparrow} - \cos\vartheta_q C^+_{-q\downarrow}\end{pmatrix}$ hence

$$C_{q\uparrow} = \cos\vartheta_q \phi_{q\uparrow} + \sin\vartheta_q \phi^+_{-q\downarrow}$$
$$C^+_{-q\downarrow} = \sin\vartheta_q \phi_{q\uparrow} - \cos\vartheta_q \phi^+_{-q\downarrow}$$
$$C_{-q\downarrow} = \sin\vartheta_q \phi^+_{q\uparrow} - \cos\vartheta_q \phi_{-q\downarrow}$$

It follows:

$$\Delta = \frac{g}{V}\sum_q \langle\Omega_{BCS}|(\underbrace{\sin\vartheta_q \phi^+_{q\uparrow}}_{=0} - \cos\vartheta_q \phi_{-q\downarrow})(\underbrace{\cos\vartheta_q \phi_{q\uparrow}}_{0} + \sin\vartheta_q \phi^+_{-q\downarrow})|\Omega_{BCS}\rangle$$

$$\langle\Omega_{BCS}| - \cos\vartheta_q \phi_{-q\downarrow} \sin\vartheta_q \phi^+_{-q\downarrow} |\Omega_{BCS}\rangle$$

finally $\Delta = -\frac{g}{V}\sum_q \cos\vartheta_q \sin\vartheta_q \underbrace{\langle\Omega_{BCS}|\phi_{-q\downarrow}\phi^+_{-q\downarrow}|\Omega_{BCS}\rangle}_{=1}$

$$\boxed{\Delta = -\frac{g}{V}\sum_q \frac{1}{2}\sin 2\vartheta_q = \frac{g}{2V}\sum_q \frac{\Delta}{\sqrt{\varepsilon_q^2+\Delta^2}}}$$

Recall: $\boxed{-\frac{\Delta}{\sqrt{\varepsilon_q^2+\Delta^2}} = \sin 2\vartheta_q}$

We arrived at BCS gap Eq!

$$\Delta = \frac{g}{2V}\sum_q \frac{\Delta}{\sqrt{\varepsilon_q^2+\Delta^2}}$$

$$\Delta \simeq \frac{g}{2}\int_{-\omega_D}^{\omega_D} D(\varepsilon)\frac{\Delta\, d\varepsilon}{\sqrt{\varepsilon^2+\Delta^2}} \approx \frac{g}{2}D(0)\Delta\int_{-\omega_D/\Delta}^{\omega_D/\Delta}\frac{du}{\sqrt{u^2+1}}$$

$$\int\frac{du}{\sqrt{u^2+1}} = \mathrm{Ash}(u)$$

$$1 = g D_0 \,\mathrm{Ash}\left(\frac{\omega_D}{\Delta}\right) \Rightarrow \Delta = \frac{\omega_D}{\mathrm{sh}\left(\frac{1}{gD_0}\right)} \underset{gD_0 \ll 1}{\approx} \frac{\omega_D}{\frac{1}{2}e^{\frac{1}{gD_0}}} = 2\omega_D e^{-\frac{1}{gD_0}}$$

At $T=0$ the gap is $\Delta \approx 2\omega_D e^{-\frac{1}{gD_0}}$ the same scale as the instability temperature of the normal state.

Left for Homework

Excitations in BCS state

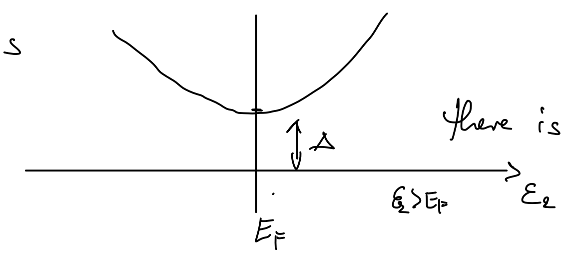
- In terms of quasiparticle states ϕ_k?

$$\tilde{G}_k = -\langle T_\tau \, \phi_{ks}(\tau)\, \phi^\dagger_{ks}(0)\rangle \quad ; \quad \text{Here } H_{BCS} = \sum_k \lambda_k \phi^\dagger_{ks}\phi_{ks} - E_0$$

$$E_0 = \sum_k (\lambda_k - \varepsilon_k)$$

This is a non-interacting problem with solution $\tilde{G}_k = \dfrac{1}{\omega - \lambda_k}$, hence

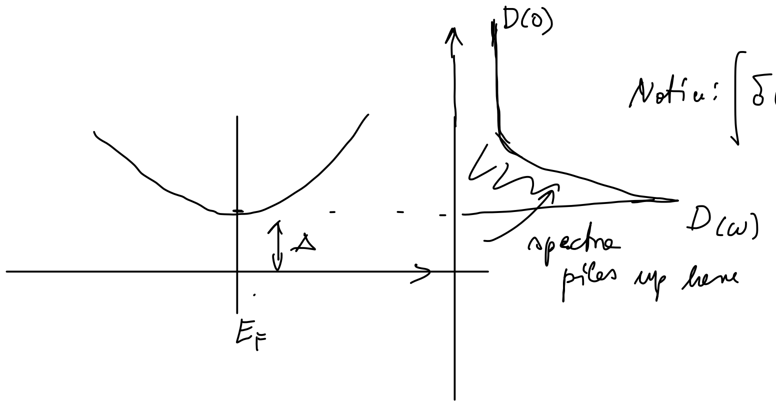
spectrum is



There is a gap for excitations, i.e., no zero energy excitation that could destabilize the state.

$$\tilde{A}_k(\varepsilon) = -\frac{1}{\pi}\,\mathrm{Im}\,\tilde{G}_k = \delta(\varepsilon - \lambda_k)$$

$$D(\omega) = \sum_k \tilde{A}_k(\omega) = \sum_k \delta(\omega - \lambda_k) = \int d\varepsilon\, D(\varepsilon)\, \delta\!\left(\omega - \sqrt{\varepsilon^2+\Delta^2}\right) \approx D(0) \left.\frac{\sqrt{\varepsilon^2+\Delta^2}}{\varepsilon}\right|_{\omega=\sqrt{\varepsilon^2+\Delta^2}} = D(0)\,\frac{\omega}{\sqrt{\omega^2-\Delta^2}}$$



Notice: $\displaystyle\int \delta(f(\varepsilon))\, d\varepsilon = \sum_{w_0} \left.\frac{1}{|f'(w_0)|}\right|_{f(w_0)=0}$

Left for Homework

Excitations in term of electrons (what ARPES measures) (HW)

$$G_k(\tau) = -\langle T_\tau \psi_k(\tau)\psi_k^+(0)\rangle = -\left\langle T_\tau \begin{pmatrix} c_{k\uparrow}(\tau) \\ c^+_{-k\downarrow}(\tau)\end{pmatrix} \cdot \left(c^+_{k\uparrow}(0),\ c_{-k\downarrow}(0)\right)\right\rangle =$$

$$= -\begin{pmatrix} \langle T_\tau c_{k\uparrow}(\tau) c^+_{k\uparrow}(0)\rangle, & \langle c_{k\uparrow}(\tau) c_{-k\downarrow}(0)\rangle \\ \langle c^+_{-k\downarrow}(\tau) c^+_{k\uparrow}(0)\rangle, & \langle c^+_{-k\downarrow}(\tau) c_{-k\downarrow}(0)\rangle \end{pmatrix} = \begin{pmatrix} G_{k\uparrow}(\tau), & \mathcal{F}_k(\tau) \\ \mathcal{F}^+_k(-\tau), & -G_{-k\downarrow}(-\tau)\end{pmatrix}$$

We started with $H_{BCS} = \sum_k \psi_k^+ \begin{pmatrix} \varepsilon_k, & -\Delta \\ -\Delta, & -\varepsilon_{-k}\end{pmatrix}\psi_k$ which is quadratic, hence

$$G_k^{-1} = I(i\omega + \underset{0}{\underset{\shortparallel}{\mu}}) - H_{BCS} = \begin{pmatrix} i\omega - \varepsilon_k, & \Delta \\ \Delta, & i\omega + \varepsilon_{-k}\end{pmatrix} \quad \text{and}$$

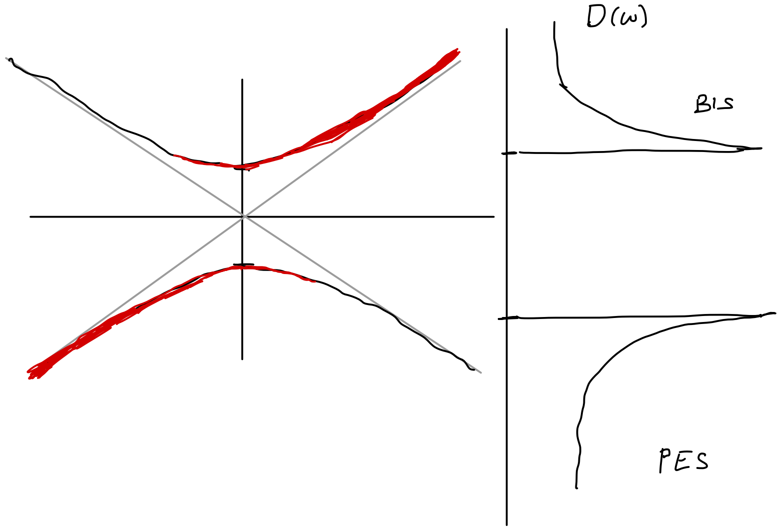
$$G_k = \frac{1}{\underbrace{(i\omega - \varepsilon_k)(i\omega + \varepsilon_{-k}) - \Delta^2}_{(i\omega)^2 - \varepsilon_k^2 - \Delta^2}}\begin{pmatrix} i\omega + \varepsilon_{-k}, & -\Delta \\ -\Delta, & i\omega - \varepsilon_k\end{pmatrix}$$

$$G_{k\uparrow}(i\omega) = \frac{i\omega + \varepsilon_k}{(i\omega)^2 - (\varepsilon_k^2 + \Delta^2)}\ ; \qquad \mathcal{F}_k(i\omega) = -\frac{\Delta}{(i\omega)^2 - (\varepsilon_k^2 + \Delta^2)}$$

$$-G_{-k\downarrow}(-i\omega) = \frac{i\omega - \varepsilon_k}{(i\omega)^2 - (\varepsilon_k^2 + \Delta^2)} \Rightarrow G_{k\downarrow}(i\omega) = \frac{i\omega + \varepsilon_k}{(i\omega)^2 - (\varepsilon_k^2 + \Delta^2)}$$

$$G_{ks}(i\omega) = \frac{\cos^2\vartheta_k}{i\omega - \lambda_k} + \frac{\sin^2\vartheta_k}{i\omega + \lambda_k}\ ; \quad \text{check: } \frac{i\omega + \lambda_k(\overbrace{\cos^2\vartheta_k - \sin^2\vartheta_k}^{\cos 2\vartheta_k = \frac{\varepsilon_k}{\lambda_k}})}{(i\omega)^2 - \lambda_k^2} \quad \checkmark$$

$$A_{ks}(i\omega) = \cos^2\vartheta_k\, \delta(\omega - \lambda_k) + \sin^2\vartheta_k(\omega + \lambda_k)$$



$$\cos\vartheta_k = \sqrt{\frac{1}{2}\left(1 + \frac{\varepsilon_k}{\sqrt{\varepsilon_k^2 + \Delta^2}}\right)}$$

$$\sin\vartheta_k = -\sqrt{\frac{1}{2}\left(1 - \frac{\varepsilon_k}{\sqrt{\varepsilon_k^2 + \Delta^2}}\right)}$$

Superconductivity from the field integral

$$S_{BCS} = \int_0^{\beta} d\tau \int d^3r \left\{ \psi_s^+(\vec r,\tau)\left[\frac{\partial}{\partial \tau} - \mu + \frac{\vec p^{\,2}}{2m}\right]\psi_s(\vec r,\tau) - g\, \underbrace{\psi_\uparrow^+(\vec r,\tau)\,\psi_\downarrow^+(\vec r,\tau)\,\psi_\downarrow(\vec r,\tau)\,\psi_\uparrow(\vec r,\tau)} \right\}$$

simplification
interaction is local
$V(\vec r-\vec r\,') = -g\,\delta(\vec r-\vec r\,')$
and constant

We will add EM field through minimal coupling

$$\vec p \to \vec p - e\vec A \ ; \quad \vec B = \vec\nabla \times \vec A$$

$$\frac{\partial}{\partial\tau} \to \frac{\partial}{\partial\tau} + ie\phi \ ; \quad \vec E = -\vec\nabla\phi - \frac{\partial \vec A}{\partial t}$$

i due to imaginary time

We check below that such coupling is gauge invariant, i.e., EM field gauge invariance translates into phase invariance of ψ operators.

$$\boxed{S_{BCS} = \int_0^{\beta} d\tau \int d^3r \left\{ \psi_s^+(\vec r,\tau)\left[\frac{\partial}{\partial \tau} - \mu + \frac{(-i\vec\nabla - e\vec A)^2}{2m} + ie\phi\right]\psi_s(\vec r,\tau) - g\, \psi_\uparrow^+(\vec r,\tau)\,\psi_\downarrow^+(\vec r,\tau)\,\psi_\downarrow(\vec r,\tau)\,\psi_\uparrow(\vec r,\tau) \right\}}$$

Changing phase to $\psi(\vec r,\tau)$:

if $\psi(\vec r,\tau) \to e^{i\vartheta(\vec r,\tau)}\psi(\vec r,\tau)$ then $(-i\vec\nabla - e\vec A)^2 e^{i\vartheta}\psi =$

$\psi^+(\vec r,\tau) \to e^{-i\vartheta}\psi^+$

$$(-i\vec\nabla - e\vec A)\, e^{i\vartheta}(-i\,i\vec\nabla\vartheta - i\vec\nabla - e\vec A)\psi$$

$$(-i\vec\nabla - e\vec A)\, e^{i\vartheta}(-i\,i\vec\nabla\vartheta - i\vec\nabla - e\vec A)\psi$$

$$e^{i\vartheta}(-i\vec\nabla - e\vec A + \vec\nabla\vartheta)^2\psi$$

If $\psi(\vec r,\tau)$ has different phase, we get:

$$\psi^+ e^{-i\vartheta}\left[\frac{\partial}{\partial\tau} - \mu + \frac{(-i\vec\nabla - e\vec A)^2}{2m} + ie\phi\right]e^{i\vartheta}\psi \to \psi^+\left[\frac{\partial}{\partial\tau} + i\dot\vartheta - \mu + \frac{(-i\vec\nabla - e\vec A + \vec\nabla\vartheta)^2}{2m} + ie\phi\right]\psi$$

hence $\boxed{\begin{aligned} \vec A &\to \vec A + \frac{\vec\nabla\vartheta}{e} \\ \Phi &\to \Phi - \frac{\dot\vartheta}{e} \end{aligned}}$ satisfied due to gauge invariance!

> Conclusion: different gauge can be achieved by changing the phase of ψ field!

We will use Hubbard-Stratonovich, in which SC-state will be saddle point approximation, and fluctuations will give Meissner effect.

Hubbard-Stratonovich:

$$e^{g\int d\tau d^3r\, \psi_\uparrow^+\psi_\downarrow^+\psi_\uparrow\psi_\downarrow} = \int \mathcal{D}[\Delta^+,\Delta]\, e^{-\int d\tau \int d^3r \underbrace{\left[\Delta^+\frac{1}{g}\Delta - \Delta^+\psi_\downarrow\psi_\uparrow - \Delta\psi_\uparrow^+\psi_\downarrow^+\right]}_{\shortparallel}}$$

check by shifting variable $(\Delta^+ - \psi_\uparrow^+\psi_\downarrow^+ g)\frac{1}{g}(\Delta - \psi_\downarrow\psi_\uparrow g) - g\,\psi_\uparrow^+\psi_\downarrow^+\psi_\downarrow\psi_\uparrow$

$$Z = \int \mathcal{D}[\psi^+\psi]\mathcal{D}[\phi^+\phi]\, e^{-\int_0^\beta d\tau\int d^3r\, \psi_s^+\left[\partial_\tau - \mu + \frac{(\vec{p}-e\vec{A})^2}{2m} + ie\phi\right]\psi_s - \int_0^\beta d\tau\int d^3r\left[\frac{|\Delta|^2}{g} - \Delta^+\psi_\downarrow\psi_\uparrow - \Delta\psi_\uparrow^+\psi_\downarrow^+\right]}$$

$$\boxed{S = \int_0^\beta d\tau\int d^3r\left\{\psi_s^+\left[\partial_\tau - \mu + \frac{(\vec{p}-e\vec{A})^2}{2m} + ie\phi\right]\psi_s + \frac{|\Delta|^2}{g} - \Delta^+\psi_\downarrow\psi_\uparrow - \Delta\psi_\uparrow^+\psi_\downarrow^+\right\}}$$

Define $\Psi(\vec{r},\tau) = \begin{pmatrix}\psi_\uparrow(\vec{r}\tau)\\ \psi_\downarrow^+(\vec{r}\tau)\end{pmatrix}$

$$\boxed{S = \int_0^\beta d\tau\int d^3r\,(\psi_\uparrow^+,\psi_\downarrow)\begin{pmatrix}\partial_\tau - \mu + \frac{(-i\vec{\nabla}-e\vec{A})^2}{2m} + ie\phi, & -\Delta\\ -\Delta^+ & , \partial_\tau + \mu - \frac{(i\vec{\nabla}-e\vec{A})^2}{2m} - ie\phi\end{pmatrix}\begin{pmatrix}\psi_\uparrow\\ \psi_\downarrow^+\end{pmatrix} + \int_0^\beta d\tau\int d^3r\,\frac{|\Delta|^2}{g}}$$

because $\psi_\downarrow^+(\tau)\left(\partial_\tau - \mu + \frac{(-i\vec{\nabla}-e\vec{A})^2}{2m} + ie\phi\right)\psi_\downarrow(\tau) = \psi_\downarrow(\tau)\left(-\partial_\tau - \mu + \frac{(i\vec{\nabla}-e\vec{A})}{2m} + ie\phi\right)\psi_\downarrow^+(\tau)$

sign change in derivatives because ψ^+ has opposite phase to ψ.

Define $\boxed{G^{-1}[\Delta](\vec{r},i\omega) = \begin{pmatrix} i\omega + \mu - \frac{p^2}{2m} - ie\phi, & \Delta\\ \Delta^+ & , i\omega - \mu + \frac{p^2}{2m} + ie\phi\end{pmatrix}}$

Integrating out fermions:

$$Z = \int \mathcal{D}[\Delta^+,\Delta]\int \mathcal{D}[\psi^+\psi]\, e^{-\int \psi^+(-G^{-1})\psi - \int\frac{|\Delta|^2}{g}} = \mathrm{Det}(-G^{-1})\, e^{-\int\frac{|\Delta|^2}{g}} = e^{\mathrm{Tr}\ln(-G^{-1}) - \int\frac{|\Delta|^2}{g}}$$

Formally:

$$\boxed{S = -\mathrm{Tr}\ln(-G^{-1}) + \int d\tau d^3r\,\frac{|\Delta|^2}{g}}$$

Saddle point approximation correspond to new mean-field, i.e., BCS state. 4

Our guess for the solution is $\Delta = \text{const}$ in $\vec{r}$ and τ and hence $\Delta = \Delta^+$

saddle point $\quad \frac{\delta S}{\delta \Delta^+} = \frac{\delta}{\delta \Delta^+}\left(\int d\tau d^3r \frac{|\Delta|^2}{g} - Tr\left(G \frac{\delta G^{-1}}{\delta \Delta} \right)\right)$

$$\begin{pmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{pmatrix} \qquad \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$\frac{\Delta}{g} = G_{12}$$

first set $\vec{A} = \phi = 0$ then $\Delta = \text{const}$

$$\frac{\Delta}{g} = \frac{1}{\beta V}\sum_{i\omega, k}\left[\begin{pmatrix} i\omega + \mu - \frac{k^2}{2m}, & \Delta \\ \Delta^+, & i\omega - \mu + \frac{k^2}{2m} \end{pmatrix}^{-1}\right]_{12} = -\frac{1}{\beta V}\sum_{k, i\omega} \frac{\Delta}{(i\omega)^2 - (\varepsilon_k^2 + \Delta^2)}$$

$$\begin{pmatrix} i\omega - \varepsilon_k, & \Delta \\ \Delta^+, & i\omega + \varepsilon_k \end{pmatrix}^{-1} = \frac{1}{(i\omega)^2 - \varepsilon_k^2 - \Delta^2}\begin{pmatrix} i\omega + \varepsilon_k, & -\Delta \\ -\Delta^+, & i\omega - \varepsilon_k \end{pmatrix}$$

$$\frac{1}{g} = -\frac{1}{\beta V}\sum_{k, i\omega} \frac{1}{(i\omega)^2 - \lambda_k^2} = -\frac{1}{\beta V}\sum_{k, i\omega}\left(\frac{1}{i\omega - \lambda_k} - \frac{1}{i\omega + \lambda_k}\right)\frac{1}{2\lambda_k} = \frac{1}{V}\sum_k \frac{[-f(\lambda_k) + f(-\lambda_k)]}{2\lambda_k}$$

BCS gap Eq at finite temp: $\boxed{\frac{1}{g} = \frac{1}{V}\sum_k \frac{1 - 2f(\lambda_k)}{2\sqrt{\varepsilon_k^2 + \Delta^2}}}$

$$\boxed{\frac{1}{g}} = \int_{-\omega_D}^{\omega_D} D(\varepsilon)\, \frac{\overbrace{1 - 2f(\lambda_\varepsilon)}^{th\frac{\beta\lambda_\varepsilon}{2}}}{2\sqrt{\varepsilon^2 + \Delta^2}}\, d\varepsilon = \int_{-\omega_D}^{\omega_D} D(\varepsilon)\, \frac{th\left(\frac{\beta\lambda_\varepsilon}{2}\right)}{2\lambda_\varepsilon}\, d\varepsilon \approx \frac{2}{2} D_0 \int_0^{\omega_D} \frac{th\left(\frac{\beta\lambda_\varepsilon}{2}\right)}{\lambda_\varepsilon}\, d\varepsilon = D_0 \int_0^{\omega_D} \frac{th\left(\frac{\sqrt{\varepsilon^2+\Delta^2}}{2T}\right)}{\sqrt{\varepsilon^2 + \Delta^2}}\, d\varepsilon = \boxed{D_0 \int_0^{\frac{\omega_D}{2T}} \frac{th\left(\sqrt{x^2 + \mathcal{H}^2}\right)}{\sqrt{x^2 + \mathcal{H}^2}}\, dx}$$

$\boxed{\frac{\varepsilon}{2T} = x \text{ and } \mathcal{H} = \left(\frac{\Delta}{2T}\right)}$

$\boxed{\text{At } T = T_c}$ $\boxed{\Delta \to 0 \text{ and } \mathcal{H} \to 0 \text{ hence:}}$

$$\boxed{\frac{1}{gD_0}} = \int_0^{\frac{\omega_D}{2T}} \frac{th(x)}{x}\, dx = \int_0^{\Lambda} \frac{th(x)}{x} dx + \int_{\Lambda}^{\frac{\omega_D}{2T_c}} \underset{\substack{\uparrow \\ th(x) \approx 1 \text{ for } \Lambda \gg 1}}{\frac{th(x)}{x}}\, dx = \underbrace{\int_0^{\Lambda} \frac{th(x)}{x} - \ln\Lambda}_{\ln(1.13 \times 2)} + \ln\frac{\omega_D}{2T_c} = \boxed{\ln\frac{\omega_D}{T_c} \times 1.13}$$

$$\boxed{T_c = 1.13\,\omega_D\, e^{-\frac{1}{gD_0}}}$$

Homework 2

- gap dependence around T_c:

$$\frac{1}{gD_0} = \int_0^{\frac{\omega_D}{2T}} \left(\frac{th\left(\sqrt{x^2+\varkappa^2}\right)}{\sqrt{x^2+\varkappa^2}} - \frac{th(x)}{x} \right) dx + \underbrace{\int_0^{\frac{\omega_D}{2T_c}} \frac{th(x)}{x}}_{= \frac{1}{gD_0}} + \underbrace{\int_{\frac{\omega_D}{2T_c}}^{\frac{\omega_D}{2T}} \frac{th(x)}{x}}_{\frac{1}{\frac{\omega_D}{2T_c}}\left(\frac{\omega_D}{2T} - \frac{\omega_D}{2T_c}\right) = \frac{T_c - T}{T}}$$

from previous calculation

hence

$$-\frac{T_c - T}{T} = \int_0^{\frac{\omega_D}{2T}} \left(\frac{th\left(\sqrt{x^2+\varkappa^2}\right)}{\sqrt{x^2+\varkappa^2}} - \frac{th(x)}{x} \right) dx$$

Estimation:

$$\underbrace{\int_0^{\Lambda} \left(\frac{th\left(\sqrt{x^2+\varkappa^2}\right)}{\sqrt{x^2+\varkappa^2}} - \frac{th(x)}{x} \right) dx}_{} + \int_{\Lambda}^{\frac{\omega_D}{2T}} \left(\frac{1}{\sqrt{x^2+\varkappa^2}} - \frac{1}{x} \right) dx$$

$$\int_0^{\Lambda} \left(-\frac{\varkappa^2}{3} + \frac{4\varkappa^2}{15} x^2 + \dots \right) dx \qquad \frac{1}{x}\left(\left(1 + \left(\frac{\varkappa}{x}\right)^2\right)^{-\frac{1}{2}} - 1 \right)$$

$$\frac{1}{x}\left(-\frac{\varkappa^2}{2x^2} + \frac{3}{8}\left(\frac{\varkappa}{x}\right)^4 \right)$$

$$-\frac{\varkappa^2}{3}\Lambda + \frac{4\varkappa^2}{15 \cdot 3}\Lambda^3 + \dots \qquad -\frac{\varkappa^2}{2}\int_{\Lambda}^{\frac{\omega_D}{2T}} \frac{1}{x^3} dx = -\frac{1}{4}\varkappa^2 \left(\frac{1}{\Lambda^2} - \left(\frac{2T}{\omega_D}\right)^2 \right)$$

$$\frac{T_c - T}{T} = \varkappa^2 \left(\underbrace{\frac{\Lambda}{3}\left(1 - \frac{4}{15}\Lambda^2 + \cdot\right) + \frac{1}{4}\left(\frac{1}{\Lambda^2} - \left(\frac{2T}{\omega_D}\right)^2\right)}_{\frac{1}{2}} \right) \approx \frac{1}{2}\left(\frac{\Delta}{2T}\right)^2 \Rightarrow \Delta \approx \sqrt{8 T_c (T_c - T)}$$

- Δ at $T = 0$:

$$\varkappa = \frac{\Delta}{2T} \to \infty$$

$$\frac{1}{gD_0} = \int_0^{\frac{\omega_D}{2T}} \frac{th\left(\sqrt{x^2+\varkappa^2}\right)}{\sqrt{x^2+\varkappa^2}} dx \approx \int_0^{\frac{\omega_D}{2T}} \frac{dx}{\sqrt{x^2+\varkappa^2}} = \ln\left(x + \sqrt{x^2+\varkappa^2}\right)\Big|_0^{\frac{\omega_D}{2T}} = \ln\left(\frac{\omega_D}{2T} + \sqrt{\left(\frac{\omega_D}{2T}\right)^2 + \left(\frac{\Delta}{2T}\right)^2}\right) - \ln\left(\frac{\Delta}{2T}\right)$$

$$\ln\left(\frac{\omega_D + \sqrt{\omega_D^2 + \Delta^2}}{\Delta}\right)$$

$$e^{-\frac{1}{gD_0}} = \frac{\Delta_0}{\omega_D + \sqrt{\omega_D^2 + \Delta_0^2}} \approx \frac{\Delta_0}{2\omega_D} \Rightarrow \Delta_0 = 2\omega_D e^{-\frac{1}{gD_0}}$$

while $T_c = 1.13\, \omega_D e^{-\frac{1}{gD_0}}$

hence $\frac{\Delta_0}{T_c} = \frac{2}{1.13}$ and $\frac{T_c}{\Delta_0} \approx 0.57$

or $\frac{\Delta}{2T_c} \sim 1$

We finished saddle point, which gave us BCS equations.
We could study fluctuations around saddle point (in the absence of EM-field) and could derive Ginzburg Landau theory (give explicit meaning and values for phenomenological coefficients).
But we will here concentrate on interaction of EM field with superconductor, i.e., derive Meissner effect.

There are two types of fluctuations of field Δ around mean field value of constant: $\Delta = |\Delta| e^{i\vartheta}$

- fluctuations of the magnitude $|\Delta|$
- fluctuations of the phase $\vartheta(\vec{r},\tau)$

The latter is a soft mode (Goldstone mode), because it costs no energy.

The grounds state of a bulk superconductor spontaneously breaks that symmetry and picks certain phase (usually around $\vartheta=0$) inside bulk superconductor. This is known as rigidity of the global phase of the condensate.

If the phase changes in space, i.e., $\nabla\vartheta \neq 0$ then condensate is flowing with nonzero supercurrent and B field is nonzero. This can happen only on the surface.

We will show that there is a Goldstone mode due to gauge freedom of the EM-field.
Any phase could be picked by the condensate in principle

We will integrate over this gauge freedom ϑ, and because of that Goldstone mode the gauge field $\vec{A}$ will acquires a mass term, which expells magnetic field from the superconductor. This mechanism is called Anderson-Higgs mechanisms.

Starting with general action in EM field:

Repetition of ☆:

$$S=\int_0^\beta d\tau\int d^3r\,(\psi_\uparrow^+,\psi_\downarrow)\underbrace{\begin{pmatrix}\frac{\partial}{\partial\tau}-\mu+\frac{(-i\vec\nabla-e\vec A)^2}{2m}+ie\phi, & -\Delta_0 e^{2i\vartheta(\vec r,\tau)}\\ -\Delta_0^+ e^{-2i\vartheta(\vec r,\tau)}, & \frac{\partial}{\partial\tau}+\mu-\frac{(i\vec\nabla-e\vec A)^2}{2m}-ie\phi\end{pmatrix}}_{-G^{-1}[\Delta]}\begin{pmatrix}\psi_\uparrow\\ \psi_\downarrow^+\end{pmatrix}+\underbrace{\int_0^\beta d\tau\int d^3r\,\frac{|\Delta|^2}{g}}_{\tilde S_0}$$

We integrate out ψ fields, to obtain

$$Z=\int D[\psi^+\psi]\,e^{-\int\psi^+(-G^{-1})\psi}=Det(-G^{-1})=e^{Tr\ln(-G^{-1})}$$ hence

$$S=-Tr\ln(-G^{-1}[\Delta])+\tilde S_0$$

In addition to phase fluctuation, we also have massive fluctuation $\delta|\Delta|$ which are expensive and less important. So integral over Δ will be only over its phase ϑ!

We introduce unitary transformation $\hat U=\begin{pmatrix}e^{-i\vartheta}&0\\0&e^{i\vartheta}\end{pmatrix}$ and change G^{-1} with this transformation, which can not change action $\hat U\begin{pmatrix}G^{-1}_{11}&G^{-1}_{12}\\G^{-1}_{21}&G^{-1}_{22}\end{pmatrix}U^+$

This is equivalent of changing phase of $\psi_s\to\psi_s e^{i\vartheta}$, which does not change action and can be freely picked.

We next show that this unitary $\hat U$ leads to action without the phase $\Delta=\Delta_0$.

$$\hat U\cdot\begin{pmatrix}G^{-1}_{11}, & G^{-1}_{12}\\ G^{-1}_{21}, & G^{-1}_{22}\end{pmatrix}\cdot\hat U^+=\begin{pmatrix}e^{-i\vartheta}G^{-1}_{11}e^{i\vartheta}, & e^{-2i\vartheta}G^{-1}_{12}\\ e^{2i\vartheta}G^{-1}_{21}, & e^{i\vartheta}G^{-1}_{22}e^{-i\vartheta}\end{pmatrix}$$

- $e^{-2i\vartheta}G^{-1}_{12}=-\Delta_0$
- $e^{-i\vartheta}G^{-1}_{11}e^{i\vartheta}=e^{-i\vartheta}\left(\frac{\partial}{\partial\tau}-\mu+\frac{(-i\vec\nabla-e\vec A)^2}{2m}+ie\phi\right)e^{i\vartheta}=$

$$=e^{-i\vartheta}e^{i\vartheta}\left(\frac{\partial}{\partial\tau}+i\dot\vartheta-\mu+\frac{(-i\vec\nabla+(\vec\nabla\vartheta)-e\vec A)^2}{2m}+ie\phi\right)$$

$$=\left(\frac{\partial}{\partial\tau}-\mu+\frac{(-i\vec\nabla-e\vec A)^2}{2m}+ie\phi\right)$$

because we have gauge freedom in choosing $(\vec A,\phi)$ and transformation $\vec A\to\vec A+\frac{\vec\nabla\vartheta}{e}$, $\vec\phi\to\vec\phi-\frac{\dot\vartheta}{e}$ removes $\vec\nabla\vartheta$ and $\dot\vartheta$.

We just proved that the phase $\Delta_0 e^{2i\vartheta}$ does not change action S and costs no energy, hence it is a Goldstone mode. 7

Since ϑ can be choosen arbitrary, Δ can not be experimentally measurable quantity.
Δ is not gauge independent quantity, hence can not be measured.

While $\vartheta(\vec r,\tau)$ can be arbitrarily choosen by the condensate, the phase can not change in space or time, i.e., we have a spontaneous symmetry breakup that picks one phase out of infinite number of possibilities (for example $\vartheta=0$).

We will show later that $S[\vartheta=0,\vec A]=e^2\int_0^\beta d\tau\int d^3r\left[D_0[\phi(\vec r,\tau)]^2+\frac{n_s}{2m}[\vec A(\vec r,\tau)]^2\right]$ where D_0 is $D(\omega=0)$ and n_s is superfluid density

It follow that under gauge transformation the action is

$$S[\vartheta,\vec A]=e^2\int_0^\beta d\tau\int d^3r\left[D_0\left(\phi+\frac{\dot\vartheta}{e}\right)^2+\frac{n_s}{2m}\left(\vec A-\frac{\vec\nabla\vartheta}{e}\right)^2\right]$$

hence variation of ϑ in space leads to finite $\vec A$ field!

Meissner Effect ϑ is arbitrary and is part of Δ, hence $\int D[\Delta]$ requires integral over ϑ and over $(\delta\Delta)$. The latter is higher in energy and less important. Hence we will integrate over ϑ:

Free field: $S^0=\int d^3r\int d\tau\,\frac{e^2}{2}B^2$ in our units $\left(\frac{B^2}{2\mu_0}\right)$

total S:

$$S[\vartheta]=e^2\beta\int d^3r\left[\frac{n_s}{2m}\left(\vec A-\vec\nabla\vartheta\right)^2+\frac{1}{2}\left(\vec\nabla\times\vec A\right)^2\right]$$

free field

Fourier transform

$$S[\vartheta]=e^2\frac{\beta}{2}\sum_q\frac{n_s}{m}\left(\vec A_q-i\vec q\vartheta_q\right)\left(\vec A_{-q}+i\vec q\vartheta_{-q}\right)+\underbrace{i\vec q\times\vec A_q\,(-i)\vec q\times\vec A_{-q}}_{q^2\vec A_q\cdot\vec A_{-q}-(\vec q\cdot\vec A_q)(\vec q\cdot\vec A_{-q})}$$

$(\vec a\times\vec b)\cdot(\vec c\times\vec d)=\vec a\cdot\vec c\;\vec b\cdot\vec d-\vec a\cdot\vec d\;\vec b\cdot\vec c$

$$S[\vartheta] = e^2 \frac{\beta}{2} \sum_q \frac{n_s}{m}\left[q^2 \vartheta_q \vartheta_{-q} + i\vec{q}(\vec{A}_q \vartheta_{-q} - \vec{A}_{-q}\vartheta_q) + \vec{A}_q \cdot \vec{A}_{-q}\right] + q^2 \vec{A}_q \cdot \vec{A}_{-q} - (\vec{q}\cdot\vec{A}_{-q})(\vec{q}\cdot\vec{A}_q)$$

$$q^2\underbrace{\left(\vec{A}_q\cdot\vec{A}_{-q} - (\vec{e}_q\cdot\vec{A}_{-q})(\vec{e}_q\cdot\vec{A}_q)\right)}{} = q^2 \vec{A}^{\perp}_q \vec{A}^{\perp}_{-q}$$

define transverse component $\vec{A}^{\perp}_q \equiv \vec{A}_q - (\vec{e}_q\cdot\vec{A}_q)\vec{e}_q$

To carry out gauss integral:

$$Z = \int D[\vartheta]\, e^{-S[\vartheta]} \; ; \quad S \equiv \vartheta_q A \vartheta_{-q} - j_q \vartheta_{-q} - j_q^{+} \vartheta_q \qquad \int D[\vartheta_q, \vartheta_{-q}]\, e^{-S} = \frac{\pi^N}{\mathrm{Det}(A)}\, e^{\vec{j}_q^{+} A^{-1} \vec{j}_q}$$

$$\left.\begin{aligned} A &= e^2\frac{\beta}{2}\frac{n_s}{m} q^2 \cdot I \\ \vec{j}_q &= e^2\frac{\beta}{2}\frac{n_s}{m}\, i\,\vec{q}\cdot\vec{A}_q \\ \vec{j}_q^{+} &= -e^2\frac{\beta}{2}\frac{n_s}{m}\, i\,\vec{q}\cdot\vec{A}_{-q} \end{aligned}\right\} \quad \begin{aligned} j_q^{+} A^{-1} j_q &= -i(\vec{q}\cdot\vec{A}_{-q})\frac{1}{q^2}\, i(\vec{q}\cdot\vec{A}_q)\, e^2\frac{\beta}{2}\frac{n_s}{m} \\ &= \frac{(\vec{q}\cdot\vec{A}_q)(\vec{q}\cdot\vec{A}_{-q})}{q^2}\, e^2\frac{\beta}{2}\frac{n_s}{m} \end{aligned}$$

$$S_{\mathrm{eff}} = e^2\frac{\beta}{2}\sum_q \underbrace{-\frac{n_s}{m}\frac{(\vec{q}\cdot\vec{A}_q)(\vec{q}\cdot\vec{A}_{-q})}{q^2} + \frac{n_s}{m}\vec{A}_q\cdot\vec{A}_{-q}}_{\frac{n_s}{m}\vec{A}^{\perp}_q\cdot\vec{A}^{\perp}_{-q}} + \underbrace{q^2 A^{\perp}_q A^{\perp}_{-q}}_{\text{free field}} = e^2\frac{\beta}{2}\sum_q \left(\frac{n_s}{m} + q^2\right)\vec{A}^{\perp}_q\cdot\vec{A}^{\perp}_{-q}$$

In real space: $S_{\mathrm{eff}} = \frac{e^2}{2}\int_0^\beta d\tau \int d^3r\; \vec{A}(\vec{r})\left(\frac{n_s}{m} - \nabla^2\right)\vec{A}(\vec{r})$

The goldstone mode ϑ was integrated out and the gauge field $\vec{A}_q$, which was massless ($S \propto q^2 A_q$) acquired a mass term ($S \propto (q^2+\lambda) A_q$)

Anderson–Higgs mechanism

Even long range ($q \to 0$) component of the field are expensive $\to$ static fields expelled

Saddle point: $\frac{\delta S_{\mathrm{eff}}}{\delta A(\vec{r})} = \left(\frac{n_s}{m} - \nabla^2\right)\vec{A}(\vec{r}) = 0$ $\boxed{\text{London Eq.}}$

$$B(z) = B_0\, e^{-z/\lambda} \qquad \frac{n_s}{m} = \frac{1}{\lambda^2} \text{ and } \lambda = \sqrt{\frac{m}{n_s}}$$

magnetic field does not penetrate into the SC sample

current $\vec{j} = \frac{\delta S_{\mathrm{eff}}}{\delta \vec{A}}$; $\vec{j} = e^2\left(\underbrace{\frac{n_s}{m}}_{\text{super current}} - \underbrace{\nabla^2}_{\text{free space}}\right)\vec{A}$

Proof that current $\vec{j} = \frac{\delta S}{\delta \vec{A}}$

$$S = S_0 + \int \psi^+ \frac{1}{2m}(-i\vec{\nabla} - e\vec{A})^2 \psi = S_0 + \int \psi^+ \frac{1}{2m}\left(-\nabla^2 + ie(\vec{\nabla}\cdot\vec{A} + \vec{A}\cdot\vec{\nabla}) + e^2\vec{A}\cdot\vec{A}\right)\psi$$

$$\int \psi^+ \frac{1}{2m}\left(-\nabla^2 + ie\,\vec{A}\cdot\vec{\nabla} + e^2\vec{A}\cdot\vec{A}\right)\psi - \int (\vec{\nabla}\psi^+)\frac{ie}{2m}\vec{A}\psi$$

$$\frac{\delta S}{\delta \vec{A}} = \psi^+ \frac{1}{2m}\left(ie\vec{A} + 2e^2\vec{A}\right)\psi - \frac{ie}{2m}(\vec{\nabla}\psi^+)\psi = \underbrace{-\frac{ie}{2m}\left[(\vec{\nabla}\psi^+)\psi - \psi^+\vec{\nabla}\psi\right]}_{j_{para}} + \frac{e^2}{m}\underbrace{\psi^+\psi}_{n}\vec{A}$$

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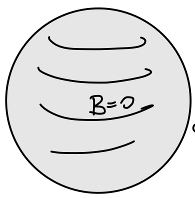

Inside superconductor there is no $\vec{B}$ field and no current $\vec{j}$

Current on the surface in depth $\lambda = \sqrt{\frac{m}{n_s}}$

Why is there no resistance?

$$\vec{j}_s = e^2\frac{n_s}{m}\vec{A}$$

$$\frac{d\vec{j}_s}{dt} = e^2\frac{n_s}{m}\frac{d\vec{A}}{dt} = e^2\frac{n_s}{m}\vec{E}$$

hence current is growing in the presence of $\vec{E}$ field.

Here we will set $\vartheta=0$ and derive the effective action

$$\boxed{S[\vartheta=0,\vec{A}] = \underbrace{\mathrm{Tr}\ln(-G_0)+\mathrm{Tr}\left(\frac{|\Delta|^2}{g}\right)}_{\approx (T-T_c)|\Delta|^2+c|\Delta|^4+\cdots} + \underbrace{e^2\int_0^\beta d\tau\int d^3r\left[-D_0\left[\phi(\vec{r},\tau)\right]^2+\frac{n_s}{2m}\left[\vec{A}(\vec{r},\tau)\right]^2\right]}_{\text{this part is interesting}}}$$

Lets split G^{-1} into three parts (we take into account $\vartheta=0$ and $\Delta_0^+=\Delta_0$)

$$G^{-1} = \underbrace{-\frac{\partial}{\partial\tau}I+\left(\mu+\frac{\nabla^2}{2m}\right)\tau_3+\tau_1\cdot\Delta_0}_{\substack{G_0^{-1}\\ \text{no EM field}}}\ \underbrace{-ie\phi\tau_3-\frac{ie}{2m}\{\vec{\nabla},\vec{A}\}I}_{\substack{X_1\\ \text{linear in fields}}}\ \underbrace{-\frac{e^2}{2m}\vec{A}^2\tau_3}_{\substack{X_2\\ \text{quadratic in fields}}}$$

$$S-\tilde{S}_0 = -\mathrm{Tr}\ln\left(-G^{-1}[\Delta]\right) = -\mathrm{Tr}\ln\left(-G_0^{-1}\left(I-G_0(X_1+X_2)\right)\right) = \underbrace{-\mathrm{Tr}\ln(-G_0^{-1})}_{S_{00}}-\mathrm{Tr}\ln\left(I-G_0(X_1+X_2)\right)$$

$$-\ln(1-x)\approx x+\tfrac{1}{2}x^2+\tfrac{1}{3}x^3$$

$$\underbrace{S-\tilde{S}_0-S_{00}}_{S_0} = \mathrm{Tr}\left(G_0(X_1+X_2)\right)+\tfrac{1}{2}\mathrm{Tr}\left(G_0(X_1+X_2)G_0(X_1+X_2)\right)+\cdots =$$

$$= \mathrm{Tr}(G_0X_1)+\mathrm{Tr}(G_0X_2)+\tfrac{1}{2}\mathrm{Tr}(G_0X_1G_0X_1)+O(\{A^2,\phi^2\})$$

$$G^0_{p_1p_2} = \left(i\omega_2 I+\left[\left(\mu-\frac{p_2^2}{2m}\right)\tau_3+\tau_1\cdot\Delta_0\right]\right)^{-1}\delta_{p_1-p_2}\delta_{\omega_1-\omega_2} \Rightarrow \delta_{p_1p_2}G^0_{p_1}$$

$$(X_1)_{p_1p_2} = \left(ie\phi\tau_3+i\frac{e}{2m}\{\vec{\nabla},\vec{A}\}\cdot I\right)_{p_1p_2} = ie\phi_{p_2-p_1}\tau_3+\frac{ie}{2m}i(\vec{p}_1+\vec{p}_2)\cdot\vec{A}_{\vec{p}_2-\vec{p}_1}\cdot I = ie\,\phi_{\vec{p}_2-\vec{p}_1}\tau_3-\frac{e}{2m}(\vec{p}_1+\vec{p}_2)\vec{A}_{\vec{p}_2-\vec{p}_1}\cdot I$$

Check $$\left(\{\vec{\nabla},\vec{A}\}\right)_{p_1p_2} = \int\frac{e^{-i\vec{p}_1\cdot\vec{r}}}{\sqrt{V}}(\vec{\nabla}\vec{A}+\vec{A}\vec{\nabla})\frac{e^{i\vec{p}_2\cdot\vec{r}}}{\sqrt{V}}d^3r = \frac{1}{V}\int e^{-i\vec{p}_1\cdot\vec{r}}\left((\vec{\nabla}\cdot\vec{A})+2\vec{A}\vec{\nabla}\right)e^{i\vec{p}_2\cdot\vec{r}}d^3r =$$

$$\frac{1}{V}\int\left(-\vec{\nabla}e^{i(\vec{p}_2-\vec{p}_1)\vec{r}}\right)\cdot\vec{A}\,d^3r+2i\vec{p}_2\frac{1}{V}\int\vec{A}\,e^{i(\vec{p}_2-\vec{p}_1)\vec{r}}d^3r = \left(-i(\vec{p}_2-\vec{p}_1)+2i\vec{p}_2\right)\vec{A}_{\vec{p}_2-\vec{p}_1} = i(\vec{p}_1+\vec{p}_2)\vec{A}_{\vec{p}_2-\vec{p}_1}$$

$$\mathrm{Tr}(G_0 X_1) = \sum_{p_1} \mathrm{Tr}_{2\times 2}(G_{0\,p_1 p_1} \; X_{1\,p_1 p_1}) = \mathrm{Tr}_{2\times 2}\Big(\frac{1}{\beta}\sum_{i\omega, p} G_{0p}(i\omega)\left[ie\,\phi_{q=0}\,\tau_3 - \frac{e}{2m}\vec{p}\,A_{q=0}\cdot I\right]$$

$$\frac{1}{\beta V}\sum_{i\omega,p}\mathrm{Tr}\Big(G_{0p}(i\omega)\Big(ie\,\phi_{q=0}\,\tau_3 - \underbrace{\frac{e}{2m}\vec{p}\,\vec{A}_{q=0}}_{\text{odd in } \vec{p} \Rightarrow 0}\cdot I\Big)\Big)$$

$$= \Big(\frac{1}{\beta V}\sum_{i\omega,p}[G_{0p}(i\omega)]_{11} - [G_{0p}(i\omega)]_{22}\Big)\cdot ie\,\phi_{q=0}$$

$$\Big(\frac{1}{V}\sum_p \underbrace{[G_{0p}(\tau=0^-)]_{11}} - [G_{0p}(\tau=0^-)]_{22}\Big)\cdot ie\,\phi_{q=0}$$

$$\underbrace{\frac{1}{V}\sum_p \langle \psi^+_{p\uparrow}\psi_{p\uparrow}\rangle - \langle \psi_{\downarrow p}\psi^+_{\downarrow p}\rangle}_{N_\uparrow + N_\downarrow}$$

$$\mathrm{Tr}(G_0\cdot X_1) = ie\,n_{tot}\cdot\phi_{q=0} = ie\int d^3r\, n(\vec{r})\,\phi(\vec{r})$$ – electrostatic potential of electrons in E-field

The ion charge should give equal and opposite constant which should cancel this term. Hence neglect.

$$\mathrm{Tr}(G_0\cdot X_2) = \frac{e^2}{2m}\mathrm{Tr}_{2\times 2}\Big(\underbrace{G_{0p}(i\omega)\cdot\tau_3}_{n_{tot}}\;\vec{A}^2(p_1-p_2=0)\Big) = \underbrace{\frac{e^2}{2m}\int d^3r\, n(\vec{r})}_{\text{will be used later}}\,A^2(\vec{r})$$ – diamagnetic term, which is also present in normal state.

$$\frac{1}{2}\mathrm{Tr}(G^0 X_1 G^0 X_1) = \frac{1}{2}\mathrm{Tr}_{2\times 2}\Big(G^0_{p_1}(i\omega_1)\,X_{1\,p_1 p_2}\,G^0_{p_2}(i\omega_2)\,X_{1\,p_2 p_1}\Big) = \qquad p_1 = p-\tfrac{q}{2} \quad p_2 = p+\tfrac{q}{2}$$

$$= \frac{1}{2}\mathrm{Tr}_{2\times 2}\Big(G^0_{p-\frac{q}{2}}\big(ie\,\phi_q\,\tau_3 - \tfrac{e}{m}\vec{p}\cdot\vec{A}_q\cdot I\big)\,G^0_{p+\frac{q}{2}}\big(ie\,\phi_{-q}\,\tau_3 - \tfrac{e}{m}\vec{p}\cdot\vec{A}_{-q}\cdot I\big)\Big) =$$

$$= \frac{1}{2}\mathrm{Tr}\big(G^0_{p-\frac{q}{2}}\tau_3 G^0_{p+\frac{q}{2}}\tau_3\big)(-e^2\phi_q\phi_{-q}) + \frac{1}{2}\mathrm{Tr}\big(G^0_{p-\frac{q}{2}}G^0_{p+\frac{q}{2}}\big)\left(\frac{e}{m}\right)^2\vec{p}\cdot\vec{A}_q\,\vec{p}\cdot\vec{A}_{-q} + \underbrace{\mathrm{Tr}\big(G^0_{p+\frac{q}{2}}\tau_3\,G^0_{p-\frac{q}{2}}\cdot I\big)}_{\text{even in } \vec{p}}\,\underbrace{ie\,\phi_{-q}\left(-\frac{e}{m}\right)\vec{p}\cdot\vec{A}_q}_{\text{odd in } \vec{p}} \to 0$$

We are interested in the limit of small $\vec{q}$ hence we will approximate $G^0_{p\pm\frac{q}{2}} \approx G^0_p$

$$\frac{1}{2}\mathrm{Tr}(G^0 X_1 G^0 X_1) = -\frac{e^2}{2}\phi_q\,\phi_{-q}\,\frac{1}{\beta}\sum_{i\omega,p}\left[(G^{11}_p(i\omega))^2 + (G^{22}_p(i\omega))^2 - 2G^{12}_p(i\omega)\,G^{21}_p(i\omega)\right]$$

$$+\frac{e^2}{2m^2}\sum_{\vec{p}}\underbrace{(\vec{p}\cdot\vec{A}_q)(\vec{p}\cdot\vec{A}_{-q})}_{\vec{A}_q\cdot\vec{A}_{-q}\cdot\frac{p^2}{3}}\frac{1}{\beta}\sum_{i\omega}\left[(G^{11}_p(i\omega))^2 + (G^{22}_p(i\omega))^2 + 2G^{12}_p(i\omega)\,G^{21}_p(i\omega)\right]$$

This identity is satisfied for any rotationally invariant $R(p^2)$:

$$\sum_{\vec{p}}(\vec{p}\cdot\vec{A}_q)(\vec{p}\cdot\vec{A}_{-q})\,R(p^2) = \frac{1}{3}\vec{A}_q\cdot\vec{A}_{-q}\sum_{\vec{p}}p^2 R(p^2)$$

Check $A_q \parallel A_{-q} \Rightarrow$ $$\int 2\pi p^2 dp\underbrace{\int_{-1}^{1} d(\cos\vartheta)\cos^2\vartheta}_{\frac{2}{3}}\; p^2 A_q^2\,R(p^2) = \frac{1}{3}\int 4\pi p^2 dp\; p^2 R(p^2)\,A_q^2 \;\checkmark$$

We previously derived

$$G_k(i\omega) = \begin{pmatrix} i\omega + \varepsilon_k , & \Delta \\ \Delta , & i\omega - \varepsilon_k \end{pmatrix} \frac{1}{(i\omega)^2 - \lambda_k^2} = \begin{pmatrix} \frac{\cos^2\theta_k}{i\omega - \lambda_k} + \frac{\sin^2\theta_k}{i\omega + \lambda_k} , & \frac{\Delta}{2\lambda}\left(\frac{1}{i\omega-\lambda} - \frac{1}{i\omega+\lambda}\right) \\ \frac{\Delta}{2\lambda}\left(\frac{1}{i\omega-\lambda} - \frac{1}{i\omega+\lambda}\right) , & \frac{\sin^2\theta_k}{i\omega - \lambda_k} + \frac{\cos^2\theta_k}{i\omega + \lambda_k} \end{pmatrix} \quad ; \quad \frac{\Delta}{2\lambda} \equiv -\sin\theta_k \cos\theta_k$$

$$(G^{11})^2 + (G^{22})^2 - 2G^{12}G^{21} = \frac{(i\omega+\varepsilon_k)^2 + (i\omega-\varepsilon_k)^2 - 2\Delta^2}{[(i\omega)^2 - \lambda_k^2]^2} = 2\frac{(i\omega)^2 + \varepsilon_k^2 - \Delta^2}{[(i\omega)^2 - \lambda_k^2]^2} = 2\frac{(i\omega)^2 + \lambda_k^2 - 2\Delta^2}{[(i\omega)^2 - \lambda_k^2]^2}$$

$$(G^{11})^2 + (G^{22})^2 + 2G^{12}G^{21} = \frac{(i\omega+\varepsilon_k)^2 + (i\omega-\varepsilon_k)^2 + 2\Delta^2}{[(i\omega)^2 - \lambda_k^2]^2} = 2\frac{(i\omega)^2 + \varepsilon_k^2 + \Delta^2}{[(i\omega)^2 - \lambda_k^2]^2} = 2\frac{(i\omega)^2 + \lambda_k^2}{[(i\omega)^2 - \lambda_k^2]^2}$$

$$\frac{1}{2}\mathrm{Tr}(G^0 X_1 G^0 X_1) = -\frac{e^2}{2}\phi_q \phi_{-q} \frac{1}{\beta}\sum_{i\omega, p} 2\frac{(i\omega)^2 + \lambda_p^2 - 2\Delta^2}{[(i\omega)^2 - \lambda_p^2]^2} + \frac{e^2}{2m^2}\vec{A}_q \cdot \vec{A}_{-q} \sum_{\vec{p}} \frac{p^2}{3} \frac{1}{\beta}\sum_{i\omega} 2\frac{(i\omega)^2 + \lambda_p^2}{[(i\omega)^2 - \lambda_p^2]^2}$$

$$= -e^2 \frac{1}{\beta}\sum_{i\omega, p} \frac{1}{[(i\omega)^2 - \lambda_p^2]^2}\left[\phi_q \phi_{-q} \left((i\omega)^2 + \lambda_p^2 - 2\Delta^2\right) - \vec{A}_q \cdot \vec{A}_{-q} \frac{p^2}{3m^2}\left((i\omega)^2 + \lambda_p^2\right)\right]$$

$$\mathrm{Tr}(G_0 X_2) + \frac{1}{2}\mathrm{Tr}(G^0 X_1 G^0 X_1) = -e^2 \underbrace{\frac{1}{\beta}\sum_{i\omega, p}\frac{\left((i\omega)^2 + \lambda_p^2 - 2\Delta^2\right)}{[(i\omega)^2 - \lambda_p^2]^2}}_{-D_0} \phi_q \phi_{-q} + e^2 A_q A_{-q} \underbrace{\left(\frac{n}{2m} + \frac{1}{\beta}\sum_{i\omega, p}\frac{p^2}{3m^2}\frac{\left((i\omega)^2 + \lambda_p^2\right)}{[(i\omega)^2 - \lambda_p^2]^2}\right)}_{\frac{n_s}{2m}}$$

add back diamagnetic term

diamagnetic term

$$\frac{1}{\beta}\sum_{i\omega}\frac{1}{(i\omega)^2 - \lambda_p^2} = \frac{1}{2\lambda_p}\frac{1}{\beta}\sum_{i\omega}\left(\frac{1}{i\omega - \lambda_p} - \frac{1}{i\omega + \lambda_p}\right) = \frac{2f(\lambda_p) - 1}{2\lambda_p}$$

; Notice: $$\frac{d}{d\lambda_p}\left(\frac{1}{\beta}\sum_{i\omega}\frac{1}{(i\omega)^2 - \lambda_p^2}\right) = \frac{1}{\beta}\sum_{i\omega}\frac{2\lambda_p}{((i\omega)^2 - \lambda_p^2)^2} = \frac{f'(\lambda_p)}{\lambda_p} - \frac{2f(\lambda_p) - 1}{2\lambda_p^2}$$

$$\frac{1}{\beta}\sum_{i\omega}\frac{(i\omega)^2 + \lambda_p^2 - 2\Delta^2}{[(i\omega)^2 - \lambda_p^2]^2} = \frac{1}{\beta}\sum_{i\omega}\frac{(i\omega)^2 - \lambda_p^2 + 2(\lambda_p^2 - \Delta^2)}{[(i\omega)^2 - \lambda_p^2]^2} = \frac{1}{\beta}\sum_{i\omega}\frac{1}{(i\omega)^2 - \lambda_p^2} + \frac{2(\lambda_p^2 - \Delta^2)}{[(i\omega)^2 - \lambda_p^2]^2} = \frac{2f(\lambda_p) - 1}{2\lambda_p} + \frac{2(\lambda_p^2 - \Delta^2)}{2\lambda_p^2}\left[f'(\lambda_p) - \frac{2f(\lambda_p) - 1}{2\lambda_p}\right]$$

$$\frac{1}{\beta}\sum_{i\omega}\frac{(i\omega)^2 + \lambda_p^2 - 2\Delta^2}{[(i\omega)^2 - \lambda_p^2]^2} = f'(\lambda_p)\left(1 - \frac{\Delta^2}{\lambda_p^2}\right) + [2f(\lambda_p) - 1]\frac{\Delta^2}{2\lambda_p^3} \xrightarrow[\substack{f'(\sqrt{\varepsilon_p^2 + \Delta^2}) \approx 0 \\ f(\sqrt{\varepsilon_p^2 + \Delta^2}) \approx 0}]{\text{for finite } \Delta} -\frac{\Delta^2}{2\lambda_p^3}$$

$$\frac{1}{\beta}\sum_{i\omega}\frac{(i\omega)^2 + \lambda_p^2}{[(i\omega)^2 - \lambda_p^2]^2} = \frac{1}{\beta}\sum_{i\omega}\frac{1}{(i\omega)^2 - \lambda_p^2} + \frac{2\lambda_p^2}{[(i\omega)^2 - \lambda_p^2]^2} = \frac{2f(\lambda_p) - 1}{2\lambda_p} + \frac{2\lambda_p^2}{2\lambda_p}\left[\frac{f'(\lambda_p)}{\lambda_p} - \frac{2f(\lambda_p) - 1}{2\lambda_p^2}\right] = f'(\lambda_p)$$

cancel

$$Tr(G_0 X_2) + \frac{1}{2} Tr(G^0 X_1 G^0 X_1) = e^2 \Phi_q \Phi_{-q} \sum_p + \frac{\Delta^2}{2\lambda_p^3} + e^2 A_{\vec q} A_{-\vec q} \left(\frac{M}{2m} - \sum_p \frac{p^2}{3m^2} f'(\lambda_p) \right)$$

$$\sum_p + \frac{\Delta^2}{2\lambda_p^3} = + \underset{\text{spin}}{\frac{1}{2}} \int d\varepsilon\, D(\varepsilon) \frac{\Delta^2}{(\varepsilon^2+\Delta^2)^{3/2}} \approx + \frac{1}{2} D(0) \int_{-\infty}^{\infty} \frac{dx}{(x^2+1)^{3/2}} = + D(0)$$

$$\frac{M}{2m} + \sum_p \frac{p^2}{3m^2} f'(\lambda_p) = \frac{M}{2m} + \sum_p \frac{2}{3m}(\xi_p + \mu) f'(\lambda_p) = \frac{M}{2m} - \frac{2}{3m} \underset{\text{spin}}{\frac{1}{2}} \int D(\varepsilon)\, (\underbrace{\varepsilon}_{\sim 0} + \mu)\, \beta f(\beta\sqrt{\varepsilon^2+\Delta^2}) f(-\beta\sqrt{\varepsilon^2+\Delta^2})\, d\varepsilon$$

$$\frac{p^2}{2m} - \mu = \xi_p$$

$$f'(\lambda_p) = -\beta f(\lambda_p) f(-\lambda_p)$$

$$= \frac{M}{2m} - \underbrace{\frac{\mu D(0)}{3m}}_{\frac{M}{2m}} \underbrace{\int d\varepsilon\, \beta f(\beta\sqrt{\varepsilon^2+\Delta^2}) f(-\beta\sqrt{\varepsilon^2+\Delta^2})}_{\substack{\text{at } T=0 \ \to 0 \\ \text{at } T > T_c \ \to 1}}$$

$$= \frac{M}{2m}\left(1 - \underbrace{\int d\varepsilon\, \beta f(\beta\sqrt{\varepsilon^2+\Delta^2}) f(-\beta\sqrt{\varepsilon^2+\Delta^2})}_{\substack{\text{at } T=0 \ \to 0 \\ \text{at } T=T_c \ \to 1}}\right) \equiv \frac{M_s}{2m}$$

Check relation between $D(0)$ and M:

$$\begin{Bmatrix} D(0) \\ M \end{Bmatrix} = \underset{\text{spin}}{\frac{2}{V}} \sum_{\vec p} \begin{Bmatrix} \delta(\mu - \varepsilon_p) \\ \Theta(\mu - \varepsilon_p) \end{Bmatrix} = \frac{2}{(2\pi)^3} \int d^3p \begin{Bmatrix} \delta(\mu - \varepsilon_p) \\ \Theta(\mu - \varepsilon_p) \end{Bmatrix} = \frac{2\pi (2m)^{3/2}}{(2\pi)^3} \int_0^\infty d\varepsilon_p \sqrt{\varepsilon_p} \begin{Bmatrix} \delta(\mu - \varepsilon_p) \\ \Theta(\mu - \varepsilon_p) \end{Bmatrix} = \frac{(2m)^{3/2}}{(2\pi)^2} \begin{Bmatrix} \sqrt{\mu} \\ \frac{2}{3}\mu^{3/2} \end{Bmatrix}$$

$$\varepsilon_p = \frac{p^2}{2m}$$

$$p = \sqrt{2m\varepsilon_p}$$

$$d^3p = 4\pi (2m\varepsilon_p) \sqrt{2m} \frac{d\varepsilon_p}{2\sqrt{\varepsilon_p}} = 2\pi (2m)^{3/2} \sqrt{\varepsilon_p}\, d\varepsilon_p$$

$$\underline{\frac{M}{D(0)} = \frac{2}{3}\mu} \Rightarrow \mu D(0) = \frac{3}{2} M$$

$$Tr(G_0 X_2) + \frac{1}{2} Tr(G^0 X_1 G^0 X_1) = \sum_q \left(e^2 D_0\, \Phi_q \Phi_{-q} + e^2 \frac{M_s}{2m} A_{\vec q} A_{-\vec q} \right)$$

$$\boxed{\text{We just proved } S[V=0, \vec A] = Tr \ln(-G_0) + Tr\left(\frac{|\Delta|^2}{g}\right) + e^2 \int_0^\beta d\tau \int d^3r \left[D_0\, [\Phi(\vec r, \tau)]^2 + \frac{M_s}{2m} [\vec A(\vec r, \tau)]^2 \right]}$$

Here we want to derive that

$$\boxed{S[\upsilon=0,\hat{A}=0] = \mathrm{Tr}\ln(-G_0) + \mathrm{Tr}\left(\frac{|\Delta|^2}{g}\right) \approx (T-T_c)|\Delta|^2 + c|\Delta|^4 + \cdots}$$

$$\mathrm{Tr}\ln(-G_0) = -\mathrm{Tr}\ln\left(-\left(\underbrace{[G_0(\Delta=0)]^{-1}}_{\text{normal state}} + \underbrace{\begin{pmatrix}0 & \Delta\\ \Delta^+ & 0\end{pmatrix}}_{\hat{\Delta}}\right)\right) = \underbrace{\mathrm{Tr}\ln(-G_{00})}_{\text{normal state}} - \mathrm{Tr}\ln(1+G_{00}\hat{\Delta})$$

$$-\mathrm{Tr}\Big(\underbrace{G_{00}\cdot\hat{\Delta}}_{0} - \tfrac{1}{2}(G_{00}\hat{\Delta})^2 + \underbrace{\tfrac{1}{3}(G_{00}\cdot\hat{\Delta})^3}_{0} - \tfrac{1}{4}(G_{00}\cdot\hat{\Delta})^4 \cdots\Big)$$

because Δ is off-diagonal, G_{00} is diagonal

Here $G_{00} = \begin{pmatrix}\frac{1}{i\omega-\xi_k}, & 0\\ 0, & \frac{1}{i\omega+\xi_k}\end{pmatrix}$ and $\hat{\Delta} = \begin{pmatrix}0, & \Delta\\ \Delta^+, & 0\end{pmatrix}$

$$\mathrm{Tr}\ln(-G_0) = S_{00} + \sum_{m=1}^{\infty}\frac{1}{2m}\mathrm{Tr}(G_{00}\cdot\hat{\Delta})^{2m}$$

$$\mathrm{Tr}((G_{00}\cdot\hat{\Delta})^2) = \mathrm{Tr}\left((G_{00})_{pp}\Delta_{pp'}(G_{00})_{p'p'}\Delta_{p'p}\right) = \frac{1}{\beta^2}\sum_{\substack{i\omega,k\\ i\Omega,q}}\mathrm{Tr}\left(G_{00}^{k}(i\omega)\,\Delta_{q\Omega}\,G_{00}^{k+q}(i\omega+i\Omega)\,\Delta_{-q-\Omega}\right), \quad q=p'-p$$

$$\mathrm{Tr}\left[\begin{pmatrix}G_{11} & 0\\ 0 & G_{22}\end{pmatrix}\begin{pmatrix}0 & \Delta\\ \Delta^+ & 0\end{pmatrix}\begin{pmatrix}G_{11} & 0\\ 0 & G_{22}\end{pmatrix}\begin{pmatrix}0 & \Delta\\ \Delta^+ & 0\end{pmatrix}\right] = G_{11}\Delta G_{22}\Delta^+ + G_{22}\Delta^+ G_{11}\Delta$$

$$\mathrm{Tr}((G_{00}\cdot\hat{\Delta})^2) = \frac{1}{\beta^2}\sum_{\substack{i\omega,k\\ i\Omega,q}}\Delta_q\Delta^+_{-q}\frac{1}{i\omega-\xi_k}\,\frac{1}{i\omega+i\Omega+\xi_{k+q}} + \Delta^+_q\Delta_{-q}\frac{1}{i\omega+\xi_k}\,\frac{1}{i\omega+i\Omega-\xi_{k+q}}$$

$$= \frac{1}{\beta}\sum_{q,\Omega}\underbrace{\Delta_q\Delta^+_q}_{\text{mimics the external field}}\;\frac{1}{\beta}\sum_{i\omega,k}\frac{1}{i\omega-\xi_k}\,\frac{1}{i\omega+i\Omega+\xi_{k+q}} + \frac{1}{i\omega+\xi_k}\,\frac{1}{i\omega-i\Omega-\xi_{k-q}}$$

$$\left[\underbrace{\frac{f(\xi_k)+f(\xi_{k+q})-1}{i\Omega+\xi_k+\xi_{k+q}}}_{-B_q(i\Omega)} + q \leftrightarrow -q\right]$$

$|\Delta_q|^2 = |\Delta_{-q}|^2$

$$= \frac{1}{\beta}\sum_{i\Omega,q}|\Delta_q|^2\cdot 2B_q(i\Omega)$$

$$S_{eff} = S_{00} + \frac{1}{\beta}\sum_{i\Omega,q}|\Delta_q|^2\Big(\underbrace{\frac{1}{g}}_{\text{from }\tilde{S}_0} - \underbrace{B_q(i\Omega)}_{\left(\frac{1}{g}+D_0\frac{T_c-T}{T_c}\right)}\Big) + O(\Delta^4) = S_{00} + \sum_q|\Delta|^2\underbrace{\frac{D_0}{T_c}(T-T_c)}_{\frac{1}{2}r(T)} + \underbrace{c|\Delta|^4}_{\text{Ginzburg Landau}}$$

Here we check what is $B_q(\Omega)$

$$B_q(i\Omega) = \frac{1 - f(\varphi_k) - f(\varphi_{k+q})}{i\Omega + \varphi_k + \varphi_{k+q}} \quad ; \quad \sum_k \delta(\omega - \varphi_k) = \int D(\varphi)\, d\varphi$$

$$B_{q\simeq 0}(\Omega \sim 0) = \int_{-\omega_D}^{\omega_D} d\varepsilon\, D(\varepsilon) \cdot \frac{1 - 2f(\varepsilon)}{2\varepsilon} = \int_0^{\omega_D} d\varepsilon\, D(\varepsilon)\, \frac{th\left(\frac{\beta\varepsilon}{2}\right)}{\varepsilon} \simeq D_0 \underbrace{\int_0^{\frac{\omega_D}{2T}} \frac{th(x)}{x}\, dx}_{\text{at } T=T_c \text{ this is } \frac{1}{g D_0}} = D_0 \int_0^{\frac{\omega_D}{2T_c}} \frac{th\, x}{x} dx + D_0 \int_{\frac{\omega_D}{2T_c}}^{\frac{\omega_D}{2T}} \frac{th(x)}{x} dx \simeq \frac{1}{g} - D_0 \ln \frac{T}{T_c}$$

$$\simeq \frac{1}{g} + D_0 \frac{T_c - T}{T_c}$$

$$\frac{1}{gD_0} = \int_0^{\frac{\omega_D}{2T}} \left(\frac{th\left(\sqrt{x^2+\varkappa^2}\right)}{\sqrt{x^2+\varkappa^2}} - \frac{th(x)}{x} \right) dx + \underbrace{\int_0^{\frac{\omega_D}{2T_c}} \frac{th(x)}{x}}_{=\frac{1}{gD_0}} + \underbrace{\int_{\frac{\omega_D}{2T_c}}^{\frac{\omega_D}{2T}} \frac{th(x)}{x}}_{\frac{1}{\frac{\omega_D}{2T_c}}\left(\frac{\omega_D}{2T} - \frac{\omega_D}{2T_c}\right) = \frac{T_c - T}{T}}$$

from previous calculation

hence

$$-\frac{T_c - T}{T} = \int_0^{\frac{\omega_D}{2T}} \left(\frac{th\left(\sqrt{x^2+\varkappa^2}\right)}{\sqrt{x^2+\varkappa^2}} - \frac{th(x)}{x} \right) dx$$

Estimation: $\underbrace{\int_0^{\Lambda} \left(\frac{th\left(\sqrt{x^2+\varkappa^2}\right)}{\sqrt{x^2+\varkappa^2}} - \frac{th(x)}{x} \right) dx}$ $+ \int_{\Lambda}^{\frac{\omega_D}{2T}} \left(\frac{1}{\sqrt{x^2+\varkappa^2}} - \frac{1}{x} \right) dx$

$$\int_0^{\Lambda} \left(-\frac{\varkappa^2}{3} + \frac{4\varkappa^2}{15} x^2 + \dots \right) dx \qquad \frac{1}{x}\left(\left(1 + \left(\frac{\varkappa}{x}\right)^2\right)^{-\frac{1}{2}} - 1 \right)$$

$$\frac{1}{x}\left(-\frac{\varkappa^2}{2x^2} + \frac{3}{8}\left(\frac{\varkappa}{x}\right)^4 \right)$$

$$-\frac{\varkappa^2}{3}\Lambda + \frac{4\varkappa^2}{15 \cdot 3}\Lambda^3 + \dots \qquad -\frac{\varkappa^2}{2}\int_{\Lambda}^{\frac{\omega_D}{2T}} \frac{1}{x^3} dx = -\frac{1}{4}\varkappa^2 \left(\frac{1}{\Lambda^2} - \left(\frac{2T}{\omega_D}\right)^2 \right)$$

$$\frac{T_c - T}{T} = \varkappa^2 \left(\underbrace{\frac{\Lambda}{3}\left(1 - \frac{4}{15}\Lambda^2 + \cdot\right) + \frac{1}{4}\left(\frac{1}{\Lambda^2} - \left(\frac{2T}{\omega_D}\right)^2\right)}_{\frac{1}{2}} \right) \approx \frac{1}{2}\left(\frac{\Delta}{2T}\right)^2 \Rightarrow \Delta \approx \sqrt{8T_c(T_c - T)}$$

– Δ at $T = 0$:

$\varkappa = \frac{\Delta}{2T} \to \infty$

$$\frac{1}{gD_0} = \int_0^{\frac{\omega_D}{2T}} \frac{th\left(\sqrt{x^2+\varkappa^2}\right)}{\sqrt{x^2+\varkappa^2}} dx \approx \int_0^{\frac{\omega_D}{2T}} \frac{dx}{\sqrt{x^2+\varkappa^2}} = \ln\left(x + \sqrt{x^2+\varkappa^2}\right)\Big|_0^{\frac{\omega_D}{2T}} = \ln\left(\frac{\omega_D}{2T} + \sqrt{\left(\frac{\omega_D}{2T}\right)^2 + \left(\frac{\Delta}{2T}\right)^2}\right) - \ln\left(\frac{\Delta}{2T}\right)$$

$$\ln\left(\frac{\omega_D + \sqrt{\omega_D^2 + \Delta^2}}{\Delta}\right)$$

$$e^{-\frac{1}{gD_0}} = \frac{\Delta_0}{\omega_D + \sqrt{\omega_D^2 + \Delta_0^2}} \approx \frac{\Delta_0}{2\omega_D} \Rightarrow \Delta_0 = 2\omega_D e^{-\frac{1}{gD_0}}$$

while $T_c = 1.13\,\omega_D e^{-\frac{1}{gD_0}}$

hence $\frac{\Delta_0}{T_c} = \frac{2}{1.13}$ and $\frac{T_c}{\Delta_0} \approx 0.57$

or $\frac{\Delta}{2T_c} \sim 1$

Homework 4, 620 Many body

December 12, 2022

1) The excitations spectra of the superconductor: Calculate the excitations spectra of quasiparticles as well as the real electrons in the BCS state wave function.
In class we derived the BCS Hamiltonian

$$H^{BCS} = \sum_{\mathbf{k}} \Psi^\dagger_{\mathbf{k}} \begin{pmatrix} \varepsilon_{\mathbf{k}} & -\Delta \\ -\Delta & -\varepsilon_{-\mathbf{k}} \end{pmatrix} \Psi_{\mathbf{k}} + \varepsilon_{-\mathbf{k}} \tag{1}$$

in which the $\Psi_{\mathbf{k}}$ spinor is

$$\Psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k},\uparrow} \\ c^\dagger_{-\mathbf{k},\downarrow}. \end{pmatrix} \tag{2}$$

The Hamiltonian is diagonalized with a unitary transformation in the form

$$\hat{U}_{\mathbf{k}} = \begin{pmatrix} \cos(\theta_{\mathbf{k}}) & \sin(\theta_{\mathbf{k}}) \\ \sin(\theta_{\mathbf{k}}) & -\cos(\theta_{\mathbf{k}}) \end{pmatrix} \tag{3}$$

where

$$\cos(\theta_{\mathbf{k}}) = \sqrt{\frac{1}{2}(1 + \frac{\varepsilon_{\mathbf{k}}}{\sqrt{\varepsilon_{\mathbf{k}} + \Delta^2}})} \tag{4}$$

$$\sin(\theta_{\mathbf{k}}) = -\sqrt{\frac{1}{2}(1 - \frac{\varepsilon_{\mathbf{k}}}{\sqrt{\varepsilon_{\mathbf{k}} + \Delta^2}})} \tag{5}$$

and the quasiparticle spinors are

$$\begin{pmatrix} \Phi_{\mathbf{k},\uparrow} \\ \Phi^\dagger_{-\mathbf{k},\downarrow} \end{pmatrix} = \hat{U}_{\mathbf{k}} \begin{pmatrix} c_{\mathbf{k},\uparrow} \\ c^\dagger_{-\mathbf{k},\downarrow}. \end{pmatrix} \tag{6}$$

The diagonal BCS Hamiltonian has the form

$$H^{BCS} = \sum_{\mathbf{k}} \lambda_{\mathbf{k}} \Phi^\dagger_{\mathbf{k},s} \Phi_{\mathbf{k},s} - E_0 \tag{7}$$

with $E_0 = \sum_{\mathbf{k}} \lambda_{\mathbf{k}} - \varepsilon_{\mathbf{k}}$ and $\lambda_{\mathbf{k}} = \sqrt{\varepsilon^2_{\mathbf{k}} + \Delta^2}$

- Show that the quasiparticle Green's function $\widetilde{G}_{\mathbf{k}} = -\langle T_\tau \Phi_{\mathbf{k},s}(\tau)\Phi^\dagger_{\mathbf{k},s}(0)\rangle$ has a gap with the size Δ. What is the spectral function corresponding to this Green's function? Show that the corresponding densities of states has the form $D(\omega) \approx D_0\ \omega/\sqrt{\omega^2-\Delta^2}$, where D_0 is density of states at the Fermi level of the normal state.
- Compute the physical Green's function (measured in ARPES)

$$G_{\mathbf{k},s} = -\langle T_\tau c_{\mathbf{k},s}(\tau) c^\dagger_{\mathbf{k},s}(0)\rangle \tag{8}$$

  and its density of states. Show that the corresponding spectral function has the form

$$A_{\mathbf{k},s}(\omega) = \cos^2\theta_{\mathbf{k}}\ \delta(\omega-\lambda_{\mathbf{k}}) + \sin^2\theta_{\mathbf{k}}\ \delta(\omega+\lambda_{\mathbf{k}}) \tag{9}$$

  Sketch the bands and their weight, and sketch the density of states.

2) In class we derived the BCS action, which takes the form

$$S = \int_0^\beta d\tau \int d^3\mathbf{r}\Psi^\dagger(\mathbf{r}) \begin{pmatrix} \frac{\partial}{\partial\tau} - \mu + \frac{(i\nabla+e\vec{A})^2}{2m} + ie\phi & -\Delta \\ -\Delta^\dagger & \frac{\partial}{\partial\tau} + \mu - \frac{(i\nabla-e\vec{A})^2}{2m} - ie\phi \end{pmatrix} \Psi(\mathbf{r}) + s_0 (10)$$

where $s_0 = \int_0^\beta d\tau \int d^3\mathbf{r}\frac{|\Delta|^2}{g}$

Show that the action can also be expressed by

$$S = s_0 + \mathrm{Tr}\log(-G) \tag{11}$$

where

$$G^{-1} = \begin{pmatrix} i\omega_n + \mu - \frac{(\mathbf{p}-e\mathbf{A})^2}{2m} - ie\phi, \Delta & \\ \Delta^\dagger & i\omega - \mu + \frac{(\mathbf{p}+e\mathbf{A})^2}{2m} + ie\phi \end{pmatrix} \tag{12}$$

Show that the transformation $UG^{-1}U^\dagger$, where U is

$$U = \begin{pmatrix} e^{-i\theta} & 0 \\ 0 & e^{i\theta} \end{pmatrix} \tag{13}$$

leads to the following change of the quantities

$$\Delta \rightarrow e^{-2i\theta}\Delta \tag{14}$$

$$\mathbf{A} \rightarrow \mathbf{A} + \frac{1}{e}\nabla\theta \tag{15}$$

$$\phi \rightarrow \phi - \frac{1}{e}\dot{\theta} \tag{16}$$

and otherwise the same form of the action. Argue that since this corresponds to the change of the EM gauge, the phase of Δ is arbitrary in BCS theory, and can always be changed. Moreover, the phase can not be experimentally measurable quantity.

In the absence of the EM field, derive the saddle point equations in field Δ, which are often written as $\Delta = gG_{12}$, and cam be expressed as

$$\frac{1}{g} = -\frac{1}{V\beta}\sum_{\mathbf{k},n} \frac{1}{(i\omega_n)^2 - \lambda_{\mathbf{k}}^2}. \tag{17}$$

Show that the same equation can also be expressed as

$$\frac{1}{g} = \frac{1}{V}\sum_{\mathbf{k}} \frac{1-2f(\lambda_{\mathbf{k}})}{2\lambda_{\mathbf{k}}} \tag{18}$$

and with D_0 being the density of the normal state at the Fermi level, it can also be expressed as

$$\frac{1}{g} \approx D_0 \int_0^{\frac{\omega_D}{2T}} dx \frac{\tanh(\sqrt{x^2+\kappa^2})}{\sqrt{x^2+\kappa^2}} \tag{19}$$

where $x = \varepsilon/(2T)$ and $\kappa = \Delta/(2T)$.

Next, derive the critical temperature by taking the limit $\Delta \to 0$ ($\kappa \to 0$). Assuming that $\omega_D/(2T) \gg 1$, break the integral into two parts $[0, \Lambda]$, and $[\Lambda, \frac{\omega}{2T}]$. Here $\Lambda \gg 1$. In the second part set $\tanh(x) = 1$, as x is large. Using numerical integration (in Mathematica or similar tool) verify that

$$\lim_{\Lambda\to\infty} \int_0^{\Lambda} dx \frac{\tanh(x)}{x} - \log(\Lambda) \approx \log(2 \times 1.13) \tag{20}$$

Next, show that T_c is determined by

$$\frac{1}{gD_0} \approx \log(2\times 1.13) + \log(\frac{\omega_D}{2T_c}) \tag{21}$$

and consequently

$$T_c \approx 1.13\, \omega_D e^{-1/(gD_0)}$$

Using Eq. 19 compute the size of the gap at $T = 0$. Show that to the leading order in Δ/ω_D the gap size is

$$\Delta(T=0) = 2\omega_D e^{-1/(gD_0)} \tag{22}$$

Finally, show that within BCS there is universal ration $\Delta(T=0)/(2T_c) \approx 1/1.13 \approx 0.88$.

3) Starting from action Eq. 10 derive the effective action for small EM field A, ϕ. Show that for a constant and time independent phase, the action takes the form

$$S_{eff} = \mathrm{Tr}\log(-G_{A=0,\phi=0}) + \mathrm{Tr}(\frac{|\Delta|^2}{g}) + e^2\int_0^\beta d\tau \int d^3\mathbf{r} \left[D_0(\phi(\mathbf{r},\tau))^2 + \frac{n_s}{2m}\left[\mathbf{A}(\mathbf{r},\tau)\right]^2\right] \tag{23}$$

Note that using EM gauge transformation, we arrive at an equivalent action

$$S_{eff} = S_0 + e^2\int_0^\beta d\tau \int d^3\mathbf{r}\left[D_0(\phi(\mathbf{r},\tau)+\dot{\theta})^2 + \frac{n_s}{2m}\left[\mathbf{A}(\mathbf{r},\tau) - \nabla\theta\right]^2\right] \tag{24}$$

Below we summarize the steps to derive this effective action.

We start by splitting G^{-1} in Eq.12 into $G_{A=0,\phi=0} \equiv G^0$ and terms linear and quadratic in EM-fields, i.e,

$$G^{-1} = \left(G^0\right)^{-1} - X_1 - X_2$$

where

$$X_1 = ie\phi\, \sigma_3 + \frac{ie}{2m}[\nabla, A]_+ I \tag{25}$$

$$X_2 = \frac{e^2}{2m}\mathbf{A}^2\, \sigma_3 \tag{26}$$

and σ_3, σ_1 are Pauli matrices. Show that action 11 can then be expressed as

$$S = s_0 + \mathrm{Tr}\log(-G^0) - \mathrm{Tr}\log(I - G^0(X_1 + X_2)) \tag{27}$$

$$\approx S_0 + \mathrm{Tr}(G^0 X_1) + \mathrm{Tr}(G^0 X_2) + \frac{1}{2}\mathrm{Tr}(G^0 X_1 G^0 X_1) + O(X^3) \tag{28}$$

where $S_0 = s_0 + \mathrm{Tr}\log(-G^0)$ (which vanishes at T_c), and the second term, which is linear in fields, while third and fourth are quadratic.

Next show that the form of G^0 is

$$G^0_{\mathbf{p}n,\mathbf{p}'n'} = \delta_{\mathbf{p},\mathbf{p}'}\delta_{nn'}\left(i\omega_n I - \left(\frac{p^2}{2m} - \mu\right)\sigma_3 + \Delta\, \sigma_1\right)^{-1} \tag{29}$$

where the inverse is in the 2×2 space only, while G^0 is diagonal in frequency& momentum space. We will use $(\mathbf{p}, n) = p$ for short notation. Similarly, show that X_1 is

$$(X_1)_{p_1,p_2} = (ie\phi\, \sigma_3 + \frac{ie}{2m}[\nabla, A]_+ I)_{p_1,p_2} = ie\phi_{p_2-p_1}\sigma_3 - \frac{e}{2m}(\mathbf{p}_1 + \mathbf{p}_2)\mathbf{A}_{p_2-p_1} \tag{30}$$

Show that

$$\mathrm{Tr}(G^0 X_1) = \frac{1}{\beta}\sum_{\omega_n,\mathbf{p}} \mathrm{Tr}_{2\times2}(G^0_{\mathbf{p}}(i\omega_n)[ie\phi_{\mathbf{q}=0}\sigma_3 - \frac{e}{m}\mathbf{p}\mathbf{A}_{\mathbf{q}=0}]).$$

Argue that the second term vanishes when inversion symmetry is present, as it is odd in $\mathbf{p}$ (with $G^0_{\mathbf{p}}$ even function). The first term than becomes $nie\phi_{\mathbf{q}=0,\omega=0}$ (n is total density), which describes the electron density in uniform electric field, which should cancel with the action between negative ions and the external field.

Next show that

$$\mathrm{Tr}(G^0 X_2) = \frac{e^2}{2m}\frac{1}{\beta}\sum_{\omega_n,\mathbf{p}} \mathrm{Tr}_{2\times2}(G^0_{\mathbf{p}}(i\omega_n)\mathbf{A}^2_{q=0}\sigma_3) = \frac{e^2}{2m} n \sum_{\mathbf{q}} \mathbf{A}_{\mathbf{q}}\mathbf{A}_{-\mathbf{q}}$$

is standard diamagnetic term, which will be used later.

Finally, we address the term $\frac{1}{2}\mathrm{Tr}(G^0 X_1 G^0 X_1)$. We find

$$\frac{1}{2}\mathrm{Tr}(G^0 X_1 G^0 X_1) = \frac{1}{2}\sum_{p_1,p_2} \mathrm{Tr}_{2\times 2}\left(G^0_{p_1}(X_1)_{p_1,p_2} G^0_{p_2}(X_1)_{p_2,p_1}\right) \quad (31)$$

$$\frac{1}{2}\sum_{p,q} \mathrm{Tr}_{2\times 2}\left(G^0_{p-q/2}(X_1)_{p-q/2,p+q/2} G^0_{p+q/2}(X_1)_{p+q/2,p-q/2}\right) \quad (32)$$

$$= \frac{1}{2}\sum_{p,q} \mathrm{Tr}_{2\times 2}\left(G^0_{p-q/2}\left(ie\phi_q\sigma_3 - \frac{e}{m}\mathbf{p}\mathbf{A}_{\mathbf{q}}\right) G^0_{p+q/2}\left(ie\phi_{-q}\sigma_3 - \frac{e}{m}\mathbf{p}\mathbf{A}_{-\mathbf{q}}\right)\right) \quad (33)$$

$$= \frac{1}{2}\sum_{p,q}\left(-e^2\phi_{\mathbf{q}}\phi_{-\mathbf{q}}\mathrm{Tr}_{2\times 2}\left(G^0_{p-q/2}\sigma_3 G^0_{p+q/2}\sigma_3\right) + \frac{e^2}{m^2}(\mathbf{p}\mathbf{A}_{\mathbf{q}})(\mathbf{p}\mathbf{A}_{-\mathbf{q}})\mathrm{Tr}_{2\times 2}\left(G^0_{p-q/2}G^0_{p+q/2}\right)\right) \quad (34)$$

In the last line we dropped the cross-terms, which are odd in $\mathbf{p}$ and vanish.

For any rotationally invariant function $R(\mathbf{p}^2)$, the following identity is satisfied

$$\sum_{\mathbf{p}}(\mathbf{p}\mathbf{A}_{\mathbf{q}})(\mathbf{p}\mathbf{A}_{-\mathbf{q}})R(\mathbf{p}^2) = \mathbf{A}_{\mathbf{q}}\mathbf{A}_{-\mathbf{q}}\sum_{\mathbf{p}}\frac{\mathbf{p}^2}{3}R(\mathbf{p}^2). \quad (35)$$

We are interested in slowly varying fields (small q), hence $p \pm q/2 \approx p$. We therefore arrive at

$$\frac{1}{2}\mathrm{Tr}(G^0 X_1 G^0 X_1) = \frac{e^2}{2}\sum_{p,q}\left(-\phi_{\mathbf{q}}\phi_{-\mathbf{q}}\mathrm{Tr}_{2\times 2}\left(G^0_p\sigma_3 G^0_p\sigma_3\right) + \mathbf{A}_{\mathbf{q}}\mathbf{A}_{-\mathbf{q}}\frac{\mathbf{p}^2}{3m^2}\mathrm{Tr}_{2\times 2}\left(G^0_p G^0_p\right)\right) \quad (36)$$

Next, show that

$$\mathrm{Tr}_{2\times 2}\left(G^0_p\sigma_3 G^0_p\sigma_3\right) = 2\frac{(i\omega_n)^2 + \lambda^2_{\mathbf{p}} - 2\Delta^2}{\left((i\omega_n)^2 - \lambda^2_{\mathbf{p}}\right)^2} \quad (37)$$

$$\mathrm{Tr}_{2\times 2}\left(G^0_p G^0_p\right) = 2\frac{(i\omega_n)^2 + \lambda^2_{\mathbf{p}}}{\left((i\omega_n)^2 - \lambda^2_{\mathbf{p}}\right)^2} \quad (38)$$

Next, carry out the frequency summations, and show that

$$\frac{1}{\beta}\sum_{\omega_n}\frac{(i\omega_n)^2 + \lambda^2_{\mathbf{p}} - 2\Delta^2}{\left((i\omega_n)^2 - \lambda^2_{\mathbf{p}}\right)^2} = f'(\lambda_{\mathbf{p}})(1 - \frac{\Delta^2}{\lambda^2_{\mathbf{p}}}) + (2f(\lambda_{\mathbf{p}}) - 1)\frac{\Delta^2}{2\lambda^3_{\mathbf{p}}} \approx -\frac{\Delta^2}{2\lambda^3_{\mathbf{p}}} \quad (39)$$

$$\frac{1}{\beta}\sum_{\omega_n}\frac{(i\omega_n)^2 + \lambda^2_{\mathbf{p}}}{\left((i\omega_n)^2 - \lambda^2_{\mathbf{p}}\right)^2} = f'(\lambda_{\mathbf{p}}) \quad (40)$$

Here $f'(\lambda_{\mathbf{p}}) = df(\lambda_{\mathbf{p}})/d\lambda_{\mathbf{p}}$ and we took only the leading terms at low temperature.

Combining all we learned so far, we get

$$\frac{1}{2}\mathrm{Tr}(G^0 X_1 G^0 X_1) = e^2\sum_{q,\mathbf{p}}\left(\phi_{\mathbf{q}}\phi_{-\mathbf{q}}\left(\frac{\Delta^2}{2\lambda^3_{\mathbf{p}}}\right) + \mathbf{A}_{\mathbf{q}}\mathbf{A}_{-\mathbf{q}}\frac{\mathbf{p}^2}{3m^2}f'(\lambda_{\mathbf{p}})\right) \quad (41)$$

Next we combine this result with the diamagnetic term, derived before, and we obtain

$$\mathrm{Tr}(G^0 X_2) + \frac{1}{2}\mathrm{Tr}(G^0 X_1 G^0 X_1) = e^2 \sum_{q,\mathbf{p}} \phi_{\mathbf{q}}\phi_{-\mathbf{q}} \left(\frac{\Delta^2}{2\lambda_{\mathbf{p}}^3}\right) + \mathbf{A}_{\mathbf{q}}\mathbf{A}_{-\mathbf{q}} \left(\frac{n}{2m} + \frac{\mathbf{p}^2}{3m^2} f'(\lambda_{\mathbf{p}})\right) \tag{42}$$

Next we show that

$$\sum_{\mathbf{p}} \frac{\Delta^2}{2\lambda_{\mathbf{p}}^3} = \int d\varepsilon D(\varepsilon) \frac{\Delta^2}{2(\varepsilon^2+\Delta^2)^{3/2}} \approx D_0 \tag{43}$$

$$f'(\lambda_{\mathbf{p}}) = -\beta f(\lambda_{\mathbf{p}}) f(-\lambda_{\mathbf{p}}) \tag{44}$$

hence $S_{eff} \equiv \mathrm{Tr}(G^0 X_2) + \frac{1}{2}\mathrm{Tr}(G^0 X_1 G^0 X_1)$ becomes

$$S_{eff} = e^2 \sum_{q} \phi_{\mathbf{q}}\phi_{-\mathbf{q}} D_0 + \mathbf{A}_{\mathbf{q}}\mathbf{A}_{-\mathbf{q}} \left(\frac{n}{2m} - \beta \sum_{\mathbf{p}} \frac{\mathbf{p}^2}{3m^2} f(\lambda_{\mathbf{p}}) f(-\lambda_{\mathbf{p}})\right) \tag{45}$$

Finally, we will prove that

$$\left(\frac{n}{2m} - \beta \sum_{\mathbf{p}} \frac{\mathbf{p}^2}{3m^2} f(\lambda_{\mathbf{p}}) f(-\lambda_{\mathbf{p}})\right) \equiv \frac{n_s}{2m} \tag{46}$$

where n_s is superfluid density.

We see that

$$\frac{n_s}{2m} = \frac{n}{2m} - \beta \sum_{\mathbf{p}} \frac{2}{3m}(\varepsilon_{\mathbf{p}} + \mu) f(\lambda_{\mathbf{p}}) f(-\lambda_{\mathbf{p}}) \tag{47}$$

$$= \frac{n}{2m} - \beta \frac{1}{2} \int d\varepsilon D(\varepsilon) \frac{2}{3m}(\varepsilon + \mu) f(\lambda_\varepsilon) f(-\lambda_\varepsilon) \tag{48}$$

$$\approx \frac{n}{2m} - \frac{D_0 \mu}{3m} \int d\varepsilon \beta f(\lambda_\varepsilon) f(-\lambda_\varepsilon) \tag{49}$$

Note that here we used $D(\omega) = 2\sum_{\mathbf{p}} \delta(\omega - \varepsilon_{\mathbf{p}})$, where 2 is due to spin. This is essential because n contains the spin degeneracy as well. It is straightforward to prove that $\mu D_0 = \frac{3}{2} n$ in our approximation, because

$$D_0 = 2 \sum_{\mathbf{p}} \delta(\mu - \frac{p^2}{2m}) = c\sqrt{\mu} \tag{50}$$

$$n = 2 \sum_{\mathbf{p}} \theta(\mu - \frac{p^2}{2m}) = c(2/3)\mu^{3/2}. \tag{51}$$

We thus conclude that

$$\frac{n_s}{2m} = \frac{n}{2m} \left(1 - \int d\varepsilon \beta f(\sqrt{\varepsilon^2 + \Delta^2}) f(-\sqrt{\varepsilon^2 + \Delta^2})\right) \tag{52}$$

At low temperature $f(\sqrt{\varepsilon^2 + \Delta^2}) \approx 0$, hence $n_s = n$ and all electrons contribute to the superfluid density. Above T_c we have

$$\int d\varepsilon \beta f(\varepsilon) f(-\varepsilon) = 1$$

and therefore $n_s = 0$ as expected. We interpret that n_s is the fraction of electrons that are parred up in superfluid, i.e., superfluid density, as promised.

We just proved that

$$S_{eff} = e^2 \sum_q \phi_{\mathbf{q}} \phi_{-\mathbf{q}} D_0 + \mathbf{A}_{\mathbf{q}} \mathbf{A}_{-\mathbf{q}} \frac{n_s}{2m}, \tag{53}$$

which is equivalent to Eq. 23.