Lecture course

INTERACTING FERMI SYSTEMS

Michael M. Scherer, Winter term 2019/2020

Contents

1. Introduction

1.1. Motivation: interacting Fermi systems

▷ solid state / condensed-matter physics

↳ quantum mechanical description of materials properties

↳ many particles / degrees of freedom (d.o.f.): atoms, ions, electrons, phonons, ...

↳ this course: focus on fermionic degrees of freedom & correlated states

▷ microscopic description is well known:

$$\mathcal{H} = \underbrace{\sum_i \frac{\vec{p}_i^{\,2}}{2m} + \frac{1}{2}\sum_{i\neq i'} \frac{e^2}{|\vec{r}_i - \vec{r}_{i'}|}}_{\text{electrons}} + \underbrace{\sum_j \frac{\vec{p}_j^{\,2}}{2M_j} + \frac{1}{2}\sum_{j\neq j'} \frac{Z_j Z_{j'} e^2}{|\vec{R}_j - \vec{R}_{j'}|}}_{\text{ions}} - \underbrace{\sum_{ij} \frac{Z_j e^2}{|\vec{r}_i - \vec{R}_j|}}_{\text{interaction}}$$

▷ many particles put together show new <u>emergent</u> collective behavior:

"... the ability to reduce everything to simple fundamental laws does not imply the ability to start from those laws and reconstruct the universe."

P. Anderson, More is different, Science 177, 393 (1972)

▷ need appropriate conceptual insight and methods to describe many-body systems

↳ effective theories / models

↳ emergent d.o.f. / symmetry

↳ Anderson-Higgs or BCS mechanisms, ...

1.2. Examples

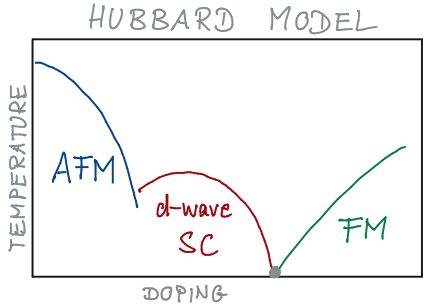
▷ Experiments reveal complex phase diagrams of interacting fermion systems:

↳ cuprate superconductors (layered materials with CuO_2 layers and spacer layers)

↳ 2D materials (graphene, van-der-Waals heterostructures, ...)

▷ high-temperature superconducting phases, magnetism, ...

- phase diagrams should be described by theory / theoretical models
- quantum many-body approaches/methods
  - numerical quantum Monte Carlo methods
  - quantum field theory & renormalization group:
    - → from mathematics to materials
    - → superconductivity from repulsive interaction ?!



1.3. Outline of the lecture course

- recap of 2nd quantization & connection between models & materials
- functional integral formalism
  - focus on two-particle interactions & channel resummations
  - explicit applications: BCS superconductivity, antiferromagnetism
- renormalization group for fermions with Fermi surface
  - competing interactions (qualitative)
  - functional renormalization group formalism } ⇒ phase diagram
  - application to Hubbard model

- advanced topics (optional):
  - Dirac fermions and the Gross-Neveu model
  - universality and critical phenomena
  - twisted bilayer graphene

2. Second quantization

▷ idea: construct Hilbert space of many-particle system, define operators & Hamiltonian

▷ central concept: Fock space

2.1. Identical particles

▷ one-particle Hilbert space $\mathbb{H}_1$ equipped with basis $|\alpha\rangle$ and wavefunctions:

$$\psi_\alpha(x) = \langle x | \alpha \rangle$$

▷ N distinguishable particles: $\mathbb{H}_N = \overbrace{\mathbb{H}_1 \otimes \mathbb{H}_1 \otimes \dots \otimes \mathbb{H}_1}^{N \text{ times}}$

↳ basis: $|\alpha_1, \dots, \alpha_N\rangle = |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \dots \otimes |\alpha_N\rangle$

↳ wavefunction: $\psi_{\alpha_1 \dots \alpha_N}(x_1, \dots, x_N) = \big(\langle x_1| \otimes \dots \otimes \langle x_N|\big)\big(|\alpha_1\rangle \otimes \dots \otimes |\alpha_N\rangle\big) = \psi_{\alpha_1}(x_1) \cdot \dots \cdot \psi_{\alpha_N}(x_N)$

▷ N indistinguishable particles: exchange of particles does not create new state:

↳ $\psi(x_1, \dots, x_i, \dots, x_j, \dots, x_N) = \zeta\, \psi(x_1, \dots, x_j, \dots, x_i, \dots, x_N)$ with $\zeta \in \mathbb{C}, |\zeta| = 1, \zeta^2 = 1$

↳ two exchanges bring back original state

↳ $\zeta = +1$: bosons – totally symmetric wave functions

↳ $\zeta = -1$: fermions – totally antisymmetric wave functions

▷ mathematical remark: wavefunction transforms by some transformation of the permutation group S_N. There are only two one-dimensional irreducible representations of S_N:

1] the identity 1 (bosons) and 2] parity $(-1)^P$ (fermions)

▷ Hilbert space of wavefunctions: $\mathbb{H}_N^\zeta = \{|\psi\rangle \in \mathbb{H}_N : P|\psi\rangle = \zeta^P |\psi\rangle \in S_N\}$

↳ here S_N is the set of all permutations P of N particles

↳ $\zeta^P = \begin{cases} +1 & \text{if } \zeta = +1 \text{ or even \#(transpositions)} \\ -1 & \text{if } \zeta = -1 \text{ or odd \#(transpositions)} \end{cases}$

▷ Slater determinant for fermions: $\begin{vmatrix} \psi_{\alpha_1}(x_1) & \cdots & \psi_{\alpha_1}(x_N) \\ \vdots & & \\ \psi_{\alpha_N}(x_1) & \cdots & \psi_{\alpha_N}(x_N) \end{vmatrix} \in \mathbb{H}_N^-$

▷ Pauli principle: $\psi = 0$ if $x_i = x_j$ or $\alpha_i = \alpha_j$ ⇒ 2 fermions cannot occupy the same state

▷ Notation: $|\psi\rangle = |\alpha_1 \dots \alpha_N\rangle$ with proper antisymmetrization implicit

▷ Problems:

↳ complicated, $\langle \psi_N' | \psi_N \rangle$ has $(N!)^2$ terms

↳ made for fixed N, would like grand canonical or coherent states (see below)

2.2. Occupation numbers and Fock space

▷ describe many-particle system in Hilbert space $\mathbb{H}_N^-$ (i.e. fermions!)

▷ given a single-particle basis $|\alpha\rangle$

↳ specify state by set of occupation numbers $\{n_\alpha\}$

↳ for fermions: $n_\alpha \in \{0, 1\}$

↳ full wavefunction: $|\phi\rangle = |\alpha_1 \dots \alpha_N\rangle \longrightarrow |n_1 n_2 \dots\rangle$

↳ with particle number: $N = \sum_i n_i$

▷ Example: $\mathbb{H}_1 = \{|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle\} \rightsquigarrow |\phi\rangle = |\psi_1 \psi_3\rangle \longrightarrow |1\ 0\ 1\rangle$

▷ Sign convention: $|\alpha_1 \dots \alpha_N\rangle \longrightarrow |n_1 n_2 \dots\rangle$ for $\alpha_1 < \alpha_2 < \dots < \alpha_N$

↳ increasing quantum numbers

▷ Fock space: $\mathcal{F} = \mathcal{F}_0 \oplus \mathcal{F}_1 \oplus \mathcal{F}_2 \oplus \dots$ with $\mathcal{F}_n = \mathbb{H}_n^-$

↳ $\mathcal{F}_0 = \{|0\rangle\}$ one-dimensional vector space spanned by vacuum vector $|0\rangle \neq 0$

↳ basis in Fock space $|n_1 n_2 \dots\rangle \in \mathcal{F}$

- general wavefunction $|\psi\rangle = \sum_{n_1 n_2 \dots} c_{n_1 n_2 \dots} |n_1 n_2 \dots\rangle$
- includes superposition of states with different particle number!

2.3. Creation and annihilation operators

▷ add particle in state α: Creation operator $\hat{a}_\alpha^\dagger$

$$\hat{a}_\alpha^\dagger |\alpha_1 \dots \alpha_N\rangle := \begin{cases} |\alpha\, \alpha_1 \dots \alpha_N\rangle & \text{if } \alpha \neq \alpha_i \ \forall i \\ 0 & \text{if } \exists i : \alpha = \alpha_i \end{cases}$$

↳ Fock representation:

$$\hat{a}_\alpha^\dagger |n_1 \dots n_\alpha \dots\rangle := \begin{cases} (-1)^{\sum_{i<\alpha} n_i} |n_1 \dots 1 \dots\rangle & \text{if } n_\alpha = 0 \\ 0 & \text{if } n_\alpha = 1 \end{cases}$$

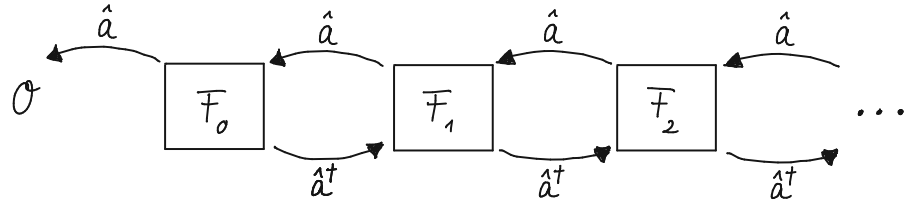
↳ sign convention: flip sign for every (occupied) particle with quantum number $i<\alpha$

▷ remove particle in state α: annihilation operator $\hat{a}_\alpha = (\hat{a}_\alpha^\dagger)^\dagger$

$$\hat{a}_\alpha |n_1 \dots n_\alpha \dots\rangle := \begin{cases} (-1)^{\sum_{i<\alpha} n_i} |n_1 \dots 0 \dots\rangle & \text{if } n_\alpha = 1 \\ 0 & \text{if } n_\alpha = 0 \end{cases}$$

▷ Summary:

$$\left.\begin{aligned} \hat{a}_\alpha |0\rangle &= 0 \qquad \text{(defines vacuum)} \\ |n_1 n_2 \dots\rangle &= \prod_\alpha \frac{(\hat{a}_\alpha^\dagger)^{n_\alpha}}{\sqrt{n_\alpha!}} |0\rangle = \prod_\alpha (\hat{a}_\alpha^\dagger)^{n_\alpha} |0\rangle \end{aligned}\right\} \text{fermions \& bosons!}$$



2.4. Algebra of creation and annihilation operators

▷ enforcement of antisymmetrization ↝ $\{\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger\} = 0$, $\{\hat{a}_\alpha, \hat{a}_\beta\} = 0$, $\{\hat{a}_\alpha, \hat{a}_\beta^\dagger\} = \delta_{\alpha\beta}$

↳ with anticommutator $\{A, B\} = [A, B]_+ = AB + BA$

↳ implies $\hat{a}_\alpha^2 = 0 = (\hat{a}_\alpha^\dagger)^2$ (Pauli principle)

↳ derivation: (1) $\hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger |\alpha_1 \dots \alpha_N\rangle = |\alpha\beta\alpha_1 \dots \alpha_N\rangle = -|\beta\alpha\,\alpha_1 \dots \alpha_N\rangle = -\hat{a}_\beta^\dagger \hat{a}_\alpha^\dagger |\alpha_1 \dots \alpha_N\rangle$

on every state $\Rightarrow$ $\hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger = -\hat{a}_\beta^\dagger \hat{a}_\alpha^\dagger$ as an operator equation

(2) analoguous: $\hat{a}_\beta^\dagger \hat{a}_\alpha = -\hat{a}_\alpha \hat{a}_\beta^\dagger$ if $\alpha \neq \beta$

(3) $\hat{a}_\alpha^\dagger \hat{a}_\alpha |\dots n_\alpha \dots\rangle = n_\alpha |\dots n_\alpha \dots\rangle$ and $\hat{a}_\alpha \hat{a}_\alpha^\dagger |\dots n_\alpha \dots\rangle = (1-n_\alpha) |\dots n_\alpha \dots\rangle$, $n_\alpha = 0, 1$

▷ occupation number operator $\hat{n}_\alpha = \hat{a}_\alpha^\dagger \hat{a}_\alpha$ ↝ total particle number $\hat{N} = \sum_\alpha \hat{n}_\alpha$

2.5. Basis transformation of creation and annihilation operators

▷ $\hat{a}_\lambda^\dagger, \hat{a}_\lambda$ are defined with respect to single-particle basis $|\lambda\rangle = \hat{a}_\lambda^\dagger |0\rangle$

▷ new single-particle basis μ: $|\mu\rangle = \sum_\lambda |\lambda\rangle\langle\lambda|\mu\rangle \Rightarrow \hat{a}_\mu^\dagger|0\rangle = |\mu\rangle = \sum_\lambda \langle\lambda|\mu\rangle \hat{a}_\lambda^\dagger|0\rangle$

↳ $\hat{a}_\mu^\dagger = \sum_\lambda \langle\lambda|\mu\rangle \hat{a}_\lambda^\dagger$, $\hat{a}_\mu = \sum_\lambda \langle\mu|\lambda\rangle \hat{a}_\lambda$

▷ real space and momentum space:

↳ momentum space basis vectors $|\vec{k}\rangle$ are eigenstates of $\hat{\vec{k}}$

↳ finite system with volume $V = L^3$ and periodic boundary conditions: $\vec{k} = \frac{2\pi}{L}(n_1, n_2, n_3)^T$, $n_i \in \mathbb{Z}$

↳ $\langle\vec{k}|\vec{k}'\rangle = \delta_{\vec{k}\vec{k}'}$, $\{\hat{a}_{\vec{k}}, \hat{a}_{\vec{k}'}^\dagger\} = \delta_{\vec{k}\vec{k}'}$

↳ analoguous: real space $|\vec{x}\rangle$, $\langle\vec{x}|\vec{x}'\rangle = \delta^{(3)}(\vec{x}-\vec{x}')$, $\langle\vec{x}|\vec{k}\rangle = V^{-\frac{1}{2}} e^{i\vec{k}\cdot\vec{x}}$

↳ "field operator" $\hat{\Psi}(\vec{x}) = V^{-\frac{1}{2}} \sum_{\vec{k}} \hat{a}_{\vec{k}} e^{i\vec{k}\cdot\vec{x}}$, $\{\hat{\Psi}(\vec{x}), \hat{\Psi}^\dagger(\vec{x}')\} = \delta^{(3)}(\vec{x}-\vec{x}')$

2.6. Representation of operators on Fock space

2.6.1. Single-particle operators

▷ operator $\hat{A} = \sum_{i=1}^N \hat{A}_i$ acts on every particle, e.g., $\hat{A}_i = \frac{-\hbar^2\vec{\nabla}_i^2}{2m}$ (kinetic energy of particle i)

↳ $\hat{T}|\vec{p}_1 \dots \vec{p}_N\rangle = \sum_{i=1}^N \frac{\vec{p}_i^{\,2}}{2m} |\vec{p}_1 \dots \vec{p}_N\rangle$

▷ find representation in Fock space!

↳ consider single-particle basis where $\hat{A}$ is diagonal: $\hat{A}|\lambda_i\rangle = A_{\lambda_i}|\lambda_i\rangle$ and $A_{\lambda_i} = \langle\lambda_i|\hat{A}|\lambda_i\rangle$

$\Rightarrow \hat{A}|\lambda_1 \dots \lambda_N\rangle = \sum_i A_{\lambda_i} n_{\lambda_i} |\lambda_1 \dots \lambda_N\rangle = \sum_i A_{\lambda_i} \hat{a}_{\lambda_i}^\dagger \hat{a}_{\lambda_i} |\lambda_1 \dots \lambda_N\rangle$ for any state

$\Rightarrow \hat{A} = \sum_\lambda A_\lambda \hat{a}_\lambda^\dagger \hat{a}_\lambda$

↳ transform to another basis $\{\alpha\}$: $\hat{A} = \sum_{\lambda\alpha\beta} \langle\alpha|\lambda\rangle\langle\lambda|\hat{A}|\lambda\rangle\langle\lambda|\beta\rangle \hat{a}_\alpha^\dagger \hat{a}_\beta = \sum_{\alpha\beta} \langle\alpha|\hat{A}|\beta\rangle \hat{a}_\alpha^\dagger \hat{a}_\beta$

$\Rightarrow \hat{A} = \sum_{i=1}^N \hat{A}_i = \sum_{\alpha\beta} A_{\alpha\beta} \hat{a}_\alpha^\dagger \hat{a}_\beta$, $A_{\alpha\beta} = \langle\alpha|\hat{A}|\beta\rangle$

▷ examples: (1) momentum: $\hat{\vec{p}} = \int d\vec{r}\, \hat{\Psi}^\dagger(\vec{r})(-i\hbar\vec{\nabla})\hat{\Psi}(\vec{r})$ (3) potential energy: $\hat{U} = \int d\vec{r}\, \hat{\Psi}^\dagger(\vec{r}) U(\vec{r}) \hat{\Psi}(\vec{r})$

(2) kinetic energy: $\hat{T} = \int d\vec{r}\, \hat{\Psi}^\dagger(-\frac{\hbar^2\vec{\nabla}^2}{2m})\hat{\Psi}(\vec{r})$ (4) local density: $\hat{n}(\vec{r}) = \hat{\Psi}^\dagger(\vec{r})\hat{\Psi}(\vec{r})$

2.6.2. Two-particle operators

▷ interaction $\hat{V} = \frac{1}{2}\sum_{i\neq j}\hat{V}_{ij} = \sum_{i<j}\hat{V}_{ij}$ acts on all distinct pairs of particles

↳ for indistinguishable particles $V_{ij} = V_{ji}$, e.g., Coulomb interaction $V_{ij} = \frac{e^2}{|\vec{r}_i - \vec{r}_j|}$

▷ consider basis where $\hat{V}$ is diagonal: $\hat{V}|\lambda\mu\rangle = V_{\lambda\mu}|\lambda\mu\rangle$, $V_{\lambda\mu} = \langle\lambda\mu|\hat{V}|\lambda\mu\rangle$

↳ $\hat{V}|\lambda_1\dots\lambda_N\rangle = \sum_{\lambda\mu} V_{\lambda\mu}\underbrace{\left(\frac{n_\lambda n_\mu - \delta_{\lambda\mu}n_\mu}{2}\right)}_{\text{number of distinct pairs: } \frac{1}{2}n(n-1) \text{ for } n \text{ particles}}|\lambda_1\dots\lambda_N\rangle$

$= \frac{1}{2}\sum_{\lambda\mu} V_{\lambda\mu}(\hat{a}_\lambda^\dagger\hat{a}_\lambda\hat{a}_\mu^\dagger\hat{a}_\mu - \delta_{\lambda\mu}\hat{a}_\mu^\dagger\hat{a}_\mu)|\lambda_1\dots\lambda_N\rangle = \frac{1}{2}\sum_{\lambda\mu}V_{\lambda\mu}\hat{a}_\lambda^\dagger\hat{a}_\mu^\dagger\hat{a}_\mu a_\lambda|\lambda_1\dots\lambda_N\rangle$ for any state

$\Rightarrow \hat{V} = \frac{1}{2}\sum_{\lambda\mu} V_{\lambda\mu}\hat{a}_\lambda^\dagger\hat{a}_\mu^\dagger\hat{a}_\mu\hat{a}_\lambda$

↳ example: $\hat{V}$ diagonal in real-space representation

$$\hat{V} = \frac{1}{2}\int d\vec{r}\,d\vec{r}\,' V(\vec{r}-\vec{r}\,')\hat{\Psi}^\dagger(\vec{r})\hat{\Psi}^\dagger(\vec{r}\,')\hat{\Psi}(\vec{r}\,')\hat{\Psi}(\vec{r})$$

↳ change of basis to $\{|\alpha\rangle\}$: $\hat{V} = \frac{1}{2}\sum_{\alpha\beta\mu\delta} V_{\mu\delta\alpha\beta}\hat{a}_\mu^\dagger\hat{a}_\delta^\dagger\hat{a}_\beta\hat{a}_\alpha$, $V_{\mu\delta\alpha\beta} = \langle\mu\delta|\hat{V}|\alpha\beta\rangle$

↳ i.a. in momentum basis with Fourier transform $v_{\vec{q}}$ of $V(\vec{r})$: $\hat{V} = \frac{1}{2V}\sum_{\vec{k}\vec{k}'\vec{q}} v_{\vec{q}}\hat{a}_{\vec{k}}^\dagger\hat{a}_{\vec{k}'}^\dagger\hat{a}_{\vec{k}'+\vec{q}}\hat{a}_{\vec{k}-\vec{q}}$

2.6.3. Many-particle Hamiltonian

$$\mathcal{H} = \sum_i\left(\frac{\vec{p}_i^{\,2}}{2m} + U(\vec{r}_i)\right) + \frac{1}{2}\sum_{i\neq j}V(\vec{r}_i - \vec{r}_j)$$

▷ we may include spin index $\sigma \in \{\uparrow,\downarrow\}$ (↓ electronic field operator)

▷ real space: $\hat{\mathcal{H}} = \sum_\sigma\int d\vec{r}\,\hat{\Psi}_\sigma^\dagger(\vec{r})\left[\frac{-\hbar^2\vec{\nabla}^2}{2m} + U(\vec{r})\right]\hat{\Psi}_\sigma(\vec{r}) + \frac{1}{2}\sum_{\sigma\sigma'}\int d\vec{r}\,d\vec{r}\,' V(\vec{r}-\vec{r}\,')\hat{\Psi}_\sigma^\dagger(\vec{r})\hat{\Psi}_{\sigma'}^\dagger(\vec{r}\,')\hat{\Psi}_{\sigma'}(\vec{r}\,')\hat{\Psi}_\sigma(\vec{r})$

▷ momentum space: $\hat{\mathcal{H}} = \sum_{\vec{k}\sigma}\varepsilon_{\vec{k}}\hat{a}_{\vec{k}\sigma}^\dagger\hat{a}_{\vec{k}\sigma} + \frac{1}{V}\sum_{\vec{k}\vec{k}'\sigma}U_{\vec{k}-\vec{k}'}\hat{a}_{\vec{k}\sigma}^\dagger\hat{a}_{\vec{k}\sigma} + \frac{1}{2V}\sum_{\substack{\vec{k}\vec{k}'\vec{q}\\\sigma\sigma'}}V_{\vec{q}}\hat{a}_{\vec{k}\sigma}^\dagger\hat{a}_{\vec{k}'\sigma'}^\dagger\hat{a}_{\vec{k}'+\vec{q}\sigma'}\hat{a}_{\vec{k}-\vec{q}\sigma}$

↳ with $\varepsilon_{\vec{k}} = \frac{\hbar^2\vec{k}^2}{2m}$ being the dispersion relation (can be different)

↳ scattering off a static potential does not conserve momentum

▷ general: $\hat{\mathcal{H}} = \sum_{ij}t_{ij}\hat{a}_i^\dagger\hat{a}_j + \sum_{ijke}V_{ijke}\hat{a}_i^\dagger\hat{a}_j^\dagger\hat{a}_k\hat{a}_e$

▷ note: all operators corresponding to measurable quantities and transformations can be expressed as a function of creation and annihilation operators $\hat{a}_\alpha^{(\dagger)}$.

↳ the grand-canonical partition fct. then is: $\mathcal{Z} = \mathrm{tr}\,e^{-\beta(\hat{\mathcal{H}}-\mu\hat{N})} = \sum_n\langle n|e^{-\beta(\hat{\mathcal{H}}-\mu\hat{N})}|n\rangle$

with $|n\rangle$ being a complete set of many-particle states, e.g., Fock basis from above.

2.7. Electrons in solids

2.7.1. Tight-binding models (for crystalline solid with ionic lattice)

▷ Consider tightly bound electrons ⇝ start with atomic problem at <u>lattice site $\vec{R}$</u>:

$$H_{atom,\vec{R}}\,\phi_n(\vec{r}-\vec{R}) = E_n\phi_n(\vec{r}-\vec{R})$$

↳ where $H_{atom,\vec{R}} = -\frac{\hbar^2\vec{\nabla}^2}{2m} + U(\vec{r}-\vec{R})$ and $U(\vec{r})$ is the binding potential.

▷ assume that we know the solutions ϕ_n (atomic orbitals, eigenfcts. of H_{atom}, i.e. isolated atom)

▷ full one-electron Hamiltonian in ion lattice of the solid

$$H(\vec{r}) = -\frac{\hbar^2\vec{\nabla}^2}{2m} + \sum_{\vec{R}} U(\vec{r}-\vec{R}) = H_{atom,\vec{R}}(\vec{r}) + \Delta U(\vec{r})$$

↳ where $\Delta U(\vec{r}) = \sum_{\vec{R}'\neq\vec{R}} U(\vec{r}-\vec{R}')$

▷ for atomic solution ϕ_n centered at $\vec{R}$

↳ extra term ΔU will be <u>small perturbation</u> if ϕ_n is tightly bound

↳ perturbation will modify slightly $\phi_n \longrightarrow \tilde{\phi}_n$

▷ there are degenerate wavefunctions $\tilde{\phi}_n$ centered at all other lattice sites $\vec{R}'$

↳ Solutions of problem: superposition of atomic orbitals in form of Bloch states:

$$\psi_{n,\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}}\,\phi_n(\vec{r}-\vec{R}) \qquad \circledast$$

↳ here we have ignored the "~" on ϕ_n as a first approximation

▷ note: if there are several (nearly) degenerate ϕ_n at single site ⇒ additional sum over orbitals!

▷ these Bloch states are built from <u>linear combination of atomic orbitals</u> (LCAO)

↳ in general: not eigenstates of lattice Hamiltonian, but good approximations if ϕ_n well-bound

▷ Bloch states $\circledast$ are not orthonormal:

$$\langle\psi_{n\vec{k}}\,|\,\psi_{n'\vec{k}'}\rangle = \delta_{\vec{k}\vec{k}'}\left(\delta_{nn'} + \sum_{\vec{R}\neq 0} e^{-i\vec{k}\cdot\vec{R}}\,\alpha_{nn'}(\vec{R})\right)$$

↳ with <u>overlap integrals</u> $\alpha_{nn'}(\vec{R}) = \int d^3\vec{r}\;\phi_n^*(\vec{r}-\vec{R})\,\phi_{n'}(\vec{r})$.

▷ tight-binding approximation (of the true band structure):

↳ expectation value of full lattice Hamiltonian in Bloch states

$$\mathcal{E}_n(\vec{k}) = \frac{\langle \psi_{n\vec{k}} | H | \psi_{n\vec{k}} \rangle}{\langle \psi_{n\vec{k}} | \psi_{n\vec{k}} \rangle} = E_n + \frac{\beta_n + \sum_{\vec{R}\neq 0} e^{-i\vec{k}\cdot\vec{R}}\,\lambda(\vec{R})}{1 + \sum_{\vec{R}\neq 0} e^{-i\vec{k}\cdot\vec{R}}\,\alpha_{nn}(\vec{R})}$$

↳ with $\beta_n = \underbrace{\int d^3r\, \phi_n^*(\vec{r})\,\Delta U(\vec{r})\,\phi_n(\vec{r})}_{\text{atomic energy shift from potential of neighboring atoms}}$ and $\lambda(\vec{R}) = \underbrace{\int d^3r\, \phi_n^*(\vec{r}-\vec{R})\,\Delta U(\vec{r})\,\phi_n(\vec{r})}_{\text{interatomic matrix element or "two-center integral"}}$

↳ Bloch energies $\mathcal{E}_n(\vec{k})$: tight-binding approximation of energies of full lattice Hamiltonian.

⟹ first qualitative understanding of band structures of tightly bound electrons in solids

▷ drawback: non-orthonormality of atomic orbitals in the lattice ↝ hard to construct Fock space

↝ more complicated commutators for creation/annihilation operators.

↝ more physical picture: Wannier states!

▷ Calculation of overlap integral: recall $\delta_{\vec{k}\vec{k}'} \sim \sum_{\vec{R}} e^{-i(\vec{k}-\vec{k}')\vec{R}}$ and $\delta(\vec{R}-\vec{R}') \sim \sum_{\vec{k}} e^{i\vec{k}(\vec{R}-\vec{R}')}$

↳ $\langle \psi_{n\vec{k}}(\vec{r}) | \psi_{n'\vec{k}'}(\vec{r}') \rangle = \frac{1}{N} \int_{\vec{r}} \sum_{\vec{R},\vec{R}'} e^{-i\vec{k}\vec{R}}\, e^{i\vec{k}'\cdot\vec{R}'}\, \phi_n^*(\vec{r}-\vec{R})\,\phi_{n'}(\vec{r}-\vec{R}')$

$$= \frac{1}{N} \sum_{\vec{R},\vec{R}'} e^{-i(\vec{k}-\vec{k}')\vec{R}}\, e^{-i\vec{k}'(\vec{R}-\vec{R}')} \int_{\vec{r}} \phi_n^*(\vec{r}-\vec{R})\,\phi_{n'}(\vec{r}-\vec{R}')$$

introduce $\vec{R}'' = \vec{R} - \vec{R}'$

$$= \frac{1}{N} \sum_{\vec{R},\vec{R}''} e^{-i(\vec{k}-\vec{k}')\vec{R}}\, e^{-i\vec{k}'\vec{R}''} \underbrace{\int_{\vec{r}} \phi_n^*(\vec{r}-\vec{R}'')\,\phi_{n'}(\vec{r})}_{\text{with } \vec{r}\to\vec{r}+\vec{R}'}$$

$$= \delta_{\vec{k}\vec{k}'} \sum_{\vec{R}''} e^{-i\vec{k}\cdot\vec{R}''} \int_{\vec{r}} \phi_n^*(\vec{r}-\vec{R}'')\,\phi_{n'}(\vec{r})$$

$$= \delta_{\vec{k}\vec{k}'} \left[\left(\sum_{\vec{R}\neq 0}{}' e^{-i\vec{k}\cdot\vec{R}} \underbrace{\int_{\vec{r}} \phi_n^*(\vec{r}-\vec{R})\,\phi_{n'}(\vec{r})}_{\alpha_{nn'}(\vec{R})} \right) + \delta_{nn'} \right]$$

2.7.2. Wannier states

▷ Wannier states contructed from (yet to be determined) properly orthonormalized Bloch eigenstates

▷ definition: $w_n(\vec{r}-\vec{R}) = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{-i\vec{k}\cdot\vec{R}} \psi_{n\vec{k}}(\vec{r})$

⇒ Wannier states orthonormal on different sites if Bloch fcts. $\psi_{n\vec{k}}(\vec{r})$ orthonormal in $\vec{k}, n$:

$\int d^3r\, w_n^*(\vec{r}-\vec{R})\, w_{n'}(\vec{r}-\vec{R}') = \delta_{nn'}\delta_{\vec{R}\vec{R}'}$ ↝ non-local overlap integrals vanish!

▷ ambiguity: localization properties and spatial spread of Wannier fcts. can be manipulated by using phase d.o.f. of Bloch fct., i.e. by multiplying the latter with arbitrary phase $e^{i\theta(\vec{k})}$.

⇒ Fourier back-transform to real space yields different $w_n(\vec{r}-\vec{R})$

↳ example: multiplying Bloch fct. with $e^{i\theta(\vec{k})} = e^{i\vec{k}\cdot\vec{a}}$ ⇒ shifts Wannier state by $\vec{a}$.

↳ minimize spatial spread of $w_{n,\vec{R}}$ by optimizing $e^{i\theta(\vec{k})}$ ⇒ <u>maximally localized Wannier fcts.</u>

▷ express Bloch states via Wannier states: $\psi_{n\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} w_n(\vec{r}-\vec{R})$

⇒ $\varepsilon_n(\vec{k}) = \frac{\langle\psi_{n\vec{k}}|H|\psi_{n\vec{k}}\rangle}{\langle\psi_{n\vec{k}}|\psi_{n\vec{k}}\rangle} = \tilde{E}_n + \sum_{R\neq 0} e^{i\vec{k}\cdot\vec{R}}\, \tilde{\lambda}_n(\vec{R})$ (two-center approx.)

↳ where $\tilde{E}_n = \int_r w_n^*(\vec{r})\left[-\frac{\hbar^2\vec{\nabla}^2}{2m} + \sum_{\vec{R}} U(\vec{r}-\vec{R})\right] w_n(\vec{r})$

↳ and $\tilde{\lambda}_n(\vec{R}) = \int_r w_n^*(\vec{r}-\vec{R})[\quad''\quad] w_n(\vec{r})$ (⇒ <u>hopping amplitudes</u> (see below))

▷ how do the properly orthonormalized Bloch/Wannier states look like?

↳ approximation starting from atomic states ↝ construct approx. Wannier fcts. from LCAO (linear combination of atomic orbitals) scheme with finite number of ϕ_m of different m (atomic quantum numbers) in subspace S ↝ ansatz: $w_n(r-R) = \sum_{m\in S} a_m \phi_m(r-R)$

↝ choose a_m such that non-local overlap $\alpha_n(R) = \int_r w_n^*(r-R)\, w_n(r)$ is minimized

↝ as ϕ_m decay rapidly ⇒ only a few nearest-neighbor overlaps need to be considered!

↳ precise calculation: use e.g. <u>density functional theory</u> (DFT) ↝ ab initio approach.

2.7.3. Hubbard Hamiltonian

▷ electronic field operators $\Psi_\sigma(\vec{r})$ in many-body Hamiltonian:

$$H = \underbrace{\sum_\sigma \int d^3r\, \Psi_\sigma^\dagger(\vec{r}) \left[\frac{-\hbar^2\vec{\nabla}^2}{2m} + U(\vec{r}) - \mu \right] \Psi_\sigma(\vec{r})}_{H_0} + \underbrace{\frac{e^2}{2} \sum_{\sigma\sigma'} \int d^3r d^3r' \frac{\Psi_\sigma^\dagger(\vec{r})\, \Psi_\sigma(\vec{r})\, \Psi_{\sigma'}^\dagger(\vec{r}')\, \Psi_{\sigma'}(\vec{r}')}{|\vec{r} - \vec{r}'|}}_{H_I}$$

↳ decompose field operator in Bloch states $\Psi_{n\vec{k}}(\vec{r})$: $\Psi_\sigma(\vec{r}) = \sum_{n,\vec{k}} \Psi_{n,\vec{k}}(\vec{r})\, c_{n\vec{k}\sigma}$

↳ creation and annihilation operators $c^{(\dagger)}_{n\vec{k}\sigma}$ for Bloch states

↳ decompose field operator in Wannier fcts. $w_{n,\vec{R}}(\vec{r}-\vec{R})$ centered at lattice sites $\vec{R}$: $\Psi_\sigma(\vec{r}) = \sum_{n\vec{R}} w_{n,\vec{R}}(\vec{r}-\vec{R})\, c_{n\vec{R}\sigma}$

▷ <u>free part of H</u>: Bloch decomposition using Bloch eigenstates of free Hamiltonian

$$H_0 = \sum_{n\vec{k}\sigma} \varepsilon_n(\vec{k})\, c^\dagger_{n\vec{k}\sigma}\, c_{n\vec{k}\sigma}$$

↳ using $\Psi_{n\vec{k}}(\vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} w_n(\vec{r}-\vec{R}) \Rightarrow c_{n\vec{k}\sigma} = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}}\, c_{n\vec{R}\sigma}$

↳ in terms of Wannier states, the free part H_0 becomes a hopping kinetic energy E_{kin}

$$H_0 = -\sum_{n\vec{R}\vec{R}'\sigma} t^{(n)}(\vec{R},\vec{R}')\, c^\dagger_{n\vec{R}\sigma}\, c_{n\vec{R}'\sigma} \text{ with hopping } t^{(n)}(\vec{R},\vec{R}') = \frac{-1}{N} \sum_{\vec{k}} \varepsilon_n(\vec{k})\, e^{i\vec{k}(\vec{R}-\vec{R}')}$$

↳ we find by inspection: $t^{(n)}(\vec{R},\vec{R}') = -\tilde{\lambda}(\vec{R}-\vec{R}')$

$$\Rightarrow t^{(n)}(0,\vec{R}) = -\int d^3r\, w_n^*(\vec{r}-\vec{R}) \left[\frac{-\hbar^2\vec{\nabla}^2}{2m} + \sum_{\vec{R}'} U(\vec{r}-\vec{R}') \right] w_n(\vec{r})$$

↳ due to maximal localization $t^{(n)}(0,\vec{R})$ decays with increasing $\vec{R}$

↳ simple approximation: just take nearest-neighbor term, denoted t

▷ <u>interaction term of H</u>: $H_I = \frac{1}{2} \sum_{\sigma\sigma'} \sum_{R_1,\dots R_4}{}' V_{n_1\dots n_4}(R_1,\dots,R_4)\, c^\dagger_{n_1R_1\sigma}\, c_{n_2R_2\sigma}\, c^\dagger_{n_3R_3\sigma'}\, c_{n_4R_4\sigma'}$

↳ with $V_{n_1\dots n_4}(R_1,\dots,R_4) = e^2 \int d^3r \int d^3r' \frac{w^*_{n_1}(r-R_1)\, w_{n_2}(r-R_2)\, w^*_{n_3}(r'-R_3)\, w_{n_4}(r'-R_4)}{|r-r'|}$

↳ onsite term ($R_1 = R_2 = R_3 = R_4$) is largest: $U := e^2 \int d^3r \int d^3r' \frac{|w(r)|^2 |w(r')|^2}{|r-r'|}$ (Hubbard U)

↘ must have $\sigma \neq \sigma'$ in H_I because of Pauli principle

↘ neglect remaining non-local terms (... depending on material)

▷ <u>Hubbard model</u>: combine nearest-neighbor hopping and onsite i.a.

$$H_{Hubbard} = \underbrace{-t \sum_{\langle R,R'\rangle} \left[c^\dagger_{R\sigma} c_{R'\sigma} + h.c. \right]}_{H_t} + \underbrace{U \sum_R c^\dagger_{R\uparrow} c_{R\uparrow}\, c^\dagger_{R\downarrow} c_{R\downarrow}}_{H_U}$$

2.7.4. Kinetic part of the Hubbard model

▷ hopping term: $H_t = -t \sum_{\langle \vec{R},\vec{R}' \rangle \sigma} \left(c^\dagger_{\vec{R}\sigma} c_{\vec{R}'\sigma} + c^\dagger_{\vec{R}'\sigma} c_{\vec{R}\sigma} \right)$

▷ consider two-dimensional square lattice with lattice spacing $a = 1$

↳ $N_x \times N_y$ sites and periodic boundary conditions

▷ diagonalization of hopping term by Fourier transform $c_{\vec{R}\sigma} = \frac{1}{\sqrt{N}} \sum_{\vec{k}} e^{i\vec{k}\cdot\vec{R}} c_{\vec{k}\sigma}$

↳ with $\vec{k}$ in the first Brillouin zone $(-\pi, \pi] \times (-\pi, \pi] \cong \mathcal{B} = \frac{\mathbb{R}^2}{2\pi\mathbb{Z}^2}$

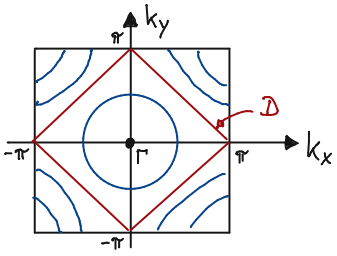
↳ wavevector components $k_{x,y} = \frac{2\pi n_{x,y}}{N_{x,y}}$ with $n_{x,y} = 1, \dots, N_{x,y}$ ↝ use $\sum_{\vec{k}} e^{i\vec{k}\cdot\vec{R}} = N\delta_{\vec{R},0}$

$\Rightarrow$ $H_t = \sum_{\vec{k}\sigma} \varepsilon(\vec{k}) c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma}$ with dispersion $\varepsilon(\vec{k}) = -2t(\cos k_x + \cos k_y)$

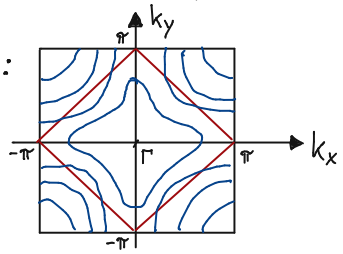
▷ include second-nearest neighbor hopping t' and chemical potential μ:

$$\varepsilon(\vec{k}) = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu$$

↳ $t' = 0$:



↳ $t' \neq 0$:



↳ $\varepsilon(\vec{k})$ parabolic for small $|\vec{k}|$, deformed for larger $|\vec{k}|$

↳ $t' = 0$: perfect square $\mathcal{D}$ for energy contour $\varepsilon(\vec{k}) = 0$ (important for magnetism)

↝ corners of square $(\pi, 0)$ and $(0, \pi)$

↝ <u>perfect nesting of Fermi surface</u>: $\mathcal{D} = \mathcal{D} + (\pi, \pi)$ for $\mu = 0, t' = 0$

▷ <u>spin-summed density of states (DOS)</u>: $g(E) = 2 \sum_{\vec{k}} \delta(E - \varepsilon(\vec{k}))$ (2: spin)

↳ determine number of states $g_E \, dE$ in $\mathcal{B}$ located in $E \leq \varepsilon(\vec{k}) \leq E + dE$

$\Rightarrow$ line integral $\int_{\varepsilon = E} dk_\parallel$ over constant ε contour around which there is shell

$$dk_\perp = \frac{dE}{|\partial E / \partial k_\perp|} = \frac{dE}{|\nabla \varepsilon|} = \frac{dE}{v_{\vec{k}}} \Rightarrow g(E) = \frac{2}{(2\pi)^2} \int_{\varepsilon = E} \frac{dk_\parallel}{v_{\vec{k}}}$$ with group velocity $v_{\vec{k}}$

▷ van-Hove singularities (VHS):

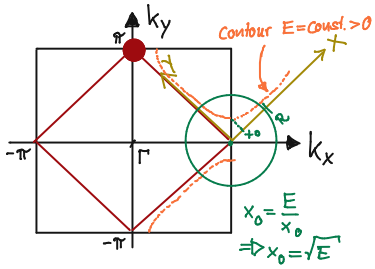
↳ $v_{\vec{k}}$ can go to zero for some points in $\mathcal{B}$ ↝ VHS

↳ saddle point where 2nd derivatives (Hesse matrix) are indefinite

↝ for $\varepsilon(\vec{k}) = -2t(\cos k_x + \cos k_y)$ near $\vec{k} = (0,\pi)$ and $(\pi,0)$: $\varepsilon(\vec{k}) \sim k_x^2 - k_y^2$

↳ in 2D: saddle points ⇒ log-divergence in DOS: $\rho(E) \sim -\log E$ (VHS)

• derivation: for $\varepsilon(\vec{k}) = -2t(\cos k_x + \cos k_y)$ ↝ consider circle around $(\pi,0)$ with radius R



• 45°-rotated coordinates x,y w.r.t. saddle point

⇒ for small R: dispersion $\varepsilon \sim x \cdot y$, velocity $v \sim \sqrt{x^2+y^2}$

↝ lines of constant energy $\varepsilon = E$: $y = E/x$ (hyperbolae)

$$\Rightarrow dk_{\parallel} = dx\sqrt{1+(\partial y/\partial x)^2} = dx\sqrt{1+(E/x^2)^2}$$

⇒ for small positive $\varepsilon = E$ two hyperbolae contribute identically between $x = x_0 = \sqrt{E}$ and $x = R$:

$$\rho(E) \sim \int_{x_0}^{R} dx \sqrt{1+E^2/x^4}\, \frac{1}{\sqrt{x^2+E^2/x^2}} = \int_{\sqrt{E}}^{R} dx\, \frac{1}{x} = \log\frac{R}{\sqrt{E}} = \frac{1}{2}\log\frac{R^2}{E}$$

⇒ for $E \to 0$ the <u>DOS diverges logarithmically $\rho(E) \sim -\log E$</u>

↳ VHS near Fermi surface ⇒ large number of states available which can be coupled by i.a.

▷ <u>generalization:</u> for two-dimensional system, cf. arXiv: 1905.05188

↳ energy dispersion: $\varepsilon(\vec{k}) = A_+ k_x^{n_x} - A_- k_y^{n_y}$ with $k_{x,y} = |k_{x,y}|$

↳ consider time-reversal symmetric case ⇒ n_x, n_y even

↳ if at least one $n_x, n_y > 2$ ⇒ $\det(\partial_{k_i}\partial_{k_j}\varepsilon(\vec{k})) = 0$ ↝ high-order VHS

↳ energy dispersion fulfills scaling relation: $\varepsilon(\vec{k}) = b\,\varepsilon(\vec{k}')$ with $\vec{k}' = (k_x/b^{1/n_x}, k_y/b^{1/n_y})$

⇒ with $\rho(\varepsilon) = 2\int_{\vec{k}} \delta(\varepsilon - \varepsilon(\vec{k}))$:

$$\rho(\varepsilon) = \begin{cases} D_+\,\varepsilon^{-\alpha} & \text{for } \varepsilon > 0 \\ D_-\,\varepsilon^{-\alpha} & \text{for } \varepsilon < 0 \end{cases}$$

$$\text{with} \quad \alpha = 1 - \frac{1}{n_x} - \frac{1}{n_y}.$$

2.7.5. Materials described by the Hubbard model

▷ effective one-band model for cuprate materials (high-T_c superconductors)

↳ cuprate: • layered material composed of Cu and O atoms } modelling by 2D system!
• 3D material but small hopping between CuO planes }

clean compound ↝ insulating AFM

chemical doping ↝ high-T_c superconductor

↳ Hubbard model: • idealization with same basic phenomenology
• not realistic for quantitative description

▷ model for graphene: Coulomb-Hubbard model on honeycomb lattice, $g(E) \sim |E|$

3. Many-fermion coherent state functional integral formalism

3.1. Fermionic coherent states

▷ so far: used occupation numbers to label states in Fock space

▷ now use eigenstates of annihilation operators: $\hat{a}_\alpha |\phi\rangle = \phi_\alpha |\phi\rangle$

↳ coherent state: • helps to transform operators into "numbers" in path integral

• superposition of infinitely many different occupation number eigenstates

3.1.1. Grassmann algebra: consider an eigenstate $\hat{a}_\alpha |\phi\rangle = \phi_\alpha |\phi\rangle$

▷ anticommutation $\{\hat{a}_\alpha, \hat{a}_\beta\} = 0$ implies anticommutation of eigenvalues ϕ_α:

$$(\hat{a}_\alpha \hat{a}_\beta + \hat{a}_\beta \hat{a}_\alpha)|\phi\rangle = (\phi_\alpha \phi_\beta + \phi_\beta \phi_\alpha)|\phi\rangle = 0 \Rightarrow \phi_\alpha^2 = 0 \quad \text{and} \quad \{\phi_\alpha, \phi_\beta\} = 0$$

↳ this doesn't work for ordinary $\mathbb{C}$ numbers $\Rightarrow$ need Grassmann numbers (H. Grassmann, 19th century)

▷ Definition: Grassmann algebra $\mathcal{A}$ of dimension N is a set of elements η_i, $i \in \{1, \dots, N\}$ with properties:

(1) the elements can be added to other elements and to complex numbers $c \in \mathbb{C}$ and can be multiplied with complex numbers. The outcome is again an element of the algebra:

$$c_0 + c_i \eta_i + c_j \eta_j \in \mathcal{A}$$

(2) the product $\mathcal{A} \times \mathcal{A} \to \mathcal{A} : (\eta_i, \eta_j) \to \eta_i \eta_j$ is associative and anticommutative:

$$\eta_i \eta_j = \eta_j \eta_i \quad \Rightarrow \quad \eta_i^2 = 0 \quad \forall\, i.$$

▷ the whole Grassmann algebra is spanned by linear combinations and with N Grassmann numbers one can form 2^N distinct products: $\{1, \eta_1, \eta_2, \dots, \eta_N, \eta_1\eta_2, \dots, \eta_1\eta_2 \dots \eta_N\}$

↳ basis for the vector space over complex numbers (Grassmann algebra)

3.1.2. Functions of Grassmann numbers

▷ define functions of Grassmann numbers via power series, for example:

↳ exponential function: $f(\eta) = \exp(\eta) = \sum_{k=0}^{\infty} \eta^k / k!$

↳ for pair η_1, η_2 due to nilpotency: $\exp(\eta_1 + \eta_2) = 1 + \eta_1 + \eta_2 + \eta_1\eta_2 + \eta_2\eta_1 = 1 + \eta_1 + \eta_2$.

3.1.3. Derivatives of Grassmann functions

▷ define derivative w.r.t. Grassmann number as $\frac{\partial}{\partial\eta_i}\eta_j = \partial_{\eta_i}\eta_j = \delta_{ij}$

↳ $\partial_{\eta_i}\exp(c_1\eta_1 + c_2\eta_2) = c_1\delta_{i1} + c_2\delta_{i2}$ for $c_i \in \mathbb{C}$

▷ derivatives inherit anticommutation property: $\partial_{\eta_1}\partial_{\eta_2}\eta_1\eta_2 = -\partial_{\eta_1}\partial_{\eta_2}\eta_2\eta_1 = -\partial_{\eta_1}\eta_1 = -1$

and $\partial_{\eta_2}\partial_{\eta_1}\eta_1\eta_2 = \partial_{\eta_2}\eta_2 = +1$

$\Rightarrow \partial_{\eta_1}\partial_{\eta_2} + \partial_{\eta_2}\partial_{\eta_1} = 0$ or $\{\partial_{\eta_i}, \partial_{\eta_j}\} = 0 \;\forall_{i,j}$, similarly $\{\partial_{\eta_i}, \eta_j\} = 0$ for $i \neq j$

3.1.4. Grassmann integrals

▷ define integral operator to be zero on a total derivative:

$$\int d\eta_i \left(\frac{\partial}{\partial\eta_i}\eta_i\right) = \int d\eta_i\, 1 \equiv 0 \quad \text{and} \quad \int d\eta_i\, \eta_j = \delta_{ij}$$

↳ Grassmann integration and derivatives have the same effect.

↳ example: $\int d\eta_1 \exp(c_1\eta_1) = \int d\eta_1 (1 + c_1\eta_1) = c_1 \;\rightsquigarrow\; \int d\eta_i = \partial_{\eta_i}$

3.1.5. Fermionic coherent states

▷ define rules: $\{\eta_i, \hat{a}_j^{(\dagger)}\} = 0$ and $\{\partial_{\eta_i}, \hat{a}_j^{(\dagger)}\} = 0$ (anticommutation)

▷ defining property of a coherent state $|\eta\rangle$: $\hat{a}_i|\eta\rangle = \eta_i|\eta\rangle$ (eigenstate of annihilation operator)

▷ consider first one single-particle level i and the state $|\eta_i\rangle = \exp(-\eta_i\hat{a}_i^\dagger)|0\rangle = (1 - \eta_i\hat{a}_i^\dagger)|0\rangle$

↳ this is an eigenstate of $\hat{a}_i$: $\hat{a}_i|\eta_i\rangle = \hat{a}_i(1 - \eta_i\hat{a}_i^\dagger)|0\rangle = \eta_i\hat{a}_i\hat{a}_i^\dagger|0\rangle = \eta_i|0\rangle$ □

↳ this is the same as η_i times the original state: $\eta_i|0\rangle = \eta_i(1-0)|0\rangle = \eta_i(1 - \eta_i\hat{a}_i^\dagger)|0\rangle = \eta_i|\eta_i\rangle$ ($0 = \eta_i^2$)

$\Rightarrow \hat{a}_i|\eta_i\rangle = \eta_i|\eta_i\rangle$ □

▷ generalization for many single-particle levels is the "right" eigenstate of the annihilation operator:

$$|\eta\rangle = \exp\left(-\sum_i \eta_i\hat{a}_i^\dagger\right)|0\rangle = \prod_i (1 - \eta_i\hat{a}_i^\dagger)|0\rangle$$

▷ note: one may have to take care of minus signs when Grassmann numbers are commuted with occupied fermion states: $\eta_j\hat{a}_i^\dagger|0\rangle = \eta_j|1_i\rangle$

$$|1_i\rangle\eta_j = a_i^\dagger|0\rangle\eta_j = \hat{a}_i^\dagger\eta_j|0\rangle = -\eta_j\hat{a}_i^\dagger|0\rangle = -\eta_j|1_i\rangle.$$

3.1.6. Adjoint of coherent state

▷ declare what "conjugation" of Grassmann variables in exponent means ⇝ not really defined!

↳ enlarge Grassmann algebra by <u>conjugate Grassmann variables</u> $\bar{\eta}_i$ ($\bar{\eta}_i$ is independent set)

↳ $\bar{\eta}_i$ defined to anticommute among themselves and with unbarred quantities

▷ $\langle \eta | = \langle 0 | \exp\left(-\sum_i \hat{a}_i \bar{\eta}_i\right) = \langle 0 | \exp\left(\sum_i \bar{\eta}_i \hat{a}_i\right)$

↳ bra vector $\langle \eta |$ is "left" eigenstate of creation operators $\langle \eta | \hat{a}_i^\dagger = \langle \eta | \bar{\eta}_i$

↳ note: while $\{\hat{a}_i, \hat{a}_i^\dagger\} = 1$, we have $\{\eta_i, \bar{\eta}_i\} = 0$.

▷ <u>scalar product</u>: $\langle \eta | \eta' \rangle = \langle 0 | \prod_i (1 - \hat{a}_i \bar{\eta}_i)(1 - \eta_i' \hat{a}_i^\dagger) | 0 \rangle = \prod_i (1 + \bar{\eta}_i \eta_i') = \exp\left(\sum_i \bar{\eta}_i \eta_i'\right)$

↳ r.h.s. commutes with all Grassmann numbers and operators.

▷ resolution of unity (closure relation): $\int \prod_i d\bar{\eta}_i d\eta_i \, e^{-\sum_i \bar{\eta}_i \eta_i} |\eta\rangle\langle\eta| = \mathbb{1}_{\text{Fock}}$

↳ check for one single-particle state: $\int d\bar{\eta} d\eta \, e^{-\bar{\eta}\eta} |\eta\rangle\langle\eta| = \int d\bar{\eta} d\eta \, (1 - \bar{\eta}\eta)[|0\rangle - \eta|1\rangle][\langle 0| - \langle 1|\bar{\eta}]$

$$= -\int d\bar{\eta} d\eta \, \bar{\eta}\eta |0\rangle\langle 0| + \int d\bar{\eta} d\eta \, \eta\bar{\eta} |1\rangle\langle 1| = |0\rangle\langle 0| + |1\rangle\langle 1| \quad \square$$

▷ notation: $\int \mathcal{D}(\bar{\eta}, \eta) \ldots = \int \prod_i d\bar{\eta}_i \prod_i d\eta_i \ldots$

3.1.7. Trace of an operator $\hat{A}$

▷ $\hat{A}$ shall be even in the number of creation/annihilation operators

▷ $\mathrm{Tr}\, \hat{A} = \sum_m \langle m | A | m \rangle = \int \mathcal{D}(\bar{\eta}, \eta) \, e^{-\sum_i \bar{\eta}_i \eta_i} \sum \overbrace{\langle m | \eta \rangle \langle \eta | A | m \rangle}^{= \langle -\eta | A | m \rangle \langle m | \eta \rangle}$

$$\Rightarrow \quad \mathrm{Tr}\, \hat{A} = \int \mathcal{D}(\bar{\eta}, \eta) e^{-\sum_i \bar{\eta}_i \eta_i} \langle -\eta | A | \eta \rangle$$

3.1.8. Gaussian integrals

▷ $\{\eta_1, \ldots, \eta_n\}$ and independent $\{\bar{\eta}_1, \ldots, \bar{\eta}_n\}$

↳ $\int d\bar{\eta} d\eta \, e^{-\bar{\eta} a \eta} = a$, $a \in \mathbb{C}$

↳ $\int d\bar{\eta}_1 d\eta_1 \ldots d\bar{\eta}_n d\eta_n \exp\{-\bar{\eta}_i H_{ij} \eta_j + \bar{\eta}_i \xi_i + \bar{\xi}_i \eta_i\} = (\det H) \exp\{\bar{\xi}_i H_{ij}^{-1} \xi_j\}$

for general complex H_{ij}, invertible H in the presence of Grassmann "sources" $\xi_i, \bar{\xi}_i$

3.1.9. Summary on coherent states (bosonic and fermionic):

▷ (anti-) commutation relations: $[a_\alpha, a_\beta^\dagger]_\zeta = \delta_{\alpha\beta}$ and $[\psi_\alpha, \psi_\beta]_\zeta = 0$

with $\zeta = \pm 1$ for bosons / fermions

▷ coherent states: $\langle\psi| = \langle 0| e^{\zeta \sum_\alpha a_\alpha \bar{\psi}_\alpha}$ and $|\psi\rangle = e^{\zeta \sum_\alpha \psi_\alpha a_\alpha^\dagger}$

$\langle\psi| a_\alpha^\dagger = \langle\psi| \bar{\psi}_\alpha$ and $a_\alpha |\psi\rangle = \psi_\alpha |\psi\rangle$

▷ overlap: $\langle\psi|\psi'\rangle = e^{\sum_\alpha \bar{\psi}_\alpha \psi'_\alpha} = e^{\bar{\psi}\psi'}$ (last "=" introduces shorthand notation)

▷ expectation value: $\langle\psi| \hat{A}(\hat{a}_\alpha^\dagger, \hat{a}_\beta) |\psi'\rangle = A(\bar{\psi}_\alpha, \psi'_\beta) \langle\psi|\psi'\rangle$

($\hat{A}$: normal ordered)

▷ closure relation: $\mathbb{1}_{\text{Fock}} = \int \mathcal{D}(\bar{\psi}, \psi) e^{-\bar{\psi}\psi} |\psi\rangle\langle\psi|$

▷ note: for bosons the "$-$" on $\bar{\psi}$ is just complex conjugation, i.e. $\bar{\psi} = \psi^*$

3.2. Coherent state functional integral

▷ partition function: $\mathcal{Z} = \mathrm{tr}\, e^{-\beta(\hat{H}-\mu\hat{N})} = \sum \langle n| e^{-\beta(\hat{H}-\mu\hat{N})} |n\rangle$

↳ Hamiltonian (general form): $\hat{H}(\hat{a}_i, \hat{a}_i^\dagger) = \sum_{ij} t_{ij}\, \hat{a}_i^\dagger \hat{a}_j + \sum_{ijkl} v_{ijkl} \underbrace{\hat{a}_i^\dagger \hat{a}_j^\dagger \hat{a}_k \hat{a}_l}_{\text{"normal ordered"}}$

↳ total particle number operator: $\hat{N} = \sum_i \hat{a}_i^\dagger \hat{a}_i$

↳ replace operators by use of coherent state resolutions of unity:

$\mathbb{1} = \int \mathcal{D}(\bar{\psi},\psi) e^{-\sum_i \bar{\psi}_i \psi_i} |\psi\rangle\langle\psi| = \int \mathcal{D}(\bar{\psi},\psi) e^{-\bar{\psi}\psi} |\psi\rangle\langle\psi|$ with $\psi = \{\psi_i\} = (\psi_1, \psi_2, \dots)$ being Grassmann variables

▷ insert unity in $\mathcal{Z}$ behind $\langle n|$:

$$\mathcal{Z} = \int \mathcal{D}(\bar{\psi},\psi)\, e^{-\sum_i \bar{\psi}_i \psi_i} \sum_n \langle n|\psi\rangle\langle\psi| e^{-\beta(\hat{H}-\mu\hat{N})} |n\rangle = \int \mathcal{D}(\bar{\psi},\psi) e^{-\sum_i \bar{\psi}_i \psi_i} \sum_n \langle -\psi| e^{-\beta(\hat{H}-\mu\hat{N})} |n\rangle\langle n|\psi\rangle$$

↳ note that the minus "−" in $\langle -\psi|$ comes from:

$$\langle i|\psi\rangle\langle\psi|j\rangle = \langle 0|\hat{a}_i|\psi\rangle\langle\psi|\hat{a}_j^\dagger|0\rangle = \psi_i \overbrace{\langle 0|\psi\rangle}^{=1}\overbrace{\langle\psi|0\rangle}^{=1}\bar{\psi}_j = \psi_i\bar{\psi}_j = -\bar{\psi}_j\psi_i = \langle -\psi|j\rangle\langle i|\psi\rangle$$

↝ holds for any pair of single-particle states i,j and $\langle -\psi| = \langle 0| e^{\sum_j \hat{a}_j \bar{\psi}_j}$

↳ more generally for N-particle states $|n\rangle$ and $|n'\rangle$ with ordering $i_1 < i_2 < \dots < i_N$ and $j_1 < \dots < j_N$:

$$\langle n|\psi\rangle = \langle 0|\hat{a}_{i_1}\dots\hat{a}_{i_N}|\psi\rangle = \psi_{i_1}\psi_{i_2}\dots\psi_{i_N}$$

$$\Rightarrow \langle n|\psi\rangle\langle\psi|n'\rangle = \psi_{i_N}\dots\psi_{i_2}\psi_{i_1}\bar{\psi}_{j_1}\bar{\psi}_{j_2}\dots\bar{\psi}_{j_N} = \psi_{i_1}\bar{\psi}_{j_1}\psi_{i_2}\bar{\psi}_{j_2}\dots\psi_{i_N}\bar{\psi}_{j_N}$$

$$= (-\bar{\psi}_{j_1}\psi_{i_1})(-\bar{\psi}_{j_2}\psi_{i_2})\dots(-\bar{\psi}_{j_N}\psi_{i_N}) = (-\bar{\psi}_{j_1})(-\bar{\psi}_{j_2})\dots(-\bar{\psi}_{j_N})(\psi_{i_N}\dots\psi_{i_1}) = \langle -\psi|n'\rangle\langle n|\psi\rangle .$$

▷ now decompose intervall $[0,\beta]$ in M equidistant steps with $\Delta\tau = \beta/M$ and factorize:

↳ $e^{-\beta(\hat{H}-\mu\hat{N})} = \prod_{n=1}^{M} e^{-\Delta\tau(\hat{H}-\mu\hat{N})}$ ↝ then introduce "$\mathbb{1}$" between all these factors

$$\Rightarrow \mathcal{Z} = \int_{\psi^{(1)} = -\psi^{(M+1)}} \mathcal{D}(\bar{\psi},\psi)\, e^{-\Delta\tau\left[\sum_{n=1}^{M} \bar{\psi}^{(n)}(\psi^{(n)} - \psi^{(n-1)})/\Delta\tau + H(\bar{\psi}^{(n)}, \psi^{(n-1)}) - \mu N(\bar{\psi}^{(n)}, \psi^{(n-1)})\right]}$$

↳ now take the limit $\Delta\tau \to 0$ and consider τ as continuous variable $\in [0,\beta]$

↳ define τ-derivative: $\dfrac{\psi^{(n)} - \psi^{(n-1)}}{\Delta\tau} = \partial_\tau \psi(\tau)$

$$\Rightarrow \mathcal{Z} = \int \mathcal{D}(\bar{\psi},\psi)\, e^{-\int_0^\beta d\tau \left[\bar{\psi}(\tau)\partial_\tau\psi(\tau) + H[\bar{\psi}(\tau),\psi(\tau)] - \mu\bar{\psi}(\tau)\psi(\tau)\right]} = \int \mathcal{D}(\bar{\psi},\psi) e^{-S(\psi,\bar{\psi})}$$

▷ exponent contains grandcanonical action (Grassmann fields $\psi, \bar{\psi}$): $S(\psi,\bar{\psi}) = \int_0^\beta d\tau \left[\bar{\psi}(\tau)\partial_\tau\psi(\tau) + H[\bar{\psi}(\tau),\psi(\tau)] - \mu\bar{\psi}(\tau)\psi(\tau)\right]$

▷ antiperiodic boundary conditions due to $\langle -\psi|$: $\psi(\tau=0) = -\psi(\tau=\beta)$ (for fermions)

3.3. Matsubara frequency representation

▷ use discrete Fourier expansion for Grassmann fields: $\psi(\tau) = T\sum_n e^{-i\omega_n\tau}\psi(\omega_n)$

↳ inverse relation: $\psi(\omega_n) = \int_0^\beta d\tau\, e^{i\omega_n\tau}\psi(\tau)$

↳ ω_n are the Matsubara frequencies: $\omega_n = (2n+1)\pi T$, $n\in\mathbb{Z}$ (for bosons: $\omega_n = 2n\pi T$)

⇒ boundary conditions relating fields at $\tau=0$ and $\tau=\beta$ are fulfilled!

▷ resolve single-particle quantum number i, again in Matsubara frequency representation:

$$S(\bar\psi,\psi) = T\sum_{i,j,n}\bar\psi_i(\omega_n)(-i\omega_n + t_{ij} - \mu\delta_{ij})\psi_j(\omega_n) + T^3\sum_{\substack{i,j,k,l\\ n_1,n_2,n_3}} V_{ijkl}\bar\psi_l(\omega_{n_4})\bar\psi_k(\omega_{n_3})\psi_j(\omega_{n_2})\psi_i(\omega_{n_1})$$

where we have used $\int_0^\beta d\tau\, e^{i(\omega_n-\omega_{n'})\tau} = \beta\delta_{n,n'}$

↳ frequency conservation is enforced in the interaction part: $\omega_{n_1}+\omega_{n_2} = \omega_{n_3}+\omega_{n_4}$

↷ delete sum over n_4 by fixing $\omega_{n_4} = \omega_{n_1}+\omega_{n_2}-\omega_{n_3}$

▷ another choice for Fourier transform to Matsubara frequencies: $\psi(\tau) = \sqrt{T}\sum_n e^{-i\omega_n\tau}\psi(\omega_n)$

↳ inverse relation: $\psi(\omega_n) = \sqrt{T}\int_0^\beta d\tau\, e^{i\omega_n\tau}\psi(\tau)$

↳ with this choice:

$$S(\psi,\bar\psi) = \sum_{i,j,n}\bar\psi_i(\omega_n)(-i\omega_n + t_{ij} - \mu\delta_{ij})\psi_j(\omega_n) + T\sum_{\substack{i,j,k,l\\ n_1,n_2,n_3}} V_{ijkl}\bar\psi_l(\omega_{n_4})\bar\psi_k(\omega_{n_3})\psi_j(\omega_{n_2})\psi_i(\omega_{n_1})$$

▷ Summary:

↳ in total we have transformed the partition function of the many-fermion system into a functional integral over Grassmann fields living on an "imaginary" time axis τ.

▷ zero-temperature limit ($T\to 0$, $\beta\to\infty$):

↳ τ integration becomes infinite in range!

↷ if $i \triangleq \vec{x}$ in D-dimensions ⇒ $\psi(\vec{x},\tau)$ lives in $(D+1)$ dimensions

↷ quantum system at $T=0$ resembles classical system in one dimension higher

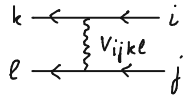
▷ quantum statistical mechanics in D-dim space at temperature T: $Z = \mathrm{tr}\, e^{-\beta(\hat H-\mu\hat N)}$

~ euclidean quantum field theory in $(D+1)$-dimensional spacetime, $0\le\tau<\beta$

3.4. Correlation functions and generating functionals

▷ assumption: time-independent Hamiltonian with spin quantum number $s \in \{\uparrow, \downarrow\}$:

$$H = H_0 + H_I = \sum_{\vec{k}} \varepsilon(\vec{k})\, \bar{\psi}(\vec{k},\tau,s)\, \psi(\vec{k},\tau,s) + H_I \quad \rightsquigarrow \text{ interaction usually quartic in } \bar{\psi}, \psi$$

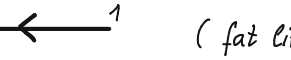


▷ quadratic part of fermionic action S_0 $\rightsquigarrow$ introduce multiindex $K = (\vec{k}, \omega_n, s)$

↳ in Matsubara rep.: $S_0 = \sum_{\vec{k},\omega_n,s} \overbrace{\left(-i\omega_n + \varepsilon(\vec{k})\right)}^{Q(K)} \bar{\psi}(\vec{k},\omega_n,s)\, \psi(\vec{k},\omega_n,s) = \sum_K Q(K)\, \bar{\psi}(K)\psi(K) = (\bar{\psi}, Q\psi)$

3.4.1. Single-particle Green's function

▷ the single-particle Green's fct. is: $G(K) = -\langle \psi(K)\bar{\psi}(K)\rangle = -\dfrac{\int \mathcal{D}(\bar{\psi},\psi)\,\psi(K)\bar{\psi}(K)\, e^{-S(\psi,\bar{\psi})}}{\int \mathcal{D}(\bar{\psi},\psi)\, e^{-S(\psi,\bar{\psi})}}$

↳ graphical representation: $-\langle \psi(K_2)\bar{\psi}(K_1)\rangle =$  (fat line)

▷ in the non-interacting case with only S_0, we get $G_0(K)$ and we have two Gaussian integrals:

(1) denominator: $\int \mathcal{D}(\bar{\psi},\psi)\, e^{-S_0} = \int \mathcal{D}(\bar{\psi},\psi)\, e^{-(\bar{\psi}, Q\psi)} = \det Q = \mathcal{Z}_0$

(2) numerator: $\int \mathcal{D}(\bar{\psi},\psi)\,\psi(K)\bar{\psi}(K)\, e^{-S_0} = \dfrac{\delta^2}{\delta\eta(K)\delta\bar{\eta}(K)} \int \mathcal{D}(\bar{\psi},\psi)\, e^{-(\bar{\psi},Q\psi)+(\bar{\eta},\psi)+(\bar{\psi},\eta)}\Big|_{\eta=\bar{\eta}=0}$

$$= \frac{\delta^2}{\delta\eta(K)\delta\bar{\eta}(K)} \left(e^{(\bar{\eta},Q^{-1}\eta)} \det Q\right)_{\eta=\bar{\eta}=0} = Q^{-1}(K)\det Q$$

$$\Rightarrow \quad G_0(K) = -Q^{-1}(K) = \frac{1}{i\omega_n - \varepsilon(\vec{k})} =$$ (thin line)

▷ therefore, we can write in the interacting case: $e^{-S(\psi,\bar{\psi})} = e^{(\bar{\psi}, G_0^{-1}\psi) - H_I(\bar{\psi},\psi)}$

3.4.2. Higher-order correlation functions

▷ definition: $G^{(2n)}(K_1,\dots,K_n,K_1',\dots,K_n') = -\langle \psi(K_1)\dots\psi(K_n)\,\bar{\psi}(K_n')\dots\bar{\psi}(K_1')\rangle$

$$= -\mathcal{Z}^{-1}\int \mathcal{D}(\bar{\psi},\psi)\,\psi(K_1)\dots\psi(K_n)\bar{\psi}(K_n')\dots\bar{\psi}(K_1')\, e^{-S(\psi,\bar{\psi})} \quad \text{with } \mathcal{Z} = \int \mathcal{D}(\bar{\psi},\psi) e^{-S(\psi,\bar{\psi})}$$

3.4.3. Generating functional

▷ correlation functions can be obtained from generating functional

$$\mathcal{G}(\eta,\bar{\eta}) = -\mathcal{Z}^{-1}\int \mathcal{D}(\bar{\psi},\psi)\, e^{-S(\psi,\bar{\psi})}\, e^{(\bar{\eta},\psi)+(\bar{\psi},\eta)} \quad \text{by taking functional derivatives}$$

▷ $G^{(2n)}(K_1,\dots,K_n,K_1',\dots,K_n') = (-1)^n \dfrac{\delta^{2n}}{\delta\bar{\eta}(K_1)\dots\delta\bar{\eta}(K_n)\delta\eta(K_n')\dots\delta\eta(K_1')}\, \mathcal{G}(\eta,\bar{\eta})\Big|_{\eta=\bar{\eta}=0}$

▷ generating functional in the non-interacting case: $\mathcal{G}_0(\eta,\bar{\eta}) = -e^{-(\bar{\eta}, G_0\eta)}$

▷ single-particle Green's fct.: $G_0^{(2)}(K) = G_0(K) = (-1)^1 \dfrac{\delta^2 \mathcal{G}_0(\eta,\bar{\eta})}{\delta\bar{\eta}(K)\delta\eta(K')}\Big|_{\eta=\bar{\eta}=0} = -Q^{-1}(K)\delta_{K,K'}$

▷ perturbation theory in $H_I \Rightarrow$ ▷ $\mathcal{G}(\eta,\bar\eta)$ generates connected AND disconnected diagrams

▷ taking logarithm removes disconnected parts ⇝ <u>generating functional for connected correlation fcts.</u>:

$$\mathcal{G}^c(\eta,\bar\eta) = -\ln[Z\,\mathcal{G}(\eta,\bar\eta)] = -\ln\left\{\int\mathcal{D}(\bar\psi,\psi)\, e^{-S(\psi,\bar\psi)}\, e^{(\bar\eta,\psi)+(\bar\psi,\eta)}\right\}$$

▷ expanding $\mathcal{G}(\eta,\bar\eta)$ in source fields leads to a formal power series with the connected Green's functions as coefficients:

$$\mathcal{G}^c(\eta,\bar\eta) = -\ln Z + (\bar\eta, G_c^{(2)}\eta) + \frac{1}{(2!)^2}\sum_{K_1,K_2,K_1',K_2'} G_c^{(4)}(K_1,K_2;K_1',K_2')\,\bar\eta(K_1)\bar\eta(K_2)\eta(K_2')\eta(K_1') + \dots$$

3.5. Wick theorem

▷ Compute Gaussian averages (i.e. with non-interacting action) over $2n$ fields as sum over all possible contractions of n pairs of fields, i.e n free Green's fcts.

▷ use general free action $S_0 = \sum_{K,K'} \bar\psi(K) Q(K,K') \psi(K')$, then:

$$\langle \psi(K_1)\dots\psi(K_n)\bar\psi(K_u')\dots\bar\psi(K_1')\rangle_0 = Z_0^{-1}\int\mathcal{D}(\bar\psi,\psi)\,\psi(K_1)\dots\psi(K_n)\bar\psi(K_u')\dots\psi(K_1')\, e^{-S_0(\psi,\bar\psi)}$$

$$= \sum_P (-1)^P Q^{-1}(K_1,K_{P_1}')\cdot\dots\cdot Q^{-1}(K_n,K_{P_n}')$$

↳ the sum over P denotes the sum over all 2^n permutations P_j of the n indices $j=1$ to $j=n$. $(-1)^P = 1$ for an even permutation and $(-1)^P = -1$ for an odd p.

▷ proof: use generating functional, cf. book by Negele & Orland

▷ $n=2$: $\langle\psi(K_1)\psi(K_2)\bar\psi(K_2')\bar\psi(K_1')\rangle_0 = Q^{-1}(K_1,K_1')Q^{-1}(K_2,K_2') - Q^{-1}(K_1,K_2')Q^{-1}(K_2,K_1')$

$$= G_0(K_1,K_1')G_0(K_2,K_2') - G_0(K_1,K_2')G_0(K_2,K_1').$$

3.6. Perturbation expansion

▷ many-body systems are complicated due to the interactions between particles, formally because interactions correspond to non-quadratic contributions to the action $S_I(\psi,\bar\psi)$

↳ functional integrals are no longer Gaussian!

▷ consider the expectation value $\langle f(\psi,\bar\psi)\rangle = \frac{\int \mathcal{D}(\bar\psi,\psi)\, f(\psi,\bar\psi)\, e^{-S_0(\psi,\bar\psi)-S_I(\psi,\bar\psi)}}{\int \mathcal{D}(\bar\psi,\psi)\, e^{-S_0(\psi,\bar\psi)-S_I(\psi,\bar\psi)}}$

↳ here, $f(\psi,\bar\psi)$ is some function in the fields $\psi,\bar\psi$.

↳ all terms in the action are of even degree in the Grassmann fields

$$\Rightarrow \langle f(\psi,\bar\psi)\rangle = \frac{\sum_{\ell=0}^{\infty}\frac{1}{\ell!}\int \mathcal{D}(\bar\psi,\psi)\, f(\psi,\bar\psi)[-S_I(\psi,\bar\psi)]^\ell e^{-S_0(\psi,\bar\psi)}}{\sum_{\ell=0}^{\infty}\frac{1}{\ell!}\int \mathcal{D}(\bar\psi,\psi)[-S_I(\psi,\bar\psi)]^\ell e^{-S_0(\psi,\bar\psi)}} = \frac{\sum_{\ell=0}^{\infty}\frac{1}{\ell!}\langle f(\psi,\bar\psi)[-S_I(\psi,\bar\psi)]^\ell\rangle_0}{\sum_{\ell=0}^{\infty}\frac{1}{\ell!}\langle[-S_I(\psi,\bar\psi)]^\ell\rangle_0} \qquad (*)$$

↳ the fields appearing in $f(\psi,\bar\psi)$ are <u>external fields</u>, in contrast to the ones in $S_I(\psi,\bar\psi)$

↳ in the last step, we have introduced free or Gaussian expectation values.

▷ Eq. $(*)$ suggests that in principle any interacting expectation value can be obtained by evaluating an infinite series of free Gaussian expectation values ⇝ for those Wick's theorem can be used!

▷ Note: ✗ convergence of the series is not guaranteed and often fails

✗ infinite summation is not doable, i.e. only low orders or subsets of sum calculable

✓ sometimes it works leading to many important physical conclusions ...

3.6.1. Perturbation theory for the single-particle Green's function

▷ see QFT1 (A. Rosch, Sec. 5.4)

↳ only connected diagrams matter

↳ Calculation of self-energy, Hartree-Fock approximation

↳ well-defined quasiparticles near Fermi level in interacting electron gas

3.6.2. Perturbation theory for the two-particle Green's function

▷ We want to study "effective interactions", i.e. the interactions that act between quasiparticles not only due to the bare interaction, but also due to multiple scattering events

↳ this information is contained in the (connected part of the) two-particle correlation function:

$$G^{(4)}(K_1,K_2;K_1',K_2') = -\langle \psi(K_1)\psi(K_2)\bar{\psi}(K_2')\bar{\psi}(K_1')\rangle$$

▷ for simplicity, we choose Hubbard-type interaction (and N lattice sites):

$$S_I = \frac{U}{N}\int_0^\beta d\tau \sum_{\vec{k},\vec{k}',\vec{q}} \bar{\psi}_\uparrow(\vec{k}+\vec{q},\tau)\bar{\psi}_\downarrow(\vec{k}'-\vec{q},\tau)\psi_\downarrow(\vec{k}',\tau)\psi_\uparrow(\vec{k},\tau) \quad \text{(constant onsite interaction!)}$$

↳ in Matsubara space: $S_I = \frac{TU}{N}\sum_{k,k',q}\bar{\psi}_\uparrow(k+q)\bar{\psi}_\downarrow(k'-q)\psi_\downarrow(k')\psi_\uparrow(k)$ with $k=(i\omega_n,\vec{k})$

▷ the perturbation expansion then reads using $K=(p,s),\dots$

$$G^{(4)}(p,s,p',s';p+\ell,s,p'-\ell,s') = -\langle\psi_s(p)\psi_{s'}(p')\bar{\psi}_{s'}(p'-\ell)\bar{\psi}_s(p+\ell)\rangle$$
$$= \frac{-\sum_n \frac{1}{n!}\langle\psi_s(p)\psi_{s'}(p')\bar{\psi}_{s'}(p'-\ell)\bar{\psi}_s(p+\ell)(-S_I)^n\rangle_0}{\sum_n\frac{1}{n!}\langle(-S_I)^n\rangle_0}$$

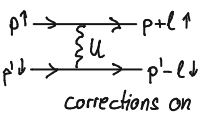
▷ Zeroth order: $G^{(4)}(p,s,p',s';p+\ell,s,p'-\ell,s')$

$$= -\langle\psi_s(p)\psi_{s'}(p')\bar{\psi}_{s'}(p'-\ell)\bar{\psi}_s(p+\ell)\rangle_0 = -G_0^{(2),s}G_0^{(2),s'}\delta_{0,\ell}+\delta_{ss'}G_0^{(2),s}(p)G_0^{(2),s'}(p')\delta_{p,p'-\ell}$$

▷ first order: choose $s=\uparrow$ and $s'=\downarrow$

↳ consider only contributions where each of the external fields are connected to the ones in S_I

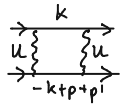
↳ these contributions are solely due to the interactions and will be called connected (subscript "c"):

$$G_c^{(4)}(p,\uparrow,p',\downarrow;p+\ell,\uparrow,p-\ell,\downarrow) = -\frac{UT}{N}G_0^{(2)}(p)G_0^{(2)}(p')G_0^{(2)}(p'-\ell)G_0^{(2)}(p+\ell)$$ "=" 

corrections on external legs

▷ second order: more involved... after using wavevector and frequency conservation:

$$\mathcal{O}(U^2) = G_0^{(2)}(p)G_0^{(2)}(p')G_0^{(2)}(p'-\ell)G_0^{(2)}(p+\ell)\frac{T}{N}U^2\Big[\underbrace{T\sum_k G_0^{(2)}(k)G_0^{(2)}(-k+p+p')}_{\text{"particle-particle" term: } L^{PP}(i\nu,\vec{Q})} + \underbrace{T\sum_k G_0^{(2)}(k)G_0^{(2)}(k+p'-\ell+p)}_{\text{"particle-hole" term: } L^{PH}(i\nu,\vec{Q})}\Big]+\dots$$



▷ third order: $\mathcal{O}(U^3)$ ... all contributions can be summed up ⇒ full Green's fct. ...

▷ general observation: effective interaction acquires wavevector & frequency dependence, i.e. becomes nonlocal in space and imaginary time through pert. corrections.

3.6.3 Particle-particle and particle-hole terms (one-loop bubbles)

▷ for later use: introduce "infrared cutoff" Λ imposed on bare single-particle Green's fct.

↳ cuts out modes near Fermi level for $|\varepsilon(\vec{k})| \leq \Lambda$

↳ full results obtained when letting $\Lambda \to 0$

↳ free propagator is then: $G_{0,\Lambda}(i\omega, \vec{k}) = \dfrac{\Theta(|\varepsilon(\vec{k})| - \Lambda)}{i\omega - \varepsilon(\vec{k})}$ ← step function!

▷ particle-particle term for incoming total frequency $i\nu$ (bosonic) and wavevector $\vec{Q}$

$$L^{PP}_{\Lambda}(i\nu, \vec{Q}) = \sum_{\vec{k}} T \sum_{i\omega_n} G_{0,\Lambda}(i\omega, \vec{k})\, G_{0,\Lambda}(-i\omega + i\nu, -\vec{k} + \vec{Q})$$

▷ Matsubara summation:

↳ study integral $I_R = \oint_R \dfrac{dz}{2\pi i} f(z)\, n_F(z) \overset{\text{Residue theorem}}{=} \sum_n \text{Res}\left[f(z_n)\, n_F(z_n)\right]$

↳ sum over poles encircled by circle integral

↳ integration contour: circle with radius R and $R \to \infty$

↳ integrand is assumed to decay fast enough such that I_R vanishes when $R \to \infty$

↳ for particle-particle term use $z = i\omega$ and $f(z) = \dfrac{\Theta(|\varepsilon(\vec{k})| - \Lambda)}{z - \varepsilon(\vec{k})} \cdot \dfrac{\Theta(|\varepsilon(-\vec{k}+\vec{Q})| - \Lambda)}{-z + i\nu - \varepsilon(-\vec{k}+\vec{Q})}$

↳ for $n_F(z)$ use the Fermi function $n_F(z) = \dfrac{1}{e^{z/T} + 1}$ ↳ poles at $z_n = i(2n-1)\pi T$

↳ poles are exactly the Matsubara frequencies with residues $-T$!

↳ for $I_R \to 0$: $T \sum_{i\omega_n} \dfrac{\Theta(|\varepsilon(\vec{k})| - \Lambda)}{i\omega_n - \varepsilon(\vec{k})} \cdot \dfrac{\Theta(|\varepsilon(-\vec{k}+\vec{Q})| - \Lambda)}{-i\omega_n + i\nu - \varepsilon(-\vec{k}+\vec{Q})} = \sum_{z_{\vec{k}}} n_F(z_{\vec{k}})\, \text{Res}\left[\dfrac{\Theta(|\varepsilon(\vec{k})| - \Lambda)\,\Theta(|\varepsilon(-\vec{k}+\vec{Q})| - \Lambda)}{(z - \varepsilon(\vec{k}))(-z + i\nu - \varepsilon(-\vec{k}+\vec{Q}))}\right]$

$$= \Theta(|\varepsilon(\vec{k})| - \Lambda)\,\Theta(|\varepsilon(-\vec{k}+\vec{Q})| - \Lambda)\, \frac{1 - n_F(\varepsilon(\vec{k})) - n_F(\varepsilon(-\vec{k}+\vec{Q}))}{-i\nu + \varepsilon(\vec{k}) + \varepsilon(-\vec{k}+\vec{Q})}$$

↳ we have used $n_F(\varepsilon + i\nu) = n_F(\varepsilon)$ ($i\nu$: multiple of $2\pi T$)

$\Longrightarrow$ particle-particle term: $L^{PP}_{\Lambda}(i\nu, \vec{Q}) = \sum_{\vec{k}} \Theta(|\varepsilon(\vec{k})| - \Lambda)\,\Theta(|\varepsilon(-\vec{k}+\vec{Q})| - \Lambda)\, \dfrac{1 - n_F(\varepsilon(\vec{k})) - n_F(\varepsilon(-\vec{k}+\vec{Q}))}{-i\nu + \varepsilon(\vec{k}) + \varepsilon(-\vec{k}+\vec{Q})}$

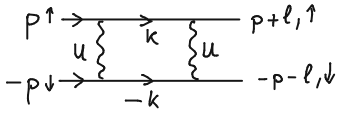
▷ particle-hole term: analoguous calculation with $Q = p' - l + p$

$\Longrightarrow$ particle-hole term: $L^{PH}_{\Lambda}(i\nu, \vec{Q}) = \sum_{\vec{k}} \Theta(|\varepsilon(\vec{k})| - \Lambda)\,\Theta(|\varepsilon(\vec{k}+\vec{Q})| - \Lambda)\, \dfrac{n_F(\varepsilon(\vec{k})) - n_F(\varepsilon(\vec{k}+\vec{Q}))}{i\nu + \varepsilon(\vec{k}) - \varepsilon(\vec{k}+\vec{Q})}$

3.6.4. Logarithmic divergence of particle-particle term

▷ focus on vanishing external frequency $i\nu = 0$ and $\vec{Q} = 0$

↳ graphical representation as particle-particle diagram



▷ inversion symmetry: $\varepsilon(\vec{k}) = \varepsilon(-\vec{k})$ (e.g.. free electron gas $\frac{\vec{k}^2}{2m}$, square lattice tight-binding $\cos k_x + \cos k_y$)

↳ $L^{pp}_{\Lambda}(0,0) = \sum_{\vec{k}} \Theta(|\varepsilon(\vec{k})|-\Lambda)\Theta(|\varepsilon(\vec{k})|-\Lambda)\frac{1-2n_F(\varepsilon(\vec{k}))}{2\varepsilon(\vec{k})} = \int_{-W}^{-\Lambda} d\varepsilon\, \rho(\varepsilon)\frac{1-2n_F(\varepsilon)}{2\varepsilon} + \int_{\Lambda}^{W} d\varepsilon\, \rho(\varepsilon)\frac{1-2n_F(\varepsilon)}{2\varepsilon}$

↳ transformed from wavevector summation $\sum_{\vec{k}}$ to energy integral $\int d\varepsilon\, \rho(\varepsilon)$ ← DOS

↳ bandwidth W and cutoff function cuts out region around Fermi level $|\varepsilon| < \Lambda$

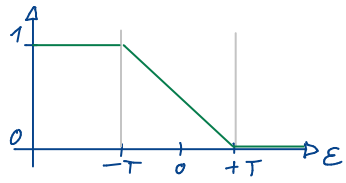
↳ for $T \ll \Lambda$: neglect thermal smearing of Fermi function and combine two integrals

↳ $L^{pp}_{\Lambda}(0,0) \approx \int_{\Lambda}^{W} d\varepsilon\, \rho(\varepsilon)\frac{1}{\varepsilon} \approx \rho(0)\ln\frac{W}{\Lambda}$ with $\rho(0)$ = DOS at Fermi level

↳ have used assumption that variation of $\rho(\varepsilon)$ can be neglected in the respective energy window!

↳ not a good idea near VHS, see below!

↳ for $T \ll W$: approximate $n_F(\varepsilon) \approx \begin{cases} 0 & \text{for } \varepsilon > T \\ 1 & \text{for } \varepsilon < -T \\ \frac{1}{2}(1-\frac{\varepsilon}{T}) & \text{for } \varepsilon \in [-T,T] \end{cases}$



↳ interval $[-T,T]$ gives finite contribution for $T \to 0$

↳ outer regions give singular contribution: $L^{pp}_{\Lambda=0}(0,0) = \int_{T}^{W} d\varepsilon\, \rho(\varepsilon)\frac{1}{\varepsilon} = \rho(0)\log\frac{W}{T}$

↳ note: Sharp step of Fermi fct. for $T \to 0$ is essential for this behavior

⟹ pp-diagram is logarithmically divergent at low T and small Λ: $L^{pp}_{\Lambda}(0) \approx \rho(0)\ln\frac{W}{\max(\Lambda,T)}$

graphene $\rho(\varepsilon) \sim |\varepsilon|$!

▷ this divergence at $i\nu = 0$ and $\vec{Q} = 0$ is common to all many-fermion systems with $\varepsilon(\vec{k}) = \varepsilon(-\vec{k})$ in any spatial dimension as long as DOS $\rho(0) > 0$!

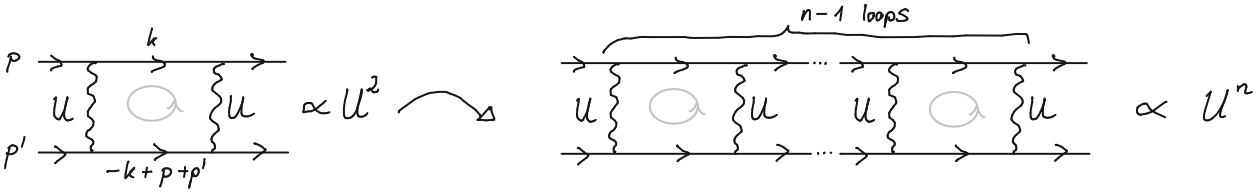
▷ analysis of particle-particle term at $i\nu = 0$ and $\vec{Q} = 0$ is worst-case scenario:

↳ other contributions from this term are usually smaller and regular at low T or Λ!

3.6.5. Summation of particle-particle channel (go beyond U^2)

▷ it is not possible to give closed expression for full perturbation series to all orders of U

▷ higher order terms $\propto U^n$ contain contributions that are chains (ladders) of particle-particle terms:



↳ each closed loop ◯ corresponds to internal k-summation from perturbation series

↳ internal k-summations within each chain segment are independent

⇒ value of chain diagram is n^{th} power of particle-particle bubble

[▷ picking out these contributions in perturbation expansion can sometimes be justified

↳ $D > 1$: when pp-bubble at $Q=0$ is the only log-div diagram ⇒ pp-ladder will dominate at any given order!]

▷ the pp-ladder $\Gamma^{(4)}_{pp,\,ladder} = V_{eff}$ is explicitly given as:

$$\Gamma^{(4)}_{pp,\,ladder}(p\uparrow, p'\downarrow; p+\ell\uparrow, p'-\ell\downarrow) = \left(-\frac{T}{N}\right)\left[U - U^2 L^{pp}_{\Lambda}(p+p') + U^3 L^{pp}_{\Lambda}(p+p')^2 + \dots\right] \overset{\text{geometric series}}{=} \left(-\frac{T}{N}\right) U \frac{1}{1 + U L^{pp}_{\Lambda}(p+p')}$$

↳ log-div for $p+p'=0$

(1) if $U>0$: $\Gamma^{(4)}_{pp}$ becomes very small for $T, \Lambda \to 0$ ↝ log-div. insignificant

(2) if $U<0$: $\Gamma^{(4)}_{pp}$ diverges ↝ effective interaction becomes infinitely strong

↳ V_{eff} develops a pole when $1 - g(0)|U| \log \frac{W}{T} \Rightarrow T_c \sim W e^{-\frac{1}{g(0)|U|}}$ (pp- or Cooper instability)

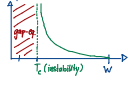
↝ instability of Fermi sea w.r.t. attractive interactions ⇒ formation of bound states "Cooper pairs"
↳ $\vec{p}+\vec{p}'=0$

↝ for phonon-mediated attractive interaction $T_c \sim \mathcal{O}(10\,K)$

▷ remark: even for repulsive i.a. ↝ divergence of pp-channel at extremely low $T>0$: Kohn-Luttinger effect

↳ usual ground state of clean metal with $\varepsilon(k) = \varepsilon(-k)$ is superconductor ↝ killed by impurities!

▷ option to proceed: introduce Hubbard-Stratonovich decoupling ↝ SC gap eq.



3.6.6. Particle-hole term and summation

▷ similar to Cooper channel, also ph-term in perturbation series for $G^{(4)}$ (vertex) can be summed:

$$\Gamma^{(4)}_{\mathrm{PH,ladder}}(p,\uparrow,p,\downarrow;p+\ell,\uparrow,p'-\ell,\downarrow) = \left(-\frac{T}{N}\right)\left[U - U^2 L^{\mathrm{PH}}_\Lambda(Q) + U^3 L^{\mathrm{PH}}_\Lambda(Q)^2 + \dots\right] = \left(-\frac{T}{N}\right) U \frac{1}{1+U L^{\mathrm{PH}}_\Lambda(Q)}$$

▷ ph-bubble is real: $L^{\mathrm{PH}}_\Lambda(i\nu,\vec{Q}) = \sum_{\vec{k}} \frac{n_F(\varepsilon(\vec{k})) - n_F(\varepsilon(\vec{k}+\vec{Q}))}{i\nu + \varepsilon(\vec{k}) - \varepsilon(\vec{k}+\vec{Q})} = \sum_{\vec{k}'=-\vec{k}-\vec{Q}} \frac{n_F(\varepsilon(-\vec{k}'-\vec{Q})) - n_F(\varepsilon(-\vec{k}'))}{i\nu + \varepsilon(-\vec{k}'-\vec{Q}) - \varepsilon(-\vec{k}')}$

$\varepsilon(\vec{k}) = \varepsilon(-\vec{k})$

$$= \sum_{\vec{k}'} \frac{n_F(\varepsilon(\vec{k}')) - n_F(\varepsilon(\vec{k}'+\vec{Q}))}{-i\nu + \varepsilon(\vec{k}') - \varepsilon(\vec{k}'+\vec{Q})} = L^{\mathrm{PH}}_\Lambda(i\nu,\vec{Q})^*$$

▷ ph-bubble is negative: $L^{\mathrm{PH}}_\Lambda(i\nu,\vec{Q}) = \sum_{\vec{k}} \frac{[n_F(\varepsilon(\vec{k})) - n_F(\varepsilon(\vec{k}+\vec{Q}))]\cdot[\varepsilon(\vec{k}) - \varepsilon(\vec{k}+\vec{Q})]}{\nu^2 + [\varepsilon(\vec{k}) - \varepsilon(\vec{k}+\vec{Q})]^2} \leq 0$

↳ if $\varepsilon_1 > \varepsilon_2 \Rightarrow n_F(\varepsilon_1) < n_F(\varepsilon_2)$
$\Rightarrow (n_F(\varepsilon_1) - n_F(\varepsilon_2))(\varepsilon_1 - \varepsilon_2) < 0.$

$\Rightarrow$ maximum of $|L^{\mathrm{PH}}_\Lambda|$ will occur at $i\nu = 0$! (X)

▷ since L^{PH}_Λ is negative ⇝ ladder $\Gamma^{(4)}_{\mathrm{PH,ladder}}$ can have a divergence for $U > 0$, when:

$$\boxed{1 - U\,|L^{\mathrm{PH}}_\Lambda(i\nu,\vec{Q})| = 0}$$ ⇝ ph instability ⇝ (generalized) Stoner criterion (◍)

(1) Consider $i\nu = 0$ and $\vec{Q} \to 0$: $L^{\mathrm{PH}}_{\Lambda=0}(0,\vec{Q}\to 0) = \sum_{\vec{k}} \frac{n_F(\varepsilon(\vec{k})) - n_F(\varepsilon(\vec{k}+\vec{Q}))}{\varepsilon(\vec{k}) - \varepsilon(\vec{k}+\vec{Q})}\Big|_{\vec{Q}\to 0}$

$$= \sum_{\vec{k}} \frac{\partial n_F(\varepsilon(\vec{k}))}{\partial \varepsilon}\Big|_{\vec{k}} \longrightarrow -\sum_{\vec{k}} \delta(\varepsilon) = -g(0) \quad \text{for } T \to 0$$

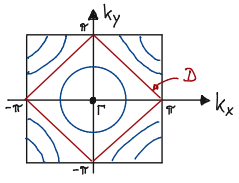
↳ for finite $g(0)$ ⇝ require critical value U_c in Stoner criterion for ph instability

↳ such a $\vec{Q} = 0$ ph-instability corresponds to ferromagnetism

(2) Consider $i\nu = 0$, $\vec{Q} = (\pi,\pi) = -\vec{Q}$ in 2D Hubbard model with nesting $\varepsilon(\vec{k}+\vec{Q}) = -\varepsilon(\vec{k})$

$\mathcal{D} = \mathcal{D}_{+(\pi,\pi)}$ for $\mu = 0$, $t' = 0$

↳ wavevector $\vec{Q}$ ⇒ alternating sign for phase factor $e^{i\vec{Q}\cdot\vec{r}}$ on neighboring lattice sites



▷ everywhere along flat sides of square Fermi surface we can let go $\varepsilon(\vec{k}+\vec{Q})$ and $\varepsilon(\vec{k})$ to zero simultaneously ⇒ ph-bubble becomes:

$$L^{\mathrm{PH}}_\Lambda(0,\vec{Q}) = \sum_{\vec{k}} \frac{2n_F(\varepsilon(\vec{k})) - 1}{2\varepsilon(\vec{k})} = -\int d\varepsilon\, g(\varepsilon)\frac{1}{2\varepsilon}\tanh\frac{\varepsilon}{2T} \quad \text{with DOS } g(\varepsilon) \sim -\log\varepsilon$$

↳ for $T \to 0$: $L^{\mathrm{PH}}_\Lambda(0,\vec{Q}) \sim \int_\Lambda^W d\varepsilon \log(\varepsilon)\cdot\frac{1}{\varepsilon} = \frac{1}{2}\left(\log\frac{W}{\Lambda}\right)^2 \Rightarrow$ log-square divergence!
(nesting + van-Hove singularity)

▷ divergence (2) is stronger than (1): $e^{i\vec{Q}\cdot\vec{r}}$ leads to antiferromagnetic order

↳ in 2D Hubbard model at $\mu = t' = 0$

3.6.7. Decoupling in the magnetic channel for $H = H_t + H_u \rightsquigarrow Z = \mathrm{tr}\, e^{-\beta(H-\mu N)} = \int \mathcal{D}\bar{c}\mathcal{D}c\, e^{-S}$

▷ draw connection between ph-instability and magnetic order!

↳ decompose Hubbard interaction: $H_u = U\sum_i n_{i\uparrow}n_{i\downarrow} = \frac{U}{4}\Big(\sum_i \overbrace{(n_{i\uparrow}+n_{i\downarrow})}^{g_i}{}^2 - \sum_i \overbrace{(n_{i\uparrow}-n_{i\downarrow})}^{S_{z,i}}{}^2\Big)$, $n_{i\sigma} = c^\dagger_{i\sigma}c_{i\sigma}$ (quartic in fermions)

↳ to consider magnetic ordering: ignore first term and go to functional integral

↳ $S_{z,i}$ is a fermion bilinear: $S_{z,i}(\tau) = \bar{c}_{i\uparrow}(\tau)c_{i\uparrow}(\tau) - \bar{c}_{i\downarrow}(\tau)c_{i\downarrow}(\tau)$ (in Grassmann fields)

▷ Hubbard-Stratonovich transformation/decoupling:

↳ recall from Gaussian integration (case of scalar fields ϕ): $\int d\phi\, e^{-\phi^2 - 2\phi J} \propto e^{J^2}$

↳ $e^{\frac{U}{4}\sum_i \int_0^\beta d\tau\, S^2_{z,i}(\tau)} = \int \mathcal{D}m(\tau,i)\, e^{-\sum_i \int_0^\beta d\tau \left[\frac{U}{4}m(i,\tau)^2 - \frac{U}{2}m(i,\tau)S_{z,i}(\tau)\right]}$ with real scalar field $m(\tau,i)$ (✳)

↝ $m(\tau,i)$ couples like magnetic field z-component to electrons $(\bar{c}_{i,\uparrow\downarrow}(\tau))$

↝ interpretation: collective magnetization field $m(\tau,i)$ (Hubbard-Stratonovich field)

▷ if m has non-vanishing expectation value ↝ dynamics of ↑ and ↓ electrons is different ↝ System is magnetic

▷ full action:
$$S(\bar{c}_{i\uparrow\downarrow}, c_{i\uparrow\downarrow}, m_i) = \int_0^\beta d\tau \Big\{ \sum_{i,s}\bar{c}_{is}(\tau)(\partial_\tau - \mu)c_{is}(\tau) - t\sum_{\langle ij\rangle s}\left[\bar{c}_{is}(\tau)c_{js}(\tau) + \bar{c}_{js}(\tau)c_{is}(\tau)\right]$$
$$+ \frac{U}{2}\sum_i m_i(\tau)\underbrace{\left[\bar{c}_{i\uparrow}(\tau)c_{i\uparrow}(\tau) - \bar{c}_{i\downarrow}(\tau)c_{i\downarrow}(\tau)\right]}_{S_{z,i}} + \frac{U}{4}\sum_i m_i(\tau)^2 \Big\}$$

↳ action is only quadratic in fermions (⇒ fermions can be integrated out with Gaussian int.)

↳ rewrite action conveniently in wavevector & Matsubara space w/ $(\vec{k}, ik_0)_s = k_s$:

$$S(\bar{c}_{k_s}, c_{k_s}, m(q)) = -\sum_{k_s}\bar{c}_{k_s}\hat{M}_{k_s;k's'}c_{k's'} + \frac{U}{4}\sum_q m(q)^2$$

where $\hat{M}_{k_s,k's'} = \underbrace{(ik_0 - \varepsilon(\vec{k}) + \mu)\delta_{ss'}\delta_{kk'}}_{\hat{G}_0^{-1}} \underbrace{- \sqrt{\tfrac{T}{V}}\tfrac{U}{2}\,\mathrm{sign}(s)\, m(k-k')\delta_{ss'}}_{\hat{V}(m)} = \hat{G}_0^{-1}(1 - \hat{G}_0\hat{V}(m))$

⇒ partition function: $Z = \int \mathcal{D}m \int \mathcal{D}\bar{c}\mathcal{D}c\, e^{-S(\bar{c},c,m)} \overset{\text{Gaussian integration over fermion fields } \bar{c},c}{=} \int \mathcal{D}m\, e^{-S_{\mathrm{eff}}(m)}$

with $S_{\mathrm{eff}}(m) = \frac{U}{4}\sum_q m(q)^2 - \mathrm{Tr}\ln(\hat{M}) = \frac{U}{4}\sum_q m(q)^2 - \mathrm{Tr}\ln(\hat{G}_0^{-1}) \underbrace{- \mathrm{Tr}\ln(1 - \hat{G}_0\hat{V}(m))}_{(▨)}$

↳ second trace (▨) contains scalar fields $m(q)$ and can be expanded...

▷ (▨) $= -\mathrm{Tr}\ln(1-\hat{G}_0\hat{V}(m)) = \underbrace{\mathrm{Tr}(\hat{G}_0\hat{V}(m))}_{=\sqrt{\frac{T}{V}}\sum_{k,s}G_0(k)\frac{\mathrm{sign}(s)U}{2}m(k=k')=0\ \text{(because } s=+1 \text{ and } s=-1 \text{ cancel)}} + \frac{1}{2}\mathrm{Tr}(\hat{G}_0\hat{V}(m)\hat{G}_0\hat{V}(m)) + \mathcal{O}(m^3)$

↳ trace over second term:

$$\frac{1}{2}\mathrm{Tr}[\hat{G}_0\hat{V}(m)\hat{G}_0V(m)] = \frac{T}{2V}\frac{U^2}{4}\sum_s\sum_{k,k'}G_0(k)\,m(k-k')\,G_0(k')\,m(k'-k)$$

$$= \sum_q \frac{U^2}{4}|m(q)|^2\left\{\frac{T}{V}\sum_k G_0(k)\,G_0(k+q)\right\} = \frac{U^2}{4}\sum_q{}' L^{PH}(q)\,|m(q)|^2$$

(ph bubble)

⇒ action for mag. field up to 2nd order in $m(q)$: $\boxed{S_{\text{eff}}^{(2)}(m) = \sum_q \frac{U}{4}\left(1+UL^{PH}(q)\right)|m(q)|^2}$

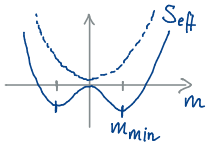
▷ as long as $(1+UL^{PH}(q)) > 0$ ⇒ larger $|m(q)|$ have larger $S_{\text{eff}}^{(2)}(m)$

⇒ statistical weight $e^{-S_{\text{eff}}(m)}$ smaller than weight for $m(q)=0$ ⇒ no difference for ↑ and ↓ electrons!

▷ Situation changes when $\underline{(1+UL^{PH}(q_m)) \leq 0}$ for some q_m ↘ generalized Stoner criterion (▨)

↳ for $(1+UL^{PH}(q_m)) < 0$: non-zero values of $|m(q)|$ have higher statistical weight

↳ higher-order terms in $S_{\text{eff}} \propto m^4, m^6, \ldots$ render action bounded from below



⇒ action is minimal at some $\pm m(q_m)_{\min}$ ↘ most probable value for $m(q)$

▷ if system is in one of the two minima: Spontaneous breaking of spin symmetry!

↳ ↑ and ↓ spins will see opposite mean-field $\pm m(q_m)_{\min}$ ⇒ magnetic state

▷ because of (x): (▨) happens first for $\nu = q_0 = 0$ ⇒ $\pm m(q_m)_{\min}$ is τ independent

▷ saddle-point approximation: ignore fluctuations of $m(q)$ ↘ $m(q) = \delta_{q_0,0}\,\delta_{\vec{q},\vec{q}_m}\,m(\vec{q}_m)_{\min}$

↳ condition for minimum of S_{eff}: $\frac{\delta}{\delta m(\vec{q}_m)}S_{\text{eff}}(m(\vec{q}_m)) = 0$ ↘ gap equation

▷ ordering wavevectors $\vec{q}_m$:

(1) $\vec{q}_m \to 0$: real space $m_i = m(\vec{q}_m)_{\min}e^{i\vec{q}_m\cdot\vec{r}_i} = m(0)_{\min}$ ↘ constant mag. field ↘ FERROMAGNETISM

(2) $\vec{q}_m \to \vec{Q}=(\pi,\pi) = -\vec{Q}$: $m_i = m(\vec{Q})_{\min}e^{i\vec{Q}\cdot\vec{r}_i}$ ↘ alternates on neighboring sites ↘ ANTIFERROMAGNETISM

↳ for perfect nesting (2) is stronger than (1) due to $\log^2$ divergence ↘ AFM ground state

3.6.8. Comments on Hubbard-Stratonovich decoupling

▷ FM order : shifts spin-dependent chemical potential ↝ $\varepsilon_{\uparrow/\downarrow}(\vec{k}) = \varepsilon(\vec{k}) - \mu \pm \frac{U m(\vec{0})_{min}}{2}$

↳ no gap for ph excitations ↝ system remains metallic (for example iron, nickel, cobalt)

▷ AFM order leads to energy dispersion for electrons of the form $E(\vec{k}) = \pm\sqrt{\varepsilon^2(\vec{k}) + \frac{U^2}{2} m(\vec{Q})^2}$

↳ excitation gap at Fermi level ↝ system is an insulator

▷ saddle point approximation completely ignored fluctuations ↝ overestimates ordering

▷ for attractive Hubbard interaction: use different collective field for decoupling

$$e^{U\int_0^\beta d\tau \frac{1}{V}\sum_{k,k'} \bar{c}_{k\uparrow}\bar{c}_{-k+q\downarrow}c_{k'+q\downarrow}c_{-k'}} \propto \int \mathcal{D}\Delta(q)\mathcal{D}\Delta^*(q)\, e^{-\int_0^\beta d\tau\left\{\sum_q \Delta^*(q)\Delta(q)\frac{1}{U} + \sqrt{\frac{1}{V}}\sum_q\left(\Delta^*(q)\sum_k c_{-k\downarrow}c_{k+q\uparrow} + \Delta(q)\sum_k \bar{c}_{k\uparrow}\bar{c}_{-k+q\downarrow}\right)\right\}}$$

↳ with auxiliary complex Hubbard-Stratonovich field $\Delta(\vec{q},\tau)$

↳ Δ couples to operator $c^\dagger_{\vec{k}+\vec{q},\uparrow} c^\dagger_{-\vec{k},\downarrow}$ ↝ Cooper pair with total momentum $\vec{q}$

3.6.9. Comment on competing instabilities

▷ for Hubbard-model dispersion, also pp-bubble diverges as $(\log)^2$ due to VHS

▷ separate summations in pp- and ph-channels ↝ both ladders can lead to instabilities

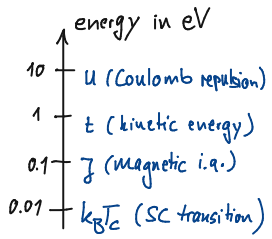
▷ full perturbation series contains many other diagrams ↝ e.g. mixed divergent pp-/ph-bubbles

↝ Question: which instability is strongest? ↝ competing instabilities

↝ (1) sum up all diagrams (at least one-loop and their products → parquet summation)

or (2) renormalization group for summation of all possibly dangerous diagrams...

4. Renormalization group (RG)



▷ interacting electron systems exhibit distinct behavior on different energy scales

↳ integrate out d.o.f.s with different energy scales successively ↝ RG

4.1. The generating functionals W, Γ and V

▷ fermionic action: $S[\psi,\bar\psi] = -(\bar\psi, G_0^{-1}\psi) + V[\psi,\bar\psi]$ (arbitrary many-body interaction (S_I))

↳ where $(\bar\psi, G_0^{-1}\psi) = \sum_{x,x'} \bar\psi(x) G_0^{-1}(x,x') \psi(x')$ and $x = (k_0, \vec k, \sigma)$ (fern. Matsubara frequency; wavevector/momentum; spin orientation)

↳ $V[\psi,\bar\psi] = \frac{1}{4} \sum_{\substack{x_1,x_2\\ x_1',x_2'}} V(x_1',x_2';x_1,x_2)\,\bar\psi(x_1')\bar\psi(x_2')\psi(x_2)\psi(x_1)$

↳ spin-rotation and translation invariant bare propagator: $G_0(x,x') = \delta_{k_0 k_0'}\,\delta_{\vec k \vec k'}\,\delta_{\sigma\sigma'}\,G_0(k_0,\vec k)$

with $G_0(k_0,\vec k) = \frac{1}{ik_0 - \xi_{\vec k}}$ where $\xi_{\vec k} = \varepsilon(\vec k) - \mu$ (single-particle energy relative to μ)

▷ generating functional of connected Green's functions:

$$W[\eta,\bar\eta] = -\ln \int \mathcal{D}(\psi,\bar\psi)\, e^{-S[\psi,\bar\psi]}\, e^{(\bar\eta,\psi)+(\bar\psi,\eta)} \qquad \text{(Schwinger functional)}$$

▷ connected m-particle Green's functions:

$$G_c^{(2m)}(x_1,\dots,x_m;x_1',\dots,x_m') = -\langle \psi(x_1)\dots\psi(x_m)\bar\psi(x_m')\dots\bar\psi(x_1')\rangle_c = (-1)^m \frac{\delta^{2m} W[\eta,\bar\eta]}{\delta\bar\eta(x_1)\dots\delta\bar\eta(x_m)\,\delta\eta(x_m')\dots\delta\eta(x_1')}\Big|_{\eta,\bar\eta=0}$$

▷ expanding $W[\eta,\bar\eta]$ in powers of fields: $W[\eta,\bar\eta] = -\ln\mathcal{Z} + (\bar\eta, G\eta) + \frac{1}{(2!)^2}\sum_{\substack{x_1,x_2\\ x_1',x_2'}} G_c^{(4)}(x_1,x_2;x_1',x_2')\bar\eta(x_1)\bar\eta(x_2)\eta(x_2')\eta(x_1') + \dots$

↳ with propagator of interacting system: $\boxed{G = G_c^{(2)}}$

4.1.1. Effective action Γ

▷ information is also efficiently stored in Legendre transform of $W(\eta,\bar\eta)$

↳ effective action: $\Gamma[\psi,\bar\psi] = (\bar\eta,\psi) + (\bar\psi,\eta) + W[\eta,\bar\eta]$ with $\psi = -\frac{\delta W}{\delta\bar\eta}$ and $\bar\psi = \frac{\delta W}{\delta\eta}$

▷ $\Gamma[\psi,\bar\psi]$ generates the so-called one-particle irreducible vertex functions (1PI vertices):

$$\Gamma^{(2m)}(x_1',\dots,x_m';x_1,\dots,x_m) = \frac{\delta^{2m}\Gamma[\psi,\bar\psi]}{\delta\bar\psi(x_1')\dots\delta\bar\psi(x_m')\,\delta\psi(x_m)\dots\delta\psi(x_1)}$$

▷ Legendre correspondence between W and Γ yields relations between $G_c^{(2m)}$ and $\Gamma^{(2m)}$, e.g.:

↳ $\Gamma^{(2)} = G^{-1} = G_0^{-1} - \Sigma$, where Σ is the <u>self-energy</u>

↳ $G_c^{(4)}(x_1,x_2;x_1',x_2') = \sum_{y_1 y_2 y_1' y_2'} G(x_1,y_1') G(x_2,y_2') \Gamma^{(4)}(y_1',y_2';y_1,y_2) G(y_1,x_1') G(y_2,x_2')$

▷ effective action obeys reciprocity relations: $\frac{\delta\Gamma}{\delta\psi} = -\bar{\eta}$ and $\frac{\delta\Gamma}{\delta\bar{\psi}} = \eta$ (4-1)

▷ second functional derivative of $W[\eta,\bar{\eta}]$: $\tilde{W}^{(2)}[\eta,\bar{\eta}] = -\begin{pmatrix} \frac{\delta W}{\delta\bar{\eta}(x)\,\delta\eta(x')} & -\frac{\delta W}{\delta\bar{\eta}(x)\,\delta\bar{\eta}(x')} \\ -\frac{\delta W}{\delta\eta(x)\,\delta\eta(x')} & \frac{\delta W}{\delta\eta(x)\,\delta\bar{\eta}(x')} \end{pmatrix}$

▷ second functional derivative of $\Gamma[\psi,\bar{\psi}]$: $\tilde{\Gamma}^{(2)}[\psi,\bar{\psi}] = \begin{pmatrix} \frac{\delta\Gamma}{\delta\bar{\psi}(x)\,\delta\psi(x')} & \frac{\delta\Gamma}{\delta\bar{\psi}(x)\,\delta\bar{\psi}(x')} \\ \frac{\delta\Gamma}{\delta\psi(x)\,\delta\psi(x')} & \frac{\delta\Gamma}{\delta\psi(x)\,\delta\bar{\psi}(x')} \end{pmatrix}$

$\Rightarrow$ $\tilde{\Gamma}^{(2)}[\psi,\bar{\psi}] = \left(\tilde{W}^{(2)}[\eta,\bar{\eta}]\right)^{-1}$ (from reciprocity relations) (4-2)

4.1.2. Effective interaction V (here: just used for intermediate step in calculation)

▷ effective interaction is another useful generating functional, which is defined as:

$$V[\chi,\bar{\chi}] = -\ln\left\{\frac{1}{Z_0}\int\mathcal{D}(\psi,\bar{\psi})\, e^{(\bar{\psi},G_0^{-1}\psi)}\, e^{-V[\psi+\chi,\bar{\psi}+\bar{\chi}]}\right\}$$

↳ substitution of variables $\rightsquigarrow$ $V[\chi,\bar{\chi}] = W[\eta,\bar{\eta}] + \ln Z_0 - (\bar{\eta},G_0\eta)$ with $\chi = G_0\eta$, $\bar{\chi} = G_0^t\bar{\eta}$ (4-3)

[▷ functional derivatives of $V[\chi,\bar{\chi}]$ w.r.t. $\chi,\bar{\chi}$ generate:

↳ connected Green's functions with bare propagators amputated from external legs in Feynman diags.

↳ term $\ln Z_0 - (\bar{\eta},G_0\eta)$ cancels non-interacting part of $W[\eta,\bar{\eta}]$ such that $V[\chi,\bar{\chi}]=0$ for $V[\psi,\bar{\psi}]=0$]

▷ representation of $V[\chi,\bar{\chi}]$ via <u>functional derivatives</u>:

$$\begin{aligned} e^{-V[\chi,\bar{\chi}]} &= \frac{1}{Z_0}\int\mathcal{D}(\psi,\bar{\psi})\, e^{(\bar{\psi},G_0^{-1}\psi) - V[\psi+\chi,\bar{\psi}+\bar{\chi}]} \\ &= \frac{1}{Z_0}\, e^{-V[\frac{\delta}{\delta\bar{\eta}},\frac{\delta}{\delta\eta}]}\int\mathcal{D}(\psi,\bar{\psi})\, e^{(\bar{\psi},G_0^{-1}\psi)}\, e^{(\bar{\eta},\psi+\chi)+(\eta,\bar{\psi}+\bar{\chi})}\Big|_{\eta=\bar{\eta}=0} \\ &= e^{-V[\frac{\delta}{\delta\bar{\eta}},\frac{\delta}{\delta\eta}]}\, e^{(\bar{\eta},G_0\eta)}\, e^{(\bar{\eta},\chi)+(\bar{\eta},\bar{\chi})}\Big|_{\eta=\bar{\eta}=0} = e^{-V[\frac{\delta}{\delta\bar{\eta}},\frac{\delta}{\delta\eta}]}\, e^{(\frac{\delta}{\delta\bar{\chi}},G_0\frac{\delta}{\delta\bar{\chi}})}\, e^{(\bar{\eta},\chi)+(\eta,\bar{\chi})}\Big|_{\eta=\bar{\eta}=0} \\ &= e^{\Delta_{G_0}}\, e^{-V[\chi,\bar{\chi}]} \end{aligned}$$

↳ with <u>functional Laplacian</u> (operator): $\Delta_{G_0} = \left(\frac{\delta}{\delta\chi},G_0\frac{\delta}{\delta\bar{\chi}}\right) = \sum_{x,x'}\frac{\delta}{\delta\chi(x)}\,G_0(x,x')\,\frac{\delta}{\delta\bar{\chi}(x')}$

4.2. Exact fermionic flow equation

▷ recall the single-particle Green's fct with infrared cutoff Λ: $G_0^\Lambda(k_0,\vec{k}) = \frac{\theta(|\xi_{\vec{k}}|-\Lambda)}{ik_0 - \xi_{\vec{k}}}$

↳ infrared singularity of propagator at $k_0 = 0$ and $\xi_{\vec{k}} = 0$ is cut off at scale Λ

↳ momenta close to the Fermi surface are excluded!

▷ bare action constructed w/ G_0^Λ is $S^\Lambda[\psi,\bar\psi]$, generating functionals $W^\Lambda[\eta,\bar\eta]$, $V^\Lambda[\chi,\bar\chi]$, $\Gamma^\Lambda[\psi,\bar\psi]$

↳ original functionals W, V, Γ recovered for $\Lambda \to 0$

▷ for finite Λ, we obtain for the effective interaction: $e^{-V^\Lambda} = e^{\Delta_{G_0^\Lambda}} e^{-V}$ (4-4)

↳ at highest scale Λ_0 s.t. $G_0^{\Lambda_0} = 0 \Rightarrow V^{\Lambda_0} = V$

$\Rightarrow V^\Lambda$ interpolates smoothly between bare interaction V and generating functional V ("flows")

4.2.1. Exact renormalization group equation for effective interaction V^Λ

▷ derivative of V^Λ w.r.t. Λ with $\dot G_0^\Lambda = \frac{d}{d\Lambda} G_0^\Lambda$ and $\mathrm{tr}\, A = \sum_x A(x,x)$:

$$\frac{d}{d\Lambda}V^\Lambda = -e^{+V^\Lambda}\frac{d}{d\Lambda}e^{-V^\Lambda} \overset{(4-4)}{=} -e^{V^\Lambda}\frac{d}{d\Lambda}\left(e^{\Delta_{G_0^\Lambda}}e^{-V}\right) = -e^{V^\Lambda}\Delta_{\dot G_0^\Lambda}e^{-V^\Lambda}$$

$$= -e^{V^\Lambda}\left(\frac{\delta}{\delta\chi}, \dot G_0^\Lambda \frac{\delta}{\delta\bar\chi}\right)e^{-V^\Lambda} = -e^{V^\Lambda}\left(\frac{\delta}{\delta\chi}, \dot G_0^\Lambda\left(-\frac{\delta V^\Lambda}{\delta\bar\chi}\right)\right)e^{-V^\Lambda}$$

$$= -e^{V^\Lambda}\left(-\frac{\delta V^\Lambda}{\delta\chi}, \dot G_0^\Lambda\left(-\frac{\delta V^\Lambda}{\delta\bar\chi}\right)\right)e^{-V^\Lambda} - e^{V^\Lambda}\mathrm{tr}\left[\dot G_0^\Lambda\left(+\frac{\delta^2 V^\Lambda}{\delta\bar\chi\delta\chi}\right)\right]e^{-V^\Lambda}$$

$\Rightarrow$ the effective interaction V^Λ satisfies the exact renormalization group equation:

$$\frac{d}{d\Lambda}V^\Lambda[\chi,\bar\chi] = -\left(\frac{\delta V^\Lambda}{\delta\chi}, \dot G_0^\Lambda \frac{\delta V^\Lambda}{\delta\bar\chi}\right) - \mathrm{tr}\left(\dot G_0^\Lambda \frac{\delta^2 V^\Lambda}{\delta\bar\chi\,\delta\chi}\right) \quad (4\text{-}5)$$

↳ requires initial condition $V^{\Lambda_0}[\chi,\bar\chi] = V[\chi,\bar\chi]$

↳ RG equation determines flow of V^Λ uniquely for all $\Lambda < \Lambda_0$

↳ for sharp momentum cutoff Λ_0 can be chosen as $\max(|\xi_{\vec{k}}|)$

4.2.2. Exact renormalization group equation for Γ^Λ

▷ combining (4-3) and (4-5) yields exact flow equation for W^Λ:

$$\frac{d}{d\Lambda} W^\Lambda[\eta,\bar\eta] = \left(\frac{\delta W^\Lambda}{\delta \eta}, \dot Q_0^\Lambda \frac{\delta W^\Lambda}{\delta \bar\eta} \right) + \mathrm{tr}\left(\dot Q_0^\Lambda \frac{\delta^2 W^\Lambda}{\delta\bar\eta\,\delta\eta} \right) \quad \text{with} \quad Q_0^\Lambda = (G_0^\Lambda)^{-1} \qquad (4\text{-}6)$$

▷ consider scale-dependent eff. action $\Gamma^\Lambda[\psi,\bar\psi] = (\bar\eta^\Lambda,\psi) + (\bar\psi,\eta^\Lambda) + W^\Lambda[\eta^\Lambda,\bar\eta^\Lambda]$

↳ $\eta^\Lambda,\bar\eta^\Lambda$ are Λ dependent functions of $\psi,\bar\psi$ determined from $-\frac{\delta W^\Lambda}{\delta\bar\eta} = \psi$ and $\frac{\delta W^\Lambda}{\delta\eta} = \bar\psi$

$$\Rightarrow \text{scale derivative}: \quad \frac{d}{d\Lambda}\Gamma^\Lambda[\psi,\bar\psi] = \left(\frac{d}{d\Lambda}\bar\eta^\Lambda,\psi\right) + \left(\bar\psi,\frac{d}{d\Lambda}\eta^\Lambda\right) + \frac{d}{d\Lambda}W^\Lambda[\eta^\Lambda,\bar\eta^\Lambda] \overset{\text{...cancellations...}}{=} \frac{d}{d\Lambda}W^\Lambda[\eta^\Lambda,\bar\eta^\Lambda]\Big|_{\eta^\Lambda,\bar\eta^\Lambda \text{ fixed}} \qquad (4\text{-}7)$$

↝ inserting (4-6) into (4-7) and using (4-2) yields an exact flow equation for the effective action:

$$\boxed{\frac{d}{d\Lambda}\Gamma^\Lambda[\psi,\bar\psi] = -(\bar\psi,\dot Q_0^\Lambda\psi) + \frac{1}{2}\mathrm{tr}\left[\begin{pmatrix}\dot Q_0^\Lambda & 0\\ 0 & -\dot Q_0^{\Lambda t}\end{pmatrix}\left(\tilde\Gamma^{(2)\Lambda}[\psi,\bar\psi]\right)^{-1}\right]} \qquad (4\text{-}8)$$

where $A^t(x,x') = A(x',x)$

4.3.3. The Wetterich equation

▷ a bit more grooming yields the most common form of the exact RG equation:

↳ define $\Gamma_R^\Lambda[\psi,\bar\psi] = \Gamma^\Lambda[\psi,\bar\psi] + (\bar\psi, R^\Lambda\psi)$ where $R^\Lambda = Q_0^\Lambda - Q_0$

$$\Rightarrow \boxed{\frac{d}{d\Lambda}\Gamma_R^\Lambda[\psi,\bar\psi] = -\frac{1}{2}\mathrm{tr}\left[\dot{\tilde R}^\Lambda\left(\tilde\Gamma_R^{(2)\Lambda}[\psi,\bar\psi] + \tilde R^\Lambda\right)^{-1}\right]} \quad \text{(Wetterich equation)}$$

with $\tilde R^\Lambda = \mathrm{diag}(R^\Lambda, -R^{\Lambda t})$

↳ Γ_R^Λ and Γ^Λ both flow to the same effective action Γ for $\Lambda \to 0$ (R^Λ vanishes)

↳ at initial scale Λ_0: $\Gamma_R^{\Lambda_0}[\psi,\bar\psi] = S[\psi,\bar\psi]$

$\Rightarrow$ Γ_R^Λ interpolates between the bare action S and the effective action Γ

▷ can be analoguously formulated for bosonic fields!

▷ exact flow eqs. can be used as starting points for calculations of correlation fcts.

4.3. Vertex expansion

▷ expand the effective action in powers of the fermion fields $\psi, \bar\psi$:

↳ $\Gamma^\Lambda[\psi,\bar\psi] = \sum_{m=0}^{\infty} \mathcal{A}^{(2m)\Lambda}[\psi,\bar\psi]$ where for $m \geq 1$ we define (4-9)

↳ $\mathcal{A}^{(2m)\Lambda}[\psi,\bar\psi] = \frac{(-1)^m}{(m!)^2} \sum_{\substack{x_1,\dots,x_m \\ x'_1,\dots,x'_m}} \Gamma^{(2m)\Lambda}(x'_1,\dots,x'_m; x_1,\dots,x_m)\, \bar\psi(x'_1)\cdots\bar\psi(x'_m)\,\psi(x_m)\cdots\psi(x_1)$ (4-10)

▷ the field independent constant $\mathcal{A}^{(0)\Lambda}$ yields the grandcanonical potential $\mathcal{A}^{(0)\Lambda} = T^{-1}\Omega^\Lambda$

▷ to expand the inverse of $\tilde\Gamma^{(2)\Lambda}$ on the r.h.s. of (4-8), we isolate the field-independent part:

$$\tilde\Gamma^{(2)\Lambda}[\psi,\bar\psi] = (\tilde G^\Lambda)^{-1} - \tilde\Sigma^\Lambda[\psi,\bar\psi]$$

(not the self-energy!)

↳ here $(\tilde G^\Lambda)^{-1} = \left(\tilde\Gamma^{(2)\Lambda}[\psi,\bar\psi]\big|_{\psi,\bar\psi=0}\right)^{-1} = \mathrm{diag}(G^\Lambda, -G^{\Lambda t})$ is the full propagator (contains the self-energy!)

↳ and $\tilde\Sigma^\Lambda[\psi,\bar\psi] = -\tilde\Gamma^{(2)\Lambda} + (\tilde G^\Lambda)^{-1}$ contains all contributions at least quadratic in the fields !

▷ now expand $\left(\tilde\Gamma^{(2)\Lambda}\right)^{-1}$ as geometric series: $(\tilde\Gamma^{(2)\Lambda})^{-1} = (1 - \tilde G^\Lambda\tilde\Sigma^\Lambda)^{-1}\tilde G^\Lambda = \left(\sum_{n=0}^{\infty}(\tilde G^\Lambda\tilde\Sigma^\Lambda)^n\right)\tilde G^\Lambda$ (4-11)

▷ insert (4-11) into (4-8): $\frac{d}{d\Lambda}\Gamma^\Lambda[\psi,\bar\psi] = -(\bar\psi, \dot Q_0^\Lambda\psi) - \mathrm{tr}(\dot Q_0^\Lambda G^\Lambda) + \frac12 \mathrm{tr}\left\{-\tilde G^\Lambda\begin{pmatrix}\dot Q_0^\Lambda & 0\\ 0 & -\dot Q_0^{\Lambda t}\end{pmatrix}\cdot\sum_{n=1}^{\infty}(\tilde G^\Lambda\tilde\Sigma^\Lambda)^n\right\}$

$$\Rightarrow \boxed{\frac{d}{d\Lambda}\Gamma^\Lambda[\psi,\bar\psi] = -\mathrm{tr}(\dot Q_0^\Lambda G^\Lambda) - (\bar\psi,\dot Q_0^\Lambda\psi) + \frac12\mathrm{tr}\left\{\tilde S^\Lambda\left(\tilde\Sigma^\Lambda[\psi,\bar\psi] + \tilde\Sigma^\Lambda[\psi,\bar\psi]\tilde G^\Lambda\tilde\Sigma^\Lambda[\psi,\bar\psi] + \dots\right)\right\}} \quad (4\text{-}12)$$

(contributions at least quadratic in $\psi,\bar\psi$)

with $\tilde S^\Lambda = \mathrm{diag}(S^\Lambda, -S^{\Lambda t}) = -\tilde G^\Lambda\begin{pmatrix}\dot Q_0^\Lambda & 0\\ 0 & -\dot Q_0^{\Lambda t}\end{pmatrix}\tilde G^\Lambda$

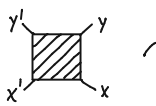
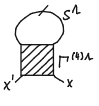
▷ using $(G^\Lambda)^{-1} = Q_0^\Lambda - \Sigma^\Lambda$, we can write $S^\Lambda = \frac{d}{d\Lambda}G^\Lambda\big|_{\Sigma^\Lambda \text{ fixed}}$ (single-scale propagator)

4.3.1. Hierarchy of flow equations

▷ compare coefficients in (4-12) of quadratic contributions $\sim \bar\psi\psi$ (see (4-9))

↳ $\frac{d}{d\Lambda}\mathcal{A}^{(2)} = -(\bar\psi,\dot Q_0^\Lambda\psi) - \mathrm{tr}\left(S^\Lambda\frac{\delta^2}{\delta\psi\delta\bar\psi}\mathcal{A}^{(4)\Lambda}\right)$

↳ insert (4-10) and use $\Gamma^{(2)\Lambda} = Q_0^\Lambda - \Sigma^\Lambda \Rightarrow$ $\boxed{\frac{d}{d\Lambda}\Sigma^\Lambda(x,x') = \sum_{y,y'} S^\Lambda(y,y')\,\Gamma^{(4)\Lambda}(x',y';x,y)}$ (4-13)

▷ diagrammatic representation: $S^\Lambda = y' \longrightarrow y$, $\Gamma^{(4)\Lambda} =$  $\rightsquigarrow$ $\frac{d}{d\Lambda}\Sigma^\Lambda =$ 

▷ comparing coefficients of quartic contributions $\sim (\bar\psi\psi)^2$

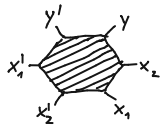
↳ $\frac{d}{d\Lambda}\mathcal{A}^{(4)\Lambda} = \frac{1}{2}\mathrm{tr}\Big\{S^\Lambda\Big(\frac{\delta}{\delta\bar\psi}\frac{\delta}{\delta\psi}\mathcal{A}^{(4)\Lambda}\Big)G^\Lambda\Big(\frac{\delta}{\delta\bar\psi}\frac{\delta}{\delta\psi}\mathcal{A}^{(4)\Lambda}\Big) + S^{\Lambda t}\Big(\frac{\delta}{\delta\psi}\frac{\delta}{\delta\bar\psi}\mathcal{A}^{(4)\Lambda}\Big)G^{\Lambda t}\Big(\frac{\delta}{\delta\psi}\frac{\delta}{\delta\bar\psi}\mathcal{A}^{(4)\Lambda}\Big)\Big\}$

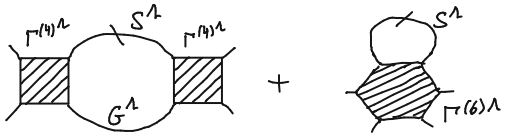
$-\frac{1}{2}\mathrm{tr}\Big\{S^\Lambda\Big(\frac{\delta}{\delta\bar\psi}\frac{\delta}{\delta\bar\psi}\mathcal{A}^{(4)\Lambda}\Big)G^{\Lambda t}\Big(\frac{\delta}{\delta\psi}\frac{\delta}{\delta\psi}\mathcal{A}^{(4)\Lambda}\Big) + S^{\Lambda t}\Big(\frac{\delta}{\delta\psi}\frac{\delta}{\delta\psi}\mathcal{A}^{(4)\Lambda}\Big)G^\Lambda\Big(\frac{\delta}{\delta\bar\psi}\frac{\delta}{\delta\bar\psi}\mathcal{A}^{(4)\Lambda}\Big)\Big\}$

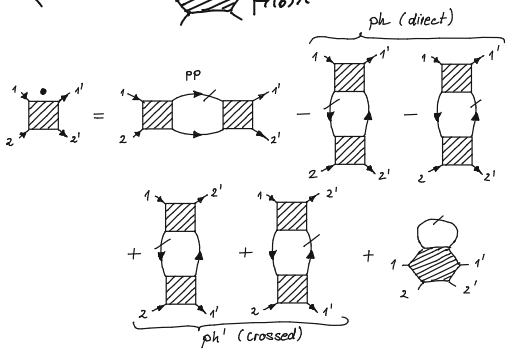
$-\mathrm{tr}\Big(S^\Lambda\frac{\delta}{\delta\bar\psi}\frac{\delta}{\delta\psi}\mathcal{A}^{(6)\Lambda}\Big)$ ↝ insert (4-10):

⇒ two-particle vertex flow

$$\frac{d}{d\Lambda}\Gamma^{(4)\Lambda}(x_1',x_2';x_1,x_2) = \sum_{y_1,y_1'}\sum_{y_2,y_2'} G^\Lambda(y_1,y_1')S(y_2,y_2')$$
$$\times\Big\{\Gamma^{(4)\Lambda}(x_1',x_2';y_1,y_2)\,\Gamma^{(4)\Lambda}(y_1',y_2';x_1,x_2) - \Big[\Gamma^{(4)\Lambda}(x_1',y_2';x_1,y_1)\,\Gamma^{(4)\Lambda}(y_1',x_2';y_2,x_2) + (y_1\leftrightarrow y_2, y_1'\leftrightarrow y_2')\Big]$$
$$+\Big[\Gamma^{(4)\Lambda}(x_2',y_2';x_1,y_1)\,\Gamma^{(4)\Lambda}(y_1',x_1';y_2,x_2) + (y_1\leftrightarrow y_2, y_1'\leftrightarrow y_2')\Big]\Big\} - \sum_{y,y'} S^\Lambda(y,y')\,\Gamma^{(6)\Lambda}(x_1',x_2',y';x_1,x_2,y) \qquad (4\text{-}14)$$

▷ diagrammatic representation: $G^\Lambda = y_1' \text{———} y_1$, $\Gamma^{(6)} =$ 

↳ flow eq. for two-particle vertex: $\frac{d}{d\Lambda}\Gamma^{(4)\Lambda} =$ 

↳ contributions involving $\Gamma^{(4)\Lambda}$ give familiar pp-/ph-diagrams: 

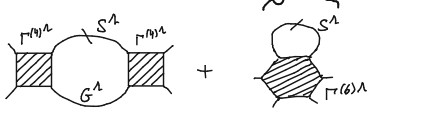
▷ similarly one obtains flow eqs. for all higher vertices $\Gamma^{(2m)\Lambda}$

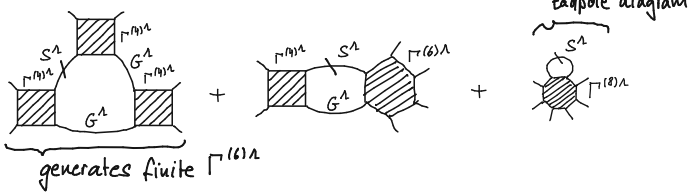
↳ flow eq. for $\Gamma^{(2m)\Lambda}$ contains contributions from "tadpole diagram" involving $\Gamma^{(2m+2)\Lambda}$

↳ m-particle vertices are generated by the flow, irrespective of their presence in bare action

⇒ <u>infinite hierarchy of flow equations</u>

$\frac{d}{d\Lambda}\Sigma^\Lambda =$ 

$\frac{d}{d\Lambda}\Gamma^{(4)\Lambda} =$ 

$\frac{d}{d\Lambda}\Gamma^{(6)\Lambda} =$ 

$\vdots$

4.3.2. Truncations

▷ exact hierarchy of flow eqs. cannot generally be solved ↝ "truncation" unavoidable

▷ level-m_0 truncation: neglect flow of all vertices $\Gamma^{(2m)\Lambda}$ beyond certain order m_0

▷ our analysis of competing instabilities in Hubbard model will be based on level-2 truncation

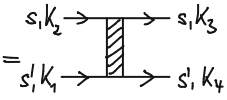
↳ analysis of flow equation (4-14) for $\Gamma^{(4)\Lambda}$
↳ set $\Gamma^{(6)\Lambda} = 0$
↳ neglect self-energy feedback

} simple approximation captures complex interplay of pp-/ph-fluctuations

▷ fermion fields carry spin index s and multiindex $K = (\omega, \vec{k})$

↳ spin-rotation invariance: $\Gamma^{(4)\Lambda}_{s_1 s_2 s_3 s_4}(K_1, K_2; K_3, K_4) = V^\Lambda(K_1, K_2; K_3, K_4)\delta_{s_1 s_3}\delta_{s_2 s_4} - V^\Lambda(K_2, K_1; K_3, K_4)\delta_{s_1 s_4}\delta_{s_2 s_3}$ (4-15)

↳ lattice- and time-translation invariance: $K_1 + K_2 = K_3 + K_4$

↳ $V^\Lambda(K_1, K_2, K_3) =$ 

(interaction vertex)

▷ Plugging (4-15) into (4-14) yields the flow equation for the interaction vertex:

$$\frac{d}{d\Lambda} V^\Lambda(K_1, K_2; K_3, K_4) = \mathcal{T}^\Lambda_{pp}(K_1, K_2; K_3, K_4) + \mathcal{T}^\Lambda_{ph,d}(K_1, K_2; K_3, K_4) + \mathcal{T}^\Lambda_{ph,cr}(K_1, K_2; K_3, K_4) \quad (4\text{-}16)$$

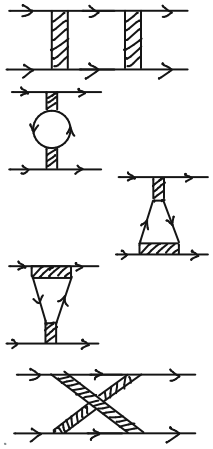
↳ can be solved numerically!

↳ with the pp-/ph-direct-/ph-crossed contributions:

$$\mathcal{T}^\Lambda_{pp}(K_1, K_2; K_3, K_4) = -\tfrac{1}{2}\int dK\, V^\Lambda(K_1, K_2, K)\, \mathcal{B}^\Lambda(K_1 - K + K_1 + K_2)\, V^\Lambda(K_1 + K_2 - K, K_1, K_3)$$

$$\mathcal{T}^\Lambda_{ph,d}(K_1, K_2; K_3, K_4) = \tfrac{1}{2}\int dK \Big[2V^\Lambda(K_1, K_2 - K_3 + K_1, K)\, V^\Lambda(K_1, K_2, K_3)$$
$$- V^\Lambda(K_1, K_2 - K_3 + K_1, K)\, V^\Lambda(K_1, K_2, K_2 - K_3 + K)$$
$$- V^\Lambda(K_1, K_2 - K_3 + K_1, K_4)\, V^\Lambda(K_1, K_2, K_3) \Big]\, \mathcal{B}^\Lambda(K_1, K + K_2 - K_3)$$

$$\mathcal{T}^\Lambda_{ph,cr}(K_1, K_2; K_3, K_4) = -\tfrac{1}{2}\int dK\, V^\Lambda(K_1, K_1, K_3)\, \mathcal{B}^\Lambda(K_1, K + K_1 - K_3)\, V^\Lambda(K_1 - K_3 + K, K_2, K)$$



↳ and $\mathcal{B}^\Lambda(K_1, K_2) = \frac{d}{d\Lambda}\big(G^\Lambda(K_1)\, G^\Lambda(K_2)\big) = \mathcal{B}^\Lambda(K_2, K_1)$ (4-17)

4.4. Application to the Hubbard model at van-Hove filling

▷ consider the Hubbard model with nearest- and 2nd-nearest neighbor hopping:

$$H = -t \sum_{\langle ij \rangle \sigma} (c^\dagger_{i,\sigma} c_{j,\sigma} + \text{h.c.}) - t' \sum_{\langle\langle ij \rangle\rangle \sigma} (c^\dagger_{i,\sigma} c_{j,\sigma} + \text{h.c.}) - \mu \sum_{i,\sigma} c^\dagger_{i,\sigma} c_{i,\sigma} + U \sum_i n_{i,\uparrow} n_{i,\downarrow}$$

↳ band dispersion: $\xi_k = \varepsilon(k) - \mu$

with $\varepsilon(k) = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y$

▷ dispersion $\varepsilon(k)$ has van-Hove points k_{VH}

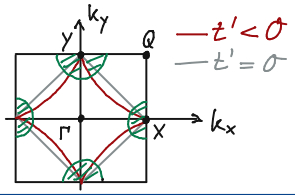
↳ DOS diverges as $\rho(\varepsilon) \propto \log \frac{W}{|\varepsilon - \varepsilon_{VH}|}$

(1) $k_{VH} = (\pi, 0) = X$ with $\varepsilon_{VH} = \varepsilon(X) = 4t'$

(2) $k_{VH} = (0, \pi) = Y$ with $\varepsilon_{VH} = \varepsilon(Y) = 4t'$

} for $\boxed{\mu = 4t'}$ ↝ Fermi surface:

Figure 4-1



↳ due to reciprocal lattice vectors $(2\pi, 0), (0, 2\pi)$: $(-\pi, 0) = X$ and $(0, -\pi) = Y$

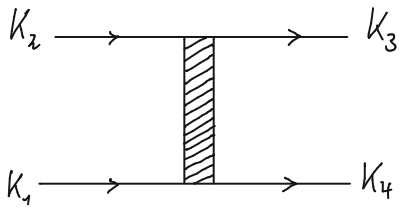
▷ strongest contributions to flow of V^Λ from momenta, where DOS is large

⟹ make "two-patch approximation" by evaluating V^Λ only at singularity momenta X, Y!

↳ momentum-conserving two-particle interactions (scattering processes) on two patches:

↝ couplings g_i, $i \in \{1,2,3,4\}$ (sometimes referred to as "g-ology")

↳ relation between interaction vertex V^Λ and g_i:



(1) $V^\Lambda_1(X,X,X,X) = V^\Lambda_1(Y,Y,Y,Y) = g_4$

(2) $V^\Lambda_1(X,Y,X,Y) = V^\Lambda_1(Y,X,Y,X) = g_1$

(3) $V^\Lambda_1(X,Y,Y,X) = V^\Lambda_1(Y,X,X,Y) = g_2$

(4) $V^\Lambda_1(X,X,Y,Y) = V^\Lambda_1(Y,Y,X,X) = g_3$

4.4.1. Flow equations for couplings g_i

▷ Start with coupling g_1 and equation (4-16):

$$\frac{d}{d\Lambda} g_1 = \frac{d}{d\Lambda} V(X_1,Y_1,X_1,Y) = \tau_{pp}(X_1,Y_1,X_1,Y) + \tau_{ph,cr}(X_1,Y_1,X_1,Y) + \tau_{ph,d}(X_1,Y_1,X_1,Y) \text{ with notation } V = V^\Lambda$$

↳ assumption: interaction vertex ~ constant in small patches p = ▨ in Figure 4-1

↳ $\tau_{pp}(X_1,Y_1,X_1,Y) = -\frac{1}{2}\int_K \mathcal{B}^\Lambda(K,X+Y-K)\, V(X_1,Y_1,K)\, V(X+Y-K,K,X)$

$$= \Big(-\frac{1}{2}\sum_{p=X,Y} \underbrace{\Big[\int_{K\in p} \mathcal{B}^\Lambda(K,X+Y-K)\Big]}_{=:\,\hat{P}(\cdot,\cdot)} V(X_1,Y_1,p)\, V(X+Y-p,p,X)\Big) \times 2^{\,\text{from } -X_1,-Y}$$

$$= -\hat{P}(X,Y)\, \overbrace{V(X_1,Y_1,X_1,Y)}^{g_1}\, \overbrace{V(Y,X_1,X_1,Y)}^{g_2} - \hat{P}(Y,X)\, \overbrace{V(X_1,Y_1,Y,X)}^{g_2}\, \overbrace{V(X_1,Y_1,X_1,Y)}^{g_1} = -2\,\underbrace{\dot{L}^\Lambda_{pp}(Q)}\,\hat{P}(X,Y)\, g_1 g_2$$

$$\Rightarrow \quad \tau_{pp}(X_1,Y_1,X_1,Y) = -2\dot{L}^\Lambda_{pp}(Q)\, g_1 g_2 \quad \text{with} \quad Q = X+Y = (\pi,\pi)$$

↳ note: K-integration in $\dot{L}^\Lambda_{pp}$ is restricted to area of the patch ▨ with radius k_c

↳ Similarly, we find: $\tau_{ph,cr}(X_1,Y_1,X_1,Y) = 2\dot{L}^\Lambda_{ph}(0) g_1 g_4$ and $\tau_{ph,d}(X_1,Y_1,X_1,Y) = 2\dot{L}^\Lambda_{ph}(Q) g_1 (g_2 - g_1)$

$$\Rightarrow \quad \frac{d}{d\Lambda} g_1 = 2\dot{L}^\Lambda_{ph}(Q) g_1 (g_2 - g_1) + 2\dot{L}^\Lambda_{ph}(0) g_1 g_4 - 2\dot{L}^\Lambda_{pp}(Q) g_1 g_2$$

▷ do analoguous calculation for g_2, g_3, g_4 to find:

$$\frac{d}{d\Lambda} g_1 = 2\dot{L}^\Lambda_{ph}(Q) g_1 (g_2 - g_1) + 2\dot{L}^\Lambda_{ph}(0) g_1 g_4 - 2\dot{L}^\Lambda_{pp}(Q) g_1 g_2 \qquad (4\text{-}17a)$$

$$\frac{d}{d\Lambda} g_2 = \dot{L}^\Lambda_{ph}(Q)(g_2^2 + g_3^2) + 2\dot{L}^\Lambda_{ph}(0)(g_1 - g_2) g_4 - \dot{L}^\Lambda_{pp}(Q)(g_1^2 + g_2^2) \qquad (4\text{-}17b)$$

$$\frac{d}{d\Lambda} g_3 = -2\dot{L}^\Lambda_{pp}(0) g_3 g_4 + 2\dot{L}^\Lambda_{ph}(Q) g_3 (2g_2 - g_1) \qquad (4\text{-}17c)$$

$$\frac{d}{d\Lambda} g_4 = -\dot{L}^\Lambda_{pp}(0)(g_3^2 + g_4^2) + \dot{L}^\Lambda_{ph}(0)(g_1^2 + 2g_1 g_2 - 2g_2^2 + g_4^2) \qquad (4\text{-}17d)$$

▷ behavior of $L^\Lambda_{pp/ph}(\cdot)$ at van-Hove filling and $|t'/t| \ll 1$ (near perfect nesting):

(1) $L^\Lambda_{pp}(0) \sim \left(\log \frac{\Lambda_0}{\Lambda}\right)^2$, (3) $L^\Lambda_{ph}(0) \sim \log \frac{\Lambda_0}{\Lambda}$

(2) $L^\Lambda_{pp}(Q) \sim -\log \frac{\Lambda_0}{\Lambda}$, (4) $L^\Lambda_{ph}(Q) \sim \begin{cases} \left(\log \frac{\Lambda_0}{\Lambda}\right)^2 & \text{for } \Lambda \gg |t'| \\ \log \left|\frac{t}{t'}\right| \log \frac{\Lambda_0}{\Lambda} & \text{for } \Lambda \ll |t'| \end{cases}$ (4-18)

always true for nesting $t'=0$

deviation from perfect nesting suppresses 2nd log-div.!

$\Rightarrow$ $L^\Lambda_{pp}(Q)$ and $L^\Lambda_{ph}(0)$ subleading ↳ neglect in (4-17)!

▷ define $y = \left(\log \frac{\Lambda}{\Lambda_0}\right)^2$ and $\dot{g}_i = \frac{dg_i}{dy}$ ↝ rewrite (4-17) with (4-18) and neglecting $\hat{L}_{pp}(Q)$ and $\hat{L}_{ph}(0)$:

$$\dot{g}_1 = 2\,d(y)\,g_1(g_2 - g_1) \quad , \quad \dot{g}_3 = -2g_3 g_4 + 2d(y)(2g_2 - g_1)g_3$$
$$\dot{g}_2 = d(y)(g_2^2 + g_3^2) \quad , \quad \dot{g}_4 = -(g_3^2 + g_4^2) \qquad (4\text{-}19)$$

↳ where $d(y) := \frac{d\hat{L}_{ph}(Q)}{dy}$ and follows $\left\{ \begin{array}{l} d(y) \longrightarrow 1 \text{ at } y \approx 1 \\ d(y) \sim \frac{1}{\sqrt{y}} \log|\frac{t}{t'}| \text{ as } y \longrightarrow \infty \end{array} \right\}$ ↝ study $\dot{g}_i$ for $0 < d(y) \leq 1$

↳ the change of g_i w.r.t. a change of y or Λ is called the "renormalization" of g_i

↳ integrating out all fluctuations means $y \longrightarrow \infty$

4.4.2. Analysis of flow equations (4-19)

▷ start from Hubbard-model initial value $g_i = U > 0$ (repulsive i.a.), $i \in \{1,2,3,4\}$

↳ inspection of (4-19): g_1, g_2, g_3 must stay positive if they start out positive!

↝ reasoning: $\dot{g}_2 > 0$ and $\dot{g}_1, \dot{g}_3$ vanish if respective couplings vanish ⇒ they remain positive

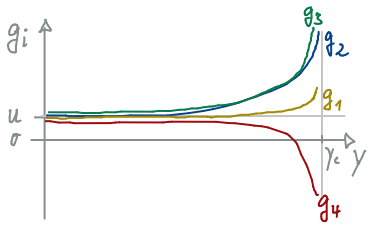
↳ however: $\dot{g}_4 < 0$ ⇒ g_4 decreases as y grows ↝ eventually changes sign and g_4 becomes negative

⇒ negative g_4 corresponds to attractive interaction component ↝ can drive SC instability

▷ leading renormalization of g_4 from Cooper-/pp-channel $\sim L_{pp}(0)$, cf. (4-17d) and (4-19)

↳ $\dot{g}_4 < 0$ reduces g_4, $\dot{g}_2 > 0$ increases g_2

↳ term $\propto d(y)\,g_2 g_3$ in $\dot{g}_3$ is positive for $g_3 > 0$ and pushes g_3 up



↳ $d(y)\,g_2 g_3$ comes from $L_{ph}(Q)$ contributions!

↳ g_2 itself is pushed up by g_3 ⇒ eventually g_3 increases

⇒ interaction $(g_4 - g_3)$ becomes negative (attractive), but $(g_4 + g_3)$ remains positive (repulsive)

▷ the described behavior and sign changes already appear for small couplings

↳ generation of attractive interaction is a qualitative result under perturbative control!

4.4.3. Divergences of flowing couplings

▷ following the RG flow towards large γ: divergence of the couplings $g_i \to \pm\infty$ for $\gamma \to \gamma_c$

▷ since "$\dot{g} \sim g^2$" $\rightsquigarrow$ $g_i = \frac{g_i^0}{\gamma_c - \gamma}$ near some γ_c (4-20)

↳ with $g_1, g_2, g_3 \to +\infty$ and $g_4 \to -\infty$

↳ divergence of g_1 only log-type w.r.t. $\gamma_c - \gamma$

▷ Substitute (4-20) into (4-19) to obtain polynomial equations:

$$g_1^0 = 2\,d(\gamma_c)\, g_1^0 (g_2^0 - g_1^0),\quad g_2^0 = d(\gamma_c)\left((g_2^0)^2 + (g_3^0)^2\right),\quad g_3^0 = -2g_3^0 g_4^0 + 2d(\gamma_c) g_3^0 (2g_2^0 - g_1^0),\quad g_4^0 = -(g_3^0)^2 - (g_4^0)^2 \qquad (4\text{-}21)$$

↳ for example for perfect nesting ($d(\gamma_c) = 1$): $g_1^0 = 0,\ g_2^0 = \frac{1}{6},\ g_3^0 = \frac{\sqrt{5}}{6},\ g_4^0 = -\frac{1}{6}$ (4-22)

4.4.4. Leading instability

▷ identify meaning of divergences of g_i in terms of order parameter (SC, magnetism, ...)

▷ introduce all potentially relevant fluctuating (order parameter) fields (e.g. by Hubbard-Strat. trafo)

↳ use OP fields to decouple 4-fermion interaction terms (AFM, SC, ...)

↳ obtain a set of terms containing <u>two fermions</u> and <u>one OP fluctuating field</u> $\rightsquigarrow$ three legs

↳ compute renormalization of "three-legged" vertices

↳ obtain susceptibilities in various channels $\rightsquigarrow$ check which one is strongest!

$\Rightarrow$ identify <u>leading instability</u>

▷ <u>Example: superconducting / pairing vertex</u>

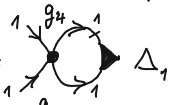
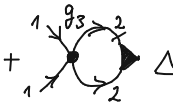
$$\delta V = \Delta_1 c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger + \Delta_1^* c_{1\uparrow} c_{1\downarrow} + \Delta_2 c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger + \Delta_2^* c_{2\uparrow} c_{2\downarrow}$$

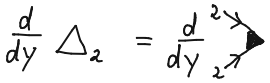
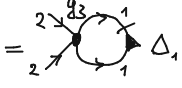
↳ here $c_i^{(\dagger)}$ is a fermion creation/annihilation operator at patch $i \in \{1,2\}$

↳ δV can be used to decouple the following part of the interaction vertex V

$$V' = g_4 (c_1^\dagger c_1^\dagger c_1 c_1 + c_2^\dagger c_2^\dagger c_2 c_2) + g_3 (c_1^\dagger c_1^\dagger c_2 c_2 + c_2^\dagger c_2^\dagger c_1 c_1)$$

↳ in RG, the Δ_i obtain 1-loop renormalization from diagrams:

$$\frac{d}{dy}\Delta_1 = \frac{d}{dy}$$  $$= \Delta_1$$  $$+ \Delta_2 = -\Delta_1 g_4 - \Delta_2 g_3$$

$$\frac{d}{dy}\Delta_2 = \frac{d}{dy}$$  $$= \Delta_1$$  $$+ \Delta_2 = -\Delta_1 g_3 - \Delta_2 g_4$$

↳ introduce $\Delta_+ = \Delta_1 + \Delta_2$ and $\Delta_- = \Delta_1 - \Delta_2$

$$\Rightarrow \frac{d}{dy}\Delta_+ = (g_4 + g_3)\Delta_+ \quad \text{and} \quad \frac{d}{dy}\Delta_- = (g_4 - g_3)\Delta_-$$

↳ with (4-20): $\Delta_+ \propto \frac{1}{(y_c - y)^{-g_3^0 - g_4^0}}$ and $\boxed{\Delta_- \propto \frac{1}{(y_c - y)^{\alpha_-}} \text{ with } \alpha_- = g_3^0 - g_4^0}$ (4-23)

▷ same procedure can be followed for AFM vertex

↳ $\frac{d}{dy}\vec{m}_{AFM} = d_1(y)(g_2 + g_3)\vec{m}_{AFM} \Rightarrow \boxed{\vec{m}_{AFM} \propto \frac{1}{(y_c - y)^{\alpha_{AFM}}} \text{ with } \alpha_{AFM} = d(y_c)(g_2^0 + g_3^0)}$ (4-24)

▷ situation at perfect nesting ($d(y_c) = 1$) ↝ use (4-21) and (4-22):

↳ $\alpha_- = g_3^0 - g_4^0 = \frac{\sqrt{5}}{6} + \frac{1}{6} = \frac{1+\sqrt{5}}{6} \approx 0.539$

↳ $\alpha_{AFM} = g_2^0 + g_3^0 = \frac{1}{6} + \frac{\sqrt{5}}{6} = \frac{1+\sqrt{5}}{6} \approx 0.539$

} divergences / instabilities of Δ_- and Δ_{AFM} are equally strong!

↳ subleading terms in (4-17) decide over leading instability! ↝ favor AFM

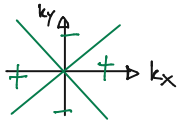
▷ situation away from perfect nesting ($d(y_c) < 1$)

↳ simple numerical evaluation of (4-21) with fixed $d(y_c) < 1$ gives: $\boxed{\alpha_- > \alpha_{AFM}}$ (4-25)

⇒ away from perfect nesting the pairing instability $\sim \Delta_-$ is stronger than AFM!

↳ the pairing field corresponding to Δ_- has opposite signs on patches 1 (X) and 2 (Y)

↳ this is in contrast to a conventional superconducting order parameter (Δ_+)

⇒ unconventional superconductivity with d-wave symmetry 

↝ the leading instability away from perfect nesting is a

d-wave SC instability

4.4.5. Summary

▷ the interaction starts out as repulsive ($g_i \sim U > 0$), but g_4 change sign at some scale γ_0

↳ system self-generates attractive pairing

↳ $\hat{L}_{PH}(Q)$-term in $\dot{g}_3$ is needed for that to push g_3 up!

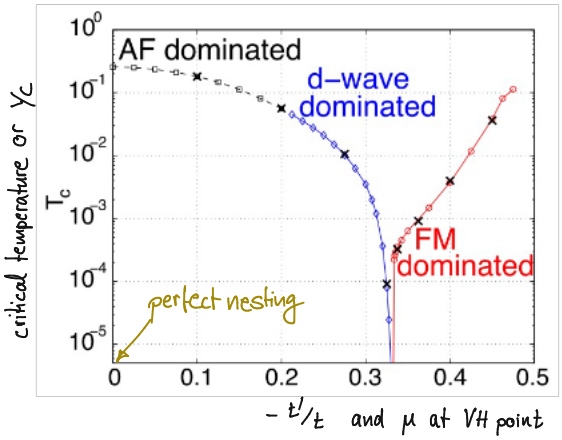
▷ both AFM and SC vertices diverge at γ_c : div $\sim \frac{1}{(\gamma_c - \gamma)^\alpha}$

↳ leading instability is the one with larger exponent α

↳ away from perfect nesting $\alpha_- > \alpha_{AFM}$

4.4.6. Outlook

▷ numerical solution of RG flow equations (4-16) yields a more detailed "phase diagram" of the t-t'-μ Hubbard model:



Honerkamp & Salmhofer PRL 87, 187004 (2001)

▷ applicable to different lattices, band structures, interactions, ...

↳ e.g., honeycomb models (graphene, ...)