

§5. Fermion

* BCS theory of superconductivity

$$\hat{H} = \sum_{\vec{k}, \sigma} \varepsilon_{\vec{k}} \hat{c}_{\vec{k}, \sigma}^+ \hat{c}_{\vec{k}, \sigma} - \frac{g}{V} \sum_{\vec{k}, \vec{k}'} \hat{c}_{\vec{k}, \uparrow}^+ \hat{c}_{-\vec{k}, \downarrow}^+ \hat{c}_{-\vec{k}', \downarrow} \hat{c}_{\vec{k}', \uparrow}$$

↓
energy band

$g > 0$: attractive interaction

$g < 0$: repulsive interaction

$$\begin{aligned} Z &= \text{Tr} e^{-\beta \hat{H}} \\ &= \int \prod_{\eta(\tau=0)} d\bar{\eta} d\eta e^{-S[\bar{\eta}, \eta]} \end{aligned}$$

$\eta(\tau=0) = \eta(\tau=\beta)$
 $\bar{\eta}(\tau=0) = \bar{\eta}(\tau=\beta)$

$$S[\bar{\eta}, \eta] = \int_0^\beta d\tau \left[\sum_{\vec{k}} \bar{\eta}_{\vec{k}, \sigma} (\omega_\tau + \varepsilon_{\vec{k}}) \eta_{\vec{k}, \sigma} - \frac{g}{V} \sum_{\vec{k}, \vec{k}'} \bar{\eta}_{\vec{k}, \uparrow} \bar{\eta}_{-\vec{k}, \downarrow} \eta_{-\vec{k}', \downarrow} \eta_{\vec{k}', \uparrow} \right]$$

- Gaussian integration for Grassmann variables:

$$\int_{\ell=1}^N d\bar{\eta}_\ell d\eta_\ell e^{-\sum_{i,j=1}^N \bar{\eta}_i A_{ij} \eta_j} = \det A$$

$\bar{\eta}^T A \eta$, $\eta = \begin{pmatrix} \eta_1 \\ \eta_2 \\ \vdots \\ \eta_N \end{pmatrix}$

Warm-up:

$$\int d\bar{\eta} d\eta \bar{\eta}\eta = \frac{d}{d\bar{\eta}} \frac{d}{d\eta} \bar{\eta}\eta = 1$$

$$\int d\bar{\eta}_1 d\eta_1 \cdots d\bar{\eta}_{N-1} d\eta_{N-1} d\bar{\eta}_N d\eta_N \bar{\eta}_N \bar{\eta}_{N-1} \bar{\eta}_{N-1} \cdots \bar{\eta}_1 \bar{\eta}_1 = 1$$

Proof of the Gaussian integration formula:

$$LHS = \int \prod_{\ell=1}^N d\bar{\eta}_\ell d\eta_\ell \prod_{i,j=1}^N e^{-\bar{\eta}_i A_{ij} \eta_j} \quad \begin{matrix} \text{Quadratic terms of} \\ \text{Grassmann numbers} \\ \text{mutually commute.} \end{matrix}$$

$$1 - \bar{\eta}_i A_{ij} \eta_j \quad \Leftarrow \bar{\eta}^2 = \eta^2 = 0$$

$$= \int \prod_{\ell=1}^N d\bar{\eta}_\ell d\eta_\ell \prod_{i,j=1}^N (1 + \eta_j \underbrace{A_{ji}^\top \bar{\eta}_i}_{\equiv A_{ij}}) \quad \Leftarrow \eta_j \bar{\eta}_i = -\bar{\eta}_i \eta_j$$

$$= \int \prod_{\ell=1}^N d\bar{\eta}_\ell d\eta_\ell \prod_{i,j=1}^N (1 + \eta_i A_{ij}^\top \bar{\eta}_j) \quad \Leftarrow i \leftrightarrow j$$

collect terms $\propto \eta_1 \bar{\eta}_1 \eta_2 \bar{\eta}_2 \cdots \eta_N \bar{\eta}_N$,
 other terms vanish after integration!

$$= \int \prod_{\ell=1}^N d\bar{\eta}_\ell d\eta_\ell \sum_{j_1+j_2+\dots+j_N} (\eta_1 A_{1j_1}^\top \bar{\eta}_{j_1}) (\eta_2 A_{2j_2}^\top \bar{\eta}_{j_2}) \cdots$$

$\{j\}$ must be a permutation of $\{1, 2, \dots, N\}$. $\times \cdots \times (\eta_N A_{Nj_N}^\top \bar{\eta}_{j_N})$

$$= \int \underbrace{\prod_{i=1}^N d\bar{\eta}_i d\eta_i}_{\text{d}\bar{\eta}_N d\eta_N \dots d\bar{\eta}_1 d\eta_1} \sum_{\sigma: \text{all permutations of } \{1, 2, \dots, N\}} \underbrace{\operatorname{sgn}(\{\sigma\}) A_{1\sigma_1}^T A_{2\sigma_2}^T \dots A_{N\sigma_N}^T}_{\times \eta_1 \bar{\eta}_1 \eta_2 \bar{\eta}_2 \dots \eta_N \bar{\eta}_N}$$

$$\operatorname{sgn}(\{\sigma\}) = \pm 1$$

signature of the permutation, due to the rearrangement of Grassmann numbers.

$$= \sum_{\sigma \in S_N} \operatorname{sgn}(\{\sigma\}) A_{1\sigma_1}^T A_{2\sigma_2}^T \dots A_{N\sigma_N}^T$$

$$= \det A^T$$

$$= \text{RHS} \quad \text{Q.E.D.}$$

Reminder: Gaussian integration for c-numbers (bosons)

$$\int \prod_{l=1}^N dz_l^* dz_l e^{-\sum_{i,j=1}^N z_i^* A_{ij} z_j} = \frac{1}{\det A}$$

For Hermitian A , the eigenvalues must be positive.
(ensuring convergence of Gaussian integration)

No such constraint for Grassmann Gaussian integrations!

Example: a determinant formula

$$\int \prod_{i=1}^N d\bar{\alpha}_i d\alpha_i \prod_{j=1}^M d\bar{\beta}_j d\beta_j e^{-(\alpha^T, \beta^T) \begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}}$$

||

$$= \det \begin{pmatrix} A & B \\ C & D \end{pmatrix} \quad \begin{matrix} \leftarrow \text{use Gaussian integration formula} \\ \text{and integrate over } \alpha, \beta \text{ at the} \\ \text{same time.} \end{matrix}$$

$$= \det D \cdot \det (A - BD^{-1}C) \quad \begin{matrix} \leftarrow \text{integrate over } \beta \\ \text{by completing square} \\ \text{and then integrate} \\ \text{over } \alpha \end{matrix}$$

- Hubbard - Stratonovich (HS) transformation:

$$Z = \int D\bar{\eta} D\eta e^{-\int_0^t d\tau \left[\sum_{\vec{k}, \sigma} \bar{\eta}_{\vec{k}\sigma} (\partial_\tau + \epsilon_{\vec{k}}) \eta_{\vec{k}\sigma} - \frac{g}{V} \sum_{\vec{k}, \vec{k}'} \bar{\eta}_{\vec{k}, \uparrow} \bar{\eta}_{-\vec{k}, \downarrow} \eta_{-\vec{k}', \downarrow} \eta_{\vec{k}', \uparrow} \right]}$$

$g \neq 0$: No longer Gaussian integration!

Expanding $e^{-S[\bar{\eta}, \eta]}$ would generate exponentially many terms.
Not efficient!

Idea: decouple four-fermion interactions.

HS transformation (also called "auxiliary field approach").

$$\begin{aligned}
 & e^{\int_0^\beta d\tau \frac{g}{V} \sum_{\vec{k},\vec{R}} \bar{\eta}_{\vec{k},\uparrow} \bar{\eta}_{-\vec{k},\downarrow} \eta_{-\vec{R},\downarrow} \eta_{\vec{R},\uparrow}} \\
 & \times \underbrace{\int D\Delta^* D\Delta e^{-\int_0^\beta d\tau \frac{V}{g} (\bar{\Delta} + \frac{g}{V} \sum_{\vec{k}} \bar{\eta}_{\vec{k},\uparrow} \bar{\eta}_{-\vec{k},\downarrow}) (\Delta + \frac{g}{V} \sum_{\vec{k}} \eta_{-\vec{k},\downarrow} \eta_{\vec{k},\uparrow})}}_{\text{Const. } [\Delta^*(\tau) \text{ and } \Delta(\tau) \text{ are complex c-number fields.}]} \\
 & = \int D\Delta^* D\Delta e^{-\int_0^\beta d\tau \left[\frac{V}{g} |\Delta|^2 + \sum_{\vec{k}} (\Delta \bar{\eta}_{\vec{k},\uparrow} \bar{\eta}_{-\vec{k},\downarrow} + \Delta^* \eta_{-\vec{k},\downarrow} \eta_{\vec{k},\uparrow}) \right]}
 \end{aligned}$$

$$\Rightarrow Z = \int D\bar{\eta} D\eta D\Delta^* D\Delta e^{-S[\bar{\eta}, \eta, \Delta^*, \Delta]}$$

$$\begin{aligned}
 S[\bar{\eta}, \eta, \Delta^*, \Delta] = & \int_0^\beta d\tau \left[\sum_{\vec{k},\sigma} \bar{\eta}_{\vec{k},\sigma} (\bar{\epsilon}_\tau + \sum_{\vec{R}}) \eta_{\vec{R},\sigma} + \frac{V}{g} |\Delta|^2 \right. \\
 & \left. + \sum_{\vec{k}} (\Delta \bar{\eta}_{\vec{k},\uparrow} \bar{\eta}_{-\vec{k},\downarrow} + \Delta^* \eta_{-\vec{k},\downarrow} \eta_{\vec{k},\uparrow}) \right]
 \end{aligned}$$

Four-fermion interaction disappears.

The price we pay is the additional function integral over c-number fields $\Delta^*(\tau)$ and $\Delta(\tau)$.

One could use Gaussian integration formula to

$$\text{integrate over } \bar{\eta} \text{ and } \eta \Rightarrow Z = \int D\Delta^* D\Delta e^{-S_{\text{eff}}[\Delta^*, \Delta]}$$

For $S_{\text{eff}}[\Delta^*, \Delta]$, one may consider saddle-point solution
(mean-field theory) : (need justification!)

$$\begin{aligned} \Delta^*(\tau) &\rightarrow \Delta^* & \text{semiclassical:} \\ \Delta(\tau) &\rightarrow \Delta & \delta S_{\text{eff}}[\Delta^*, \Delta] = 0 \end{aligned}$$

If fermions were not integrated over, the saddle-point approximation yields

$$Z \simeq \int d\bar{\eta} D\eta e^{-\int_0^B d\tau \left[\sum_{\vec{k},\sigma} \bar{\eta}_{\vec{k},\sigma} (\epsilon_\tau + \varepsilon_{\vec{k}}) \eta_{\vec{k},\sigma} + \frac{V}{g} |\Delta|^2 \right.} \\ \left. + \sum_{\vec{k}} (\Delta \bar{\eta}_{\vec{k},\uparrow} \bar{\eta}_{-\vec{k},\downarrow} + \Delta^* \eta_{-\vec{k},\downarrow} \eta_{\vec{k},\uparrow}) \right]}$$

Δ and Δ^* have no τ -dependence now,
but their value have to be determined self-consistently,
i.e. minimize free-energy (ground-state energy)
for $T > 0$ ($T = 0$) [variational method]

Corresponding Hamiltonian :

$$\hat{H}_{\text{MF}} = \sum_{\vec{k},\sigma} \varepsilon_{\vec{k}} \hat{C}_{\vec{k}\sigma}^\dagger \hat{C}_{\vec{k}\sigma} + \sum_{\vec{k}} (\Delta \hat{C}_{\vec{k},\uparrow}^\dagger \hat{C}_{-\vec{k},\downarrow}^\dagger + \Delta^* \hat{C}_{-\vec{k},\downarrow} \hat{C}_{\vec{k},\uparrow})$$

"mean-field" $+ \frac{V}{g} |\Delta|^2$ ↑
BCS mean-field Hamiltonian

The BCS Hamiltonian can be diagonalize by using the Bogoliubov transformation. Below we do it by introducing the Nambu spinor:

$$\hat{H}_{MF} = \sum_{\vec{k}} \left(\begin{array}{cc} \hat{c}_{\vec{k}\uparrow}^+ & \hat{c}_{-\vec{k}\downarrow}^- \end{array} \right) \left(\begin{array}{cc} \varepsilon_{\vec{k}} & \Delta \\ \Delta^* & -\varepsilon_{\vec{k}} \end{array} \right) \left(\begin{array}{c} \hat{c}_{\vec{k},\uparrow} \\ \hat{c}_{-\vec{k}}^+ \end{array} \right) + \frac{V}{g} |\Delta|^2 + \sum_{\vec{k}} \varepsilon_{\vec{k}}$$

$\hat{\psi}_{\vec{k}}^+ \quad \varepsilon_{\vec{k}} = \varepsilon_{-\vec{k}} \text{ assumed} \quad \hat{\psi}_{\vec{k}}$
(reflection symmetry)

// const.

Nambu spinor $\hat{\psi}_{\vec{k}} = \begin{pmatrix} \hat{c}_{\vec{k},\uparrow} \\ \hat{c}_{-\vec{k},\downarrow}^+ \end{pmatrix}$

$$\{\hat{\psi}_{\vec{k},\nu}, \hat{\psi}_{\vec{k}',\nu'}^+\} = \delta_{\vec{k},\vec{k}'} \delta_{\nu,\nu'} \quad (\nu=1,2)$$

standard fermionic commutation relation!

$$\Rightarrow \hat{H}_{MF} = \sum_{\vec{k}} \hat{\psi}_{\vec{k}}^+ U_{\vec{k}}^+ U_{\vec{k}} \left(\begin{array}{cc} \varepsilon_{\vec{k}} & \Delta \\ \Delta^* & -\varepsilon_{\vec{k}} \end{array} \right) U_{\vec{k}}^+ U_{\vec{k}} \hat{\psi}_{\vec{k}} + \frac{V}{g} |\Delta|^2$$

$I_{2 \times 2} \quad \hat{\psi}'_{\vec{k}} \text{ (new Nambu spinor)}$

$$U_{\vec{k}} = \begin{pmatrix} U_{\vec{k}} & V_{\vec{k}} \\ -V_{\vec{k}}^* & U_{\vec{k}} \end{pmatrix}, \quad E_{\vec{k}} = \sqrt{\varepsilon_{\vec{k}}^2 + |\Delta|^2}$$

unitary matrix $U_{\vec{k}} = \begin{pmatrix} U_{\vec{k}} & V_{\vec{k}} \\ -V_{\vec{k}}^* & U_{\vec{k}} \end{pmatrix}, \quad U_{\vec{k}} = \sqrt{\frac{1}{2}} \left(1 + \frac{\varepsilon_{\vec{k}}}{E_{\vec{k}}} \right)$

$V_{\vec{k}} = \frac{\Delta}{|E_{\vec{k}}|} \sqrt{\frac{1}{2} \left(1 - \frac{\varepsilon_{\vec{k}}}{E_{\vec{k}}} \right)}$

"BCS coherent factors"

The new Nambu spinor $\hat{\psi}'_{\vec{k}}$ also satisfy the fermionic commutation relation. It can be written as

$$\begin{aligned}\hat{\psi}'_{\vec{k}} &= \begin{pmatrix} \hat{\alpha}_{\vec{k}} \\ \hat{\beta}_{\vec{k}} \end{pmatrix} & \hat{\alpha}_{\vec{k}} \text{ & } \hat{\beta}_{\vec{k}} : \text{ standard fermionic annihilation operators} \\ &= U_{\vec{k}} \hat{\psi}_{\vec{k}} \\ &= \begin{pmatrix} u_{\vec{k}} & v_{\vec{k}} \\ -v_{\vec{k}}^* & u_{\vec{k}} \end{pmatrix} \begin{pmatrix} \hat{c}_{\vec{k},\uparrow} \\ \hat{c}_{-\vec{k},\downarrow} \end{pmatrix} \\ &= \begin{pmatrix} u_{\vec{k}} \hat{c}_{\vec{k},\uparrow} + v_{\vec{k}} \hat{c}_{-\vec{k},\downarrow} \\ -v_{\vec{k}}^* \hat{c}_{\vec{k},\uparrow} + u_{\vec{k}} \hat{c}_{-\vec{k},\downarrow} \end{pmatrix} \end{aligned}$$

$\xrightarrow{\hat{\alpha}_{\vec{k}}}$

$\xrightarrow{\hat{\beta}_{\vec{k}}}$

$$\begin{aligned}\Rightarrow H_{MF} &= \sum_{\vec{k}} \hat{\psi}'_{\vec{k}}^\dagger \begin{pmatrix} E_{\vec{k}} & 0 \\ 0 & -E_{\vec{k}} \end{pmatrix} \hat{\psi}'_{\vec{k}} + \frac{V}{g} |\Delta|^2 \\ &= \sum_{\vec{k}} E_{\vec{k}} (\hat{\alpha}_{\vec{k}}^\dagger \hat{\alpha}_{\vec{k}} - \hat{\beta}_{\vec{k}}^\dagger \hat{\beta}_{\vec{k}}) + \frac{V}{g} |\Delta|^2\end{aligned}$$

BCS ground state $|BCS\rangle$: "vacuum of $\hat{\alpha}_{\vec{k}}$, full occupation of $\hat{\beta}_{\vec{k}}$ "

$\hat{\alpha}_{\vec{k}}^+$ & $\hat{\beta}_{\vec{k}}^+$ create "Bogoliubov quasiparticles" on top of $|BCS\rangle$.

How to write $|BCS\rangle$ in terms of original fermions?

$$\hat{H}_{MF} = \sum_{\vec{k}} \hat{h}_{\vec{k}}$$

$$\begin{aligned}\hat{h}_{\vec{k}} &= \varepsilon_{\vec{k}} (\hat{c}_{\vec{k},\uparrow}^+ \hat{c}_{\vec{k},\uparrow} + \hat{c}_{-\vec{k},\downarrow}^+ \hat{c}_{-\vec{k},\downarrow}) \\ &\quad + \Delta \hat{c}_{\vec{k},\uparrow}^+ \hat{c}_{-\vec{k},\downarrow} + \Delta^* \hat{c}_{-\vec{k},\downarrow}^+ \hat{c}_{\vec{k},\uparrow}\end{aligned}$$

$[\hat{h}_{\vec{k}}, \hat{h}_{\vec{k}'}] = 0$, diagonalize each $\hat{h}_{\vec{k}}$ separately

Four-dimensional Hilbert space for each \vec{k} :

$$\underbrace{|0\rangle, \hat{c}_{\vec{k},\uparrow}^+ \hat{c}_{-\vec{k},\downarrow}^+ |0\rangle}_{\text{even parity}}, \underbrace{\hat{c}_{\vec{k},\uparrow}^+ |0\rangle, \hat{c}_{-\vec{k},\downarrow}^+ |0\rangle}_{\text{odd parity}}$$

The ground state appears in even-parity subspace.

Represent $\hat{h}_{\vec{k}}$ as a 2×2 matrix in this subspace:

$$\hat{h}_{\vec{k}} \rightarrow \begin{pmatrix} 0 & \Delta^* \\ \Delta & 2\varepsilon_{\vec{k}} \end{pmatrix} \xrightarrow{\text{Diagonalize}} \Delta^* = \langle 0 | \hat{h}_{\vec{k}} | \hat{c}_{\vec{k},\uparrow}^+ \hat{c}_{-\vec{k},\downarrow}^+ | 0 \rangle$$

Diagonalize this matrix to obtain ground state of $\hat{h}_{\vec{k}}$:

$$(U_{\vec{k}} - V_{\vec{k}} \hat{c}_{\vec{k},\uparrow}^+ \hat{c}_{-\vec{k},\downarrow}^+) |0\rangle$$

So the BCS ground state of $\hat{H}_{MF} = \sum_{\vec{k}} \hat{h}_{\vec{k}}$ is

$$|BCS\rangle = \prod_{\vec{k}} (U_{\vec{k}} - V_{\vec{k}} \hat{c}_{\vec{k},\uparrow}^+ \hat{c}_{-\vec{k},\downarrow}^+) |0\rangle$$

This is "the vacuum of $\hat{\alpha}_{\vec{k}}$ and full occupation of $\hat{\beta}_{\vec{k}}$ "!