Quantum Theory of Many Particle Systems

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Contents

Preface

Overview

- An introductory course for the quantum theory of many-body systems;
- A survey of general principles and language;
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- Bridging the gap between the quantum many-body theory and real material calculations;

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Resources

There are many excellent books on the quantum theory of many-particle systems. The following is a list of the books upon which this lecture is based. They will be referred in main text/side notes by using the following abbreviations:

NO J. W. Negele and H. Orland, *Quantum Many-Particle Systems* (Addison-Wesley, 1988).
–Functional integral formalism

AS Alexander Altland and Ben D. Simons, *Condensed Matter Field Theory* (Cambridge University Press, 2010).
–Various applications in condensed matter physics

GV G. Giuliani and G. Vignale, *Quantum Theory of the Electron Liquid* (Cambridge University Press, 2005).
–Theory of the electron liquid

HJ Hartmut Haug and Antti-Pekka Jauho, *Quantum Kinetics in Transport and Optics of Semiconductors* (Springer, 2008).
–Non-equilibrium Green's function

FW A. L. Fetter and J. D. Walecka, *Quantum Theory of Many-Particle Systems* (McGraw Hill, 2003).

MH G. D. Mahan, *Many-Particle Physics* (Kluwer Academic, 2000).

FR E. Fradkin, *Field Theories of Condensed Matter Physics* (Cambridge University Press, 2013).

Acknowledgements

谭奕 typos in Eq. (1.107)

林益浩 sign errors in Eq. (2.8) and (2.9); ambiguities in the energy references of Eq. (5.24) and (5.26)

尹超 inconsistency in the fluctuation-dissipation relations; a typo in Eq. (3.29)

陆易 ϵ in Eq. (3.51) should be less than $\hbar\beta$

刘震寰 a typo in Eq. (3.12)

王法杰 a typo in Eq. (3.45)

李德馨 typos in Eq. (5.27), Eq. (7.45), and Eq. (7.144)

刘鹏飞 a typo in Eq. (5.60)

刘怡然 Eq. (6.17a) is independent of the density only for its on-shell value

张凡 a typo in Eq. (6.58)

黄鑫懿 a typo in Eq. (1.27)

娄琴剑 typos in Eq. (4.10), Eq. (7.87), Eq. (2.66), Eq. (7.148), Eq. (2.32), and Problem 4 of §4

梁靖雲 a typo in Eq. (6.89)

林织星 typos in Eq. (6.79)

胡世昕 typos in Eq. (5.43), Eq. (7.19), and Eq. (7.31)

王晨冰 a typo in Eq. (6.144)

贡晓荀 typos in Eqs. (7.106, 7.109), Eq. (7.142), Eq. (7.91), and electromagnetic units in §7.3.4

陈天扬 typos in Eq. (4.47), Eq. (5.6), and Eq. (5.92).

薛泽洋 typos in Eq. (2.49) and Eq. (6.99)

杨天骅 typos in Eq. (6.89) and Eq. (7.107)

颜子涵 typos in Eq. (6.119) and Eq. (6.131)

洪源 typo in Eq. (3.37) and margin note in §1.5

冯杰超 typos in Eqs. (4.38,5.80–5.82,5.86,6.37,6.144) and the margin note for Eq.6.15)

Chapter 1

Second quantization and coherent states

1.1 Quantum mechanics

NO§1.1

Basic concepts

- States and observables: position eigenstates $|\boldsymbol{r}\rangle$, momentum eigenstates $|\boldsymbol{p}\rangle$:

$$\hat{\boldsymbol{r}}\,|\boldsymbol{r}\rangle = \boldsymbol{r}\,|\boldsymbol{r}\rangle\,, \tag{1.1}$$
$$\hat{\boldsymbol{p}}\,|\boldsymbol{p}\rangle = \boldsymbol{p}\,|\boldsymbol{p}\rangle\,. \tag{1.2}$$

  The concept of STATE can be generalized to eigenstates of *any* observables/operators, not limited to the position/momentum. An example is the spin eigenstate:

$$\hat{s}_z\,|\pm\rangle = \pm\frac{\hbar}{2}\,|\pm\rangle\,. \tag{1.3}$$

- Hilbert space: all states with finite norms.
- Completeness (closure) relations:

$$\int \mathrm{d}\boldsymbol{r}\,|\boldsymbol{r}\rangle\,\langle\boldsymbol{r}| = 1, \tag{1.4}$$
$$\int \mathrm{d}\boldsymbol{p}\,|\boldsymbol{p}\rangle\,\langle\boldsymbol{p}| = 1, \tag{1.5}$$
$$|\psi\rangle = \int \mathrm{d}\boldsymbol{r}\,|\boldsymbol{r}\rangle\,\langle\boldsymbol{r}|\,\psi\rangle \equiv \int \mathrm{d}\boldsymbol{r}\,|\boldsymbol{r}\rangle\,\psi(\boldsymbol{r}). \tag{1.6}$$

  – Note that 1 here (with or without a subscript) denotes an identity *operator*. It is associated with a particular Hilbert space. Identity operators associated with different Hilbert spaces are *not* equal:

$$|+\rangle\,\langle+| + |-\rangle\,\langle-| = 1_{\mathrm{S}}. \tag{1.7}$$
$$1 \neq 1_{\mathrm{S}}. \tag{1.8}$$

- Overlaps between states:

$$\langle\boldsymbol{r}|\boldsymbol{r}'\rangle = \delta(\boldsymbol{r}-\boldsymbol{r}'), \tag{1.9}$$
$$\langle\boldsymbol{p}|\boldsymbol{p}'\rangle = \delta(\boldsymbol{p}-\boldsymbol{p}'), \tag{1.10}$$
$$\langle\boldsymbol{r}|\boldsymbol{p}\rangle = \left(\frac{1}{2\pi\hbar}\right)^{3/2}\exp\left(\frac{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}}{\hbar}\right). \tag{1.11}$$

Schrödinger equation

- Wave function

$$\psi(\boldsymbol{r}) \equiv \langle \boldsymbol{r} \,|\, \psi \rangle \,. \tag{1.12}$$

- Momentum operator in the position basis:

$$\langle \boldsymbol{r} \,|\hat{\boldsymbol{p}}|\, \psi \rangle = \int \mathrm{d}\boldsymbol{p} \,\langle \boldsymbol{r} \,|\, \boldsymbol{p} \rangle \,\langle \boldsymbol{p} \,|\hat{\boldsymbol{p}}|\, \psi \rangle = \left(\frac{1}{2\pi\hbar}\right)^{3/2} \int \mathrm{d}\boldsymbol{p} e^{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}/\hbar} \boldsymbol{p} \,\langle \boldsymbol{p} \,|\, \psi \rangle \tag{1.13}$$

$$= -\mathrm{i}\hbar \frac{\partial}{\partial \boldsymbol{r}} \int \mathrm{d}\boldsymbol{p} \,\langle \boldsymbol{r} \,|\, \boldsymbol{p} \rangle \,\langle \boldsymbol{p} \,|\, \psi \rangle = -\mathrm{i}\hbar \frac{\partial}{\partial \boldsymbol{r}} \,\langle \boldsymbol{r} | \,\psi \rangle \equiv -\mathrm{i}\hbar \frac{\partial \psi(\boldsymbol{r})}{\partial \boldsymbol{r}}. \tag{1.14}$$

- Schrödinger equation:

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\psi\rangle = \left[\frac{\hat{\boldsymbol{p}}^2}{2m} + V\left(\hat{\boldsymbol{r}}\right)\right] |\psi\rangle \,, \tag{1.15}$$

$$\mathrm{i}\hbar \frac{\partial \psi(\boldsymbol{r}t)}{\partial t} = \langle \boldsymbol{r}| \left[\frac{\hat{\boldsymbol{p}}^2}{2m} + V\left(\hat{\boldsymbol{r}}\right)\right] |\psi\rangle = \left[\frac{1}{2m}\left(-\mathrm{i}\hbar \frac{\partial}{\partial \boldsymbol{r}}\right)^2 + V(\boldsymbol{r})\right] \psi(\boldsymbol{r}). \tag{1.16}$$

Heisenberg and Schrödinger representations

- In the Schrödinger representation, states evolve with time:

$$|\psi(t)\rangle = e^{-\mathrm{i}\hat{H}t/\hbar} \,|\psi(0)\rangle \,. \tag{1.17}$$

- In the Heisenberg representation, operators (observables) evolve with time:

$$\hat{\boldsymbol{p}}^{(\mathrm{H})}(t) = e^{\mathrm{i}\hat{H}t/\hbar} \hat{\boldsymbol{p}} e^{-\mathrm{i}\hat{H}t/\hbar}. \tag{1.18}$$

- The two representations are equivalent:

$$\langle \psi(t) \,|\, \hat{\boldsymbol{p}} \,|\, \psi(t) \rangle = \left\langle \psi(0) \,\middle|\, e^{\mathrm{i}\hat{H}t/\hbar} \hat{\boldsymbol{p}} e^{-\mathrm{i}\hat{H}t/\hbar} \,\middle|\, \psi(0) \right\rangle \tag{1.19}$$

$$= \left\langle \psi(0) \,\middle|\, \hat{\boldsymbol{p}}^{(\mathrm{H})}(t) \,\middle|\, \psi(0) \right\rangle . \tag{1.20}$$

1.2 Quantum statistical mechanics

NO§2.1

Statistical ensembles

- Micro-canonical ensemble: fixed energy and particle number. The system is assumed to be *ergodic*.
- Canonical ensemble: fixed particle number, exchange energy with a thermal reservoir

$$\hat{\rho} \propto e^{-\beta \hat{H}}, \tag{1.21}$$

where $\beta \equiv 1/k_{\mathrm{B}}T$. Note that $e^{-\beta\hat{H}}$ could be interpreted as an imaginary-time evolution operator with $t = -\mathrm{i}\hbar\beta$:

$$e^{-\beta\hat{H}} = e^{-\mathrm{i}\hat{H}(-\mathrm{i}\hbar\beta)/\hbar}. \tag{1.22}$$

- Grand canonical ensemble: exchange both the energy and particles.

$$\hat{\rho} \propto e^{-\beta\left(\hat{H} - \mu\hat{N}\right)}. \tag{1.23}$$

$\hat{K} \equiv \hat{H} - \mu\hat{N}$ is called grand-canonical Hamiltonian.

Thermodynamic limit $N, V \to \infty$, $N/V \to \rho$.

- All three ensembles are equivalent in the thermodynamic limit .
- Except when some observable has divergent fluctuations –phase transitions and symmetry-breaking systems.

Partition function

$$Z = \mathrm{Tr} e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}.$$

Grand canonical potential

$$\Omega = -\frac{1}{\beta}\ln Z. \tag{1.24}$$

Expectation values

$$\left\langle \hat{R} \right\rangle = \mathrm{Tr}\hat{\rho}\hat{R}, \tag{1.25}$$

$$\hat{\rho} = \frac{1}{Z} e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}, \tag{1.26}$$

Thermodynamic relations can be inferred from the statistical mechanics

$$-\frac{\partial\Omega}{\partial\mu} = \frac{1}{Z}\mathrm{Tr}\hat{N}e^{-\beta\left(\hat{H}-\mu\hat{N}\right)} \equiv N, \tag{1.27}$$

$$-\frac{\partial\Omega}{\partial T} = -\frac{\Omega - \left\langle \hat{H}-\mu\hat{N} \right\rangle}{T} \equiv S, \tag{1.28}$$

$$-\frac{\partial\Omega}{\partial V} = P. \tag{1.29}$$

Note that in the thermodynamic limit, Ω must be proportional to V. Therefore $\Omega = -PV$.

1.3 Identical particles

NO§1.2

The quantum mechanics can be generalized for many-particle systems.

Product states can be constructed from orthonormal single particle states $|\alpha\rangle$:

$$|\alpha_1 \ldots \alpha_N) \equiv |\alpha_1\rangle \otimes |\alpha_2\rangle \otimes \cdots \otimes |\alpha_N\rangle\,. \tag{1.30}$$

Note that we use $|)$ to denote the product states.

Overlap between product states:

$$(\alpha_1 \ldots \alpha_N\,|\alpha'_1 \ldots \alpha'_N) = \langle\alpha_1\,|\,\alpha'_1\rangle\,\langle\alpha_2\,|\,\alpha'_2\rangle \ldots \langle\alpha_N\,|\,\alpha'_N\rangle\,, \tag{1.31}$$

$$\begin{aligned}\psi_{\alpha_1\ldots\alpha_N}(\boldsymbol{r}_1 \ldots \boldsymbol{r}_N) &\equiv (\boldsymbol{r}_1 \ldots \boldsymbol{r}_N\,|\alpha_1 \ldots \alpha_N) \\ &= \psi_{\alpha_1}(\boldsymbol{r}_1)\psi_{\alpha_2}(\boldsymbol{r}_2)\ldots\psi_{\alpha_N}(\boldsymbol{r}_N).\end{aligned} \tag{1.32}$$

Closure relation

$$\sum_{\alpha_1\ldots\alpha_N} |\alpha_1 \ldots \alpha_N)\,(\alpha_1 \ldots \alpha_N| = 1. \tag{1.33}$$

Exchange symmetry

Only totally symmetric (Bosons) and anti-symmetric states (Fermions) are observed in nature:

$$\psi\left(\boldsymbol{r}_{P1}, \boldsymbol{r}_{P2}, \ldots, \boldsymbol{r}_{PN}\right) = \psi\left(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N\right) \quad \text{(Bosons)}, \tag{1.34}$$

$$\psi\left(\boldsymbol{r}_{P1}, \boldsymbol{r}_{P2}, \ldots, \boldsymbol{r}_{PN}\right) = (-1)^P \psi\left(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N\right) \quad \text{(Fermions)}. \tag{1.35}$$

Statistics theorem: Bosons (Fermions) have integer (half-integer) spins.

Normalize symmetrized states are constructed from the product states by applying symmetrizations:

$$\hat{\mathcal{P}}\psi\left(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N\right) = \frac{1}{N!}\sum_P \zeta^P \psi\left(\boldsymbol{r}_{P1}, \boldsymbol{r}_{P2}, \ldots, \boldsymbol{r}_{PN}\right), \tag{1.36}$$

$$|\alpha_1 \ldots \alpha_N\rangle = \sqrt{\frac{N!}{\prod_\alpha n_\alpha!}}\hat{\mathcal{P}}\,|\alpha_1 \ldots \alpha_N)\,, \tag{1.37}$$

$$\psi^{\mathrm{Sym.}}_{\alpha_1\ldots\alpha_N}(\boldsymbol{r}_1 \ldots \boldsymbol{r}_N) = \frac{1}{\sqrt{N!\prod_\alpha n_\alpha!}}\sum_P \zeta^P \psi_{\alpha_1}(\boldsymbol{r}_{P1})\psi_{\alpha_2}(\boldsymbol{r}_{P2})\ldots\psi_{\alpha_N}(\boldsymbol{r}_{PN}) \tag{1.38}$$

where we introduce the symbol

$$\zeta = \begin{cases} 1 & \text{(Bosons)} \\ -1 & \text{(Fermions)} \end{cases}. \tag{1.39}$$

Note that $\hat{\mathcal{P}}$ is a projection operator:

$$\hat{\mathcal{P}}^2 = \hat{\mathcal{P}}. \tag{1.40}$$

Overlap

$$\langle \beta_1 \cdots \beta_N | \alpha_1 \cdots \alpha_N \rangle = \frac{1}{\sqrt{\prod_\beta n_\beta! \prod_\alpha n_\alpha!}} S\left(\langle \beta_i | \alpha_j \rangle\right), \tag{1.41}$$

where S is a permanent or determinant for Bosons and Fermions, respectively, defined by

$$\mathrm{Per}\,(M) = \sum_P M_{1,P1} M_{2,P2} \ldots M_{N,PN}, \tag{1.42}$$

$$\det(M) = \sum_P (-1)^P M_{1,P1} M_{2,P2} \ldots M_{N,PN}. \tag{1.43}$$

Closure relation can be obtained from Eq. (1.33) by applying the projection $\hat{\mathcal{P}}$:

$$\sum_{\alpha_1 \ldots \alpha_N} \hat{\mathcal{P}} \left|\alpha_1 \ldots \alpha_N\right\rangle \left(\alpha_1 \ldots \alpha_N\right| \hat{\mathcal{P}} = \hat{\mathcal{P}}. \tag{1.44}$$

$$\sum_{\alpha_1 \ldots \alpha_N} \frac{\prod_\alpha n_\alpha!}{N!} \left|\alpha_1 \ldots \alpha_N\right\rangle \left\langle \alpha_1 \ldots \alpha_N\right| = 1_{\mathrm{P}}, \tag{1.45}$$

where $1_{\mathrm{P}} \equiv \hat{\mathcal{P}}$ is the identity operator of the projected space.

1.4 Creation and annihilation operators

1.4.1 Basics

NO§1.4

Creation operator adds a particle

$$a_\alpha^\dagger \left|\alpha_1 \ldots \alpha_N\right\rangle = \sqrt{n_\alpha + 1} \left|\alpha \alpha_1 \ldots \alpha_N\right\rangle, \text{(Boson)}, \tag{1.46}$$

$$a_\alpha^\dagger \left|\alpha_1 \ldots \alpha_N\right\rangle = \begin{cases} \left|\alpha \alpha_1 \ldots \alpha_N\right\rangle & \alpha \notin \{\alpha_1, \ldots, \alpha_N\} \\ 0 & \alpha \in \{\alpha_1, \ldots, \alpha_N\} \end{cases}, \text{(Fermion)}. \tag{1.47}$$

Vacuum state $|0\rangle$: a state with no particle. Note that it is *not* a zero state! A symmetrized state can be created from the vacuum state by

$$\left|\alpha_1 \ldots \alpha_N\right\rangle = \frac{1}{\sqrt{\prod_\alpha n_\alpha!}} a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger \ldots a_{\alpha_N}^\dagger \left|0\right\rangle. \tag{1.48}$$

Commutation relations: the symmetry or antisymmetry properties of the many-particle states impose commutation or anticommutation relations between the creation operators:

$$\hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger - \hat{a}_\beta^\dagger \hat{a}_\alpha^\dagger \equiv [\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger]_- = 0 \,\text{(Bosons)} \tag{1.49}$$

$$\hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger + \hat{a}_\beta^\dagger \hat{a}_\alpha^\dagger \equiv [\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger]_+ = 0 \,\text{(Fermions)} \tag{1.50}$$

Fock space: the creation operator changes the number of particles. Therefore, the space of all states should include all Hilbert spaces with different numbers of particles:

$$\mathcal{B} = \mathcal{B}_0 \oplus \mathcal{B}_1 \oplus \ldots, \tag{1.51}$$

$$\mathcal{F} = \mathcal{F}_0 \oplus \mathcal{F}_1 \oplus \ldots. \tag{1.52}$$

Closure relations: (1.45)

$$|0\rangle\langle 0| + \sum_{N=1}^{\infty} \sum_{\alpha_1 \ldots \alpha_N} \frac{\prod_\alpha n_\alpha!}{N!} |\alpha_1 \ldots \alpha_N\rangle\langle \alpha_1 \ldots \alpha_N| = 1. \tag{1.53}$$

Annihilation operator a_α is the adjoint of $a_\alpha^\dagger$, and removes a particle:

$$a_\alpha |\alpha_1 \ldots \alpha_N\rangle = \frac{1}{\sqrt{n_\alpha}} \sum_{i=1}^{N} \zeta^{i-1} \delta_{\alpha,\alpha_i} |\alpha_1 \ldots \alpha_{i-1}\alpha_{i+1} \ldots \alpha_N\rangle . \tag{1.54}$$

Commutator between the creation and annihilation operators is NO *p.* 14

$$[a_\alpha, a_\beta^\dagger]_- \equiv a_\alpha a_\beta^\dagger - a_\beta^\dagger a_\alpha = \delta_{\alpha\beta}, \text{(Bosons)} \tag{1.55}$$

$$[a_\alpha, a_\beta^\dagger]_+ \equiv a_\alpha a_\beta^\dagger + a_\beta^\dagger a_\alpha = \delta_{\alpha\beta}. \text{(Fermions)} \tag{1.56}$$

Number representation labels states with the numbers of particles occupying single-particle states:

$$|\alpha_1 \ldots \alpha_N\rangle \Rightarrow |n_{\alpha_1} n_{\alpha_2} \ldots\rangle , \tag{1.57}$$

- Bosons:

$$a_{\alpha_i} |n_{\alpha_1} n_{\alpha_2} \ldots\rangle = \sqrt{n_{\alpha_i}}\, |n_{\alpha_1} n_{\alpha_2} \ldots (n_{\alpha_i} - 1) \ldots\rangle , \tag{1.58}$$

$$a_{\alpha_i}^\dagger |n_{\alpha_1} n_{\alpha_2} \ldots\rangle = \sqrt{n_{\alpha_i} + 1}\, |n_{\alpha_1} n_{\alpha_2} \ldots (n_{\alpha_i} + 1) \ldots\rangle . \tag{1.59}$$

- Fermions

$$a_{\alpha_i} |n_{\alpha_1} n_{\alpha_2} \ldots\rangle = \begin{cases} (-1)^{\sum_{j=1}^{i-1} n_{\alpha_j}} |n_{\alpha_1} n_{\alpha_2} \ldots (n_{\alpha_i} \to 0) \ldots\rangle & n_{\alpha_i} = 1 \\ 0 & n_{\alpha_i} = 0 \end{cases}, \tag{1.60}$$

$$a_{\alpha_i}^\dagger |n_{\alpha_1} n_{\alpha_2} \ldots\rangle = \begin{cases} (-1)^{\sum_{j=1}^{i-1} n_{\alpha_j}} |n_{\alpha_1} n_{\alpha_2} \ldots (n_{\alpha_i} \to 1) \ldots\rangle & n_{\alpha_i} = 0 \\ 0 & n_{\alpha_i} = 1 \end{cases}. \tag{1.61}$$

Basis transformation: The creation/annihilation operators with respect to two bases $|\alpha\rangle$ and $|\tilde{\alpha}\rangle$ are related by:

$$\hat{a}_{\tilde{\alpha}}^\dagger = \sum_\alpha \langle \alpha \,|\, \tilde{\alpha}\rangle\, \hat{a}_\alpha^\dagger, \tag{1.62}$$

$$\hat{a}_{\tilde{\alpha}} = \sum_\alpha \langle \tilde{\alpha} \,|\, \alpha\rangle\, \hat{a}_\alpha. \tag{1.63}$$

Field operators are creation/annihilation operators in the position basis:

$$\hat{\psi}(\boldsymbol{r}) = \sum_\alpha \phi_\alpha(\boldsymbol{r}) \hat{a}_\alpha. \tag{1.64}$$

It is obtained by setting $|\tilde{\alpha}\rangle = |\boldsymbol{r}\rangle$.

$$[\hat{\psi}(\boldsymbol{r}), \hat{\psi}(\boldsymbol{r}')]_{-\zeta} = [\hat{\psi}^\dagger(\boldsymbol{r}), \hat{\psi}^\dagger(\boldsymbol{r}')]_{-\zeta} = 0, \tag{1.65}$$

$$[\hat{\psi}(\boldsymbol{r}), \hat{\psi}^\dagger(\boldsymbol{r}')]_{-\zeta} = \delta(\boldsymbol{r} - \boldsymbol{r}'). \tag{1.66}$$

Second quantization expresses a physical quantity in terms of the creation and annihilation operators:

Number operator:

$$\hat{n}_\alpha = a_\alpha^\dagger a_\alpha. \tag{1.67}$$

One-body operator $\hat{U} = \sum_i \hat{u}_i$:

$$\hat{U} = \sum_{\alpha\beta} \langle \alpha \,|\, \hat{u} \,|\, \beta\rangle\, a_\alpha^\dagger a_\beta. \tag{1.68}$$

Proof

- We choose the eigenstates of $\hat{u}_i$ as the single-particle basis:

$$\hat{u}\,|u\rangle = u\,|u\rangle\,. \tag{1.69}$$

- We can calculate a general matrix element:

$$\left\langle u'_1 \dots u'_N \middle| \hat{U} \middle| u_1 \dots u_N \right\rangle = \left(\sum_i u_i\right) \langle u'_1 \dots u'_N \,|\, u_1 \dots u_N\rangle \tag{1.70}$$

$$= \left(\sum_u n_u u\right) \langle u'_1 \dots u'_N \,|\, u_1 \dots u_N\rangle\,. \tag{1.71}$$

- Therefore

$$\hat{U} = \sum_u \langle u \,|\, \hat{u} \,|\, u\rangle\, \hat{n}_u = \sum_u \langle u \,|\, \hat{u} \,|\, u\rangle\, \hat{a}^\dagger_u a_u. \tag{1.72}$$

- Transform from the diagonal basis to a general basis by applying Eqs. (1.62, 1.63).

Kinetic energy and single-body potential

$$\hat{T} = -\frac{\hbar^2}{2m} \int \mathrm{d}\boldsymbol{r} \hat{\psi}^\dagger(\boldsymbol{r}) \nabla^2 \hat{\psi}(\boldsymbol{r}), \tag{1.73}$$

$$\hat{U} = \int \mathrm{d}\boldsymbol{r} U\,(\boldsymbol{r})\, \hat{\psi}^\dagger(\boldsymbol{r}) \hat{\psi}(\boldsymbol{r}). \tag{1.74}$$

Two-body operator $\hat{V} = (1/2)\sum_{ij} \hat{v}_{ij}$:

$$\hat{V} = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} (\alpha\beta\,|\hat{v}|\,\gamma\delta)\, a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma. \tag{1.75}$$

Note the order of the state indexes, and that the matrix element is calculated with product states instead of symmetrized states.

Proof

- We assume that a two-body operator $\hat{V}$ may be diagonalized in product states:

$$\hat{v}\,|\alpha\beta) = v_{\alpha\beta}\,|\alpha\beta)\,. \tag{1.76}$$

- We can calculate a general matrix element:

$$\langle \alpha'_1 \dots \alpha'_N \,|\, \hat{v} \,|\, \alpha_1 \dots \alpha_N\rangle = \left(\frac{1}{2}\sum_{i\neq j} v_{\alpha_i\alpha_j}\right) \langle \alpha'_1 \dots \alpha'_N \,|\, \alpha_1 \dots \alpha_N\rangle\,. \tag{1.77}$$

- The number of times that $v_{\alpha\beta}$ appears in the summation is $n_\alpha n_\beta$ for $\alpha \neq \beta$ and $n_\alpha(n_\alpha - 1)$ for $\alpha = \beta$. We can thus define a operator to count the number:

$$\hat{P}_{\alpha\beta} = \hat{n}_\alpha \hat{n}_\beta - \delta_{\alpha\beta}\hat{n}_\alpha = \hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta \hat{a}_\beta \hat{a}_\alpha. \tag{1.78}$$

and

$$\hat{V} = \frac{1}{2}\sum_{\alpha\beta} v_{\alpha\beta}\hat{P}_{\alpha\beta}. \tag{1.79}$$

- Transform from the diagonal basis to a general basis by applying Eqs. (1.62, 1.63).

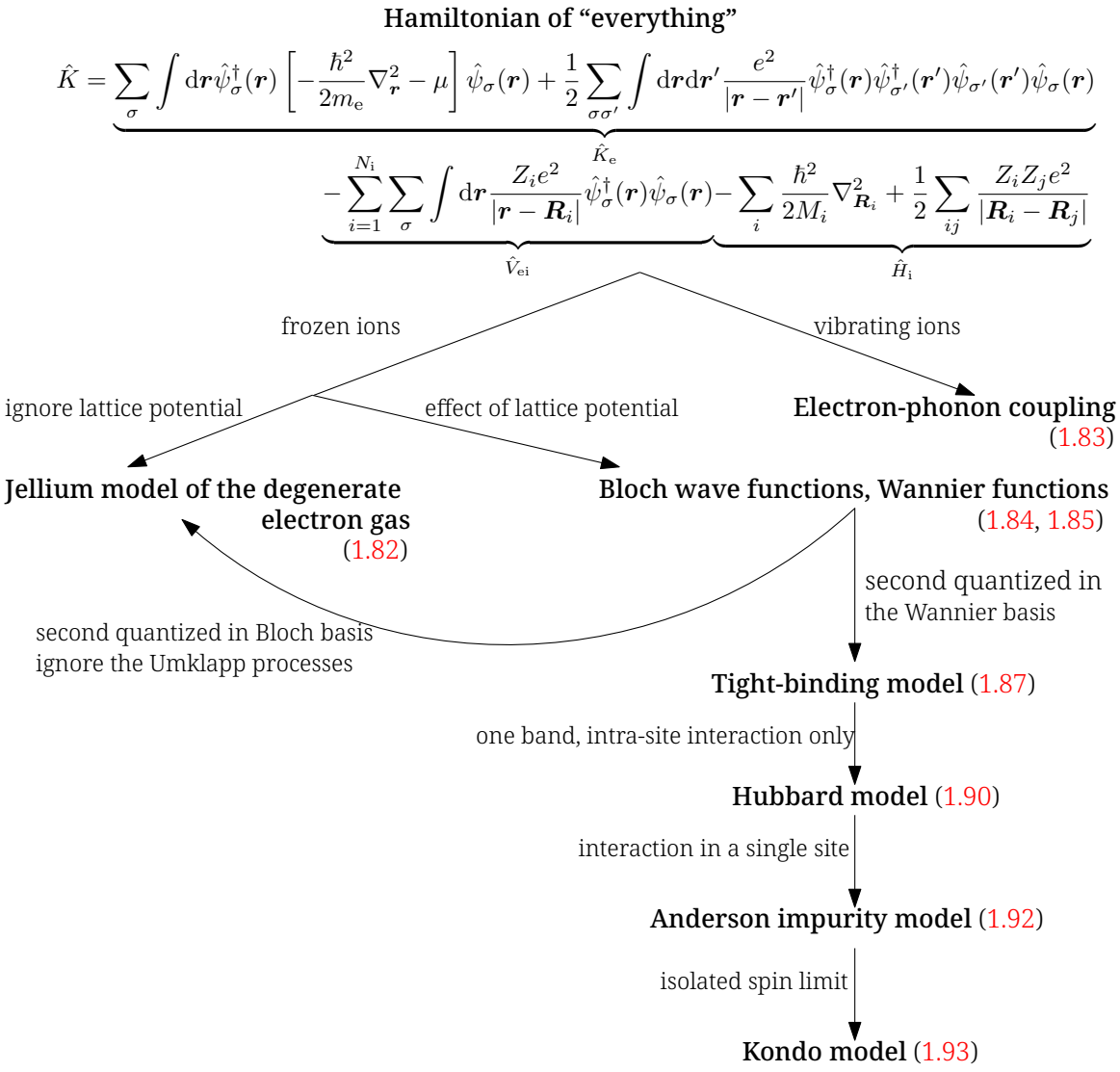
Interaction

$$\hat{V} = \frac{1}{2}\int \mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{r}' v(\boldsymbol{r}-\boldsymbol{r}')\hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}^\dagger(\boldsymbol{r}')\hat{\psi}(\boldsymbol{r}')\hat{\psi}(\boldsymbol{r}). \tag{1.80}$$

Normal ordering: all creation operators are to the left of annihilation operators.

1.4.2 Second quantized Hamiltonians

From the "Hamiltonian of everything", one can deduce various model Hamiltonians appropriate for different physical circumstances. The hierarchy of these models is shown in the following diagram:



Degenerate Electron gas FW§3

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_\sigma\int \mathrm{d}\boldsymbol{r}\hat{\psi}^\dagger_\sigma(\boldsymbol{r})\nabla^2\hat{\psi}_\sigma(\boldsymbol{r}) + \sum_\sigma\int \mathrm{d}\boldsymbol{r}V_b(\boldsymbol{r})\hat{\psi}^\dagger_\sigma(\boldsymbol{r})\hat{\psi}_\sigma(\boldsymbol{r}) + \frac{1}{2}\sum_{\sigma\sigma'}\int \mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{r}'\frac{e^2}{|\boldsymbol{r}-\boldsymbol{r}'|}\hat{\psi}^\dagger_\sigma(\boldsymbol{r})\hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}')\hat{\psi}_{\sigma'}(\boldsymbol{r}')\hat{\psi}_\sigma(\boldsymbol{r}), \quad (1.81)$$

where $V_b(\boldsymbol{r})$ denotes the potential exerted by a uniform positive charge background (jellium model). In the momentum basis $\varphi_{\boldsymbol{k}} = \mathcal{V}^{-1/2}e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}$, the Hamiltonian can be written as:

$$\hat{H} = \sum_{\boldsymbol{k}\sigma}\frac{\hbar^2k^2}{2m}\hat{a}^\dagger_{\boldsymbol{k}\sigma}\hat{a}_{\boldsymbol{k}\sigma} + \frac{e^2}{2\mathcal{V}}\sum_{\boldsymbol{q}\neq 0}\sum_{\boldsymbol{k}\sigma,\boldsymbol{p}\sigma'}\frac{4\pi}{q^2}\hat{a}^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma}\hat{a}^\dagger_{\boldsymbol{p}-\boldsymbol{q}\sigma'}\hat{a}_{\boldsymbol{p}\sigma'}\hat{a}_{\boldsymbol{k}\sigma}. \quad (1.82)$$

Note that the $\boldsymbol{q} = 0$ component of the interaction is *canceled* by the potential of the positive charge background.

Electron-phonon coupling describes the interaction between electrons and the vibrations of ions in a solid: HJ§3.1

$$\hat{H}_{\mathrm{el-ph}} = \frac{1}{\sqrt{\mathcal{V}}}\sum_{\boldsymbol{kq}} M_{\boldsymbol{q}}\hat{a}^\dagger_{\boldsymbol{k}+\boldsymbol{q}}\hat{a}_{\boldsymbol{k}}\hat{c}_{\boldsymbol{q}} + \mathrm{h.c.} \quad (1.83)$$

with $M_{\boldsymbol{q}}$ being the matrix element of the electron-phonon coupling.

Electrons in periodic potential are relevant for solids. The counterparts of the momentum basis and the position basis are the Bloch states $\varphi_{n\boldsymbol{k}}(\boldsymbol{r})$ and the Wannier states $w_n(\boldsymbol{r}-\boldsymbol{R}_i)$, respectively. They are related by:

$$w_n(\boldsymbol{r}-\boldsymbol{R}_i)=\frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}\in\text{B.Z.}} e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_i}\varphi_{n\boldsymbol{k}}(\boldsymbol{r}), \tag{1.84}$$

$$\varphi_{n\boldsymbol{k}}(\boldsymbol{r})=\frac{1}{\sqrt{N}}\sum_{\boldsymbol{R}_i} e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_i}w_n(\boldsymbol{r}-\boldsymbol{R}_i). \tag{1.85}$$

Note that the momentum conservation is modified to:

$$\boldsymbol{k}_1+\boldsymbol{k}_2=\boldsymbol{k}_1'+\boldsymbol{k}_2'+\boldsymbol{K}, \tag{1.86}$$

with a reciprocal wave-vector $\boldsymbol{K}$. It leads to the UMKLAPP scattering process when $|\boldsymbol{K}|\neq 0$.

Tight-binding models are Hamiltonians second quantized in the Wannier function basis. A general *single-band* tight-binding Hamiltonian can be written as: AS§2.2

$$\hat{H}=-\sum_{ij,\sigma}t_{ij}\hat{a}^\dagger_{i\sigma}\hat{a}_{j\sigma}+\sum_{ii'jj'}U_{ii'jj'}\hat{a}^\dagger_{i\sigma}\hat{a}^\dagger_{i'\sigma'}\hat{a}_{j'\sigma'}\hat{a}_{j\sigma}. \tag{1.87}$$

In particular, interacting terms are classified as:

Direct coupling: $U_{ii'ii'}=V_{ii'}$, and $H_U=\sum_{ii'}V_{ii'}\hat{n}_i\hat{n}_{i'}$;

Exchange coupling: $J_{ij}\equiv U_{ijji}$, and $\hat{H}_U=-2\sum_{ij}J_{ij}\left(\hat{\boldsymbol{S}}_i\cdot\hat{\boldsymbol{S}}_j+\frac{1}{4}\hat{n}_i\hat{n}_j\right)$, where $\hat{\boldsymbol{S}}_i$ is the "spin operator":

$$\hat{\boldsymbol{S}}_i=\frac{1}{2}\sum_{\sigma\sigma'}\hat{a}^\dagger_{i\sigma}\hat{\boldsymbol{\tau}}_{\sigma\sigma'}\hat{a}_{i\sigma'}, \tag{1.88}$$

with Pauli matrices

$$\hat{\tau}_x=\begin{bmatrix}0&1\\1&0\end{bmatrix},\ \hat{\tau}_y=\begin{bmatrix}0&-\mathrm{i}\\\mathrm{i}&0\end{bmatrix},\ \hat{\tau}_z=\begin{bmatrix}1&0\\0&-1\end{bmatrix}. \tag{1.89}$$

Hubbard model The single band tight-binding model with well localized atomic orbits could be approximated as: FR§2

$$\hat{H}=-t\sum_{\langle ij\rangle,\sigma}\left[\hat{a}^\dagger_{i\sigma}\hat{a}_{j\sigma}+\text{h.c.}\right]+U\sum_i\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, \tag{1.90}$$

where $\langle ij\rangle$ denotes that i and j are nearest neighbors.
The interacting part can be alternatively written as:

$$\hat{H}_U\equiv U\sum_i\hat{n}_{i\uparrow}\hat{n}_{i\downarrow}=-\frac{2U}{3}\sum_i\left|\hat{\boldsymbol{S}}_i\right|^2+\frac{N_eU}{2}, \tag{1.91}$$

Anderson impurity model describes the interaction between conduction band electrons and an impurity:

$$\hat{H}=\sum_\sigma\epsilon_f\hat{f}^\dagger_\sigma\hat{f}_\sigma+U\hat{n}_{f\uparrow}\hat{n}_{f\downarrow}+\sum_{\boldsymbol{k}\sigma}\left[V_{\boldsymbol{k}}\hat{f}^\dagger_\sigma\hat{a}_{\boldsymbol{k}\sigma}+\text{h.c.}\right]+\sum_{\boldsymbol{k}\sigma}\epsilon_{\boldsymbol{k}}\hat{a}^\dagger_{\boldsymbol{k}\sigma}\hat{a}_{\boldsymbol{k}\sigma}. \tag{1.92}$$

Kondo model describes the interaction between conduction band electrons and a local spin:

$$\hat{H}=\sum_{\boldsymbol{k}\sigma}\epsilon_{\boldsymbol{k}}\hat{a}^\dagger_{\boldsymbol{k}\sigma}\hat{a}_{\boldsymbol{k}\sigma}-J\hat{\boldsymbol{S}}^{(i)}\cdot\hat{\boldsymbol{S}}^{(e)}_0, \tag{1.93}$$

where $\hat{\boldsymbol{S}}^{(e)}_0$ denotes an electron-spin operator Eq. (1.88) at the origin. The Anderson impurity model is reduced to the Kondo model in the limit $U\to\infty$ for a deeply buried impurity. The physics of the Kondo model is the origin of correlation effects in heavy-Fermion systems. See Ref. [10].

1.5 Coherent states

NO§1.5

Coherent states are the eigenstates of the annihilation operators:

$$\hat{a}_\alpha |\phi\rangle = \phi_\alpha |\phi\rangle . \tag{1.94}$$

Note that one cannot define the eigenstates of the creation operators.

For Fermions, the eigenvalues cannot be ordinary numbers because annihilation operators anti-commute. They must be GRASSMANN NUMBERS:

$$\phi_\alpha \phi_\beta + \phi_\beta \phi_\alpha = 0. \tag{1.95}$$

1.5.1 Boson coherent states

Definition

$$|\phi\rangle = e^{\sum_\alpha \phi_\alpha a_\alpha^\dagger} |0\rangle. \tag{1.96}$$

Overlap

$$\langle\phi|\phi'\rangle = \left\langle 0 \middle| e^{\sum_\alpha \phi_\alpha^* \hat{a}_\alpha} \middle| \phi' \right\rangle = e^{\sum_\alpha \phi_\alpha^* \phi'_\alpha} \langle 0 \,|\, \phi'\rangle = \exp\left(\phi^* \cdot \phi'\right). \tag{1.97}$$

Note that coherent states do not form an orthonormal basis. Instead, they form an *over-complete* basis.

Closure relation

$$\int \mathrm{d}\mu(\phi) |\phi\rangle\langle\phi| = 1. \tag{1.98}$$

$$\mathrm{d}\mu(\phi) \equiv \prod_\alpha \frac{\mathrm{d}\phi_\alpha \mathrm{d}\phi_\alpha^*}{2\pi \mathrm{i}} e^{-\sum_\alpha |\phi_\alpha|^2} \equiv \prod_\alpha \frac{\mathrm{d}(\mathrm{Re}\phi_\alpha)\mathrm{d}(\mathrm{Im}\phi_\alpha)}{\pi} e^{-\sum_\alpha |\phi_\alpha|^2}. \tag{1.99}$$

Proof

- One can show that the right hand side of the relation commutes with all creation and annihilation operators. According to Schur's lemma, it must be proportional to the identity operator.
- To prove the commutability, one can show

$$\hat{a}_\alpha^\dagger |\phi\rangle = \hat{a}_\alpha^\dagger e^{\sum_\alpha \phi_\alpha \hat{a}_\alpha^\dagger} |0\rangle = \frac{\partial}{\partial \phi_\alpha} e^{\sum_\alpha \phi_\alpha \hat{a}_\alpha^\dagger} |0\rangle = \frac{\partial}{\partial \phi_\alpha} |\phi\rangle , \tag{1.100}$$

$$\left[\hat{a}_\alpha^\dagger,\, |\phi\rangle\langle\phi|\right] = \left(\frac{\partial}{\partial \phi_\alpha} - \phi_\alpha^*\right) |\phi\rangle\langle\phi| , \tag{1.101}$$

then inserts the relation into the integral and integrates by parts.

Trace

$$\begin{aligned} \mathrm{Tr}\hat{A} = \sum_n \left\langle n \middle| \hat{A} \middle| n \right\rangle &= \sum_n \int \mathrm{d}\mu(\phi) \langle n \,|\, \phi\rangle \left\langle \phi \middle| \hat{A} \middle| n \right\rangle \\ &= \sum_n \int \mathrm{d}\mu(\phi) \left\langle \phi \middle| \hat{A} \middle| n \right\rangle \langle n \,|\, \phi\rangle = \int \mathrm{d}\mu(\phi) \left\langle \phi \middle| \hat{A} \middle| \phi \right\rangle . \end{aligned} \tag{1.102}$$

Coherent state representation

$$|\psi\rangle = \int \mathrm{d}\mu(\phi) |\phi\rangle \langle\phi \,|\, \psi\rangle \equiv \int \mathrm{d}\mu(\phi) |\phi\rangle \psi(\phi^*), \tag{1.103}$$

where we define a wave function $\psi(\phi^*) \equiv \langle\phi|\psi\rangle$. It is an anti-holomorphic function of ϕ^*.

- All coherent states form a Segal-Bargmann space [9].

- One can set up a "Schrödinger equation" for $\psi(\phi^*)$. An application of the representation can be found in Ref. [8].

Representation of operators:

$$\hat{a}_\alpha \to \frac{\partial}{\partial \phi_\alpha^*}, \tag{1.104}$$

$$\hat{a}_\alpha^\dagger \to \phi_\alpha^*. \tag{1.105}$$

Proof

$$\left\langle \phi \left| \hat{a}_\alpha^\dagger \right| \psi \right\rangle = \phi^* \left\langle \phi \,|\, \psi \right\rangle \equiv \phi^* \psi\left(\phi^*\right), \tag{1.106}$$

$$\left\langle \phi \,|\, \hat{a}_\alpha \,|\, \psi \right\rangle = \int \mathrm{d}\mu(\phi') \left\langle \phi \,|\, \hat{a}_\alpha \,|\, \phi' \right\rangle \left\langle \phi' \,|\, \psi \right\rangle = \int \mathrm{d}\mu(\phi') \phi'_\alpha e^{\phi^* \cdot \phi'} \psi\left(\phi'^*\right) \tag{1.107}$$

$$= \frac{\partial}{\partial \phi_\alpha^*} \int \mathrm{d}\mu(\phi') e^{\phi^* \cdot \phi'} \psi\left(\phi'^*\right) = \frac{\partial \psi\left(\phi^*\right)}{\partial \phi_\alpha^*}. \tag{1.108}$$

Unit-operator: One can prove the identity

$$\psi\left(\phi'^*\right) = \int \mathrm{d}\mu(\phi) e^{\phi'^* \cdot \phi} \psi\left(\phi^*\right) \tag{1.109}$$

by appending $\langle \phi' |$ to both sides of Eq. (1.103).

Matrix-elements of *normal-ordered* operators:

$$\left\langle \phi \left| \hat{A}\left(\hat{a}^\dagger, \hat{a}\right) \right| \phi' \right\rangle = A\left(\phi^*, \phi'\right) e^{\phi^* \cdot \phi'}. \tag{1.110}$$

Average and variance of the particle number

$$\bar{N} \equiv \frac{\left\langle \phi \left| \hat{N} \right| \phi \right\rangle}{\langle \phi \,|\, \phi \rangle} = \sum_\alpha \left|\phi_\alpha\right|^2, \tag{1.111}$$

$$(\Delta N)^2 \equiv \frac{\left\langle \phi \left| \left(\hat{N} - \bar{N}\right)^2 \right| \phi \right\rangle}{\langle \phi \,|\, \phi \rangle} = \bar{N}. \tag{1.112}$$

In the limit of $\bar{N} \to \infty$, $\Delta N / \bar{N} \to 0$, a coherent state can be interpreted as a *classical field*. For instances, the coherent states of phonons correspond to classical sound waves, and the coherent states of photons correspond to classical electromagnetic fields.

1.5.2 Grassmann algebra

Grassmann algebra is defined by a set of generators $\{\xi_\alpha\}, \alpha = 1 \ldots n$ which anti-commute:

$$\xi_\alpha \xi_\beta + \xi_\beta \xi_\alpha = 0. \tag{1.113}$$

A matrix representation of Grassmann numbers requires matrices of dimension at least $2^n \times 2^n$ [1]. It is obvious:

$$\xi_\alpha^2 = 0. \tag{1.114}$$

Number in the Grassmann algebra is a linear combination with coefficients of the generators:

$$\{1, \xi_\alpha, \xi_{\alpha_1}\xi_{\alpha_2}, \ldots, \xi_{\alpha_1}\xi_{\alpha_2}\ldots\xi_{\alpha_n}\}. \tag{1.115}$$

Note that a complex number could also be regarded as a linear combination of generators $\{1, \mathrm{i}\}$.

Conjugate has properties:

$$(\xi_\alpha)^* = \xi^*_\alpha, \tag{1.116}$$
$$(\xi^*_\alpha)^* = \xi_\alpha, \tag{1.117}$$
$$(\lambda\xi_\alpha)^* = \lambda^*\xi^*_\alpha, \tag{1.118}$$
$$(\xi_{\alpha_1}\dots\xi_{\alpha_n})^* = \xi^*_{\alpha_n}\dots\xi^*_{\alpha_1}. \tag{1.119}$$

Function

$$f(\xi) = f_0 + f_1\xi, \tag{1.120}$$
$$A(\xi^*,\xi) = a_0 + a_1\xi + \bar{a}_1\xi^* + a_{12}\xi^*\xi. \tag{1.121}$$

Derivative is defined to be identical to the complex derivative, except that ∂_ξ has to be anti-commuted through until it reaches to act on ξ:

$$\frac{\partial}{\partial\xi}(\xi^*\xi) = -\xi^*. \tag{1.122}$$

Note that ∂_ξ and ∂_{ξ^*} also anti-commute.

Integral is defined by the rules:

$$\int \mathrm{d}\xi\, 1 = \int \mathrm{d}\xi^*\, 1 = 0, \tag{1.123}$$
$$\int \mathrm{d}\xi\, \xi = \int \mathrm{d}\xi^*\, \xi^* = 1. \tag{1.124}$$

- Note that $\int \mathrm{d}\xi^*\xi$ is not defined! Just treat ξ and ξ^* as two independent variables.
- Anti-commute between an integral and another integral, or an integral and a Grassmann variable.
- The integral coincides with the derivative.

Reproducing kernel (Dirac function)

$$\delta(\xi,\xi') = -(\xi-\xi'), \tag{1.125}$$
$$f(\xi) = \int \mathrm{d}\xi'\delta(\xi,\xi')f(\xi'). \tag{1.126}$$

Scalar product of Grassmann functions:

$$\langle f \mid g\rangle \equiv \int \mathrm{d}\xi^*\mathrm{d}\xi\, e^{-\xi^*\xi} f^*(\xi)g(\xi^*) \tag{1.127}$$
$$= \int \mathrm{d}\xi^*\mathrm{d}\xi\, (1-\xi^*\xi)\,(f_0^* + f_1^*\xi)\,(g_0 + g_1\xi^*) \tag{1.128}$$
$$= -\int \mathrm{d}\xi^*\mathrm{d}\xi\, \xi^*\xi f_0^* g_0 + \int \mathrm{d}\xi^*\mathrm{d}\xi\, \xi\xi^* f_1^* g_1 \tag{1.129}$$
$$= f_0^* g_0 + f_1^* g_1. \tag{1.130}$$

1.5.3 Fermion coherent states

Definition

$$|\xi\rangle = e^{-\sum_\alpha \xi_\alpha \hat{a}^\dagger_\alpha}|0\rangle = \prod_\alpha \left(1-\xi_\alpha\hat{a}^\dagger_\alpha\right)|0\rangle. \tag{1.131}$$

$$\hat{a}_\alpha|\xi\rangle = \xi_\alpha|\xi\rangle, \tag{1.132}$$
$$\langle\xi|\hat{a}^\dagger_\alpha = \langle\xi|\xi^*_\alpha, \tag{1.133}$$
$$\hat{a}^\dagger_\alpha|\xi\rangle = -\frac{\partial}{\partial\xi_\alpha}|\xi\rangle, \tag{1.134}$$
$$\langle\xi|\hat{a}_\alpha = +\frac{\partial}{\partial\xi^*_\alpha}\langle\xi|. \tag{1.135}$$

- ξ_α is a Grassmann number –The Fermion Fock space must be enlarged to define a coherent state.
- ξ, ξ^*, $\hat{a}$, and $\hat{a}^\dagger$ anti-commute, and $(\xi\hat{a})^\dagger = \hat{a}^\dagger\xi^*$.

Proof

$$\hat{a}_\alpha |\xi\rangle = \prod_{\beta\neq\alpha}\left(1-\xi_\beta\hat{a}_\beta^\dagger\right)\left(\hat{a}_\alpha+\xi_\alpha\hat{a}_\alpha\hat{a}_\alpha^\dagger\right)|0\rangle = \prod_{\beta\neq\alpha}\left(1-\xi_\beta\hat{a}_\beta^\dagger\right)\xi_\alpha|0\rangle$$
$$= \prod_{\beta\neq\alpha}\left(1-\xi_\beta\hat{a}_\beta^\dagger\right)\xi_\alpha\left(1-\xi_\alpha\hat{a}_\alpha^\dagger\right)|0\rangle = \xi_\alpha|\xi\rangle \quad (1.136)$$

$$\hat{a}_\alpha^\dagger |\xi\rangle = \prod_{\beta\neq\alpha}\left(1-\xi_\beta\hat{a}_\beta^\dagger\right)\left(\hat{a}_\alpha^\dagger+\xi_\alpha\hat{a}_\alpha^\dagger\hat{a}_\alpha^\dagger\right)|0\rangle = \prod_{\beta\neq\alpha}\left(1-\xi_\beta\hat{a}_\beta^\dagger\right)\hat{a}_\alpha^\dagger|0\rangle$$
$$= \prod_{\beta\neq\alpha}\left(1-\xi_\beta\hat{a}_\beta^\dagger\right)\left(-\frac{\partial}{\partial\xi_\alpha}\right)\left(1-\xi_\alpha\hat{a}_\alpha^\dagger\right)|0\rangle = -\frac{\partial}{\partial\xi_\alpha}|\xi\rangle \quad (1.137)$$

Overlap

$$\langle\xi\,|\,\xi'\rangle = e^{\xi^*\cdot\xi'} \quad (1.138)$$

Closure relation

$$\int\prod_\alpha \mathrm{d}\xi_\alpha^*\mathrm{d}\xi_\alpha e^{-\xi^*\cdot\xi}|\xi\rangle\langle\xi| = 1. \quad (1.139)$$

Trace of an operator:

$$\mathrm{Tr}\hat{A} = \sum_n\left\langle n\middle|\hat{A}\middle|n\right\rangle = \int\prod_\alpha \mathrm{d}\xi_\alpha^*\mathrm{d}\xi_\alpha e^{-\xi^*\cdot\xi}\sum_n\langle n\,|\,\xi\rangle\left\langle\xi\middle|\hat{A}\middle|n\right\rangle$$
$$= \int\prod_\alpha \mathrm{d}\xi_\alpha^*\mathrm{d}\xi_\alpha e^{-\xi^*\cdot\xi}\sum_n\left\langle -\xi\middle|\hat{A}\middle|n\right\rangle\langle n\,|\,\xi\rangle$$
$$\equiv \int\prod_\alpha \mathrm{d}\xi_\alpha^*\mathrm{d}\xi_\alpha e^{-\xi^*\cdot\xi}\left\langle -\xi\middle|\hat{A}\middle|\xi\right\rangle. \quad (1.140)$$

The extra minus sign is due to

$$\int \mathrm{d}\xi^*\mathrm{d}\xi\, e^{-\xi^*\cdot\xi}g(\xi)f(\xi^*) = \int \mathrm{d}\xi^*\mathrm{d}\xi\, e^{-\xi^*\cdot\xi}f(-\xi^*)g(\xi). \quad (1.141)$$

Coherent state representation

$$|\psi\rangle = \int\prod_\alpha \mathrm{d}\xi_\alpha^*\mathrm{d}\xi_\alpha e^{-\xi^*\cdot\xi}|\xi\rangle\langle\xi\,|\,\psi\rangle \equiv \int\prod_\alpha \mathrm{d}\xi_\alpha^*\mathrm{d}\xi_\alpha e^{-\xi^*\cdot\xi}|\xi\rangle\,\psi(\xi^*). \quad (1.142)$$
$$\langle\xi\,|\,\hat{a}_\alpha\,|\,\psi\rangle = \frac{\partial}{\partial\xi_\alpha^*}\psi(\xi^*), \quad (1.143)$$
$$\left\langle\xi\middle|\hat{a}_\alpha^\dagger\middle|\psi\right\rangle = \xi_\alpha^*\psi(\xi^*), \quad (1.144)$$

Matrix element of a normal-ordered operator

$$\left\langle\xi\middle|\hat{A}\left(\hat{a}^\dagger,\hat{a}\right)\middle|\xi'\right\rangle = e^{\xi^*\cdot\xi'}A\left(\xi^*,\xi'\right). \quad (1.145)$$

Caveats

- There are no classical interpretation of the coherent states of Fermions.
- No viable approximation (e.g., stationary-phase approximation) exists.

1.5.4 Gaussian integrals

For complex variables

$$\int \prod_i \frac{\mathrm{d}z_i^* \mathrm{d}z_i}{2\pi \mathrm{i}} e^{-z^\dagger H z + J^\dagger z + z^\dagger J} = [\det H]^{-1} \, e^{J^\dagger H^{-1} J}. \tag{1.146}$$

H is a matrix with a positive-definite Hermitian part.

For Grassmann variables

$$\int \prod \mathrm{d}\eta_i^* \mathrm{d}\eta_i e^{-\eta^\dagger H \eta + J^\dagger \eta + \eta^\dagger J} = [\det H] \, e^{J^\dagger H^{-1} J}. \tag{1.147}$$

Both $\{\eta_i, \eta_i^*\}$ and $\{J_i, J_i^*\}$ are Grassmann variables. H is not necessary to be positive definite.

- The law for linear transformations of Grassmann variables:

$$\int \prod \mathrm{d}\zeta_i^* \mathrm{d}\zeta_i P\left(\zeta^*, \zeta\right) = \left| \frac{\partial(\eta^*, \eta)}{\partial(\zeta^*, \zeta)} \right| \int \prod \mathrm{d}\eta_i^* \mathrm{d}\eta_i P\left(\zeta^*(\eta^*, \eta), \zeta(\eta^*, \eta)\right). \tag{1.148}$$

  Note that the Jacobian is *inverted*.

- For more general cases involving $\eta_i \eta_j$ and $\eta_i^* \eta_j^*$ quadratic terms, a generalized Gaussian integral formula can be found in Ref. [20].

1.6 Summary

Commutation relation $\left[\hat{a}_\alpha, \hat{a}_\beta^\dagger\right]_{-\zeta} = \delta_{\alpha\beta}$, $\left[\hat{a}_\alpha, \hat{a}_\beta\right]_{-\zeta} = \left[\hat{a}_\alpha^\dagger, \hat{a}_\beta^\dagger\right]_{-\zeta} = 0$.

Coherent state $|\xi\rangle = \exp\left(\zeta \sum_\alpha \xi_\alpha \hat{a}_\alpha^\dagger\right)|0\rangle$

Operations $\hat{a}_\alpha |\xi\rangle = \xi_\alpha |\xi\rangle$, $\hat{a}_\alpha^\dagger |\xi\rangle = \zeta \partial_{\xi_\alpha} |\xi\rangle$, $\langle\xi| \hat{a}_\alpha^\dagger = \langle\xi| \xi_\alpha^*$, $\langle\xi| \hat{a}_\alpha = \partial_{\xi_\alpha^*} \langle\xi|$

Matrix element $\langle\xi|\hat{A}(\hat{a}^\dagger, \hat{a})|\xi'\rangle = e^{\xi^* \cdot \xi'} A(\xi^*, \xi')$

Closure relation $1 = \int \mathrm{d}\mu(\xi) |\xi\rangle \langle\xi|$

Trace $\mathrm{Tr}\hat{A} = \int \mathrm{d}\mu(\xi) \langle\zeta\xi|\hat{A}|\xi\rangle$

Representation $|\psi\rangle = \int \mathrm{d}\mu(\xi) |\xi\rangle \psi(\xi^*)$, $\psi(\xi^*) = \langle\xi|\psi\rangle$, $\langle\xi|\hat{a}_\alpha^\dagger|\psi\rangle = \xi_\alpha^* \psi(\xi^*)$, $\langle\xi|\hat{a}_\alpha|\psi\rangle = \partial_{\xi_\alpha^*} \psi(\xi^*)$

Gaussian integral

$$\int \prod_\alpha \frac{\mathrm{d}\xi_\alpha^* \mathrm{d}\xi_\alpha}{\mathcal{N}} e^{-\sum_{\alpha\beta} \xi_\alpha^* H_{\alpha\beta} \xi_\beta + \sum_\alpha (\eta_\alpha^* \xi_\alpha + \xi_\alpha^* \eta_\alpha)} = [\det H]^{-\zeta} \, e^{\sum_{\alpha\beta} \eta_\alpha^* H_{\alpha\beta}^{-1} \eta_\beta}$$

$$\zeta = \begin{cases} 1 & \text{Bosons} \\ -1 & \text{Fermions} \end{cases}$$

$$\mathrm{d}\mu(\xi) = \prod_\alpha \frac{\mathrm{d}\xi_\alpha^* \mathrm{d}\xi_\alpha}{\mathcal{N}} e^{-\xi^* \cdot \xi}$$

$$\mathcal{N} = \begin{cases} 2\pi\mathrm{i} & \text{Bosons} \\ 1 & \text{Fermions} \end{cases}$$

$$\xi^* \cdot \xi' = \sum_\alpha \xi_\alpha^* \xi_\alpha'$$

Problems

1. A set of N particles are in single-particle states $|\beta_1\rangle \dots |\beta_N\rangle$. The single-particle states have the coordinate representation $\langle \boldsymbol{r}|\beta_i\rangle = \psi_{\beta_i}(\boldsymbol{r})$. Show the coordinate representations of the normalized symmetrized many-body states for Bosons and Fermions by using the overlap formula Eq. (1.41).

2. Second quantization:

   (a) Derive Eq. (1.82).

   (b) Determine the commutation relations of $\hat{\boldsymbol{S}}_i$ defined in (1.88). Are they the same as those for angular momentum operators?

   (c) Prove Eq. (1.91) by making use of the identity $\boldsymbol{\tau}_{ab} \cdot \boldsymbol{\tau}_{cd} = 2\delta_{ad}\delta_{bc} - \delta_{ab}\delta_{cd}$.

3. Derive the closure relation Eq. (1.98) by

   (a) showing

   $$\int \mathrm{d}\mu(\phi) \, |\phi\rangle \langle\phi| = \sum_n |n\rangle \langle n| \, . \tag{1.149}$$

   (b) and the closure relation Eq. (1.45) can be written as

   $$\sum_{\{n_\alpha\}} |n_{\alpha_1} n_{\alpha_2} \dots \rangle \langle n_{\alpha_1} n_{\alpha_2} \dots | = 1. \tag{1.150}$$

4. Boson coherent states in the large N limit could be interpreted as classical fields. For example, a classical electromagnetic field can be viewed as a coherent state of photons. This can also be seen in another system, i.e., the harmonic oscillator with

   $$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2 \tag{1.151}$$

   (a) Show

   $$\hat{H} = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) \tag{1.152}$$

   with

   $$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} \left(\hat{a}^\dagger + \hat{a} \right) \tag{1.153}$$

   $$\hat{p} = \mathrm{i}\sqrt{\frac{\hbar\omega m}{2}} \left(\hat{a}^\dagger - \hat{a} \right) \tag{1.154}$$

   and $\hat{a}$ and $\hat{a}^\dagger$ satisfy the commutation relations of Boson annihilation and creation operators. Therefore, a harmonic oscillator can be viewed as a *phonon* system.

   (b) Assume that the system is in the coherent state $|\phi_0\rangle$ at $t = 0$. Show that the state at the finite time t is

   $$|\psi(t)\rangle = e^{-\mathrm{i}\omega t/2} \, |\phi_0 e^{-\mathrm{i}\omega t}\rangle \, . \tag{1.155}$$

   (c) Determine the expectation value $\langle\hat{x}\rangle$, $\langle\hat{p}\rangle$, and $\left\langle \hat{H} \right\rangle$ with respect to $|\psi(t)\rangle$. Compare the results with those for a classical harmonic oscillator with initial values $x(t=0) = \sqrt{2\hbar/m\omega}|\phi_0|$ and $p(t=0) = 0$.

5. Prove the identity of integral by part for *Grassmann* variables:

   $$\int \mathrm{d}\xi^* \mathrm{d}\xi e^{-\xi^*\xi} \left(\xi - \frac{\partial}{\partial \xi^*} \right) A(\xi, \xi^*) = 0, \tag{1.156}$$

   for any A.

Chapter 2

Green's functions

We define a set of quantities called Green's functions:

- Properties of a many-particle system, e. g., quasi-excitations and spectral weights, can be extracted from the Green's functions.
- A wide range of observables of direct experimental interest may also be related to them.

We first introduce *time-ordered Green's functions*, which are special because they could be conveniently evaluated by using the functional integrals (see §3). For general circumstances, one has to introduce *more species of Green's functions*. In equilibrium, the different species of the Green's functions can be related by the *fluctuation-dissipation theorem*. More generally, they can be unified into a single *Green's function defined on a time contour*.

2.1 Green's functions and observables

2.1.1 Time-ordered Green's functions

Real-time Green's function

$$G^{(n)}\left(\alpha_1 t_1, \ldots \alpha_n t_n; \alpha_1' t_1', \ldots \alpha_n' t_n'\right) = (-\mathrm{i})^n \left\langle \hat{T}\left[\hat{a}_{\alpha_1}^{(\mathrm{H})}(t_1)\ldots \hat{a}_{\alpha_n}^{(\mathrm{H})}(t_n)\hat{a}_{\alpha_n'}^{(\mathrm{H})\dagger}(t_n')\ldots \hat{a}_{\alpha_1'}^{(\mathrm{H})\dagger}(t_1')\right]\right\rangle, \tag{2.1}$$

where the superscript (H) denotes the Heisenberg representation. The Green's function could be evaluated by using the functional integrals for *an equilibrium system at the zero temperature*. (See §4.3) (1.18)

Time-ordered product rearranges operators in descending order of time:

$$\hat{T}\left[\hat{O}^{(\mathrm{H})}(t_1)\hat{O}^{(\mathrm{H})}(t_2)\ldots\hat{O}^{(\mathrm{H})}(t_n)\right] = \zeta^P \hat{O}^{(\mathrm{H})}(t_{P1})\hat{O}^{(\mathrm{H})}(t_{P2})\ldots\hat{O}^{(\mathrm{H})}(t_{Pn}). \tag{2.2}$$

P is a permutation which orders the time such that $t_{P1} > t_{P2} > \ldots t_{Pn}$, and yields *normal order* at equal times.

Single-particle Green's function

$$G\left(\alpha t; \alpha' t'\right) = -\mathrm{i}\left\langle \hat{T}\left[\hat{a}_{\alpha}^{(\mathrm{H})}(t)\hat{a}_{\alpha'}^{(\mathrm{H})\dagger}(t')\right]\right\rangle. \tag{2.3}$$

It can be interpreted as the propagation amplitude of an added particle/hole:

$$G\left(\alpha t; \alpha' t'\right) = -\mathrm{i}\begin{cases} \left\langle \hat{a}_{\alpha}^{(\mathrm{H})}(t)\hat{a}_{\alpha'}^{(\mathrm{H})\dagger}(t')\right\rangle = \sum_n \rho_n \left\langle \hat{a}_{\alpha}^{\dagger}\Psi_n(t)|e^{-\mathrm{i}\hat{H}(t-t')/\hbar}|\hat{a}_{\alpha'}^{\dagger}\Psi_n(t')\right\rangle & t > t' \\ \zeta\left\langle \hat{a}_{\alpha'}^{(\mathrm{H})\dagger}(t')\hat{a}_{\alpha}^{(\mathrm{H})}(t)\right\rangle = \zeta\sum_n \rho_n \left\langle \hat{a}_{\alpha'}\Psi_n(t')|e^{-\mathrm{i}\hat{H}(t'-t)/\hbar}|\hat{a}_{\alpha}\Psi_n(t)\right\rangle & t \le t' \end{cases}. \tag{2.4}$$

Equation of motion of a *non-interacting* system: By assuming the Hamiltonian $\hat{K}_0 = \sum_\alpha (\epsilon_\alpha - \mu)\, \hat{a}^\dagger_\alpha \hat{a}_\alpha$, we have

$$\mathrm{i}\hbar \frac{\partial}{\partial t} G_0(\alpha t; \alpha' t') = \hbar \left\langle \left[\hat{a}_\alpha, \hat{a}^\dagger_{\alpha'}\right]_{-\zeta} \right\rangle \delta(t-t') + (\epsilon_\alpha - \mu)\, G_0(\alpha t; \alpha' t') \\ = \hbar \delta_{\alpha\alpha'} \delta(t-t') + (\epsilon_\alpha - \mu)\, G_0(\alpha t; \alpha' t'), \quad (2.5)$$

where we make use of the relation:

$$\mathrm{i}\hbar \frac{\partial \hat{a}^{(\mathrm{H})}_\alpha(t)}{\partial t} = \left[\hat{a}^{(\mathrm{H})}_\alpha(t), \hat{K}_0\right] = (\epsilon_\alpha - \mu)\, \hat{a}^{(\mathrm{H})}_\alpha(t). \quad (2.6)$$

The equation of motion can be solved by imposing the boundary conditions:

$$G_0(\alpha t, \alpha' t') = -\mathrm{i}\delta_{\alpha\alpha'} \begin{cases} 1 + \zeta n_\alpha & t \to t' + 0^+ \\ \zeta n_\alpha & t \to t' \end{cases}, \quad (2.7)$$

where $n_\alpha \equiv \langle \hat{a}^\dagger_\alpha \hat{a}_\alpha \rangle$is the occupation number of the state α.
The solution is

$$G_0(\alpha t; \alpha' t') = -\mathrm{i}\delta_{\alpha\alpha'} e^{-\frac{\mathrm{i}}{\hbar}(\epsilon_\alpha - \mu)(t-t')} \left[\theta(t-t'-\eta)\,(1+\zeta n_\alpha) + \theta(t'-t+\eta)\zeta n_\alpha\right], \quad (2.8)$$

where $\eta \equiv 0^+$ in the θ-function is to fix the value of the Green's function at the equal time.
The Fourier transform is

$$\tilde{G}_{0\alpha\alpha'}(\omega) \equiv \int_{-\infty}^{\infty} \mathrm{d}t G_0(\alpha t; \alpha' t') e^{\mathrm{i}\omega(t-t')} \\ = \delta_{\alpha\alpha'} \left[\frac{1+\zeta n_\alpha}{\omega - (\epsilon_\alpha - \mu)/\hbar + \mathrm{i}\eta} - \frac{\zeta n_\alpha}{\omega - (\epsilon_\alpha - \mu)/\hbar - \mathrm{i}\eta}\right] e^{\mathrm{i}\omega\eta}. \quad (2.9)$$

For interacting systems, the equation of motion is related to higher order Green's functions and not closed by itself.

Thermal Green's function is the Green's function for the imaginary time $t = -\mathrm{i}\tau$, $\tau \in [0, \hbar\beta)$:[1]

$$\mathcal{G}^{(n)}(\alpha_1\tau_1, \ldots \alpha_n\tau_n; \alpha'_1\tau'_1, \ldots \alpha'_n\tau'_n) = (-1)^n \left\langle T\left[\hat{a}^{(\mathrm{H})}_{\alpha_1}(\tau_1) \ldots \hat{a}^{(\mathrm{H})}_{\alpha_n}(\tau_n) \hat{a}^{(\mathrm{H})\dagger}_{\alpha'_n}(\tau'_n) \ldots \hat{a}^{(\mathrm{H})\dagger}_{\alpha'_1}(\tau'_1)\right]\right\rangle, \quad (2.10)$$

where

$$\hat{a}^{(\mathrm{H})}_\alpha(\tau) \equiv e^{\frac{\hat{K}}{\hbar}\tau} \hat{a}_\alpha e^{-\frac{\hat{K}}{\hbar}\tau}, \quad (2.11)$$

$$\hat{a}^{(\mathrm{H})\dagger}_\alpha(\tau) \equiv e^{\frac{\hat{K}}{\hbar}\tau} \hat{a}^\dagger_\alpha e^{-\frac{\hat{K}}{\hbar}\tau}. \quad (2.12)$$

Note that $\hat{a}^{(\mathrm{H})\dagger}_\alpha(\tau)$ and $\hat{a}^{(\mathrm{H})}_\alpha(\tau)$ are *not* Hermitian adjoints.
The thermal-Green's function can be evaluated by using the functional integrals for *an equilibrium system at the finite temperature*.

- It is introduced for facilitating the calculations of finite-temperature equilibrium systems.
- It exploits the property that the *equilibrium* density matrix can be regarded as a time-evolution operator for a time-interval $t = -\mathrm{i}\hbar\beta$. (1.22)
- It displays the (anti-)periodicity: FW§24

$$\mathcal{G}|_{\tau_i=0} = \zeta\, \mathcal{G}|_{\tau_i=\hbar\beta}, \quad (2.13)$$

where τ_i denotes one of the time arguments of the Green's function.

[1] The definition has an extra factor $(-1)^n$, to be consistent with Fetter-Walecka's definition. See FW Eq. (23.6).

Proof

$$\mathcal{G}(\alpha 0;\alpha'\tau') = -\frac{\zeta}{Z}\mathrm{Tr}\left[e^{-\beta\hat{K}}\hat{a}_{\alpha'}^{(\mathrm{H})\dagger}(\tau')\hat{a}_{\alpha}\right] = -\frac{\zeta}{Z}\mathrm{Tr}\left[e^{-\beta\hat{K}}\left(e^{\beta\hat{K}}\hat{a}_{\alpha}e^{-\beta\hat{K}}\right)\hat{a}_{\alpha'}^{(\mathrm{H})\dagger}(\tau')\right]$$
$$\equiv -\frac{\zeta}{Z}\mathrm{Tr}\left[e^{-\beta\hat{K}}\hat{a}_{\alpha}^{(\mathrm{H})}(\hbar\beta)\,\hat{a}_{\alpha'}^{(\mathrm{H})\dagger}(\tau')\right] = \zeta\mathcal{G}(\alpha\,\hbar\beta;\alpha'\tau')\,. \quad (2.14)$$

Matsubara frequency: Because of the periodicity Eq. (2.13), the thermal Green's function can be related to its Fourier transform by

$$\mathcal{G}(\alpha\tau,\alpha'\tau') = \frac{1}{\hbar\beta}\sum_{n} e^{-\mathrm{i}\omega_n(\tau-\tau')}\mathcal{G}_{\alpha\alpha'}(\omega_n)\,, \quad (2.15)$$

$$\mathcal{G}_{\alpha\alpha'}(\omega_n) = \int_0^{\hbar\beta}\mathrm{d}\tau e^{\mathrm{i}\omega_n(\tau-\tau')}\mathcal{G}(\alpha\tau,\alpha'\tau')\,, \quad (2.16)$$

where we assume that the system is time-independent, and hence $\mathcal{G}(\alpha\tau,\alpha'\tau') = \mathcal{G}(\alpha\,\tau-\tau',\alpha' 0)$. The discrete set of frequencies is defined by

$$\omega_n = \begin{cases} \frac{2\pi n}{\hbar\beta} & \text{Boson} \\ \frac{(2n+1)\pi}{\hbar\beta} & \text{Fermion} \end{cases},\ n\in Z \quad (2.17)$$

Equation of motion: For a non-interacting system, we can establish: (2.5)

$$\left(-\frac{\partial}{\partial\tau}-\frac{\epsilon_\alpha-\mu}{\hbar}\right)\mathcal{G}_0(\alpha\tau,\alpha'\tau') = \delta_{\alpha\alpha'}\delta(\tau-\tau'). \quad (2.18)$$

- The solution is (2.7)

$$\mathcal{G}_0(\alpha\tau,\alpha'\tau') = -\delta_{\alpha\alpha'}e^{-(\epsilon_\alpha-\mu)(\tau-\tau')/\hbar}\left[\theta(\tau-\tau'-\eta)\left(1+\zeta n_\alpha\right)+\zeta\theta(\tau'-\tau+\eta)n_\alpha\right]. \quad (2.19)$$

- The periodicity Eq. (2.13) yields

$$\zeta n_\alpha = \zeta e^{-\beta(\epsilon_\alpha-\mu)}\left(1+\zeta n_\alpha\right), \quad (2.20)$$

$$n_\alpha = \frac{1}{e^{\beta(\epsilon_\alpha-\mu)}-\zeta}, \quad (2.21)$$

  which is the Bose-Einstein ($\zeta=1$) or Fermi-Dirac ($\zeta=-1$) distribution function.

- The Fourier transform is

$$\mathcal{G}_{0\alpha\alpha'}(\omega_n) = \delta_{\alpha\alpha'}\frac{e^{\mathrm{i}\omega_n\eta}}{\mathrm{i}\omega_n-(\epsilon_\alpha-\mu)/\hbar}. \quad (2.22)$$

2.1.2 Evaluation of Observables

NO§5.1

Kinetic energy

$$\left\langle\hat{T}\right\rangle = \mathrm{i}\zeta\int\mathrm{d}^3\boldsymbol{r}\left[-\frac{\hbar^2}{2m}\nabla_{\boldsymbol{r}}^2 G\left(\boldsymbol{r}t;\boldsymbol{r}'t^+\right)\right]_{\boldsymbol{r}'=\boldsymbol{r}} \quad (2.23)$$ (1.73)

$$= \mathrm{i}\zeta\mathcal{V}\int\frac{\mathrm{d}^3\boldsymbol{k}\mathrm{d}\omega}{(2\pi)^4}\frac{\hbar^2k^2}{2m}\tilde{G}(\boldsymbol{k},\omega)e^{\mathrm{i}\omega\eta}, \quad (2.24)$$

where $t^+\equiv t+0^+$, and

$$G\left(\boldsymbol{r}t;\boldsymbol{r}'t^+\right) = -\mathrm{i}\left\langle\hat{T}\left[\hat{\psi}^{(\mathrm{H})}(\boldsymbol{r}t)\hat{\psi}^{(\mathrm{H})\dagger}(\boldsymbol{r}'t^+)\right]\right\rangle, \quad (2.25)$$

$$\tilde{G}(\boldsymbol{k},\omega) = \int\mathrm{d}\boldsymbol{r}\int\mathrm{d}tG\left(\boldsymbol{r}t;\boldsymbol{r}'t'\right)e^{-\mathrm{i}\boldsymbol{k}\cdot\left(\boldsymbol{r}-\boldsymbol{r}'\right)+\mathrm{i}\omega\left(t-t'\right)}. \quad (2.26)$$

Interaction energy

$$\left\langle \hat{V} \right\rangle = \frac{\mathrm{i}\zeta}{2} \int \mathrm{d}^3\boldsymbol{r} \left[\left(\mathrm{i}\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m}\nabla_{\boldsymbol{r}}^2 + \mu \right) G\left(\boldsymbol{r}t; \boldsymbol{r}'t'\right) \right]_{\boldsymbol{r}'=\boldsymbol{r}, t'=t^+} \tag{2.27}$$

$$= \frac{\mathrm{i}\zeta}{2} \mathcal{V} \int \frac{\mathrm{d}^3\boldsymbol{k}\mathrm{d}\omega}{(2\pi)^4} e^{\mathrm{i}\omega\eta} \left(\hbar\omega - \frac{\hbar^2 k^2}{2m} + \mu \right) \tilde{G}(\boldsymbol{k}, \omega). \tag{2.28}$$

To derive the formula, we make use of the identity:

$$\hat{\psi}^\dagger(\boldsymbol{r}t)\mathrm{i}\hbar\frac{\partial\hat{\psi}(\boldsymbol{r}t)}{\partial t} = \hat{\psi}^\dagger(\boldsymbol{r}t)\left(-\frac{\hbar^2}{2m}\nabla^2 - \mu\right)\hat{\psi}(\boldsymbol{r}t) + \int \mathrm{d}\boldsymbol{r}'\hat{\psi}^\dagger(\boldsymbol{r}t)\hat{\psi}^\dagger(\boldsymbol{r}'t)v(\boldsymbol{r}-\boldsymbol{r}')\hat{\psi}(\boldsymbol{r}'t)\hat{\psi}(\boldsymbol{r}t). \tag{2.29}$$

Total energy

$$E_0 = \left\langle \hat{T} + \hat{V} \right\rangle = \frac{\mathrm{i}\zeta}{2} \int \mathrm{d}^3\boldsymbol{r} \left[\left(\mathrm{i}\hbar \frac{\partial}{\partial t} - \frac{\hbar^2}{2m}\nabla_{\boldsymbol{r}}^2 + \mu \right) G\left(\boldsymbol{r}t; \boldsymbol{r}'t'\right) \right]_{\boldsymbol{r}'=\boldsymbol{r}, t'=t^+} \tag{2.30}$$

$$= \frac{\mathrm{i}\zeta}{2} \mathcal{V} \int \frac{\mathrm{d}^3\boldsymbol{k}\mathrm{d}\omega}{(2\pi)^4} e^{\mathrm{i}\omega\eta} \left(\hbar\omega + \frac{\hbar^2 k^2}{2m} + \mu \right) \tilde{G}(\boldsymbol{k}, \omega) \tag{2.31}$$

$$= \frac{1}{2}\zeta\mathcal{V}\frac{1}{\hbar\beta}\sum_{\omega_n} \int \frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3} e^{\mathrm{i}\omega_n\eta} \left(\mathrm{i}\hbar\omega_n + \frac{\hbar^2 k^2}{2m} + \mu \right) \tilde{\mathcal{G}}(\boldsymbol{k}, \omega_n) \tag{2.32}$$

Note: The use of the one-particle Green's function for evaluating the total energy could be dangerous: a seemingly innocuous approximation having little effect on one-particle properties may have a large uncontrolled effect on the energy.

2.1.3 Response functions

NO§2.1

Linear Responses

Conductivity To calculate the conductivity of a system, we introduce an external electric field, and see how much the electric current is generated:

- The external electric field induces a modification to the Hamiltonian

$$\Delta\hat{H} = -e\int \mathrm{d}\boldsymbol{r}\hat{\rho}(\boldsymbol{r})\phi(\boldsymbol{r}), \tag{2.33}$$

  where $\phi(\boldsymbol{r})$ is the electric potential, and $\hat{\rho}(\boldsymbol{r}) \equiv \hat{\psi}^\dagger(\boldsymbol{r})\hat{\psi}(\boldsymbol{r})$ is the density operator.
- We need to calculate the expectation value of the electric current density operator

$$\hat{\boldsymbol{j}}(\boldsymbol{r}) = \frac{\mathrm{i}e\hbar}{2m}\left\{\hat{\psi}^\dagger(\boldsymbol{r})\left[\boldsymbol{\nabla}\hat{\psi}(\boldsymbol{r})\right] - \left[\boldsymbol{\nabla}\hat{\psi}^\dagger(\boldsymbol{r})\right]\hat{\psi}(\boldsymbol{r})\right\}, \tag{2.34}$$

  to the *linear* order of the electric field, or $\phi(\boldsymbol{r})$.
- A linear response has a useful property: the total response to multiple fields is the sum of the responses to each field.

Linear response formula We consider a time-dependent infinitesimally small external field:

$$\hat{H}_U(t) = \hat{H} + \hat{O}U(t). \tag{2.35}$$

Evolution operator $|\psi(t_\mathrm{f})\rangle = \hat{\mathcal{U}}(t_\mathrm{f}, t_\mathrm{i})\,|\psi(t_\mathrm{i})\rangle$:

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathcal{U}}(t, t_\mathrm{i}) = \hat{H}_U(t)\hat{\mathcal{U}}(t, t_\mathrm{i}), \tag{2.36}$$

$$\hat{\mathcal{U}}(t_\mathrm{f}, t_\mathrm{i}) = \hat{T}\exp\left[-\frac{\mathrm{i}}{\hbar}\int_{t_\mathrm{i}}^{t_\mathrm{f}}\hat{H}_U(t)\mathrm{d}t\right] \equiv \lim_{M\to\infty} e^{-\mathrm{i}\epsilon\hat{H}_U(t_M)/\hbar}e^{-\mathrm{i}\epsilon\hat{H}_U(t_{M-1})/\hbar}\ldots e^{-\mathrm{i}\epsilon\hat{H}_U(t_1)/\hbar}, \tag{2.37}$$

where we split the time interval $[t_\mathrm{i}, t_\mathrm{f}]$ into M infinitesimally small time intervals $\epsilon \equiv (t_\mathrm{f} - t_\mathrm{i})/M$, and $t_k = t_\mathrm{i} + (k-1)\epsilon$, $k = 1\ldots M$. The evolution operator for the full time interval is obtained by accumulating the action of the evolution operator for each small time interval.

Response of a wave-function

$$\delta\left|\psi(t)\right\rangle = \int_{t_{\rm i}}^{t} {\rm d}t_1 U(t_1)\left.\frac{\delta\hat{\mathcal{U}}(t,t_{\rm i})}{\delta U(t_1)}\right|_{U\to 0}\left|\psi(t_{\rm i})\right\rangle, \tag{2.38}$$

$$\left.\frac{\delta\hat{\mathcal{U}}(t,t_{\rm i})}{\delta U(t_1)}\right|_{U\to 0} = -\frac{\rm i}{\hbar}\hat{\mathcal{U}}(t,t_1)\hat{O}\hat{\mathcal{U}}(t_1,t_{\rm i})\Big|_{U\to 0} = -\frac{\rm i}{\hbar}e^{-\frac{\rm i}{\hbar}\hat{H}(t-t_{\rm i})}\hat{O}^{(\rm H)}(t_1), \tag{2.39}$$

$$\delta\left|\psi(t)\right\rangle = -\frac{\rm i}{\hbar}e^{-\frac{\rm i}{\hbar}\hat{H}(t-t_{\rm i})}\int_{t_i}^{t}{\rm d}t_1\hat{O}^{(\rm H)}(t_1)\left|\psi\left(t_{\rm i}\right)\right\rangle U(t_1). \tag{2.40}$$

where

$$\hat{O}^{(H)}(t) \equiv e^{\frac{\rm i}{\hbar}\hat{H}(t-t_{\rm i})}\hat{O}e^{-\frac{\rm i}{\hbar}\hat{H}(t-t_{\rm i})}. \tag{2.41}$$

Expectation value of an observable $\hat{R}$:

$$\delta R(t) = \sum_n \rho_n\left[\left\langle\psi_n(t)\right|\hat{R}\left|\delta\psi_n(t)\right\rangle + \left\langle\delta\psi_n(t)\right|\hat{R}\left|\psi_n(t)\right\rangle\right] \tag{2.42}$$

$$= -\frac{\rm i}{\hbar}\int_{-\infty}^{\infty}{\rm d}t_1\theta(t-t_1)\left\langle\left[\hat{R}^{(\rm H)}(t),\hat{O}^{(\rm H)}(t_1)\right]\right\rangle U(t_1), \tag{2.43}$$

$$D^{\rm r}_{RO}(t,t') \equiv \frac{\delta R(t)}{\delta U(t')} = -\frac{\rm i}{\hbar}\theta(t-t')\left\langle\left[\hat{R}^{(\rm H)}(t),\hat{O}^{(\rm H)}(t')\right]\right\rangle. \tag{2.44}$$

We see that:

- The response function is a retarded one.
- It is related to a correlation function between operators.

Scattering experiments

- An external particle interacts weakly with the constituents of a many-body system through an interaction $v(\boldsymbol{r}-\boldsymbol{r}')$. Examples include electron energy loss spectroscopy (EELS) and neutron scattering. The scattering cross section is related to the density correlation function:

$$\sigma(\boldsymbol{q},\omega) = |v_{\boldsymbol{q}}|^2\int{\rm d}t e^{{\rm i}\omega t}\left\langle\hat{\rho}^{\dagger}_{\boldsymbol{q}}(t)\,\hat{\rho}_{\boldsymbol{q}}\right\rangle, \tag{2.45}$$

where $\hat{\rho}_{\boldsymbol{q}} = \sum_i \exp\left(-{\rm i}\boldsymbol{q}\cdot\hat{\boldsymbol{r}}_i\right)$ is the Fourier transform of the density operator, and $v_{\boldsymbol{q}}$ is the Fourier transform of the interaction.

Proof

– We determine the transition matrix element of an external particle scattered from wave-vector $\boldsymbol{k}$ to $\boldsymbol{k}+\boldsymbol{q}$, and the probed system from $|\alpha\rangle$to $|\beta\rangle$:

$$T_{\alpha\beta}(\boldsymbol{q}) = \int{\rm d}\boldsymbol{r}\left\langle\beta\left|e^{-{\rm i}(\boldsymbol{k}+\boldsymbol{q})\cdot\boldsymbol{r}}\sum_i v\left(\boldsymbol{r}-\boldsymbol{r}_i\right)e^{{\rm i}\boldsymbol{k}\cdot\boldsymbol{r}}\right|\alpha\right\rangle$$

$$= v_{\boldsymbol{q}}\left\langle\beta\left|\sum_i e^{-{\rm i}\boldsymbol{q}\cdot\boldsymbol{r}_i}\right|\alpha\right\rangle = v_{\boldsymbol{q}}\left\langle\beta\left|\,\hat{\rho}_{\boldsymbol{q}}\,\right|\alpha\right\rangle. \tag{2.46}$$

– The scattering cross-section is determined by Fermi's Golden rule:

$$\sigma_\alpha\left(\boldsymbol{q},\omega\right) = \frac{2\pi}{\hbar}\left|v_{\boldsymbol{q}}\right|^2\sum_\beta\delta\left(E_\beta-E_\alpha-\hbar\omega\right)\left|\left\langle\beta\left|\,\hat{\rho}_{\boldsymbol{q}}\,\right|\alpha\right\rangle\right|^2 \tag{2.47}$$

$$= \left|v_{\boldsymbol{q}}\right|^2\sum_\beta\int{\rm d}t\,e^{-{\rm i}(E_\beta-E_\alpha)t/\hbar+{\rm i}\omega t}\left|\left\langle\beta\left|\,\hat{\rho}_{\boldsymbol{q}}\,\right|\alpha\right\rangle\right|^2 \tag{2.48}$$

$$= \left|v_{\boldsymbol{q}}\right|^2\sum_\beta\int{\rm d}t\,e^{{\rm i}\omega t}\left\langle\alpha\left|e^{{\rm i}\hat{H}t/\hbar}\hat{\rho}^{\dagger}_{\boldsymbol{q}}e^{-{\rm i}\hat{H}t/\hbar}\right|\beta\right\rangle\left\langle\beta\left|\,\hat{\rho}_{\boldsymbol{q}}\,\right|\alpha\right\rangle \tag{2.49}$$

$$= \left|v_{\boldsymbol{q}}\right|^2\int{\rm d}t\,e^{{\rm i}\omega t}\left\langle\alpha\left|\,\hat{\rho}^{\dagger}_{\boldsymbol{q}}(t)\hat{\rho}_{\boldsymbol{q}}\,\right|\alpha\right\rangle. \tag{2.50}$$

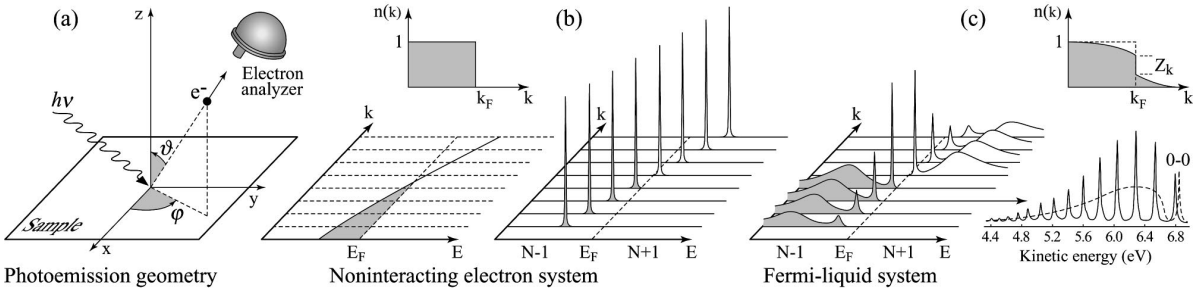


Figure 2.1: The spectral function can be measured by the angle-resolved photoemission spectroscopy (ARPES) technique. The measured intensity is proportional to $f(\omega)A(\boldsymbol{k},\omega)$, where $f(\omega)$ is the Fermi distribution function. (b) and (c) illustrate the spectral functions of non-interacting systems and interacting Fermi-liquid system, respectively. Ref. [7]

  - Average over the initial state α.
- Angle-resolved photoemission spectroscopy (ARPES): a photon excites a photoelectron out of a many-body system (see Fig. 2.1) [7]:

$$I_{\boldsymbol{k}}(\omega) \propto \int \mathrm{d}t e^{\mathrm{i}\omega t} \left\langle \hat{a}^{\dagger}_{\boldsymbol{k}}(0)\, \hat{a}_{\boldsymbol{k}}(t) \right\rangle . \tag{2.51}$$

2.1.4 Species of Green's functions

HJ§3.2

Time-ordered Green's function

$$G(\boldsymbol{r}t;\boldsymbol{r}'t') = -\mathrm{i}\left\langle T\left[\hat{\psi}(\boldsymbol{r}t)\hat{\psi}^{\dagger}(\boldsymbol{r}'t')\right]\right\rangle \tag{2.52}$$

Retarded Green's function

$$G^{\mathrm{r}}(\boldsymbol{r}t;\boldsymbol{r}'t') = -\mathrm{i}\theta(t-t')\left\langle \left[\hat{\psi}(\boldsymbol{r}t),\hat{\psi}^{\dagger}(\boldsymbol{r}'t')\right]_{-\zeta}\right\rangle . \tag{2.53}$$

Advanced Green's function

$$G^{\mathrm{a}}(\boldsymbol{r}t;\boldsymbol{r}'t') = \mathrm{i}\theta(t'-t)\left\langle \left[\hat{\psi}(\boldsymbol{r}t),\hat{\psi}^{\dagger}(\boldsymbol{r}'t')\right]_{-\zeta}\right\rangle . \tag{2.54}$$

Lesser Green's function

$$G^{<}(\boldsymbol{r}t;\boldsymbol{r}'t') = -\mathrm{i}\zeta\left\langle \hat{\psi}^{\dagger}(\boldsymbol{r}'t')\hat{\psi}(\boldsymbol{r}t)\right\rangle . \tag{2.55}$$

Greater Green's function

$$G^{>}(\boldsymbol{r}t;\boldsymbol{r}'t') = -\mathrm{i}\left\langle \hat{\psi}(\boldsymbol{r}t)\hat{\psi}^{\dagger}(\boldsymbol{r}'t')\right\rangle . \tag{2.56}$$

Relations

$$G^{\mathrm{r}} - G^{\mathrm{a}} = G^{>} - G^{<}, \tag{2.57}$$

$$G = \theta(t-t')G^{>} + \theta(t'-t)G^{<} = G^{<} + G^{\mathrm{r}} = G^{>} + G^{\mathrm{a}}, \tag{2.58}$$

$$G^{\mathrm{r}} = \theta\left(t-t'\right)\left[G^{>} - G^{<}\right], \tag{2.59}$$

$$G^{\mathrm{a}} = -\theta\left(t'-t\right)\left[G^{>} - G^{<}\right], \tag{2.60}$$

where the Green's functions all have the argument $(\boldsymbol{r}t;\boldsymbol{r}'t')$.

Conjugate relations

$$G^{\mathrm{a}}(\boldsymbol{r}t;\boldsymbol{r}'t') = \left[G^{\mathrm{r}}(\boldsymbol{r}'t';\boldsymbol{r}t)\right]^{*}, \tag{2.61}$$

$$G^{<}(\boldsymbol{r}t;\boldsymbol{r}'t') = -\left[G^{<}(\boldsymbol{r}'t';\boldsymbol{r}t)\right]^{*}, \tag{2.62}$$

$$G^{>}(\boldsymbol{r}t;\boldsymbol{r}'t') = -\left[G^{>}(\boldsymbol{r}'t';\boldsymbol{r}t)\right]^{*}. \tag{2.63}$$

Why?

- G has a systematic perturbation theory in an equilibrium system.
- $G^{\mathrm{r/a}}$ have a nicer analytic structure and are directly related to physical responses.
- $G^{<,>}$ are directly related to observables and the interpretations of scattering experiments.

2.2 Fluctuation-dissipation theorem

For *equilibrium* systems, all the Green's functions can be linked via the fluctuation-dissipation theorem.

2.2.1 Real time Green's functions

HJ§3.3

Spectral function

$$A(\boldsymbol{k},\omega) = \mathrm{i}\left[G^{\mathrm{r}}(\boldsymbol{k},\omega) - G^{\mathrm{a}}(\boldsymbol{k},\omega)\right] = -2\mathrm{Im}G^{\mathrm{r}}(\boldsymbol{k},\omega) \tag{2.64}$$

$$= \mathrm{i}\left[G^{>}(\boldsymbol{k},\omega) - G^{<}(\boldsymbol{k},\omega)\right] \tag{2.65}$$

$$= \int_{-\infty}^{\infty} \mathrm{d}t\, e^{\mathrm{i}\omega t}\left\langle \hat{a}_{\boldsymbol{k}}(t)\hat{a}_{\boldsymbol{k}}^{\dagger} - \zeta\hat{a}_{\boldsymbol{k}}^{\dagger}\hat{a}_{\boldsymbol{k}}(t)\right\rangle. \tag{2.66}$$

- The spectral function can be directly measured by using ARPES technique [7].
- Sum rule:
$$\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}A(\boldsymbol{k},\omega) = \left\langle\left[\hat{a}_{\boldsymbol{k}}(t),\hat{a}_{\boldsymbol{k}}^{\dagger}(t)\right]_{-\zeta}\right\rangle = 1. \tag{2.67}$$
- The density of states can be computed by
$$\rho(\omega) = \int\frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3}A(\boldsymbol{k},\omega). \tag{2.68}$$
- For a non-interacting system,
$$A\left(\boldsymbol{k},\omega\right) = 2\pi\delta\left(\omega - \frac{\epsilon_{\boldsymbol{k}}-\mu}{\hbar}\right). \tag{2.69}$$
It indicates that a particle with the momentum $\hbar\boldsymbol{k}$ has a definite energy $\epsilon_{\boldsymbol{k}}$.
- In an interacting electron system, $A\left(\boldsymbol{k},\omega\right)$ for $\boldsymbol{k}$ near the Fermi surface usually shows the peak-dip-hump structure: a peak (coherent peak) near $\omega = 0$, a dip, and a high-energy broad hump (incoherent peak). The finite width of the coherent peak indicates the finite lifetime of a quasi-particle. See Fig. 2.1(c).
- In equilibrium, all the Green's functions can be related to the spectral function.

Fluctuation-Dissipation relations

$$G^{<}(\boldsymbol{k},\omega) = -\zeta\frac{\mathrm{i}}{Z}\int\mathrm{d}t\, e^{\mathrm{i}\omega t}\sum_{n,m}e^{-\beta K_n}e^{\mathrm{i}(K_m-K_n)t/\hbar}\left\langle n\left|\,\hat{a}_{\boldsymbol{k}}^{\dagger}\,\right|m\right\rangle\left\langle m\left|\,\hat{a}_{\boldsymbol{k}}\,\right|n\right\rangle \tag{2.70}$$

$$= -\zeta\frac{\mathrm{i}}{Z}\sum_{n,m}2\pi\delta\left(\omega - \frac{K_n-K_m}{\hbar}\right)e^{-\beta K_n}\left|\left\langle m\left|\,\hat{a}_{\boldsymbol{k}}\,\right|n\right\rangle\right|^2, \tag{2.71}$$

$$G^{>}(\boldsymbol{k},\omega) = -\frac{\mathrm{i}}{Z}\sum_{n,m}2\pi\delta\left(\omega - \frac{K_n-K_m}{\hbar}\right)e^{-\beta K_m}\left|\left\langle m\left|\,\hat{a}_{\boldsymbol{k}}\,\right|n\right\rangle\right|^2. \tag{2.72}$$

We obtain

$$G^{>}(\boldsymbol{k},\omega) = \zeta e^{\beta\hbar\omega}G^{<}(\boldsymbol{k},\omega). \tag{2.73}$$

- Making use of the definition Eq. (2.65), we have

$$G^{<}(\boldsymbol{k},\omega) = -\mathrm{i}\zeta n_\zeta(\omega) A(\boldsymbol{k},\omega), \tag{2.74}$$
$$G^{>}(\boldsymbol{k},\omega) = -\mathrm{i}\left[1+\zeta n_\zeta(\omega)\right] A(\boldsymbol{k},\omega), \tag{2.75}$$
$$n_\zeta(\omega) \equiv \frac{1}{e^{\beta\hbar\omega}-\zeta}. \tag{2.76}$$

- Making use of Eqs. (2.58-2.60), we have

$$\begin{Bmatrix} G(\boldsymbol{k},\omega) \\ G^{\mathrm{r}}(\boldsymbol{k},\omega) \\ G^{\mathrm{a}}(\boldsymbol{k},\omega) \end{Bmatrix} = \int \frac{\mathrm{d}\omega_1}{2\pi} A(\boldsymbol{k},\omega_1) \begin{Bmatrix} -\frac{\zeta n_\zeta(\omega_1)}{\omega-\omega_1-\mathrm{i}\eta} + \frac{1+\zeta n_\zeta(\omega_1)}{\omega-\omega_1+\mathrm{i}\eta} \\ \frac{1}{\omega-\omega_1+\mathrm{i}\eta} \\ \frac{1}{\omega-\omega_1-\mathrm{i}\eta} \end{Bmatrix}. \tag{2.77}$$

- It follows:

$$\mathrm{Re}\begin{Bmatrix} G(\boldsymbol{k},\omega) \\ G^{\mathrm{r}}(\boldsymbol{k},\omega) \\ G^{\mathrm{a}}(\boldsymbol{k},\omega) \end{Bmatrix} = \mathcal{P}\int \frac{\mathrm{d}\omega_1}{2\pi} \frac{A(\boldsymbol{k},\omega_1)}{\omega-\omega_1}, \tag{2.78}$$

$$\mathrm{Im}\begin{Bmatrix} G(\boldsymbol{k},\omega) \\ G^{\mathrm{r}}(\boldsymbol{k},\omega) \\ G^{\mathrm{a}}(\boldsymbol{k},\omega) \end{Bmatrix} = \begin{Bmatrix} -\left[\tanh\frac{\beta\hbar\omega}{2}\right]^{-\zeta} \\ - \\ + \end{Bmatrix} \frac{1}{2} A(\boldsymbol{k},\omega). \tag{2.79}$$

2.2.2 Thermal Green's function and analytic continuation

FW§31

The thermal Green's function can also be related to the spectral function by:

$$\mathcal{G}(\boldsymbol{k},\omega_n) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega_1}{2\pi} \frac{A(\boldsymbol{k},\omega_1)}{\mathrm{i}\omega_n-\omega_1} \tag{2.80}$$

The derivation is similar to that for the real-time Green's functions.

Analytic continuation: The real-time Green's functions *at the finite temperature* can be obtained from the thermal Green's function via the process of the ANALYTIC CONTINUATION:

1. We have: (2.77)

$$G^{\mathrm{r}}(\boldsymbol{k},\omega) = \mathcal{G}(\boldsymbol{k},\omega_n)|_{\mathrm{i}\omega_n\to\omega+\mathrm{i}\eta}\,, \tag{2.81}$$
$$G^{\mathrm{a}}(\boldsymbol{k},\omega) = \mathcal{G}(\boldsymbol{k},\omega_n)|_{\mathrm{i}\omega_n\to\omega-\mathrm{i}\eta}\,. \tag{2.82}$$

2. With an analytic form of the thermal Green's function, the spectral function can be determined by (2.64)

$$A(\boldsymbol{k},\omega) = \mathrm{i}\left[\mathcal{G}(\boldsymbol{k},\omega_n)|_{\mathrm{i}\omega_n\to\omega+\mathrm{i}\eta} - \mathcal{G}(\boldsymbol{k},\omega_n)|_{\mathrm{i}\omega_n\to\omega-\mathrm{i}\eta}\right]. \tag{2.83}$$

3. Other real-time Green's function can then be obtained by applying the fluctuation-dissipation relations Eqs. (2.74–2.77).

2.3 Non-equilibrium Green's function

HJ§4

Motivation We introduce the non-equilibrium (Keldysh's, or time contour-ordered) Green's function because:

- The real-time Green's function are directly related to physical observables. Unfortunately, they are difficult to calculate.
- The analytic continuation is only useful when we have an analytic expression for the thermal Green's function. If determined numerically, the thermal Green's function is only defined for a discrete set of the Matsubara frequencies.

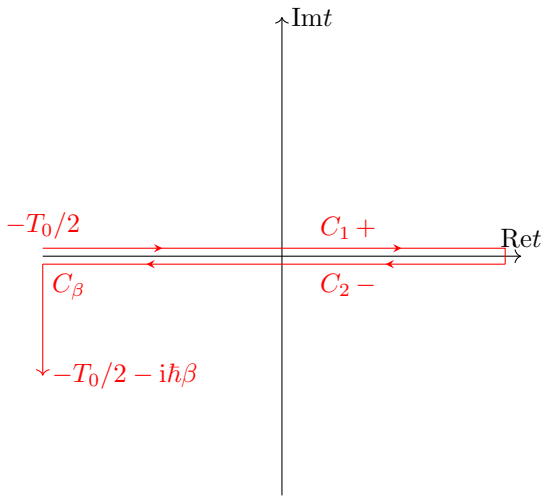


Figure 2.2: Time contour C for defining the non-equilibrium Green's functions. Note that Green's functions in the vertical part of the contour have the (anti-) periodicity Eq. (2.13). Adapted from HJ§4.3.

- When the system is not an equilibrium one (e.g., a system driven by a strong external field beyond the linear response regime), the analytic continuation cannot apply.
- By introducing the non-equilibrium Green's function, all real-time Green's functions can be unified into a single Green's function.
- It is motivated by the observation that all real-time Green's function (e.g., $G^>$) can be converted to a *contour-ordered* trace:

$$\begin{aligned} G^>(\boldsymbol{r}t;\boldsymbol{r}'t') &= -\mathrm{i}\left\langle \hat{\psi}^{(\mathrm{H})}(\boldsymbol{r}t)\hat{\psi}^{(\mathrm{H})\dagger}(\boldsymbol{r}'t')\right\rangle = -\mathrm{i}\frac{\mathrm{Tr}\left[e^{-\beta\hat{H}}\hat{\mathcal{U}}\left(-\frac{T_0}{2},t\right)\hat{\psi}(\boldsymbol{r})\hat{\mathcal{U}}\left(t,t'\right)\hat{\psi}^\dagger(\boldsymbol{r}')\hat{\mathcal{U}}\left(t',-\frac{T_0}{2}\right)\right]}{\mathrm{Tr}e^{-\beta\hat{H}}} \\ &= -\mathrm{i}\frac{\mathrm{Tr}\left[\hat{\mathcal{U}}\left(-\frac{T_0^-}{2}-\mathrm{i}\hbar\beta,-\frac{T_0^-}{2}\right)\hat{\mathcal{U}}\left(-\frac{T_0^-}{2},t^-\right)\hat{\psi}(\boldsymbol{r})\hat{\mathcal{U}}\left(t^-,t'^+\right)\hat{\psi}^\dagger(\boldsymbol{r}')\hat{\mathcal{U}}\left(t'^+,-\frac{T_0^+}{2}\right)\right]}{\mathrm{Tr}e^{-\beta\hat{H}}} \\ &= -\mathrm{i}\frac{\mathrm{Tr}\left[\hat{T}_{\mathrm{C}}e^{-\frac{\mathrm{i}}{\hbar}\int_C \mathrm{d}t\hat{H}(t)}\hat{\psi}(\boldsymbol{r}t^-)\hat{\psi}^\dagger(\boldsymbol{r}'t'^+)\right]}{\mathrm{Tr}\left[\hat{T}_{\mathrm{C}}e^{-\frac{\mathrm{i}}{\hbar}\int_C \mathrm{d}t\hat{H}(t)}\right]}, \end{aligned} \tag{2.84}$$

  where $\hat{\psi}(\boldsymbol{r}t^-)$ and $\hat{\psi}^\dagger(\boldsymbol{r}'t'^+)$ in the last line are not Heisenberg operators: their time arguments just indicate where they should appear. A time (contour) ordered trace can be conveniently evaluated by using functional integrals.

Time contour is defined in Fig. 2.2.

Contour-ordered Green's function is defined as

$$G_{\mathrm{C}}(\boldsymbol{r}t,\boldsymbol{r}'t') = -\mathrm{i}\frac{1}{Z}\mathrm{Tr}\left[\hat{T}_{\mathrm{C}}e^{-\frac{\mathrm{i}}{\hbar}\int_C \mathrm{d}t\hat{H}(t)}\hat{\psi}(\boldsymbol{r}t)\hat{\psi}^\dagger(\boldsymbol{r}'t')\right]. \tag{2.85}$$

- There are two-branches of the real time: C_1 and C_2. The real-time Green's functions can be obtained by assigning appropriate branches to their time arguments:

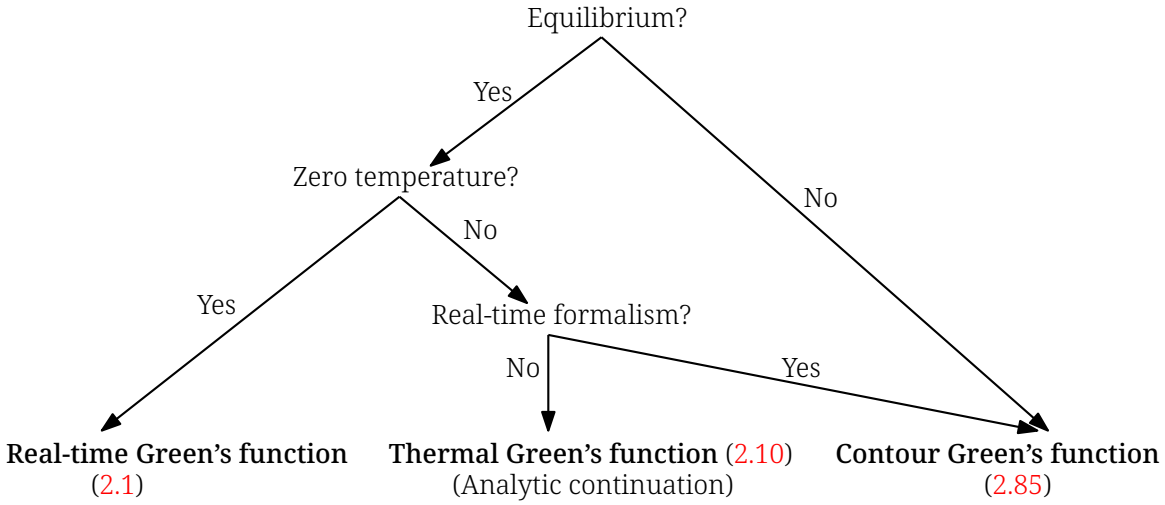
$$G(\boldsymbol{r}t,\boldsymbol{r}'t') = G_{\mathrm{C}}^{11}(\boldsymbol{r}t,\boldsymbol{r}'t'), \tag{2.86}$$
$$G^>(\boldsymbol{r}t,\boldsymbol{r}'t') = G_{\mathrm{C}}^{21}(\boldsymbol{r}t,\boldsymbol{r}'t'), \tag{2.87}$$
$$G^<(\boldsymbol{r}t,\boldsymbol{r}'t') = G_{\mathrm{C}}^{12}(\boldsymbol{r}t,\boldsymbol{r}'t'). \tag{2.88}$$

- The four components of G_{C} are not independent:

$$G_{\mathrm{C}}^{11}+G_{\mathrm{C}}^{22} = G_{\mathrm{C}}^{12}+G_{\mathrm{C}}^{21}. \tag{2.89}$$

2.4 Summary

The following diagram shows the choices of the Green's functions for different circumstances:



Problems

1. Determine the Fourier transform of Eq. (2.8). A useful identity is:

$$\theta(t) = \int \frac{\mathrm{d}\omega}{2\pi \mathrm{i}} \frac{e^{\mathrm{i}\omega t}}{\omega - \mathrm{i}\eta}, \tag{2.90}$$

   where $\eta \equiv 0^+$ is an infinitesimal positive constant.

2. Derive Eq. (2.74–2.79) and (2.80).

3. There also exist fluctuation-dissipation relations for response functions. Consider the density response function

$$D^{\mathrm{r}}(\boldsymbol{q}, t - t') = -\frac{\mathrm{i}}{\hbar \mathcal{V}} \theta(t - t') \left\langle [\hat{\rho}_{\boldsymbol{q}}(t), \hat{\rho}_{-\boldsymbol{q}}(t')] \right\rangle, \tag{2.91}$$

   where $\hat{\rho}_{\boldsymbol{q}}(t)$ is the Fourier transform of the particle density operator, and $\hat{\rho}_{-\boldsymbol{q}} = \hat{\rho}_{\boldsymbol{q}}^\dagger$.

   (a) Obtain an expression similar to Eq. (2.70) by inserting a complete set of basis.

   (b) Define a spectral function which gives rise to D^{r} through a relation similar to Eq. (2.77).

   (c) Define a time-ordered density correlation function

$$D(\boldsymbol{q}, t - t') = -\frac{\mathrm{i}}{\hbar \mathcal{V}} \left\langle T \left[\hat{\rho}_{\boldsymbol{q}}(t) \hat{\rho}_{-\boldsymbol{q}}(t') \right] \right\rangle. \tag{2.92}$$

   Establish a relation with the spectral function defined in (b).

   (d) What is the relation between the spectral function and the scattering cross section Eq. (2.45)?

Chapter 3

Functional integrals

NO§2.2

We first introduce the Feynman path integrals. The functional integrals are nothing but the "path integrals" for the coherent basis.

3.1 Feynman path integrals

To evaluate the time evolution function

$$\mathcal{U}\left(x_{\mathrm{f}}t_{\mathrm{f}}, x_{\mathrm{i}}t_{\mathrm{i}}\right) = \left\langle x_{\mathrm{f}} \left| e^{-\frac{i}{\hbar}\hat{H}(t_{\mathrm{f}}-t_{\mathrm{i}})} \right| x_{\mathrm{i}} \right\rangle. \tag{3.1}$$

The path integrals are constructed as follows:

- Time-slicing: break a finite time interval into infinitesimal slices $\Delta t = \epsilon \equiv (t_{\mathrm{f}} - t_{\mathrm{i}})/M$, and insert the closure relation between the time slices:

$$\mathcal{U}(x_{\mathrm{f}}t_{\mathrm{f}}, x_{\mathrm{i}}t_{\mathrm{i}}) = \int \prod_{k=1}^{M-1} \mathrm{d}x_k \left\langle x_{\mathrm{f}} \left| e^{-\frac{i\epsilon}{\hbar}\hat{H}} \right| x_{M-1} \right\rangle \left\langle x_{M-1} \left| e^{-\frac{i\epsilon}{\hbar}\hat{H}} \right| x_{M-2} \right\rangle \ldots \left\langle x_1 \left| e^{-\frac{i\epsilon}{\hbar}\hat{H}} \right| x_{\mathrm{i}} \right\rangle. \tag{3.2}$$

- Evaluate the evolution operator for each of the time slices
  - Insert a complete momentum basis:

$$\left\langle x_n \left| e^{-\mathrm{i}\frac{\epsilon}{\hbar}\hat{H}} \right| x_{n-1} \right\rangle = \int d^3p_n \left\langle x_n \,|\, p_n \right\rangle \left\langle p_n \left| e^{-\mathrm{i}\frac{\epsilon}{\hbar}\hat{H}} \right| x_{n-1} \right\rangle; \tag{3.3}$$

  - Express $\hat{H}$ in the *normal form*: all the $\hat{p}$'s appear to the left of all the $\hat{x}$'s;
  - $\left\langle p_n \left| e^{-\mathrm{i}\frac{\epsilon}{\hbar}\hat{H}} \right| x_{n-1} \right\rangle \approx \left\langle p_n \left| 1 - \mathrm{i}\frac{\epsilon}{\hbar}\hat{H} \right| x_{n-1} \right\rangle \approx e^{-\mathrm{i}\frac{\epsilon}{\hbar}H(p_n, x_{n-1})} \left\langle p_n | x_{n-1} \right\rangle + \mathcal{O}(\epsilon^2)$;
  - Carry out the integral over p_n: for a system with $\hat{H} = \hat{p}^2/2m + V(x)$,

$$\begin{aligned} \int \mathrm{d}p_n \left\langle x_n \,|\, p_n \right\rangle \left\langle p_n \left| e^{-\mathrm{i}\epsilon\hat{H}/\hbar} \right| x_{n-1} \right\rangle &= \frac{1}{2\pi\hbar} \int \mathrm{d}p_n e^{\frac{\mathrm{i}}{\hbar}\left[p_n(x_n - x_{n-1}) - \epsilon p_n^2/2m - \epsilon V(x_{n-1})\right]} \\ &= \sqrt{\frac{m}{2\pi\mathrm{i}\epsilon\hbar}} \exp\left\{ \frac{\mathrm{i}}{\hbar}\epsilon \left[\frac{1}{2}m\left(\frac{x_n - x_{n-1}}{\epsilon} \right)^2 - V(x_{n-1}) \right] \right\}. \end{aligned} \tag{3.4}$$

  - The approximation has some arbitrariness:
    - $e^{-\mathrm{i}\epsilon H/\hbar}$ or $1 - \mathrm{i}\epsilon H/\hbar$? –The p_n integral should be convergent.
    - $V(x_{n-1})$, $V(x_n)$, or $[V(x_{n-1}) + V(x_n)]/2$? –They are equivalent in the continuous limit $\epsilon \to 0$, but $[V(x_{n-1}) + V(x_n)]/2$ yields better precision for a finite ϵ.

- Chain the evolution operators of the slices together

$$\mathcal{U}(x_\mathrm{f}t_\mathrm{f}, x_\mathrm{i}t_\mathrm{i}) = \lim_{M\to\infty} \int \prod_{k=1}^{M-1} \mathrm{d}x_k \left(\frac{m}{2\pi \mathrm{i}\epsilon\hbar}\right)^{3M/2} e^{\frac{\mathrm{i}}{\hbar}\epsilon\sum_{k=1}^{M}\left[\frac{1}{2}m\left(\frac{x_k-x_{k-1}}{\epsilon}\right)^2 - V(x_{k-1})\right]}$$
$$\equiv \int_{x_\mathrm{i},t_\mathrm{i}}^{x_\mathrm{f}t_\mathrm{f}} \mathrm{D}\left[x(t)\right] e^{\frac{\mathrm{i}}{\hbar}\int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t\left(\frac{1}{2}m\dot{x}^2 - V(x(t))\right)} \equiv \int_{x_\mathrm{i},t_\mathrm{i}}^{x_\mathrm{f}t_\mathrm{f}} \mathrm{D}\left[x(t)\right] e^{\frac{\mathrm{i}}{\hbar}S[x(t)]}, \tag{3.5}$$

where $x_M = x_\mathrm{f}$ and $x_0 = x_\mathrm{i}$ are implied, and

$$S\left[x(t)\right] = \int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t L\left[\dot{x}(t), x(t)\right] \tag{3.6}$$

is the classical action of the system, and L is the Lagrangian. We note that the continuous form is *defined* by the discrete form.

Hamiltonian form

$$\mathcal{U}(x_\mathrm{f}t_\mathrm{f}, x_\mathrm{i}t_\mathrm{i}) = \lim_{M\to\infty} \int \prod_{k=1}^{M-1} \mathrm{d}x_k \prod_{k=1}^{M} \frac{\mathrm{d}p_k}{2\pi\hbar} e^{\frac{\mathrm{i}}{\hbar}\epsilon\sum_{k=1}^{M}\left[p_k\frac{x_k-x_{k-1}}{\epsilon} - \frac{p_k^2}{2m} - V(x_{k-1})\right]} \tag{3.7}$$
$$\equiv \int_{x_\mathrm{i},t_\mathrm{i}}^{x_\mathrm{f}t_\mathrm{f}} \mathrm{D}\left[x(t), p(t)\right] e^{\frac{\mathrm{i}}{\hbar}\int_{t_\mathrm{i}}^{t_\mathrm{f}} \mathrm{d}t(p(t)\dot{x}(t) - H(p(t),x(t)))}. \tag{3.8}$$

Note that there are $M-1$ intermediate positions and M momenta.

Matrix element of a time ordered operator can be expressed as a path-integral:

$$\int_{x_i t_i}^{x_f t_f} \mathrm{D}\left[x(t)\right] O_1\left(x(t_1)\right) O_2\left(x(t_2)\right) e^{\frac{\mathrm{i}}{\hbar}S[x(t)]} \tag{3.9}$$
$$= \int \mathrm{d}x_1 \mathrm{d}x_2 \begin{cases} \mathcal{U}\left(x_\mathrm{f}t_\mathrm{f}, x_1t_1\right) O_1\left(x_1\right) \mathcal{U}\left(x_1t_1, x_2t_2\right) O_2\left(x_2\right) \mathcal{U}\left(x_2t_2, x_\mathrm{i}t_\mathrm{i}\right) & t_1 > t_2 \\ \mathcal{U}\left(x_\mathrm{f}t_\mathrm{f}, x_2t_2\right) O_2\left(x_2\right) \mathcal{U}\left(x_2t_2, x_1t_1\right) O_1\left(x_1\right) \mathcal{U}\left(x_1t_1, x_\mathrm{i}t_\mathrm{i}\right) & t_1 < t_2 \end{cases} \tag{3.10}$$
$$\equiv \left\langle x_f \left| \hat{T}\left[\hat{O}_1(t_1)\hat{O}_2(t_2) e^{-\frac{\mathrm{i}}{\hbar}\int_{t_i}^{t_f}\mathrm{d}t\hat{H}(t)}\right] \right| x_i \right\rangle \tag{3.11}$$
$$= \begin{cases} \left\langle x_f \left| \hat{\mathcal{U}}(t_\mathrm{f},t_1)\hat{O}_1\hat{\mathcal{U}}(t_1,t_2)\hat{O}_2\hat{\mathcal{U}}(t_2,t_\mathrm{i}) \right| x_i \right\rangle & t_1 > t_2 \\ \left\langle x_f \left| \hat{\mathcal{U}}(t_\mathrm{f},t_2)\hat{O}_2\hat{\mathcal{U}}(t_2,t_1)\hat{O}_1\hat{\mathcal{U}}(t_1,t_\mathrm{i}) \right| x_i \right\rangle & t_1 < t_2 \end{cases} \tag{3.12}$$
$$= \left\langle x_f \left| \hat{\mathcal{U}}(t_\mathrm{f},t_\mathrm{i})\hat{T}\left[\hat{O}_1^{(\mathrm{H})}(t_1)\hat{O}_2^{(\mathrm{H})}(t_2)\right] \right| x_i \right\rangle \tag{3.13}$$

where $t_\mathrm{f} \geq t_1,\, t_2 \geq t_\mathrm{i}$. We note that:

- $\hat{O}_1(t_1)$ and $\hat{O}_2(t_2)$ in the second line are *not* Heisenberg operators. The time arguments just indicate which time-slides the operators act on.
- In case of $\hat{O}_{1,2}$ also depending on $\hat{p}$, first express the operator in the normal form, then use the Hamiltonian form of the path integrals, and apply the substitution $\hat{O}\left(\hat{p},\hat{x}\right) \to O\left(p_{k+1}, x_k\right)$.
- The time-order product of two (or more) Heisenberg operators is *not* a time-ordered operator!

3.2 Imaginary time path integrals and the partition function

- The partition function is just the trace of the *imaginary time* evolution operator:

$$Z = \mathrm{Tr}e^{-\beta\hat{H}} = \int \mathrm{d}x \left\langle x \left| e^{-\beta\hat{H}} \right| x \right\rangle = \int \mathrm{d}x\, \mathcal{U}\left(x, -\mathrm{i}\hbar\beta; x0\right). \tag{3.14}$$

- The imaginary time path integral can be obtained by analytic continuation $t \to -\mathrm{i}\tau$:

$$\mathcal{U}(x_\mathrm{f}\tau_\mathrm{f}, x_\mathrm{i}\tau_\mathrm{i}) = \lim_{M\to\infty} \int \prod_{k=1}^{M-1} \mathrm{d}x_k \left(\frac{m}{2\pi\epsilon\hbar}\right)^{\frac{3M}{2}} \exp\left\{-\frac{\epsilon}{\hbar}\sum_{k=1}^{M}\left[\frac{1}{2}m\left(\frac{x_k - x_{k-1}}{\epsilon}\right)^2 + V(x_{k-1})\right]\right\} \tag{3.15}$$

$$\equiv \int_{x_\mathrm{i}\tau_\mathrm{i}}^{x_\mathrm{f}\tau_\mathrm{f}} \mathrm{D}\left[x(\tau)\right] \exp\left\{-\frac{1}{\hbar}\int_{\tau_\mathrm{i}}^{\tau_\mathrm{f}} \mathrm{d}\tau \left[\frac{m}{2}\left(\dot{x}(\tau)\right)^2 + V\left(x(\tau)\right)\right]\right\}, \tag{3.16}$$

where $x_0 = x_\mathrm{i}$ and $x_M = x_\mathrm{f}$ are implied.

- The partition function is a sum over all *periodic trajectories* in $\tau \in [0, \hbar\beta)$: (3.14)

$$Z = \lim_{M\to\infty} \int \prod_{k=1}^{M} \mathrm{d}x_k \left(\frac{m}{2\pi\epsilon\hbar}\right)^{\frac{3M}{2}} \exp\left\{-\frac{\epsilon}{\hbar}\sum_{k=1}^{M}\left[\frac{1}{2}m\left(\frac{x_k - x_{k-1}}{\epsilon}\right)^2 + V(x_{k-1})\right]\right\} \tag{3.17}$$

$$\equiv \int_{x(\hbar\beta)=x(0)} \mathrm{D}\left[x(\tau)\right] \exp\left\{-\frac{1}{\hbar}\int_{0}^{\hbar\beta} \mathrm{d}\tau \left[\frac{m}{2}\left(\dot{x}(\tau)\right)^2 + V\left(x(\tau)\right)\right]\right\}, \tag{3.18}$$

where $x_0 = x_M$ is implied.

Thermodynamic expectation value of an *imaginary-time-ordered* product of Heisenberg operators can be expressed as an imaginary-time path-integral:

$$\left\langle \hat{T}\left[\hat{O}_1^{(\mathrm{H})}(\tau_1)\,\hat{O}_2^{(\mathrm{H})}(\tau_2)\right]\right\rangle = \frac{1}{Z}\mathrm{Tr}\left\{e^{-\beta\hat{H}}\hat{T}\left[\hat{O}_1^{(\mathrm{H})}(\tau_1)\,\hat{O}_2^{(\mathrm{H})}(\tau_2)\right]\right\} \tag{3.19}$$

$$= \frac{1}{Z}\mathrm{Tr}\begin{cases} e^{-\hat{H}(\hbar\beta-\tau_1)/\hbar}\hat{O}_1 e^{-\hat{H}(\tau_1-\tau_2)/\hbar}\hat{O}_2 e^{-\hat{H}(\tau_2-0)/\hbar} & \tau_1 > \tau_2 \\ e^{-\hat{H}(\hbar\beta-\tau_2)/\hbar}\hat{O}_2 e^{-\hat{H}(\tau_2-\tau_1)/\hbar}\hat{O}_1 e^{-\hat{H}(\tau_1-0)/\hbar} & \tau_2 \geq \tau_1 \end{cases} \tag{3.20}$$ (3.13)

$$\equiv \frac{1}{Z}\mathrm{Tr}\left\{\hat{T}\left[\hat{O}_1(\tau_1)\,\hat{O}_2(\tau_2)\,e^{-\frac{1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\hat{H}(\tau)}\right]\right\} \tag{3.21}$$

$$= \frac{1}{Z}\int_{x(\hbar\beta)=x(0)} \mathrm{D}\left[x(\tau)\right] O_1\left(x(\tau_1)\right) O_2\left(x(\tau_2)\right) e^{-\frac{1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\left[\frac{m}{2}(\dot{x}(\tau))^2 + V(x(\tau))\right]}. \tag{3.22}$$

Classical isomorphism maps a quantum particle into a classical ring:

$$H_\mathrm{iso}\left[x(\tau)\right] = \frac{1}{\hbar\beta}\int_0^{\hbar\beta}\mathrm{d}\tau\left[\frac{m}{2}\left(\dot{x}(\tau)\right)^2 + V\left(x(\tau)\right)\right] \tag{3.23}$$

$$\approx \frac{1}{M}\sum_{k=1}^{M}\left[\frac{1}{2}m\left(\frac{x_k - x_{k-1}}{\epsilon}\right)^2 + V(x_{k-1})\right] \tag{3.24}$$

with $x_0 = x_M$.

- τ could be interpreted as the internal coordinate of the classical ring.
- After discretization, a quantum particle is mapped into a classical ring polymer with M beads [4]. The first term becomes the elastic energy of the ring polymer. See Fig. 3.1. The mapping underlies the path-integral Monte-Carlo/molecular dynamics (PIMC/PIMD) approaches for simulating quantum systems.

Exchange symmetry for systems with identical particles modifies the result to

$$Z = \frac{1}{N!}\sum_P \zeta^P \int_{x_i(\hbar\beta)=x_{Pi}(0)} \prod_i \mathrm{D}\left[x_i(\tau)\right] e^{-\frac{1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau H(x(\tau))}. \tag{3.25}$$

There are two choices for intermediate states:

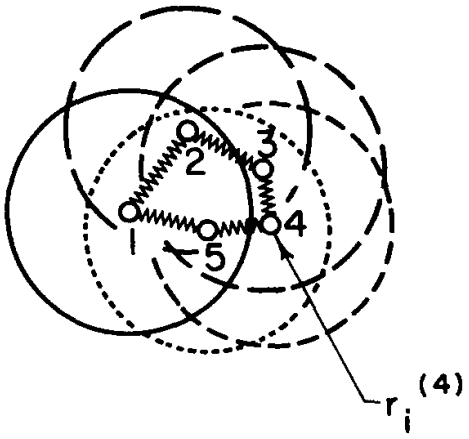


Figure 3.1: In the classical isomorphism, a quantum particle is mapped into a ring polymer with M beads. Each of the beads corresponds to the particle at an imaginary time instance. Here we show the case of $M = 5$. Adapted from Ref. [4].

- un-symmetrized product states
- (anti-)symmetrized states

The two approaches are equivalent. However, in stochastic evaluations, it may be advantageous to use the anti-symmetrized states for Fermions.

It is extremely difficult, if not impossible, to implement the exchange symmetry using path integrals.

3.3 Functional integrals

The functional integral are the "path integrals" for the coherent states (instead of the position eigenstates). The effect of the exchange symmetry is automatically taken care by the *second-quantized* form of the Hamiltonian.

With the coherent basis, the time evolution function is defined by

$$\mathcal{U}\left(\psi_{\mathrm{f}}^{*} t_{\mathrm{f}}, \psi_{\mathrm{i}} t_{\mathrm{i}}\right)=\left\langle \psi_{\mathrm{f}}\left| e^{-\frac{i}{\hbar} \hat{H}\left(t_{\mathrm{f}}-t_{\mathrm{i}}\right)}\right| \psi_{\mathrm{i}}\right\rangle . \tag{3.26}$$

The functional integral approach proceeds as follows:

- Apply the time-slicing and insert the closure relation of the coherent states:

$$\mathcal{U}(\psi_{\mathrm{f}}^{*} t_{\mathrm{f}}, \psi_{\mathrm{i}} t_{\mathrm{i}})=\int \prod_{k=1}^{M-1}\left[\frac{\mathrm{d}\psi_{k}^{*} \mathrm{d}\psi_{k}}{\mathcal{N}}\right] e^{-\psi_{k}^{*} \cdot \psi_{k}} \prod_{k=1}^{M}\left\langle \psi_{k}\left| e^{-\frac{i \epsilon}{\hbar} \hat{H}}\right| \psi_{k-1}\right\rangle , \tag{3.27}$$

  where $\psi_{M}^{*}=\psi_{\mathrm{f}}^{*}$ and $\psi_{0}=\psi_{\mathrm{i}}$ are implied.

- Transform the second quantized Hamiltonian to the *normal form*: all creation operators appear to the left of annihilation operators. The matrix element of a times slice is

$$\left\langle \psi_{k}\left| e^{-\frac{i \epsilon}{\hbar} \hat{H}\left(\hat{a}^{\dagger}, a\right)}\right| \psi_{k-1}\right\rangle \approx \exp\left[\psi_{k}^{*} \cdot \psi_{k-1}-\mathrm{i} \frac{\epsilon}{\hbar} H\left(\psi_{k}^{*}, \psi_{k-1}\right)\right] . \tag{3.28}$$

- Evolution function is:

$$\begin{aligned}\mathcal{U}(\psi_{\mathrm{f}}^{*} t_{\mathrm{f}} ; \psi_{\mathrm{i}} t_{\mathrm{i}})=\lim_{M \rightarrow \infty} \int \prod_{k=1}^{M-1}\left[\frac{\mathrm{d}\psi_{k}^{*} \mathrm{d}\psi_{k}}{\mathcal{N}}\right] \exp\Big\{ & \psi_{M}^{*} \cdot \psi_{M-1}-\mathrm{i} \frac{\epsilon}{\hbar} H\left(\psi_{M}^{*}, \psi_{M-1}\right) \\ & +\mathrm{i} \frac{\epsilon}{\hbar} \sum_{k=1}^{M-1}\left[\mathrm{i} \hbar \psi_{k}^{*} \cdot \frac{\psi_{k}-\psi_{k-1}}{\epsilon}-H\left(\psi_{k}^{*}, \psi_{k-1}\right)\right]\Big\} \end{aligned} \tag{3.29}$$

$$\equiv e^{\psi_{\mathrm{f}}^{*} \cdot \psi_{\mathrm{f}}} \int \mathrm{D}\left[\psi^{*}, \psi\right] \exp\left(\frac{\mathrm{i} S\left[\psi, \psi^{*}\right]}{\hbar}\right) , \tag{3.30}$$

$$S[\psi,\psi^*]=\int_{t_\mathrm{i}}^{t_\mathrm{f}}\mathrm{d}t\left[\mathrm{i}\hbar\psi^*(t)\cdot\frac{\partial\psi(t)}{\partial t}-H\left(\psi^*(t),\psi(t)\right)\right]. \tag{3.31}$$

The boundary conditions $\psi_M^*=\psi^*(t_\mathrm{f})\equiv\psi_\mathrm{f}^*$ and $\psi_0=\psi(t_\mathrm{i})\equiv\psi_\mathrm{i}$ are implied.

- Note that the continuous form Eq. (3.30) is *defined* by the discrete form Eq. (3.29). Adopting different discrete forms may lead to wrong results. NO Problem 2.6
- Note that the subscripts index the time slices. The field variables ψ and ψ^* may have multiple components ψ^α, $\psi^{\alpha*}$. Depending on what the component index α refers to, the fields are interpreted as:
  - for position $\alpha\equiv\boldsymbol{r}$: $\psi^\alpha\to\psi(\boldsymbol{r}t)$, $A\cdot B\equiv\int\mathrm{d}\boldsymbol{r}A(\boldsymbol{r}t)B(\boldsymbol{r}t)$;
  - for momentum $\alpha\equiv\boldsymbol{p}$: $\psi^\alpha\to\psi_{\boldsymbol{p}}(t)$, $A\cdot B\equiv\sum_{\boldsymbol{p}}A_{\boldsymbol{p}}(t)B_{\boldsymbol{p}}(t)$.

3.4 Partition function and Green's functions

One can express various quantities as functional integrals.

Partition function is just the trace of the imaginary time evolution operator. By applying the trace formula of coherent states:

$$Z=\mathrm{Tr}e^{-\beta\hat{K}}=\int\left[\frac{\mathrm{d}\psi^*\mathrm{d}\psi}{\mathcal{N}}\right]e^{-\psi^*\cdot\psi}\left\langle\zeta\psi\left|e^{-\beta\hat{K}}\right|\psi\right\rangle \tag{3.32}$$ (1.140)

$$=\lim_{M\to\infty}\int\prod_{k=1}^{M}\left[\frac{\mathrm{d}\psi_k^*\mathrm{d}\psi_k}{\mathcal{N}}\right]e^{-(\epsilon/\hbar)\sum_{k=1}^{M}\left[\hbar\psi_k^*\left(\frac{\psi_k-\psi_{k-1}}{\epsilon}-\mu\psi_{k-1}/\hbar\right)+H(\psi_k^*,\psi_{k-1})\right]} \tag{3.33}$$

$$\equiv\int\limits_{\psi(0)=\zeta\psi(\hbar\beta)}\mathrm{D}\left[\psi^*,\psi\right]\exp\left(-\frac{S\left[\psi,\psi^*\right]}{\hbar}\right), \tag{3.34}$$

$$S\left[\psi,\psi^*\right]\equiv\int_0^{\hbar\beta}\mathrm{d}\tau\left[\psi^*(\tau)\cdot\left(\hbar\partial_\tau-\mu\right)\psi(\tau)+H\left(\psi^*(\tau),\psi(\tau)\right)\right]. \tag{3.35}$$

Boundary condition is a result of the trace formula of coherent states: §1.6

$$\psi_0=\zeta\psi_M, \tag{3.36}$$

Thermal Green's functions can be expressed as the average of ϕ_α's and ϕ_α^*'s:

$$\mathcal{G}^{(n)}\left(\alpha_1\tau_1,\ldots\alpha_n\tau_n;\alpha_1'\tau_1',\ldots\alpha_n'\tau_n'\right)=\frac{(-1)^n}{Z}\int\mathrm{D}\left[\psi^*,\psi\right]\exp\left(-\frac{S\left[\psi,\psi^*\right]}{\hbar}\right)\times\psi_{\alpha_1}(\tau_1)\ldots\psi_{\alpha_n}(\tau_n)\psi_{\alpha_n'}^*(\tau_n')\ldots\psi_{\alpha_1'}^*(\tau_1'). \tag{3.37}$$ (3.22)

The periodic boundary condition $\psi(\hbar\beta)=\zeta\psi(0)$ is implied.

Contour ordered Green's function Eq. (2.85) can also be expressed as functional integrals: (2.84)

$$G_\mathrm{C}\left(\boldsymbol{r}t,\boldsymbol{r}'t'\right)=-\frac{\mathrm{i}}{Z}\int\mathrm{D}\left[\psi^*,\psi\right]\psi\left(\boldsymbol{r}t\right)\psi^*\left(\boldsymbol{r}'t'\right)\exp\left(\mathrm{i}\frac{S_\mathrm{C}\left[\psi,\psi^*\right]}{\hbar}\right), \tag{3.38}$$

$$S_\mathrm{C}\left[\psi,\psi^*\right]=\int_C\mathrm{d}t\left[\mathrm{i}\hbar\psi^*(t)\cdot\frac{\partial\psi(t)}{\partial t}-H\left(\psi^*(t),\psi(t)\right)\right], \tag{3.39}$$

where the time is defined in the contour shown in Fig. 2.2. The periodic boundary condition between the two end-points of the contour is

$$\psi\left(-\frac{T_0}{2}\right)=\zeta\psi\left(-\frac{T_0}{2}-\mathrm{i}\hbar\beta\right). \tag{3.40}$$

Non-interacting system

Partition function for $\hat{K}_0 = \sum_\alpha (\epsilon_\alpha - \mu)\, \hat{a}^\dagger_\alpha \hat{a}_\alpha$

$$Z_0 = \lim_{M\to\infty} \prod_\alpha \int \prod_{k=1}^{M} \frac{\mathrm{d}\psi_k^{\alpha *} \mathrm{d}\psi_k^\alpha}{\mathcal{N}} e^{-\sum_{k=1}^{M} \psi_k^{\alpha *}\left[\left(\psi_k^\alpha - \psi_{k-1}^\alpha\right) + \frac{\beta(\epsilon_\alpha - \mu)}{M}\psi_{k-1}^\alpha\right]} \tag{3.41}$$ (3.33)

$$\equiv \lim_{M\to\infty} \prod_\alpha \int \prod_{k=1}^{M} \frac{\mathrm{d}\psi_k^{\alpha *} \mathrm{d}\psi_k^\alpha}{\mathcal{N}} \exp\left[-\psi^{(\alpha)\dagger} S^{(\alpha)} \psi^{(\alpha)}\right] \tag{3.42}$$

$$= \lim_{M\to\infty} \prod_\alpha \left[\det S^{(\alpha)}\right]^{-\zeta} = \prod_\alpha \left(1 - \zeta e^{-\beta(\epsilon_\alpha - \mu)}\right)^{-\zeta}, \tag{3.43}$$ NO (2.71)

$$S^{(\alpha)} = \begin{bmatrix} 1 & 0 & & & 0 & -\zeta a \\ -a & 1 & 0 & & & 0 \\ 0 & -a & 1 & \ddots & & \vdots \\ & 0 & -a & \ddots & & \\ & & 0 & \ddots & 1 & 0 \\ 0 & & & \dots & -a & 1 \end{bmatrix}, \psi^{(\alpha)} = \begin{bmatrix} \psi_1^\alpha \\ \psi_2^\alpha \\ \vdots \\ \psi_M^\alpha \end{bmatrix}, a = 1 - \frac{\beta(\epsilon_\alpha - \mu)}{M}, \tag{3.44}$$

where we make use of the Gaussian integral formula. §1.6

Thermal Green's function

$$\mathcal{G}_0(\alpha\tau_q; \alpha'\tau_r) = -\delta_{\alpha\alpha'} \frac{\zeta}{Z_0^{(\alpha)}} \frac{\partial^2}{\partial J_q^* \partial J_r} \int \prod_{k=1}^{M} \frac{\mathrm{d}\psi_k^{(\alpha)*} \mathrm{d}\psi_k^{(\alpha)}}{\mathcal{N}} e^{-\sum_{jk} \psi_k^{(\alpha)*} S_{kj}^{(\alpha)} \psi_j^{(\alpha)} + \sum_i \left(J_i^* \psi_i^{(\alpha)} + \psi_i^{(\alpha)*} J_i\right)} \Big|_{J=J^*=0} \tag{3.45}$$

$$= -\delta_{\alpha\alpha'} \zeta \frac{\partial^2}{\partial J_q^* \partial J_r} \exp\left(\sum_{jk} J_j^* \left[S^{(\alpha)}\right]^{-1}_{jk} J_k\right)\Big|_{J=J^*=0} \tag{3.46}$$ §1.6

$$= -\delta_{\alpha\alpha'} \left(S^{(\alpha)}\right)^{-1}_{qr} \tag{3.47}$$ NO (2.74)

$$= -\delta_{\alpha\alpha'} e^{-(\epsilon_\alpha - \mu)(\tau_q - \tau_r)/\hbar} \left[\theta(\tau_q - \tau_r)\left(1 + \zeta n_\alpha\right) + \zeta\theta(\tau_r - \tau_q) n_\alpha\right]. \tag{3.48}$$ (2.19)

where $Z_0^{(\alpha)} \equiv \left[\det S^{(\alpha)}\right]^{-\zeta}$.

Matrix formula The partition function can be expressed as a matrix form which is independent of the choice of basis. By making use of the matrix identity $\det S = \exp\left(\mathrm{Tr}\ln S\right)$ and Eq. (3.47), we have:

$$Z_0 = \exp\left[-\zeta \mathrm{Tr}\ln\left(-\hat{\mathcal{G}}_0^{-1}\right)\right]. \tag{3.49}$$ (3.43, 3.47)

$-\hat{\mathcal{G}}_0^{-1}$ should be interpreted as a matrix similar to Eq. (3.44) with $a \to \hat{a} \equiv 1 - \beta(\hat{h}_0 - \mu)/M$, where $\hat{h}_0$ denotes the single-particle Hamiltonian operator.

Problems

1. Derive the path-integral formulation for a particle in a magnetic field with the Hamiltonian

$$\hat{H} = \frac{\left|\hat{\boldsymbol{p}} - qA(\boldsymbol{r})\right|^2}{2m}, \tag{3.50}$$

where $A(\boldsymbol{r})$ is a magnetic vector potential. NO Problem 2.5

2. Derive the Gross-Pitaevskii (GP) equation:

   (a) Determine the second quantized Hamiltonian for Bosons with interaction $V(\boldsymbol{r}, \boldsymbol{r}') = g\delta(\boldsymbol{r} - \boldsymbol{r}')$.

(b) Determine the GP equation by applying the variation principle $\delta S = 0$ (see Eq. (3.31) with respect to $\psi^*(\boldsymbol{r})$.

3. Can the ordinary real-time-ordered Green's functions Eq. (2.1) be expressed as functional integrals without using the time contour? Why?

4. Derive the frequency-sum formula by applying Cauchy's residue theorem: FW (25.38)

$$\frac{1}{\hbar\beta}\sum_{\omega_n}\frac{e^{\mathrm{i}\omega_n\epsilon}}{\mathrm{i}\omega_n - x} = -\frac{\zeta e^{\epsilon x}}{e^{\hbar\beta x} - \zeta}, \text{ for } 0 < \epsilon < \hbar\beta. \tag{3.51}$$

Chapter 4

Perturbation theory

NO§2.3

4.1 General strategy

NO§2.3

1. Decompose a Hamiltonian into two parts:

$$\hat{K} = \hat{K}_0 + \hat{V}, \tag{4.1}$$

where $\hat{K}_0$ is solvable, and can be written as a *diagonalized quadratic* form

$$\hat{K}_0 = \sum_{\alpha} (\epsilon_\alpha - \mu)\, \hat{a}^\dagger_\alpha \hat{a}_\alpha, \tag{4.2}$$

and $\hat{V}\left(\hat{a}^\dagger, \hat{a}\right)$ is the interacting part.

Choices of the zeroth order Hamiltonian: Properly choosing $\hat{K}_0$ is t*he most important step* of solving a many-body problem. *It is not always obvious* what would be an appropriate choice. For instance, there are (at least) two choices of $\hat{K}_0$ for the electron gas Hamiltonian Eq. (1.82):

- An obvious one: the kinetic part of the second-quantized Hamiltonian

$$\hat{K}_0 = \sum_{\boldsymbol{k}\sigma} \left(\frac{\hbar^2 k^2}{2m} - \mu \right) \hat{a}^\dagger_{\boldsymbol{k}\sigma} \hat{a}_{\boldsymbol{k}\sigma} \tag{4.3}$$

$$\hat{V} = \frac{e^2}{2\mathcal{V}} \sum_{\boldsymbol{q}\neq 0} \sum_{\boldsymbol{k}\sigma, \boldsymbol{p}\sigma'} \frac{4\pi}{q^2} \hat{a}^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma} \hat{a}^\dagger_{\boldsymbol{p}-\boldsymbol{q}\sigma'} \hat{a}_{\boldsymbol{p}\sigma'} \hat{a}_{\boldsymbol{k}\sigma}. \tag{4.4}$$

  This is the appropriate choice for the electron liquid phase.

- Assume electrons are localized spatially and form a regular lattice (Wigner crystal) $\boldsymbol{r}_i = \boldsymbol{u}_i + \boldsymbol{R}^0_i$. Using the first-quantized form, we have:

$$\hat{H} = -\sum_i \frac{\hbar^2}{2m} \nabla_i^2 + \sum_i V_{\mathrm{b}}(\boldsymbol{r}_i) + \frac{1}{2} \sum_{i\neq j} \frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} \tag{4.5}$$

$$= E_0 + \underbrace{\left\{ -\sum_i \frac{\hbar^2}{2m} \nabla_i^2 + \frac{1}{2} \sum_{ij} D_{i\alpha,j\beta} u_{i\alpha} u_{j\beta} \right\}}_{\hat{H}_0} + \ldots, \tag{4.6}$$

  where E_0 is the Coulomb energy of the regular lattice of electrons, $\hat{H}_0$ is obtained by expanding the Coulomb interaction to the second order with respect to $\boldsymbol{u}_i$ (harmonic approximation), and $\ldots$ denotes all higher order terms. $\hat{H}_0$ can be diagonalized, and becomes a *phonon* Hamiltonian:,

$$\hat{H}_0 = \sum_{\boldsymbol{k},a} \hbar\omega_{\boldsymbol{k}a} \hat{b}^\dagger_{\boldsymbol{k}a} \hat{b}_{\boldsymbol{k}a}, \tag{4.7}$$

where $\hat{b}_{\boldsymbol{k}a}$ and $\hat{b}^\dagger_{\boldsymbol{k}a}$ are Bosonic annihilation and creation operators, respectively. We note that the exchange symmetry of electrons can be ignored in this case. This is the appropriate choice the electron solid phase.

The two choices represent two distinct phases of electrons. *Starting from an inappropriate choice of $\hat{K}_0$, one can never reach a correct answer just by applying the perturbation approach we are about to discuss.*

2. Express physical quantities as functional integrals: (3.34)

$$Z = \int_{\psi(0)=\zeta\psi(\hbar\beta)} \mathrm{D}\left[\psi^*,\psi\right] \exp\left(-\frac{S_0\left[\psi,\psi^*\right]+S_V\left[\psi,\psi^*\right]}{\hbar}\right), \tag{4.8}$$

$$= Z_0 \left\langle \exp\left(-\frac{S_V\left[\psi^*,\psi\right]}{\hbar}\right)\right\rangle_0, \tag{4.9}$$

where

$$S_0\left[\psi,\psi^*\right] \equiv \int_0^{\hbar\beta} \mathrm{d}\tau \left[\psi^*(\tau)\cdot\hbar\partial_\tau\psi(\tau) + \sum_\alpha \left(\epsilon_\alpha-\mu\right)\psi^*_\alpha(\tau)\,\psi_\alpha(\tau)\right], \tag{4.10}$$

$$S_V\left[\psi,\psi^*\right] \equiv \int_0^{\hbar\beta} \mathrm{d}\tau V\left(\psi^*(\tau),\psi(\tau)\right), \tag{4.11}$$

$$\left\langle \hat{F}\left(\psi^*,\psi\right)\right\rangle_0 \equiv \frac{1}{Z_0}\int_{\psi(\hbar\beta)=\zeta\psi(0)} \mathrm{D}\left[\psi^*,\psi\right] e^{-S_0/\hbar} F\left(\psi^*,\psi\right). \tag{4.12}$$

Note that $V\left(\psi^*(\tau),\psi(\tau)\right)$ is obtained by applying the substitutions $\hat{a}_\alpha \to \psi_\alpha$, $\hat{a}^\dagger_\alpha \to \psi^*_\alpha$ to the second-quantized form of $\hat{V}$ *in the normal order*.

3. Expand Eq. (4.9) in a power series of V:

$$\frac{Z}{Z_0} = \sum_{n=0}^{\infty} \frac{(-1/\hbar)^n}{n!} \int_0^{\hbar\beta} d\tau_1 \ldots d\tau_n \left\langle V(\tau_1)\ldots V(\tau_n)\right\rangle_0. \tag{4.13}$$

4. Evaluate the expansion by applying the formula (3.47)

$$\left\langle \psi_{\alpha_1}(\tau_1)\ldots\psi_{\alpha_n}(\tau_n)\psi^*_{\beta_n}(\tau'_n)\ldots\psi^*_{\beta_1}(\tau'_1)\right\rangle_0 = (-1)^n \sum_P \zeta^P \mathcal{G}_{0\alpha_{Pn}\beta_n}\left(\tau_{Pn},\tau'_n\right)\ldots\mathcal{G}_{0\alpha_{P1}\beta_1}\left(\tau_{P1},\tau'_1\right), \tag{4.14}$$

which is a result of the Gaussian integral formula NO (2.84)

$$\frac{\int \mathrm{D}\left[\psi^*,\psi\right]\psi_{i_1}\psi_{i_2}\ldots\psi_{i_n}\psi^*_{j_n}\ldots\psi^*_{j_2}\psi^*_{j_1} e^{-\sum_{ij}\psi^*_i S_{ij}\psi_j}}{\int \mathrm{D}\left[\psi^*,\psi\right] e^{-\sum_{ij}\psi^*_i S_{ij}\psi_j}} = \sum_P \zeta^P S^{-1}_{i_{Pn},j_n}\ldots S^{-1}_{i_{P1},j_1}. \tag{4.15}$$

We note that $S^{-1}_{ij} = -[\mathcal{G}_0]_{ij}$ when applied to Eq. (4.12).. (3.47)

Wick's theorem is basically a re-statement of Eq. (4.15):

- Pair each ψ_i with a ψ^*_j (a complete *contraction*). Each of the pairs contributes a factor S^{-1}_{ij}.
- The sign ζ^P is determined by the permutation P that brings ψ_i with ψ^*_j in all pairs to adjacent positions.

$$\left\langle \psi_{\alpha_1}(\tau_1)\ldots\psi_{\alpha_n}(\tau_n)\psi^*_{\beta_n}(\tau'_n)\ldots\psi^*_{\beta_1}(\tau'_1)\right\rangle_0 = \sum \text{all complete contractions}. \tag{4.16}$$

Convergency A perturbation theory usually yields an *asymptotic* rather than convergent series, as demonstrated by a simple example: NO§2.1

$$Z(g) = \int \frac{\mathrm{d}x}{\sqrt{2\pi}} e^{-\frac{x^2}{2}-\frac{g}{4}x^4} \approx \sum_n g^n Z_n. \tag{4.17}$$

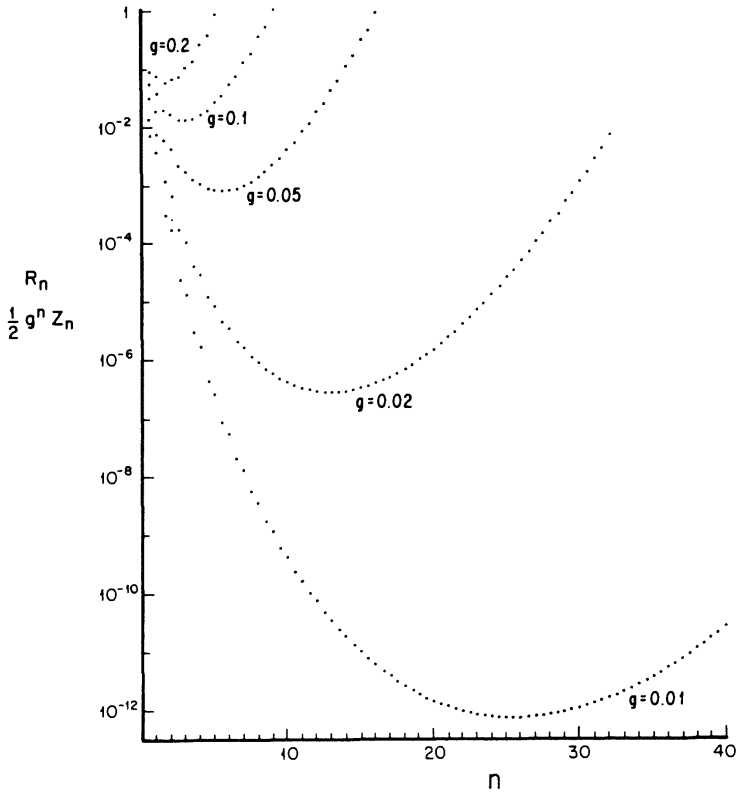


Figure 4.1: Asymptotic expansion of $Z(g)$.

- The series is not convergent because $g^n Z_n \sim (4gn/e)^n/\sqrt{n\pi} \to \infty$ when $n \to \infty$.

  Asymptotic convergence: A finite number of terms sometimes gives a better approximation: minimum $g^n Z_n \sim \sqrt{4g/\pi}\exp(-1/4g)$ occurs at $n \sim 1/4g$. See Fig. 4.1.
- Appropriate re-summations could improve the convergence. See §5.2.
- A non-convergent perturbative expansion often hints an inappropriate choice of $\hat{K}_0$ –the possibility of a non-trivial phase.

4.2 Finite temperature formalism

We explicitly evaluate the expansion for a two-body interaction:

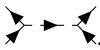
$$V\left(\psi^*(\tau),\psi(\tau)\right) = \frac{1}{2}\sum_{\alpha\beta\gamma\delta}\left(\alpha\beta\left|\hat{v}\right|\gamma\delta\right)\psi^*_\alpha(\tau)\psi^*_\beta(\tau)\psi_\delta(\tau)\psi_\gamma(\tau). \tag{4.18}$$

It leads to the Feynman diagram technique.

4.2.1 Labeled Feynman diagrams

We can represent $\langle V(\tau_1)\dots V(\tau_n)\rangle_0$ with a set of diagrams.

General idea

- A contraction, i. e., a Green's function, is represented by a propagator line .
- Each interaction matrix element $(\alpha\beta\left|\hat{v}\right|\gamma\delta)$ is represented by a vertex with two incoming and two outgoing lines  .
- The n-th order term of Eq. (4.13) is represented by a diagram with n vortexes and $2n$ propagator lines.

- Connect interaction vertexes with propagator lines, by all possible ways.
- Draw all distinct diagrams, and determine signs and coefficients.

Distinct labeled diagrams

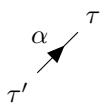
- Labeling each vertex with a time τ and a direction.
- Labeling each propagator with a direction.
- Two labeled diagrams are distinct if one cannot be deformed so as to coincide completely with the other, including both:
  - the time labels of the vertexes;
  - the directions of the vertexes and the propagation lines.

Signs and coefficients

- Each closed Fermion loop of *propagator lines* contributes a sign -1.
- An n-th order diagram has an overall factor $(-1/\hbar)^n/2^n n!$.

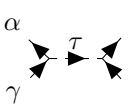
Rules for labeled diagrams

1. Draw all distinct labeled diagrams composed of n vertices  connected by $2n$ propagator lines .
2. Assign a state index to each propagator line and include the factor



$$= \mathcal{G}_{0\alpha}(\tau-\tau') = -e^{-(\epsilon_\alpha-\mu)(\tau-\tau')/\hbar}\left[(1+\zeta n_\alpha)\theta(\tau-\tau')+\zeta n_\alpha\theta(\tau'-\tau)\right]. \quad (4.19)$$

   - Equal time propagators with $\tau=\tau'$ are interpreted as $\tau'=\tau+0^+$, because the time order is the same as the normal order for equal times.
3. For each vertex, include the factor



$$= (\alpha\beta\,|\hat{v}|\,\gamma\delta) \quad (4.20)$$

4. Sum over all state indices and integrate all times over the interval $[0,\hbar\beta)$.
5. Multiply the result by the factor

$$\frac{(-1/\hbar)^n}{n!}\times\frac{1}{2^n}\times\zeta^{n_L}\times(-1)^{2n}=\frac{(-1/\hbar)^n}{2^n n!}\zeta^{n_L} \quad (4.21)$$

   where n_L is the number of closed Fermion loops. The origins of the different factors are:
   (a) $(-1/\hbar)^n/n!$: the expansion coefficient in Eq. (4.13) ;
   (b) $1/2^n$: the ceffiencient in the interacting potential Eq. (4.18);
   (c) ζ^{n_L}: the sign associated with the Wick contraction.
   (d) $(-1)^{2n}$: each contraction corresponds to a $-\mathcal{G}$. There are $2n$ contractions in total.

The labeled diagram approach is not efficient because the number of the labeled diagrams is huge, and many distinct labeled diagrams have the same contribution. It is desirable to simplify the approach.

4.2.2 Unlabeled Feynman Diagrams

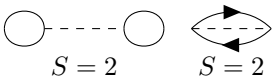
We seek for the simplification of eliminating all τ labels and the directions of the vertices. This is because *distinct labelled diagrams with only these differences* have the same contribution.

Symmetry factor S

- There are total $2^n n!$ permutations of the *time labels* and *vertex directions*.
- Not all the permutations generate distinct diagram. For a given *labeled* diagram, there is a subgroup of the permutations which just yield deformations.
- The symmetry factor S is the rank of the subgroup. The number of distinct labelled diagrams with respect to an unlabelled diagram is

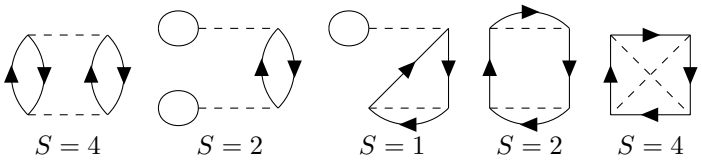
$$\frac{2^n n!}{S}. \tag{4.22}$$

- As a result, one only needs to calculate distinct labelled diagrams with respect to an unlabelled diagram only once, and then multiply the result with the above factor.
- Examples
  - First order:



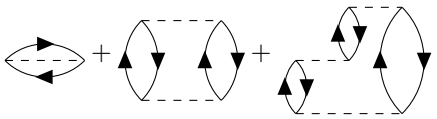
(4.23)

  - Second order (connected):



(4.24)

  - $S = 2n$ for the first-order exchange graph and all direct ring diagrams:



$$+ \cdots = -\frac{1}{2}\mathrm{Tr}\left[\ln(1+\zeta v g g/\hbar)\right] \tag{4.25}$$

- Simple rules for determining S:
  - Successively remove one of the $2n$ propagator lines to obtain $2n$ self-energy diagrams.
  - Not all the resulting self-energy diagrams are distinct. A diagram may occur many times.
  - The symmetry factor S is the number of times that a diagram occurs.

  The proof of the rules will become obvious in §5.2.1.

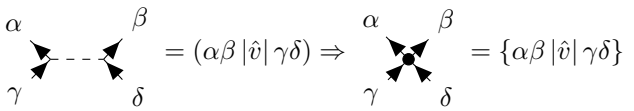
Rules for unlabeled diagrams

1. Draw all distinct diagrams without the time labels and the directions of the vertices;
2. Multiply the factor

$$\frac{(-1/\hbar)^n}{2^n n!} \times \zeta^{n_L} \times \frac{2^n n!}{S} = \frac{(-1/\hbar)^n \zeta^{n_L}}{S}. \tag{4.26}$$

4.2.3 Hugenholtz diagrams

We can make further simplification: eliminate the interaction lines by using (anti-)symmetrized interaction matrix element:



$$= \{\alpha\beta\,|\hat{v}|\,\gamma\delta\} \tag{4.27}$$

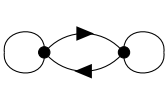
$$\{\,\alpha\beta\mid\hat{v}|\gamma\delta\,\} \equiv (\alpha\beta\,|\hat{v}|\,\gamma\delta) + \zeta\,(\alpha\beta\,|\hat{v}|\,\delta\gamma) \tag{4.28}$$

Note the orders of $\alpha\beta$ and $\gamma\delta$ in the matrix element. The diagrams become

- First order:

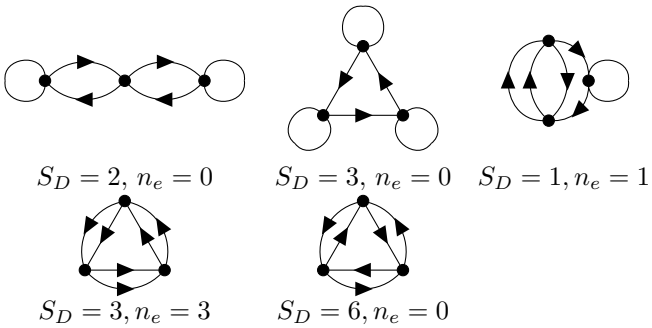
$S_D = 1, n_e = 1$ (4.29)

- Second order (connected):



$S_D = 2,\ n_e = 0$ $S_D = 2,\ n_e = 2$ (4.30)

- Third order (connected):



$S_D = 2,\ n_e = 0$ $S_D = 3,\ n_e = 0$ $S_D = 1, n_e = 1$

$S_D = 3, n_e = 3$ $S_D = 6, n_e = 0$ (4.31)

Symmetry factor

$$S = 2^{n_e} S_D \tag{4.32}$$

where S_D is the number of time-label permutations which only yield deformations, and n_e is the number of equivalent pairs of propagator lines.

Equivalent pair refers to two propagator lines that begin at the same vertex, end at the same vertex, and point in the same direction.

Simple rules for determining S_D:

- Successively remove one of *non-equivalent* propagator lines to generate a set of self-energy diagrams. Note that the two propagator lines in an equivalent pair only needs to be removed once.
- S_D is the number of times that a diagram occurs.

Number of closed loops n_L is determined by:

- expanding a Hugenholtz diagram to (any) one of corresponding Feynman diagrams;
- writing down interacting matrix elements according to the rules of Feynman diagrams, and upgrading them to symmetrized ones;
- counting the number of closed loops.

See NO Eq. (2.122a, b) for an example.

Overall factor:

$$\frac{(-1/\hbar)^n \zeta^{n_L}}{S} \tag{4.33}$$

4.2.4 Frequency and momentum representation

Momentum/frequency representation For systems homogeneous in space/time, it is advantageous to work in Momentum/frequency representation.

- The diagonal α-basis is the plane-wave basis

$$\phi_{\boldsymbol{k}}(\boldsymbol{r}) = \frac{1}{\sqrt{\mathcal{V}}} e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{4.34}$$

i.e., α should be interpreted as $\boldsymbol{k}$.

- Interaction matrix element with respect to the plane-wave basis is

$$(\boldsymbol{k}_1\boldsymbol{k}_2\,|\hat{v}|\,\boldsymbol{k}_3\boldsymbol{k}_4) = \frac{1}{\mathcal{V}}\delta_{\boldsymbol{k}_1+\boldsymbol{k}_2,\boldsymbol{k}_3+\boldsymbol{k}_4}\tilde{v}\left(\boldsymbol{k}_1-\boldsymbol{k}_3\right). \tag{4.35}$$

  - Because of the (anti-)periodicity, a time-dependent function can be expressed as a Fourier series (2.13, 3.36)

$$f(\tau) = \frac{1}{\hbar\beta}\sum_{\omega_n} f_{\omega_n} e^{-\mathrm{i}\omega_n\tau}, \tag{4.36}$$ (2.22)

    where ω_n is the Matsubara frequency. (2.17)
  - A Green's function has the form $\mathcal{G}\left(\boldsymbol{r}-\boldsymbol{r}',\tau-\tau'\right)$, which is diagonal in the time-dependent plane-wave basis:

$$\phi_{\boldsymbol{k},\omega_n}\left(\boldsymbol{r},\tau\right) = \frac{1}{\sqrt{\hbar\beta\mathcal{V}}}e^{-\mathrm{i}\omega_n\tau+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{4.37}$$ (2.15)

$$\mathcal{G}\left(\boldsymbol{r}\tau,\boldsymbol{r}'\tau'\right) = \mathcal{G}\left(\boldsymbol{r}-\boldsymbol{r}',\tau-\tau'\right) = \sum_{\omega_n\omega_{n'}}\sum_{\boldsymbol{k}\boldsymbol{k}'}\mathcal{G}_{\boldsymbol{k}\omega_n,\boldsymbol{k}'\omega_n'}\phi_{\boldsymbol{k},\omega_n}\left(\boldsymbol{r},\tau\right)\phi^*_{\boldsymbol{k}',\omega_{n'}}\left(\boldsymbol{r}',\tau'\right) \tag{4.38}$$

$$\mathcal{G}_{\boldsymbol{k}\omega_n,\boldsymbol{k}'\omega_{n'}} = \mathcal{G}\left(\boldsymbol{k},\omega_n\right)\delta_{\omega_n,\omega_{n'}}\delta_{\boldsymbol{k},\boldsymbol{k}'},$$

$$\mathcal{G}\left(\boldsymbol{k},\omega_n\right) = \int \mathrm{d}\boldsymbol{r}\int_0^{\hbar\beta}\mathrm{d}\tau\mathcal{G}\left(\boldsymbol{r}-\boldsymbol{r}',\tau-\tau'\right)e^{\mathrm{i}\omega_n\left(\tau-\tau'\right)-\mathrm{i}\boldsymbol{k}\cdot\left(\boldsymbol{r}-\boldsymbol{r}'\right)}. \tag{4.39}$$

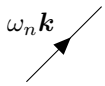
    The free Green's function in momentum-frequency representation is

$$\mathcal{G}_0\left(\boldsymbol{k},\omega_n\right) = \frac{1}{\mathrm{i}\omega_n-\left(\epsilon_{\boldsymbol{k}}-\mu\right)/\hbar}. \tag{4.40}$$ (2.22)

- After applying internal time integrals, frequencies are also conserved at each vertex.

Diagram rules NO *p.* 94, 96

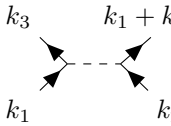
1. Assign momentum/frequency labels to each directed line in such a way that momenta/frequencies are conserved at each vertex, and include a factor:



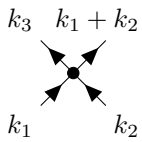
$$= \tilde{\mathcal{G}}_0(\boldsymbol{k},\omega_n) = \frac{1}{\mathrm{i}\omega_n-\left(\epsilon_{\boldsymbol{k}}-\mu\right)/\hbar}. \tag{4.41}$$

   For propagators beginning and ending at the same vertex, include an additional factor $e^{\mathrm{i}\omega_n\eta}$.

2. For each vertex include a factor:



$$= \tilde{v}(\boldsymbol{k}_1-\boldsymbol{k}_3), \tag{4.42}$$



$$= \tilde{v}(\boldsymbol{k}_1-\boldsymbol{k}_3)+\zeta\tilde{v}(\boldsymbol{k}_2-\boldsymbol{k}_3). \tag{4.43}$$

   Note that both the momenta and the frequencies are conserved at each vertex.

3. For each independent momentum/frequency, perform the integral and sum

$$\frac{1}{\hbar\beta}\sum_{\omega_n}\int\frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^d}. \tag{4.44}$$

4. Beside the overall factor, multiply an extra factor $(\hbar\beta\mathcal{V})^{n_c}$, where n_c is the number of connected parts in the diagram.

4.2.5 The linked cluster theorem

The grand potential is determined by the sum of all *connected diagrams*:

$$\Omega = -\frac{1}{\beta}\ln Z = \Omega_0 - \frac{1}{\beta}\sum(\text{all connected graphs}). \tag{4.45}$$

Proof

- Replica approach
  - Exploit the identity:
$$\lim_{n\to 0}\frac{\mathrm{d}}{\mathrm{d}n}Z^n = \ln Z. \tag{4.46}$$
  - Z^n can be obtained by calculating the partition function of a system with n replicating fields. Different species of the replicating fields do not interact.
  - For a graph with n_c connected parts, each part has n choices of the replicating field species. In total, there are n^{n_c} choices. As a result, the contribution of the graph is proportional to n^{n_c}.
  - One expands Z^n as a Taylor series of n, and $\ln Z$ is the coefficient of the linear term. Therefore, $\ln Z$ is the sum of all graphs with $n_c = 1$, i.e., connected graphs.
- Standard approach (See NO Problem 2.10).

4.2.6 Green's functions

The Green's functions can be expressed as functional integrals:

$$\begin{aligned}\mathcal{G}^{(n)}(\alpha_1\tau_2,\dots\alpha_n\tau_n;\alpha_1'\tau_1',\dots\alpha_n'\tau_n') &= (-1)^n\left\langle T\left[\hat{a}_{\alpha_1}(\tau_1)\dots\hat{a}_{\alpha_n}(\tau_n)\hat{a}^\dagger_{\alpha_n}(\tau_n)\dots\hat{a}^\dagger_{\alpha_1}(\tau_1)\right]\right\rangle \\ &= (-1)^n\frac{\left\langle e^{-\frac{1}{\hbar}\int \mathrm{d}\tau V(\psi^*(\tau),\psi(\tau))}\psi_{\alpha_1}(\tau_1)\dots\psi_{\alpha_n}(\tau_n)\psi^*_{\alpha_n'}(\tau_n')\dots\psi^*_{\alpha_1'}(\tau_1')\right\rangle_0}{\left\langle e^{-\frac{1}{\hbar}\int \mathrm{d}\tau V(\psi^*(\tau),\psi(\tau))}\right\rangle_0}.\end{aligned} \tag{4.47}$$

(3.37)

The evaluation of the Green's function is similar to that for $\ln Z$:

- Only connected graphs contribute to the Green's function. A connected diagram is a diagram with all parts connected to external vertices.
- The symmetry factor S is always one.

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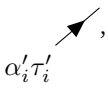
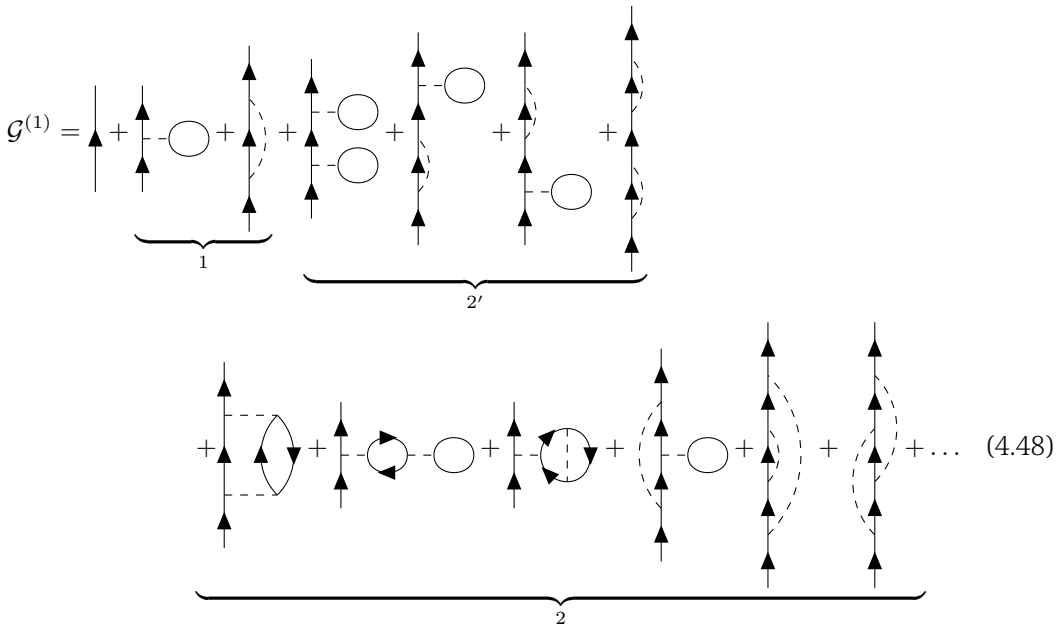
Diagram Rules: For an order r graph:

- Draw all distinct *connected* diagrams composed of n external outgoing propagators 

, n external incoming propagators 

, as well as r interaction vertices. There are

$n + 2r$ propagators in total.

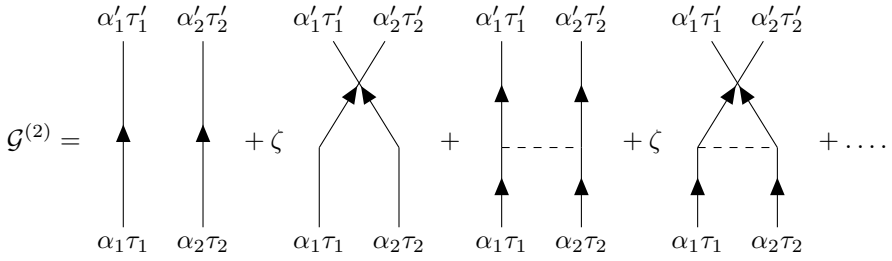


(4.48)

- Assign the usual factors to vertices and propagators.
- Sum over all *internal* single-particle indices and integrate the r *internal* times over the interval $[0, \hbar\beta]$.
- Multiply the result by the factor

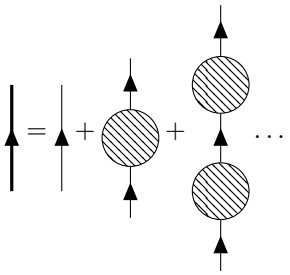
$$\left(-\frac{1}{\hbar}\right)^r \zeta^P \zeta^{n_L}, \tag{4.49}$$

where n_L is the number of closed propagator loops, and P is the permutation of out-going particles with respect to incoming particles.

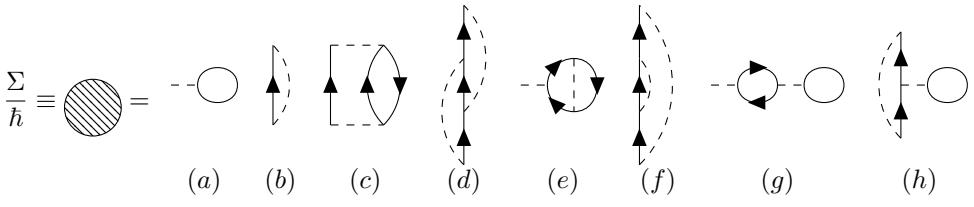


(4.50)

Proper self energy The diagrams of the single-particle Green's function has the structure:



(4.51)



(4.52)

$$\mathcal{G} = \mathcal{G}_0 + \frac{1}{\hbar}\mathcal{G}_0\Sigma\mathcal{G}_0 + \frac{1}{\hbar^2}\mathcal{G}_0\Sigma\mathcal{G}_0\Sigma\mathcal{G}_0 + \dots. \tag{4.53}$$

$$= \mathcal{G}_0 + \frac{1}{\hbar}\mathcal{G}_0\Sigma\mathcal{G} \tag{4.54}$$

Note that the products should be interpreted as matrix-products/convolutions.

The resulting equation is called the DYSON EQUATION. The solution of the equation

$$\mathcal{G} = \left(I - \frac{1}{\hbar}\mathcal{G}_0\Sigma\right)^{-1}\mathcal{G}_0. \tag{4.55}$$

is an example of the re-summation.

4.3 Zero temperature formalism

NO§3.1

For Fermion systems at *zero* temperature, it is possible to develop a *real-time* formalism. It is closely analogous to the finite temperature imaginary-time formalism with modifications in

- redefining the time domain;
- replacing the average over the density matrix with the expectation value in a *non-interacting* ground state.

It results in slight modifications to the rules of Feynman diagrams.

A Boson system will have the Bose-Einstein condensation at the zero temperature, i.e., it is a *symmetry breaking system*. It needs a special treatment.

4.3.1 Ground state energy and Green's function

We seek for analogous expressions of

- ground state energy (4.9)
- Green's function (4.47)

Ground state energy

Basic idea: We exploit the relation

$$\frac{\left\langle \Phi_0 \middle| e^{-\frac{\mathrm{i}}{\hbar}\hat{H}T_0} \middle| \Phi_0 \right\rangle}{\left\langle \Phi_0 \middle| e^{-\frac{\mathrm{i}}{\hbar}\hat{H}_0T_0} \middle| \Phi_0 \right\rangle} = \sum_n |\langle \Phi_0 \,|\, \Psi_n\rangle|^2 \, e^{-\frac{\mathrm{i}}{\hbar}(E_n - W_0)T_0} \tag{4.56}$$

$$\xrightarrow[\mathrm{Im}T_0 \to -\infty]{} |\langle \Phi_0 \,|\, \Psi_0\rangle|^2 \, e^{-\frac{\mathrm{i}}{\hbar}(E_0 - W_0)T_0}, \tag{4.57}$$

where $|\Phi_n\rangle, W_n$ ($|\Psi_n\rangle, E_n$) are the eigenstate and eigenenergy of the non-interacting Hamiltonian $\hat{H}_0$ (full Hamiltonian $\hat{H}$), respectively. The relation holds when

- $|\Phi_0\rangle$ is not orthogonal to Ψ_0;
- $|\Psi_0\rangle$ is non-degenerate.

Time-domain is redefined as C_t of Fig. 4.2.

- C_β: $t = -\mathrm{i}\tau$, $\tau \in [0, \hbar\beta)$, is the choice of the finite temperature formalism.
- C_t: $t = (1 - \mathrm{i}\eta)\, t_\mathrm{R}$ with $\eta = 0^+$, $t_\mathrm{R} \in [-T_0/2, T_0/2]$, is the choice of the zero-temperature real-time formalism.

Ground state energy

$$E_0 - W_0 = \lim_{T_0 \to (1-\mathrm{i}\eta)\infty} \frac{\mathrm{i}\hbar}{T_0} \ln \frac{\mathcal{Z}}{\mathcal{Z}_0}. \tag{4.58}$$

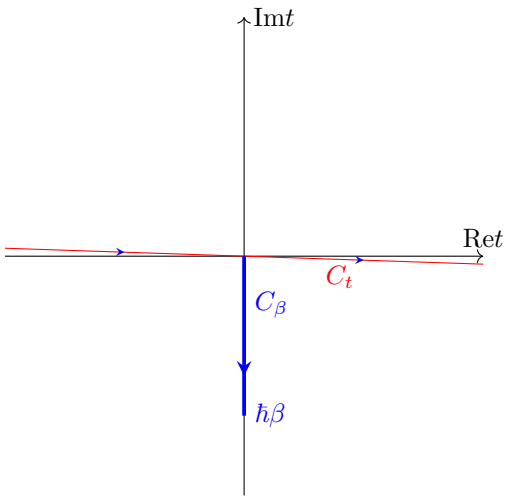


Figure 4.2: Time domains for defining Green's functions.

Partition function We define the "partition function" as

$$\mathcal{Z} = \left\langle \Phi_0 \left| e^{-\frac{\mathrm{i}}{\hbar}\hat{H}T_0} \right| \Phi_0 \right\rangle = \left\langle \Phi_0 \left| \hat{\mathcal{U}}\left(\frac{T_0}{2}, -\frac{T_0}{2}\right) \right| \Phi_0 \right\rangle \tag{4.59}$$

$$= \int \mathrm{d}\mu\left(\psi_\mathrm{f}\right) \int \mathrm{d}\mu\left(\psi_\mathrm{i}\right) \mathcal{U}\left(\psi_\mathrm{f}^*, \frac{T_0}{2}; \psi_\mathrm{i}, -\frac{T_0}{2}\right) \left\langle \Phi_0 \,|\, \psi_\mathrm{f} \right\rangle \left\langle \psi_\mathrm{i} \,|\, \Phi_0 \right\rangle \tag{4.60}$$

$$= \mathcal{U}\left(0, \frac{T_0}{2}; 0, -\frac{T_0}{2}\right). \tag{4.61}$$ (3.30)

To obtain the last line, annihilation operators should annihilate $|\Phi_0\rangle$ instead of the empty state $|0\rangle$, so that $\langle\Phi_0|\psi_\mathrm{f}\rangle = \langle\psi_\mathrm{i}|\Phi_0\rangle = 1$. See Eq. (4.79) for the definition of the annihilation operator with respect to $|\Phi_0\rangle$.

We have

$$\mathcal{Z} = \int \mathrm{D}\left[\psi^*, \psi\right] \exp\left[\frac{\mathrm{i}}{\hbar} S_0\left[\psi^*, \psi\right] - \frac{\mathrm{i}}{\hbar} \int_{-\frac{T_0}{2}}^{\frac{T_0}{2}} \mathrm{d}t V\left(\psi^*(t), \psi(t)\right)\right] \tag{4.62}$$

$$= \mathcal{Z}_0 \left\langle e^{-\frac{\mathrm{i}}{\hbar}\int_{-\frac{T_0}{2}}^{\frac{T_0}{2}} \mathrm{d}t\, V(\psi^*(t),\psi(t))} \right\rangle_{H_0}, \tag{4.63}$$ (4.9)

where

$$S_0\left[\psi^*, \psi\right] \equiv \int_{-\frac{T_0}{2}}^{\frac{T_0}{2}} \mathrm{d}t \left[\psi^*(t) \cdot \left(\mathrm{i}\hbar\partial_t + \mu\right)\psi(t) - H_0\left(\psi^*, \psi\right)\right], \tag{4.64}$$

$$\mathcal{Z}_0 \equiv \int \mathrm{D}\left[\psi^*, \psi\right] e^{\frac{\mathrm{i}}{\hbar} S_0[\psi^*,\psi]}, \tag{4.65}$$

$$\left\langle F\left(\hat{a}^\dagger(t_\alpha), \hat{a}(t_\beta)\right)\right\rangle_{H_0} = \frac{1}{\mathcal{Z}_0} \int \mathrm{D}\left[\psi^*, \psi\right] e^{\frac{\mathrm{i}}{\hbar} S_0[\psi^*,\psi]} F\left(\psi^*, \psi\right), \tag{4.66}$$ (4.12)

with the boundary conditions

$$\psi^*\left(T_0/2\right) = \psi\left(-T_0/2\right) = 0. \tag{4.67}$$

Green's function (4.47)

$$G^{(n)}\left(\alpha_1 t_1 \ldots \alpha_n t_n; \alpha_1' t_1' \ldots \alpha_n' t_n'\right) = (-\mathrm{i})^n \lim_{T_0 \to (1-\mathrm{i}\eta)\infty} \frac{\left\langle e^{-\frac{\mathrm{i}}{\hbar}\int_{-\frac{T_0}{2}}^{\frac{T_0}{2}} \mathrm{d}t\, V(\psi^*(t),\psi(t))} \psi_{\alpha_1}(t_1)\ldots\psi_{\alpha_n}(t_n)\psi^*_{\alpha_n'}(t_n')\ldots\psi^*_{\alpha_1'}(t_1')\right\rangle_{H_0}}{\left\langle e^{-\frac{\mathrm{i}}{\hbar}\int_{-\frac{T_0}{2}}^{\frac{T_0}{2}} \mathrm{d}t \hat{V}(\hat{a}^\dagger(t),\hat{a}(t))}\right\rangle_{H_0}}. \tag{4.68}$$

Proof We just consider the single-particle Green's function:

$$-\mathrm{i}\lim_{T_0 \to (1-\mathrm{i}\eta)\infty} \frac{\left\langle e^{-\frac{\mathrm{i}}{\hbar}\int_{-\frac{T_0}{2}}^{\frac{T_0}{2}} \mathrm{d}t\, V(\psi^*(t),\psi(t))} \psi_{\alpha_1}(t_1)\psi^*_{\alpha_1'}(t_1')\right\rangle_{H_0}}{\left\langle e^{-\frac{\mathrm{i}}{\hbar}\int_{-\frac{T_0}{2}}^{\frac{T_0}{2}} \mathrm{d}t \hat{V}(\hat{a}^\dagger(t),\hat{a}(t))}\right\rangle_{H_0}} \tag{4.69}$$

$$= -\mathrm{i}\lim_{T_0 \to (1-\mathrm{i}\eta)\infty} \frac{\left\langle \Phi_0 \middle| \hat{T}\left[e^{-\frac{\mathrm{i}}{\hbar}\int_{-\frac{T_0}{2}}^{\frac{T_0}{2}} \mathrm{d}t\, \hat{H}\left(\hat{a}^\dagger(t),\hat{a}(t)\right)} \hat{a}_{\alpha_1}(t_1)\hat{a}^\dagger_{\alpha_1'}(t_1')\right]\middle|\Phi_0\right\rangle}{\left\langle \Phi_0 \middle| e^{-\mathrm{i}\hat{H}T_0/\hbar}\middle|\Phi_0\right\rangle} \tag{4.70}$$

$$= -\mathrm{i}\lim_{T_0 \to (1-\mathrm{i}\eta)\infty} \frac{\left\langle \Phi_0 \middle| e^{-\mathrm{i}\hat{H}T_0/2\hbar}\hat{T}\left[\hat{a}^{(\mathrm{H})}_{\alpha_1}(t_1)\hat{a}^{(\mathrm{H})\dagger}_{\alpha_1'}(t_1')\right] e^{-\mathrm{i}\hat{H}T_0/2\hbar}\middle|\Phi_0\right\rangle}{\left\langle \Phi_0 \middle| e^{-\mathrm{i}\hat{H}T_0/\hbar}\middle|\Phi_0\right\rangle} \tag{4.71}$$

$$= -\mathrm{i}\lim_{T_0 \to (1-\mathrm{i}\eta)\infty} \sum_{lm} \frac{\langle\Phi_0\,|\,\Psi_l\rangle\langle\Psi_m\,|\,\Phi_0\rangle}{|\langle\Phi_0\,|\,\Psi_0\rangle|^2} e^{-\mathrm{i}(E_l+E_m-2E_0)T_0/2}\left\langle\Psi_l\middle|\hat{T}\left[\hat{a}^{(\mathrm{H})}_{\alpha_1}(t_1)\hat{a}^{(\mathrm{H})\dagger}_{\alpha_1'}(t_1')\right]\middle|\Psi_m\right\rangle \tag{4.72}$$

$$\to -\mathrm{i}\left\langle\Psi_0\middle|\hat{T}\left[\hat{a}^{(\mathrm{H})}_{\alpha_1}(t_1)\hat{a}^{(\mathrm{H})\dagger}_{\alpha_1'}(t_1')\right]\middle|\Psi_0\right\rangle \tag{4.73}$$ (2.1)

4.3.2 Diagram Rules

The finite temperature Feynman diagram rules can be adapted for the zero-temperature with the substitutions:

- Time substitutions

$$\int_0^{\hbar\beta}\mathrm{d}\tau \to \int_{-T_0/2}^{T_0/2}\mathrm{d}t,\quad \frac{1}{\hbar\beta}\sum_{\omega_n}\to\int\frac{\mathrm{d}\omega}{2\pi},\quad \hbar\beta\to T_0. \tag{4.74}$$

- The overall factor

$$\frac{(-1/\hbar)^n\zeta^{n_L}}{S}\to\frac{(-\mathrm{i}/\hbar)^n\zeta^{n_L}}{S}. \tag{4.75}$$

- Green's function

$$-\mathcal{G}_{0\alpha}(\tau-\tau')\to\mathrm{i}G_{0\alpha}(t-t'), \tag{4.76}$$

$$-\tilde{\mathcal{G}}_{0\alpha}(\omega_n)\to\mathrm{i}\tilde{G}_{0\alpha}(\omega), \tag{4.77}$$

where G_0 is the real-time free Green's function. (2.8, 4.90)

The expectation value of ground state energy can be obtained by

$$E_0 - W_0 = \lim_{T_0\to\infty}\frac{\mathrm{i}\hbar}{T_0}\sum \text{all connected diagrams}. \tag{4.78}$$ (4.45)

4.3.3 Free Fermion propagators

Particle-hole operators are introduced to deal with the issue that the electron annihilation operators do *not* annihilate $|\Phi_0\rangle$, i.e., $\hat{a}_\alpha |\Phi_0\rangle \neq 0$ for $\epsilon_\alpha \leq \mu$. This is because $|\Phi_0\rangle$ is *not* an empty state but a filled Fermi sea. We introduce

$$\hat{b}_\alpha = \begin{cases} \hat{a}_\alpha & \epsilon_\alpha > \mu \\ \hat{a}_\alpha^\dagger & \epsilon_\alpha \leq \mu \end{cases}. \tag{4.79}$$

$$\hat{K}_0 \equiv \hat{H}_0 - \mu \hat{N} = \sum_{\epsilon_\alpha \leq \mu} (\epsilon_\alpha - \mu) + \sum_\alpha |\epsilon_\alpha - \mu| \, \hat{b}_\alpha^\dagger \hat{b}_\alpha, \tag{4.80}$$

- It satisfies the usual commutation rules of annihilation/creation operators.
- It annihilates the non-interacting ground state: $\hat{b}_\alpha |\Phi_0\rangle = 0$.

Generating functional for free Fermion propagator:

$$\mathscr{G}_0 [J^*, J] = \left\langle e^{\int \mathrm{d}t \left[J_\alpha^*(t) \hat{a}_\alpha(t) + \hat{a}_\alpha^\dagger(t) J_\alpha(t) \right]} \right\rangle_{H_0}, \tag{4.81}$$

$$\mathrm{i}G_0 (\alpha t; \alpha' t') = - \left. \frac{\delta^2 \mathscr{G}_0 [J^*, J]}{\delta J_\alpha^*(t) \delta J_{\alpha'}(t')} \right|_{J^* = J = 0}. \tag{4.82}$$

Free Fermion propagator

$$\mathscr{G}_0 [J^*, J] = \mathscr{G}_0^{(+)} [J^*, J] \, \mathscr{G}_0^{(-)} [J^*, J], \tag{4.83}$$

$$\mathscr{G}_0^{(+)} [J^*, J] = \prod_{\epsilon_\alpha > \mu} \left\langle e^{\int \mathrm{d}t \left[J_\alpha^*(t) \hat{b}_\alpha(t) + \hat{b}_\alpha^\dagger(t) J_\alpha(t) \right]} \right\rangle_{K_0} = \prod_{\epsilon_\alpha > \mu} e^{\sum_{jk} J_{\alpha,j}^* S_{ik}^{(\alpha)-1} J_{\alpha,k}}, \tag{4.84}$$

$$\mathscr{G}_0^{(-)} [J^*, J] = \prod_{\epsilon_\alpha \leq \mu} \left\langle e^{\int \mathrm{d}t \left[J_\alpha^*(t) \hat{b}_\alpha^\dagger(t) + \hat{b}_\alpha(t) J_\alpha(t) \right]} \right\rangle_{K_0} = \prod_{\epsilon_\alpha \leq \mu} e^{\sum_{jk} J_{\alpha,j} S_{ik}^{(\alpha)-1} J_{\alpha,k}^*}. \tag{4.85}$$

$$S^{(\alpha)} = \begin{bmatrix} 1 & 0 & & & 0 & 0 \\ -a & 1 & 0 & & & 0 \\ 0 & -a & 1 & \ddots & & \vdots \\ & 0 & -a & \ddots & & \\ & & 0 & \ddots & 1 & 0 \\ 0 & & & \dots & -a & 1 \end{bmatrix}, \; a = 1 - \mathrm{i} \frac{T_0 \, |\epsilon_\alpha - \mu|}{\hbar M}. \tag{4.86}$$

(3.44)

- For $\epsilon_\alpha > \mu$

$$\mathrm{i}G_0(\alpha t_q; \alpha' t_r) = \delta_{\alpha\alpha'} \left[S^{(\alpha)} \right]_{qr}^{-1} = \delta_{\alpha\alpha'} e^{-\frac{\mathrm{i}}{\hbar}(\epsilon_\alpha - \mu)(t_q - t_r)} \theta(t_q - t_r - 0^+), \tag{4.87}$$

- For $\epsilon_\alpha \leq \mu$

$$\mathrm{i}G_0(\alpha t_q; \alpha' t_r) = -\delta_{\alpha\alpha'} \left[S^{(\alpha)} \right]_{rq}^{-1} = -\delta_{\alpha\alpha'} e^{-\frac{\mathrm{i}}{\hbar}(\epsilon_\alpha - \mu)(t_q - t_r)} \theta(t_r - t_q + 0^+). \tag{4.88}$$

  Note an extra minus sign due to the exchange of J^* and J.

- Complete form:

(2.8)

$$\mathrm{i}G_0(\alpha t; \alpha' t') = \delta_{\alpha\alpha'} e^{-\frac{\mathrm{i}}{\hbar}(\epsilon_\alpha - \mu)(t - t')} \left[\theta(t - t' - \eta) \, (1 - n_\alpha) - \theta(t' - t + \eta) n_\alpha \right], \tag{4.89}$$

  where $n_\alpha = \theta(\mu - \epsilon_\alpha)$.

- Fourier transform:

$$\tilde{G}_{0\alpha}(\omega) = \int \mathrm{d}t G_0(\alpha t, \alpha 0) e^{\mathrm{i}\omega t} = \frac{e^{\mathrm{i}\omega\eta}}{\omega - (\epsilon_\alpha - \mu)/\hbar + \mathrm{i}\eta \mathrm{sgn}(\epsilon_\alpha - \mu)} \tag{4.90}$$

$$= \left[\frac{1 - n_\alpha}{\omega - (\epsilon_\alpha - \mu)/\hbar + \mathrm{i}\eta} + \frac{n_\alpha}{\omega - (\epsilon_\alpha - \mu)/\hbar - \mathrm{i}\eta} \right] e^{\mathrm{i}\omega\eta}. \tag{4.91}$$

  – Fourier transform of $\theta(t)$

$$\theta(\pm t) = \mp \int \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{e^{-\mathrm{i}\omega t}}{\omega \pm \mathrm{i}\eta}. \tag{4.92}$$

4.4 Contour formalism

HJ §4.3

The contour ordered Green's function can also be expressed as path integrals:: (3.38)

$$G_{\mathrm{C}}^{(n)}\left(\alpha_1 t_1 \ldots \alpha_n t_n; \alpha_1' t_1' \ldots \alpha_n' t_n'\right) = (-\mathrm{i})^n \frac{\left\langle e^{-\frac{\mathrm{i}}{\hbar}\int_C \mathrm{d}t\, V(\psi^*(t),\psi(t))} \psi_{\alpha_1}(t_1)\ldots\psi_{\alpha_n}(t_n)\psi^*_{\alpha_n'}(t_n')\ldots\psi^*_{\alpha_1'}(t_1')\right\rangle_0}{\left\langle e^{-\frac{\mathrm{i}}{\hbar}\int_C \mathrm{d}t \hat{V}(\hat{a}^\dagger(t),\hat{a}(t))}\right\rangle_0}. \quad (4.93)$$

Resulting Feynman diagram rules are the same as those for the zero-temperature real-time Green's function, except that the time is defined on the contour shown in Fig. 2.2.

Adiabatic assumption: We assume that the interaction vanishes at $t = -T_0/2 \to -\infty$, and is adiabatically turned on in C_1 and off in C_2. As a result, contributions from the vertical segment C_β vanish in the perturbative expansion. The assumption is plausible for (equilibrium or non-equilibrium) steady state problems. However, it may not be valid for transient problems.

Langreth theorem expresses contour defined quantities in real-time ones. See Table. 4.1 for the rules of translation. In deriving these relations, the contribution from the vertical segment C_β of the contour is ignored, and all quantities are assumed to be in the Keldysh space.

Keldysh space A function $A(t,t')$ belongs to the Keldysh space if it can be written as [26] §5.5

$$A(t,t') = A^\delta(t)\delta(t,t') + \theta(t,t')\,A^>(t,t') + \theta(t',t)\,A^<(t,t'), \quad (4.94)$$

where both t and t' are defined on the contour, $A^\delta(t)$, $A^>(t,t')$ and $A^<(t,t')$ have values independent of the branches of their time arguments, and $\delta(t,t')$ and $\theta(t,t')$ are the δ-function and Heaviside function for the contour, respectively. We note that the δ-function is non-zero only when the two times belong to the same branch of the contour, i.e., $\delta(t^\pm, t'^\mp) = 0$.

The retarded and advanced components are defined by

$$A^{\mathrm{r}}(t,t') = A^\delta(t)\delta(t-t') + \theta(t-t')\left[A^>(t,t') - A^<(t,t')\right], \quad (4.95)$$ (2.59)

$$A^{\mathrm{a}}(t,t') = A^\delta(t)\delta(t-t') - \theta(t'-t)\left[A^>(t,t') - A^<(t,t')\right]. \quad (4.96)$$ (2.60)

Convolution If the two function $A(t,t')$ and $B(t,t')$ are in the Keldysh space, their convolution

$$C(t,t') = \int_C \mathrm{d}t_1 A(t,t_1)\,B(t_1,t') \quad (4.97)$$

is also in the Keldysh space.

Product If the two function $A(t,t')$ and $B(t,t')$ are in the Keldysh space, and *their δ-components A^δ and B^δ are identically zero*, their products

$$C(t,t') = A(t,t')B(t,t'), \quad (4.98)$$

$$D(t,t') = A(t,t')B(t',t) \quad (4.99)$$

are also in the Keldysh space.

4.5 Summary

- To unify the imaginary time (finite temperature) formalism and the real-time (zero temperature) formalism, we introduce the symbol

$$\iota = \begin{cases} -1 & \text{thermal Green's function} \\ \mathrm{i} & \text{real time Green's function} \end{cases}. \quad (4.100)$$

Contour	Real axis
$C = \int_C AB$	$C^< = \int_t [A^{\mathrm{r}} B^< + A^< B^{\mathrm{a}}]$ $C^> = \int_t [A^{\mathrm{r}} B^> + A^> B^{\mathrm{a}}]$ $C^{\mathrm{r}} = \int_t A^{\mathrm{r}} B^{\mathrm{r}}$ $C^{\mathrm{a}} = \int_t A^{\mathrm{a}} B^{\mathrm{a}}$
$D = \int_C ABC$	$D^< = \int_t [A^{\mathrm{r}} B^{\mathrm{r}} C^< + A^{\mathrm{r}} B^< C^{\mathrm{a}} + A^< B^{\mathrm{a}} C^{\mathrm{a}}]$ $D^> = \int_t [A^{\mathrm{r}} B^{\mathrm{r}} C^> + A^{\mathrm{r}} B^> C^{\mathrm{a}} + A^> B^{\mathrm{a}} C^{\mathrm{a}}]$ $D^{\mathrm{r}} = \int_t A^{\mathrm{r}} B^{\mathrm{r}} C^{\mathrm{r}}$ $D^{\mathrm{a}} = \int_t A^{\mathrm{a}} B^{\mathrm{a}} C^{\mathrm{a}}$
$C(t,t') = A(t,t')B(t,t')$	$C^<(t,t') = A^<(t,t')B^<(t,t')$ $C^>(t,t') = A^>(t,t')B^>(t,t')$ $C^{\mathrm{r}}(t,t') = A^>(t,t')B^{\mathrm{r}}(t,t') + A^{\mathrm{r}}(t,t')B^<(t,t')$ $C^{\mathrm{a}}(t,t') = A^>(t,t')B^{\mathrm{a}}(t,t') + A^{\mathrm{a}}(t,t')B^<(t,t')$
$D(t,t') = A(t,t')B(t',t)$	$D^<(t,t') = A^<(t,t')B^>(t',t)$ $D^>(t,t') = A^>(t,t')B^<(t',t)$ $D^{\mathrm{r}}(t,t') = A^<(t,t')B^{\mathrm{a}}(t',t) + A^{\mathrm{r}}(t,t')B^<(t',t)$ $D^{\mathrm{a}}(t,t') = A^<(t,t')B^{\mathrm{r}}(t',t) + A^{\mathrm{a}}(t,t')B^<(t',t)$

Table 4.1: Langreth rules of contour defined quantities. The integral $C = \int AB$ is interpreted as $C(t,t') = \int \mathrm{d}t_1 A(t,t_1)B(t_1,t')$, and similarly for $\int ABC$. All quantities are assumed to be in the Keldysh space and have vanishing δ-components.

- The free Green's function can be written as a unified form:

$$\imath\mathcal{G}_{0\alpha} = e^{(\epsilon_\alpha-\mu)(\tau-\tau')/\imath\hbar}\left[(1+\zeta n_\alpha)\theta(\tau-\tau') + \zeta n_\alpha\theta(\tau'-\tau)\right], \tag{4.101}$$

  where n_α is the occupation number of the state α. For the real-time formalism, $\mathcal{G}_0$ should be interpreted as G_0, and τ as t. In the frequency/momentum domain, the free Green's function has the form:

$$\mathcal{G}_0(\boldsymbol{k},\omega_n) = \frac{1}{\mathrm{i}\omega_n - (\epsilon_{\boldsymbol{k}}-\mu)/\hbar}, \tag{4.102}$$

$$G_0(\boldsymbol{k},\omega) = \frac{1+\zeta n_{\boldsymbol{k}}}{\omega-(\epsilon_{\boldsymbol{k}}-\mu)/\hbar+\mathrm{i}\eta} - \frac{\zeta n_{\boldsymbol{k}}}{\omega-(\epsilon_{\boldsymbol{k}}-\mu)/\hbar-\mathrm{i}\eta}, \tag{4.103}$$

  where ω_n is the Matsubara frequency:

$$\omega_n = \begin{cases} \frac{2\pi n}{\hbar\beta} & \text{(Bosons)} \\ \frac{(2n+1)\pi}{\hbar\beta} & \text{(Fermions)} \end{cases}. \tag{4.104}$$

- The factor associated a vertex/propagator line is summarized in Table 4.2.
- An n-th order diagram has an overall factor:

$$\frac{1}{S}\left(\frac{\iota}{\hbar}\right)^n \zeta^{n_L}, \tag{4.105}$$

  where S is the symmetry factor of the diagram, and n_L is the number of Fermion loops in the diagram.
- In the frequency/momentum representation, there is an extra factor

$$\mathcal{T}_0\mathcal{V} \tag{4.106}$$

  for a connected closed diagram (for calculating the grand potential/ground state energy), where $\mathcal{T}_0$ is the span of the (imaginary) time domain:

$$\mathcal{T}_0 = \begin{cases} \hbar\beta & \text{imaginary time} \\ T_0 & \text{real time} \end{cases}. \tag{4.107}$$

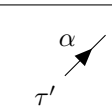
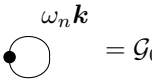
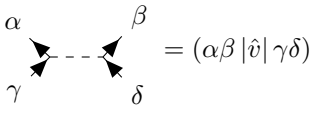
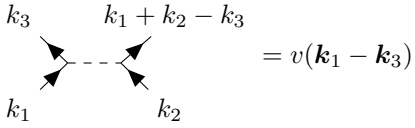
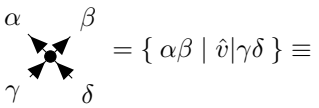
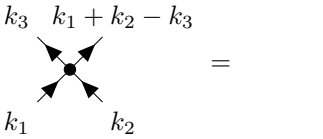
		State/time	Momentum/Frequency
Propagator		 $= \mathcal{G}_{0\alpha}(\tau - \tau')$  $= \mathcal{G}_{0\alpha}(0^-) = \iota^{-1}\zeta n_\alpha$	 $= \mathcal{G}_0(\boldsymbol{k}, \omega_n)$  $= \mathcal{G}_0(\boldsymbol{k}, \omega_n)e^{\mathrm{i}\omega_n\eta}$
Vertex	Feynman	 $= (\alpha\beta \vert \hat{v} \vert \gamma\delta)$	 $= v(\boldsymbol{k}_1 - \boldsymbol{k}_3)$
	Hugenholtz	 $= \{\, \alpha\beta \mid \hat{v} \mid \gamma\delta \,\} \equiv$ $(\alpha\beta \vert \hat{v} \vert \gamma\delta) + \zeta\, (\alpha\beta \vert \hat{v} \vert \delta\gamma)$	 $=$ $v(\boldsymbol{k}_1 - \boldsymbol{k}_3) + \zeta v(\boldsymbol{k}_2 - \boldsymbol{k}_3)$
Sums	$T \neq 0$	$\sum_\alpha \int_0^{\hbar\beta} \mathrm{d}\tau$	$\frac{1}{\hbar\beta} \sum_{\omega_n} \int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^d}$
	$T = 0$	$\sum_\alpha \int_{-T_0/2}^{T_0/2} \mathrm{d}t$	$\int \frac{\mathrm{d}\omega}{2\pi} \int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^d}$

Table 4.2: Diagram rules. For the zero-temperature formalism, $\mathcal{G}_0$ should be interpreted as G_0, ω_n as continuous ω, and τ as t.

The grand potential/ground state energy can be obtained by:

$$\left.\begin{matrix}\Omega - \Omega_0 \\ E - E_0\end{matrix}\right\} = \frac{\iota\hbar}{\mathcal{T}_0} \sum \text{all connected diagrams.} \tag{4.108}$$

- For evaluating Green's functions, an extra factor ζ^P should be incorporated, where P is the permutation of out-going particle lines with respect to incoming particle lines. (4.50)
- A useful formula for summing the Matsubara frequency:

$$\frac{1}{\hbar\beta} \sum_{\omega_n} \frac{e^{\mathrm{i}\omega_n\eta}}{\mathrm{i}\omega_n - x} = -\frac{\zeta e^{\eta x}}{e^{\hbar\beta x} - \zeta} \text{ for } \eta > 0. \tag{4.109}$$

- Determine the symmetry factor:

  Feynman diagram: generate $2n$ self-energy diagrams by successively removing one of propagator lines, and count the number of times that a self-energy diagram occurs.

  Hugenholtz diagram: $S = 2^{n_e} S_D$, where n_e is the number of the equivalent pairs of the propagator lines, S_D is number of times that a self-energy diagram occurs. The self-energy diagrams are generated by successively removing one of *non-equivalent* propagator lines.

  Green's function: $S = 1$ for Feynman diagrams and $S_D = 1$ for Hugenholtz diagrams.

Problems

1. Verify the symmetry factors shown in Eq. (4.24).
2. Determine the expressions of the diagrams shown in Eq. (4.29) and (4.30) in the momentum-frequency domain. How are the second order diagrams corresponded to the unlabeled diagrams shown in Eq. (4.24)?
3. Determine the sum of the direct ring diagrams Eq. (4.25) in the frequency/momentum representation for a homogeneous system.

4. Develop a set of diagram rules for the electron-phonon coupling Eq. (1.83). Assume that the phonon subsystem has the non-interaction Hamiltonian

$$H_0^{\mathrm{ph}} = \sum_{\boldsymbol{q}} \hbar\omega_{\boldsymbol{q}} \hat{c}_{\boldsymbol{q}}^\dagger \hat{c}_{\boldsymbol{q}}. \tag{4.110}$$

Hints:

(a) the EPC Hamiltonian can be rewritten as the form ($M_{-\boldsymbol{q}}^* = M_{\boldsymbol{q}}$):

$$\hat{H}_{\mathrm{el-ph}} = \frac{1}{\sqrt{\mathcal{V}}} \sum_{\boldsymbol{kq}} M_{\boldsymbol{q}} \hat{a}_{\boldsymbol{k}+\boldsymbol{q}}^\dagger \hat{a}_{\boldsymbol{k}} \left(\hat{c}_{\boldsymbol{q}} + \hat{c}_{-\boldsymbol{q}}^\dagger \right). \tag{4.111}$$

(b) One may adopt one of two alternative approaches: (i) Treat $\hat{H}_{\mathrm{el-ph}}$ as $\hat{V}$, and repeat the derivations of the perturbative expansions; (ii) Try to complete the functional integrals over the phonon fields, and obtain an expression analog to the ordinary two-body interaction.

5. The electron self-energy of an electron-phonon coupled system can be written as

$$\Sigma_{\mathrm{ph}}(\boldsymbol{k}, t-t') = \mathrm{i} \sum_{\boldsymbol{q}} |M_{\boldsymbol{q}}|^2 \, G(\boldsymbol{k}-\boldsymbol{q}, t-t') D(\boldsymbol{q}, t-t'), \tag{4.112}$$

where G is the free-electron Green's function and D is proportional to the density correlation function (see Problem 3, §2), and the time is defined on the contour.

(a) Determine the real-time form of the self-energy $\Sigma_{\mathrm{ph}}^{\mathrm{r}}(\boldsymbol{k}, t-t')$ by applying the Langreth theorem.

(b) Relate G and D with their respective spectral functions, and obtain an expression for $\tilde{\Sigma}_{\mathrm{ph}}^{\mathrm{r}}(\boldsymbol{k}, \omega)$.

Chapter 5

Effective action theory and energy functionals

In the effective action theory, we introduce an energy (grand potential) *functional of the Green's function*. Within the framework, determining the Green's function becomes the problem of finding the stationary point of the functional. In principle, one can determine the Green's function *exactly* as long as we know the exact form of the functional. In the real world, however, one has to rely on approximations:

- Perturbative construction
  - self-consistent re-summation of diagrams (conserving approximation)
  - integral equations (Dyson equation and GW approximation)
- Empirical approaches for limiting cases
  - Landau-Fermi liquid theory
  - Density functional theory
  - Dynamic mean-field theory (DMFT)

We will present the formalism in terms of the thermal Green's function. By using the notations introduced in §4.5, the formalism can also be applied to the real-time Green's function (and the contour Green's function).

5.1 Effective action

The effective action is defined as follows:

1. Introduce an **external source** coupling to the system:

$$S_{\text{ext.}}[\psi] = \imath^{-2} \sum_{\alpha\beta} \int \mathrm{d}\tau_1 \mathrm{d}\tau_2 \psi^*_\alpha(\tau_1)\psi_\beta(\tau_2)\phi_{\alpha\beta}(\tau_1,\tau_2). \tag{5.1}$$

   The particular choice of the external source will give rise to a functional of the *Green's function and two-particle irreducible vertices*. Depending on physical circumstances interested in, other choices are also possible:

   Linear source

$$S_{\text{ext.}} = \imath^{-2} \sum_{\alpha} \int \mathrm{d}\tau \left[J^*_\alpha(\tau)\psi_\alpha(\tau) + \psi^*_\alpha(\tau)J_\alpha(\tau)\right]. \tag{5.2}$$

   For Fermions, $J(\tau)$ is a Grassmann function. This will give rise to a functional of $\langle\psi_\alpha\rangle$ and one-particle irreducible vertices. NO§2.4

Pairing source

$$S_{\text{ext.}} = \iota^{-2} \sum_{\alpha\beta} \int \mathrm{d}\tau_1 \mathrm{d}\tau_2 \left[\psi^*_\alpha(\tau_1)\psi^*_\beta(\tau_2)\Delta_{\alpha\beta}(\tau_1,\tau_2) + \text{c.c.}\right]. \tag{5.3}$$

The source could emerge in a superconducting system. It will give rise to a functional of the abnormal Green's function

$$\mathcal{F}\left(\alpha\tau, \alpha'\tau'\right) = -\left\langle \hat{T}\left[\hat{a}^{(\mathrm{H})}_\alpha\left(\tau\right)\hat{a}^{(\mathrm{H})}_{\alpha'}\left(\tau'\right)\right]\right\rangle. \tag{5.4}$$

Mixed source Different kinds of the sources can be mixed. For instance, to describe a superconducting system, one needs to introduce both the ordinary source and the pairing source. A theory incorporating both the linear source and the bilinear source can be found in Ref. [6].

2. Determine the **partition function** in the presence of the external source:

$$\begin{aligned} Z\left[\phi\right] &= \int \mathrm{D}\left[\psi,\psi^*\right] \exp\left[\frac{\iota}{\hbar}\left(S + S_{\text{ext.}}\right)\right] \\ &= Z\left\langle \exp\left[\frac{1}{\iota\hbar}\int \mathrm{d}\tau_1\mathrm{d}\tau_2 \sum_{\alpha\beta}\psi^*_\alpha(\tau_1)\psi_\beta(\tau_2)\phi_{\alpha\beta}(\tau_1,\tau_2)\right]\right\rangle, \end{aligned} \tag{5.5}$$

where we define the average as

$$\left\langle F\left(\psi^*,\psi\right)\right\rangle = \frac{1}{Z}\int \mathrm{D}\left[\psi,\psi^*\right] F\left(\psi^*,\psi\right) \exp\left(\frac{\iota}{\hbar}S\right). \tag{5.6}$$

Generating functional

$$\mathscr{G}\left[\phi\right] \equiv \frac{Z\left[\phi\right]}{Z} = \left\langle \exp\left[\frac{1}{\iota\hbar}\int \mathrm{d}\tau_1\mathrm{d}\tau_2 \sum_{\alpha\beta}\psi^*_\alpha(\tau_1)\psi_\beta(\tau_2)\phi_{\alpha\beta}(\tau_1,\tau_2)\right]\right\rangle. \tag{5.7}$$

3. Determine the grand potential or the **connected generating functional**:

$$W\left[\phi\right] \equiv \ln \mathscr{G}\left[\phi\right] + C \equiv -\beta\left(\Omega\left[\phi\right] - \Omega_0\right), \tag{5.8}$$

where $C \equiv \ln Z - \ln Z_0$, [1] and Ω_0 (Z_0) is the grand potential (partition function) of the system at the non-interacting limit.

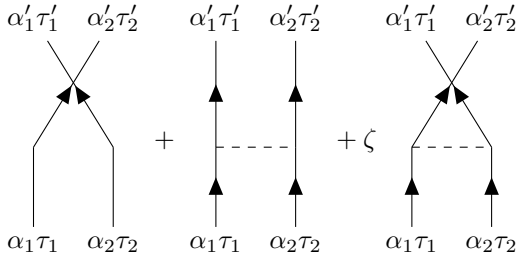
4. The Green's functions can be generated by the generating functional by

$$\mathcal{G}^{(n)}\left(\alpha_1\tau_1,\ldots\alpha_n\tau_n;\alpha'_1\tau'_1,\ldots\alpha'_n\tau'_n\right) = \left(\zeta\hbar\right)^n \left.\frac{\delta^n\mathscr{G}\left[\phi\right]}{\delta\phi_{\alpha'_1\alpha_1}\left(\tau'_1,\tau_1\right)\ldots\delta\phi_{\alpha'_n\alpha_n}\left(\tau'_n,\tau_n\right)}\right|_{\phi\to 0}. \tag{5.9}$$

The connected generating functional generates the *connected Green's functions* [2]:

$$\mathcal{G}^{(n)}_{\text{c}}\left(\alpha_1\tau_1,\ldots\alpha_n\tau_n;\alpha'_1\tau'_1,\ldots\alpha'_n\tau'_n\right) = \left(\zeta\hbar\right)^n \left.\frac{\delta^n W\left[\phi\right]}{\delta\phi_{\alpha'_1\alpha_1}\left(\tau'_1,\tau_1\right)\ldots\delta\phi_{\alpha'_n\alpha_n}\left(\tau'_n,\tau_n\right)}\right|_{\phi\to 0}. \tag{5.10}$$

The cumulant expansion leads to

$\mathcal{G}^{(2)}_{\text{c}} =$  (5.11)

[1] The particular choice of the constant is to accommodate with the construction of the Luttinger-Ward functional shown in §5.2.2.

[2] Note that the connected Green's function defined here is different from that defined in NO Eq. (2.154) by using linear sources.

$$\mathcal{G}^{(2)}\left(12;1'2'\right)=\mathcal{G}_{\mathrm{c}}^{(2)}\left(12;1'2'\right)+\mathcal{G}(11')\mathcal{G}(22'), \tag{5.12}$$

where $\mathcal{G}(11')\equiv\mathcal{G}^{(1)}(1;1')$, and the arguments are abbreviated as numbers: $1\equiv\alpha_1\tau_1$, $1'\equiv\alpha_1'\tau_1'$.

5. We define the **conjugate field** with respect to ϕ as

$$\mathcal{G}\left[\phi\right]\left(11'\right)=\zeta\hbar\frac{\delta W\left[\phi\right]}{\delta\phi\left(1'1\right)}, \tag{5.13}$$

which is nothing but the single-particle Green's function *in the presence of the external source* ϕ. The relation map ϕ to $\mathcal{G}[\phi]$.

6. We define the **effective action** (**Baym–Kadanoff functional**) by applying the Legendre transformation:

$$\Gamma\left[\mathcal{G}\right]=-\left\{W\left[\phi\right]-\sum_{11'}\frac{\delta W\left[\phi\right]}{\delta\phi\left(1'1\right)}\phi\left(1'1\right)\right\}=-W\left[\phi\right]+\frac{\zeta}{\hbar}\mathrm{Tr}\left[\mathcal{G}\phi\right] \tag{5.14}$$

$$\equiv-W\left[\phi\right]+\frac{\zeta}{\hbar}\sum_{\alpha\alpha'}\int_0^{\hbar\beta}\mathrm{d}\tau\mathrm{d}\tau'\,\mathcal{G}_{\alpha\alpha'}(\tau,\tau')\phi_{\alpha'\alpha}(\tau',\tau) \tag{5.15}$$

In defining the functional, we assume that the map $\phi\to\mathcal{G}[\phi]$ defined by Eq. (5.13) is *invertible*, i.e., we have a map $\mathcal{G}\to\phi[\mathcal{G}]$.

Why?

- It assigns a grand-potential/free energy to the *physical state/order parameter* of the system, and gives rise to a variational principle.
- It has better analytic properties than $W[\phi]$ and thus be preferable to approximate.
- It provides a unified foundation for constructing various approximations consistently.
- One may devise non-perturbative or empirical approaches for constructing the functional.

7. With the functional, we have:

$$\frac{\delta\Gamma\left[\mathcal{G}\right]}{\delta\mathcal{G}(1'1)}=\frac{\zeta}{\hbar}\phi\left(11'\right). \tag{5.16}$$

In the absence of the external source, it yields the **variational principle**:

$$\delta\Gamma\left[\mathcal{G}\right]=0, \tag{5.17}$$

i. e., the physical Green's function is the stationary point of the effective action .

8. We introduce the **Luttinger-Ward functional** $\Phi\left[\mathcal{G}\right]$ to characterize the effect of the interaction. It is defined by the decomposition

$$\Gamma\left[\mathcal{G}\right]=\Gamma_0\left[\mathcal{G}\right]-\Phi\left[\mathcal{G}\right], \tag{5.18}$$

where $\Gamma_0\left[\mathcal{G}\right]$ is the effective action of a noninteracting system.

Free effective action for a non-interacting system:

$$W_0[\phi]=-\zeta\mathrm{Tr}\left[\ln\left(-\mathcal{G}^{-1}\right)-\ln\left(-\mathcal{G}_0^{-1}\right)\right]=\zeta\mathrm{Tr}\left[\ln\left(\mathcal{G}_0^{-1}\mathcal{G}\right)\right], \tag{5.19}$$ (3.49)

$$\mathcal{G}_0^{-1}\equiv-\frac{\partial}{\partial\tau}-\frac{\hat{h}_0-\mu}{\hbar}, \tag{5.20}$$

$$\mathcal{G}^{-1}=-\frac{\partial}{\partial\tau}-\frac{\hat{h}_0+\phi-\mu}{\hbar}=\mathcal{G}_0^{-1}-\frac{\phi}{\hbar}, \tag{5.21}$$

where $\mathcal{G}_0$ and $\mathcal{G}$ are the Green's functions in the absence and presence of the external source ϕ, respectively, and $\hat{h}_0$ is the single-particle operator defining $\hat{H}_0$ (e.g., $-(\hbar^2/2m)\nabla^2$). Equation (5.21) also defines a map from ϕ to $\mathcal{G}$: $\phi\left[\mathcal{G}\right]=\hbar\left(\mathcal{G}_0^{-1}-\mathcal{G}^{-1}\right)$. By inserting the relation into Eq. (5.14), we obtain the non-interacting effective action functional:

$$\zeta\Gamma_0\left[\mathcal{G}\right]=-\mathrm{Tr}\left[\ln\mathcal{G}_0^{-1}\mathcal{G}\right]+\mathrm{Tr}\left[\mathcal{G}_0^{-1}\mathcal{G}-I\right]. \tag{5.22}$$

Energy functional is proportional to the effective action functional

$$\Omega[\mathcal{G}] - \Omega_0 \equiv \frac{1}{\beta}\Gamma = -\frac{\zeta}{\beta}\left\{\mathrm{Tr}\left[\ln \mathcal{G}_0^{-1}\mathcal{G}\right] - \mathrm{Tr}\left[\mathcal{G}_0^{-1}\mathcal{G} - I\right]\right\} - \frac{1}{\beta}\Phi[\mathcal{G}] \tag{5.23}$$

$$= -\frac{\zeta}{\beta}\sum_{\boldsymbol{k}}\sum_{\omega_n}\left\{\ln \mathcal{G}_0^{-1}(\boldsymbol{k},\omega_n)\,\mathcal{G}(\boldsymbol{k},\omega_n) - \mathcal{G}_0^{-1}(\boldsymbol{k},\omega_n)\,\mathcal{G}(\boldsymbol{k},\omega_n) + 1\right\} - \frac{1}{\beta}\Phi[\mathcal{G}]\,. \tag{5.24}$$

At the zero temperature, the ground state energy can be similarly defined as a functional of the *real-time* Green's function: (4.78)

$$E[G] - W_0 = \frac{\mathrm{i}\hbar}{T_0}\zeta\left\{\mathrm{Tr}\left[\ln G_0^{-1}G\right] - \mathrm{Tr}\left[G_0^{-1}G - I\right]\right\} + \frac{\mathrm{i}\hbar}{T_0}\Phi[G] \tag{5.25}$$

$$= \mathrm{i}\hbar\zeta\sum_{\boldsymbol{k}}\int\frac{\mathrm{d}\omega}{2\pi}\left\{\ln\left[G_0^{-1}(\boldsymbol{k},\omega)\,G(\boldsymbol{k},\omega)\right] - G_0^{-1}(\boldsymbol{k},\omega)\,G(\boldsymbol{k},\omega) + 1\right\} + \frac{\mathrm{i}\hbar}{T_0}\Phi[G]\,, \tag{5.26}$$

where W_0 is the ground state energy of the system at the free limit. GV A13

5.2 Irreducible diagrams and integral equations NO§2.4

Based on the functional, one can derive a set of *exact* self-consistent integral equations. The Luttinger-Ward functional can be constructed approximately by choosing a set of diagrams. It leads to practical calculation schemes such as the GW approximation.

Vertex functions are defined by

$$\Pi^{(n)}(\alpha_1\tau_1,\ldots\alpha_n\tau_n;\alpha_1'\tau_1',\ldots\alpha_n'\tau_n') = \zeta^n\left.\frac{\delta^n\Gamma[\mathcal{G}]}{\delta\mathcal{G}_{\alpha_1'\alpha_1}(\tau_1',\tau_1)\ldots\delta\mathcal{G}_{\alpha_n'\alpha_n}(\tau_n',\tau_n)}\right|_{\mathcal{G}\to\mathcal{G}_{\mathrm{phy.}}}. \tag{5.27}$$

Based on the analyses of the vertex functions in successive orders. one may derive a set of self-consistent integral equations.

5.2.1 Self-energy and Dyson's equation

In the absence of the external source,

$$\Pi^{(1)} = \zeta\frac{\delta\Gamma[\mathcal{G}]}{\delta\mathcal{G}} = 0. \tag{5.28}$$ (5.17)

where $\mathcal{G} = \mathcal{G}_{\mathrm{phy.}}$ is implied. With the decomposition Eq. (5.18), we have

$$\Pi^{(1)}(11') \equiv \zeta\frac{\delta\Gamma[\mathcal{G}]}{\delta\mathcal{G}(1'1)} = \left[\mathcal{G}_0^{-1}\right](11') - \left[\mathcal{G}^{-1}\right](11') - \zeta\frac{\delta\Phi[\mathcal{G}]}{\delta\mathcal{G}(1'1)} = 0, \tag{5.29}$$

where we make use of the matrix derivative identity [23](49)

$$\frac{\delta\mathrm{Tr}\ln\mathcal{G}}{\delta\mathcal{G}(1'1)} = \frac{\delta\ln(\det\mathcal{G})}{\delta\mathcal{G}(1'1)} = \left[\mathcal{G}^{-1}\right](11'). \tag{5.30}$$

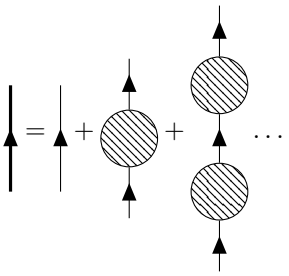
Proper self energy functional is defined to be

$$\frac{\Sigma[\mathcal{G}](11')}{\hbar} = \zeta\frac{\delta\Phi[\mathcal{G}]}{\delta\mathcal{G}(1'1)}. \tag{5.31}$$

Dyson equation:

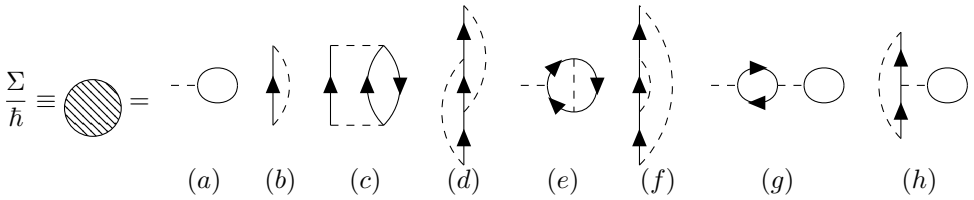
$$[\mathcal{G}]^{-1} = [\mathcal{G}_0]^{-1} - \frac{\Sigma[\mathcal{G}]}{\hbar}, \tag{5.32}$$ (4.53)

$$\mathcal{G} = \mathcal{G}_0 + \frac{1}{\hbar}\mathcal{G}_0\Sigma\mathcal{G}_0 + \frac{1}{\hbar^2}\mathcal{G}_0\Sigma\mathcal{G}_0\Sigma\mathcal{G}_0 + \ldots. \tag{5.33}$$



(5.34)

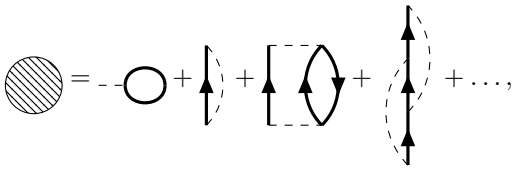
Diagrams of the proper self-energy are one-particle irreducible, i.e., they cannot be separated into two parts by cutting a particle line:



(5.35) (4.52)

Skeleton diagrams are diagrams that cannot be generated from lower order diagrams by inserting self-energy blobs in particle lines: (a–d) are skeleton diagrams, (e–h) are not.

- Alternative definition: all two-particle irreducible diagrams, i.e., the diagrams which cannot be separated by cutting two particle lines.
- With skeleton diagrams, we can construct a *self-consistent equation* for Σ (or $\mathcal{G}$):

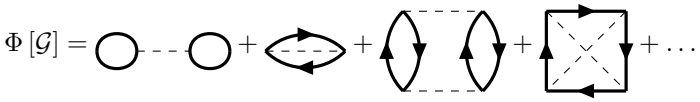


(5.36)

where the bold lines represent the Green's function $\mathcal{G}$ (instead of $\mathcal{G}_0$).

5.2.2 Perturbative construction of the Luttinger-Ward functional

The diagrams of the Luttinger-Ward functional can be constructed from the self-energy skeleton diagrams Eq. (5.36) by applying Eq. (5.31). They are *closed*, *bold*, *two-particle irreducible* (skeleton) diagrams:



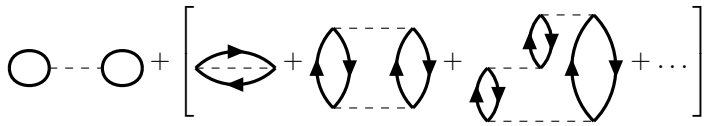
(5.37)

- Derivative with respect to $\mathcal{G}$ is to remove successively one of the particle propagators and append a factor ζ. The latter is due to the fact that removing one propagator will reduce n_L by one. It should give rise to the skeleton diagrams of the self-energy Eq. (5.36). (5.31)
- Rules for unlabeled Feynman diagrams should be applied. [3] Note that the symmetry factors S is automatically cancelled when applying the derivative which generates S copies for each of distinct self-energy diagrams.
- From Eq. (5.31), $\Phi[\mathcal{G}]$ is determined only up to a constant independent of $\mathcal{G}$. By combining GV (A13.9, A13.14), one can show that the constant is independent of the strength of the interaction. Therefore, we can set the constant to zero.

[3] The symmetry factor suggested by Luttinger and Ward is $S = 2n$ [17] (see also GV §6.3.3). This is not true for high order diagrams with $n > 2$, for instance,  .

Conserving approximation derives the self-energy and high order vertices from an approximated Luttinger-Ward functional via derivatives. The approximation will be automatically consistent with conservation laws on particle number, momentum, and energy [3].

GW approximation approximates the Luttinger-Ward functional with a subset of diagrams:

$$\Phi_{\mathrm{GW}}[\mathcal{G}] =$$  (5.38)

$$= \bigcirc\!\!-\!\!-\!\!\bigcirc - \frac{1}{2}\mathrm{Tr}\left[\ln\left(1-\frac{\iota\zeta}{\hbar}v\mathcal{G}\mathcal{G}\right)\right]. \tag{5.39}$$ (4.25)

Besides the Hartree (first) and Fock (second) terms, they include direct ring diagrams which are the most diverging diagrams of the perturbative expansion for a system with the Coulomb interaction. §6.1.2

5.2.3 Second order vertex function

By applying Eq. (5.27) and (5.29), we have

$$\zeta\Pi^{(2)}(12,1'2') = \frac{\delta\Pi^{(1)}(11')}{\delta\mathcal{G}(2'2)} = \left[\mathcal{G}^{-1}\right](12')\left[\mathcal{G}^{-1}\right](21') - \zeta\frac{\delta^2\Phi[\mathcal{G}]}{\delta\mathcal{G}(1'1)\delta\mathcal{G}(2'2)}, \tag{5.40}$$

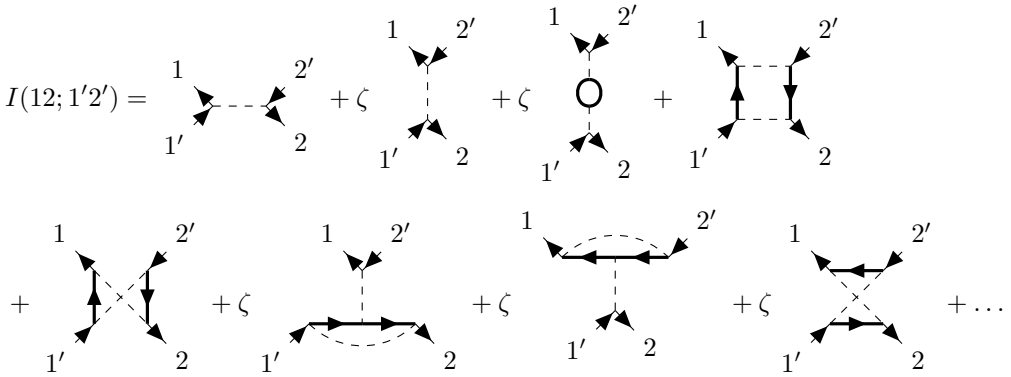
where the first term is contributed by $-\delta\mathcal{G}^{-1}(11')/\delta\mathcal{G}(2'2)$, and we make use the matrix derivative identity [23](60)

$$\frac{\delta\left[\mathcal{G}^{-1}\right](11')}{\delta\mathcal{G}(2'2)} = -\left[\mathcal{G}^{-1}\right](12')\left[\mathcal{G}^{-1}\right](21'). \tag{5.41}$$

Irreducible electron-hole interaction We define the irreducible interaction I in the direct particle-hole channel:

$$I(12;1'2') = \left(\frac{\iota}{\hbar}\right)^{-1}\frac{\delta^2\Phi[\mathcal{G}]}{\delta\mathcal{G}(1'1)\delta\mathcal{G}(2'2)} = \frac{\zeta}{\iota}\frac{\delta\Sigma(11')}{\delta\mathcal{G}(2'2)}. \tag{5.42}$$

It includes all scattering diagrams that are two-particle irreducible in the direct particle-hole channel:

$$I(12;1'2') =$$  (5.43)

It can be interpreted as the effective interaction between a particle and a hole.

Two particle Dyson Equation We have the identity

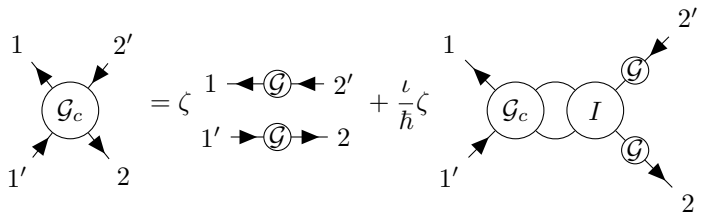
$$\delta(12)\delta(1'2') = \frac{\delta\mathcal{G}(11')}{\delta\mathcal{G}(22')} = \int \mathrm{d}3\mathrm{d}3'\frac{\delta\mathcal{G}(11')}{\delta\phi(3'3)}\frac{\delta\phi(3'3)}{\delta\mathcal{G}(22')}, \tag{5.44}$$

$$= \hbar^2\int \mathrm{d}3\mathrm{d}3'\frac{\delta^2 W[\phi]}{\delta\phi(3'3)\delta\phi(1'1)}\frac{\delta^2\Gamma[\mathcal{G}]}{\delta\mathcal{G}(22')\delta\mathcal{G}(33')}, \tag{5.45}$$ (5.13, 5.16)

$$\equiv \int \mathrm{d}3\mathrm{d}3'\,\mathcal{G}_c^{(2)}(13;1'3')\,\Pi^{(2)}(3'2',32). \tag{5.46}$$ (5.10, 5.27)

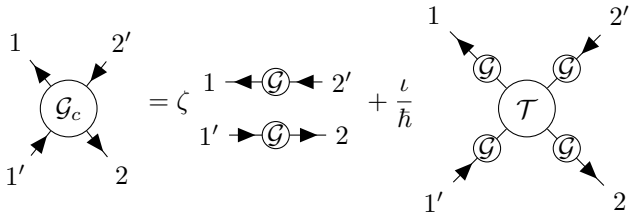
Combining it with Eq. (5.40), we have

$$\mathcal{G}_c^{(2)}(12;1'2') = \zeta\mathcal{G}(12')\mathcal{G}(21') + \frac{\iota}{\hbar}\zeta\int \mathrm{d}3\mathrm{d}3'\mathrm{d}4\mathrm{d}4'\mathcal{G}_c^{(2)}(13;1'3')I(3'4';34)\mathcal{G}(24')\mathcal{G}(42'). \tag{5.47}$$



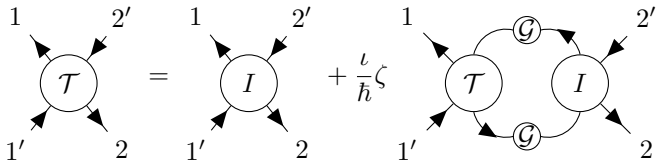
(5.48)

Scattering amplitude $\mathcal{T}$ between a pair of particle and hole is defined by [4]:



(5.49) NO (2.188a)

Bethe-Salpeter equation in the particle-hole channel relates the scattering amplitude with the irreducible interaction I:



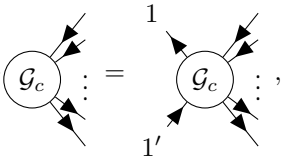
(5.50)

$$\mathcal{T}(12;1'2') = I(12;1'2') + \frac{\iota}{\hbar}\zeta\int \mathrm{d}3\mathrm{d}3'\mathrm{d}4\mathrm{d}4'\mathcal{T}(13;1'3')\,\mathcal{G}(4'3)\,\mathcal{G}(3'4)\,I(42;4'2'). \tag{5.51}$$

5.2.4 Higher order equations

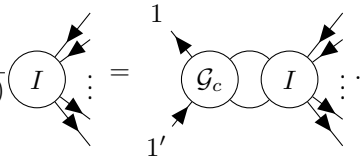
Higher order equations can be obtained by successively applying the derivative $\delta/\delta\phi$ to Eq. (5.47) or (5.48). Useful identities:

$$\zeta\hbar\frac{\delta\mathcal{G}_c^{(n)}}{\delta\phi} = \mathcal{G}_c^{(n+1)}, \quad \zeta\hbar\frac{\delta}{\delta\phi(1'1)}$$



(5.52) (5.13)

$$\zeta\hbar\frac{\delta I^{(n)}}{\delta\phi} = I^{(n+1)} \star \mathcal{G}_c^{(2)}, \quad \zeta\hbar\frac{\delta}{\delta\phi(1'1)}$$



(5.53) (5.42)

where $I^{(n)} \equiv (\iota/\hbar)^{-1}\delta^n\Phi[\mathcal{G}]/\delta\mathcal{G}(1'1)\ldots\delta\mathcal{G}(n'n)$ denotes the n-body effective interaction.

[4] Note that $\mathcal{T}$ is denoted as Γ in many books. It is actually the T-matrix of two-particle scattering.

5.2.5 Keldysh Formulation

HJ§5.2

For the case that the real-time formalism is desirable, the contour formalism should be employed. The Dyson equation Eq. (5.32) can be generalized for the contour Green's function:

$$G_{\mathrm{C}} = G_{\mathrm{C}0} + \frac{1}{\hbar} G_{\mathrm{C}0} \Sigma_{\mathrm{C}} G_{\mathrm{C}}. \tag{5.54}$$

Note that one should interpret all quantities as matrices, and the multiplications as matrix multiplications/convolutions.

By applying the Langreth rules, the equation can be expressed in terms of the real-time Green's functions: Tab. 4.1

Retarded/Advanced Green's function

$$G^{\mathrm{r/a}} = G_0^{\mathrm{r/a}} + \frac{1}{\hbar} G_0^{\mathrm{r/a}} \Sigma^{\mathrm{r/a}} G^{\mathrm{r/a}}, \tag{5.55}$$

$$G^{\mathrm{r/a}} = \left(I - \frac{1}{\hbar} G_0^{\mathrm{r/a}} \Sigma^{\mathrm{r/a}} \right)^{-1} G_0^{\mathrm{r/a}}. \tag{5.56}$$

Less Green's function

$$G^{<} = G^{\mathrm{r}} \frac{\Sigma^{<}}{\hbar} G^{\mathrm{a}} + \left(I + \frac{1}{\hbar} G^{\mathrm{r}} \Sigma^{\mathrm{r}} \right) G_0^{<} \left(I + \frac{1}{\hbar} \Sigma^{\mathrm{a}} G^{\mathrm{a}} \right). \tag{5.57}$$

It has a non-trivial form.

Poof:

- By applying the Langreth rules:

$$G^{<} = G_0^{<} + G_0^{\mathrm{r}} \frac{\Sigma^{r}}{\hbar} G^{<} + G_0^{\mathrm{r}} \frac{\Sigma^{<}}{\hbar} G^{\mathrm{a}} + G_0^{<} \frac{\Sigma^{\mathrm{a}}}{\hbar} G^{\mathrm{a}}. \tag{5.58}$$

- Solve the equation:

$$G^{<} = \left(I - \frac{1}{\hbar} G_0^{\mathrm{r}} \Sigma^{\mathrm{r}} \right)^{-1} \left(G_0^{<} + G_0^{\mathrm{r}} \frac{\Sigma^{<}}{\hbar} G^{\mathrm{a}} + G_0^{<} \frac{\Sigma^{\mathrm{a}}}{\hbar} G^{\mathrm{a}} \right) \tag{5.59}$$

$$= G^{\mathrm{r}} \frac{\Sigma^{<}}{\hbar} G^{\mathrm{a}} + \left(I - \frac{1}{\hbar} G_0^{\mathrm{r}} \Sigma^{\mathrm{r}} \right)^{-1} G_0^{<} \left(I + \frac{\Sigma^{\mathrm{a}}}{\hbar} G^{\mathrm{a}} \right). \tag{5.60}$$

(5.56)

- We have

$$\left(I - \frac{1}{\hbar} G_0^{\mathrm{r}} \Sigma^{\mathrm{r}} \right)^{-1} = G^{\mathrm{r}} \left(G_0^{\mathrm{r}} \right)^{-1} = \left(G_0^{\mathrm{r}} + \frac{1}{\hbar} G^{\mathrm{r}} \Sigma^{\mathrm{r}} G_0^{\mathrm{r}} \right) \left(G_0^{\mathrm{r}} \right)^{-1} = I + \frac{1}{\hbar} G^{\mathrm{r}} \Sigma^{\mathrm{r}}. \tag{5.61}$$

After inserting the identity to Eq. (5.60), we reach the final form.

5.2.6 Other sources

Linear source can also be used to define a set of vertex functions. It results in a set of tree diagrams and corresponding equations that relate Green's functions and vertex functions. This is particularly useful for the renormalization theory in which divergences can be isolated in a small number of low order vertex functions. See NO§2.4.

Pairing field Δ and Δ^* can also be included as external sources. The resulting Bethe-Salpeter equation will be in the particle-particle channel. The generalization is necessary for treating superconducting systems. GV§6.3.4

5.3 Landau Fermi-liquid theory

GV§8

Motivation: Physical properties of metals/Helium III liquid suggest that electrons/Helium III atoms behave like independent particles, even though the interaction in these systems are rather strong.

Basic idea: a low lying excited state of an interacting Fermion system can be constructed by:

1. preparing a low lying excited state of non-interacting ideal Fermi-liquid (e.g., adding an electron/hole above/below the Fermi level);
2. switching on the interaction *suitably slowly*: it should be switched on before the state is totally damped –It is possible because an electron/hole near the Fermi surface damps very slowly: for 3D systems, the damping rate is proportional to $(k-k_F)^2$.

Energy functional: The energy of an interacting Fermion system is a functional of the occupation number $\mathcal{N}_{\boldsymbol{k}}$ of *the non-interacting ideal* system:

- According to Eq. (5.26), the energy is a functional of G.
- It is assumed that G can be determined by the perturbative expansion shown in §4.3.
- The perturbative expansion in §4.3 is constructed from $|\Phi_0\rangle$ –the non-interacting ground state, i.e., a filled Fermi sea. To establish the Landau Fermi-liquid theory, one needs to assume that the expansion is also valid for low excited states of the non-interacting system, i.e., $|\Phi_0\rangle \to |\Phi_n\rangle$.
- The Green's function G_0 for a low excited state can be written as

$$G_0(\boldsymbol{k},\omega) = \frac{1-\mathcal{N}_{\boldsymbol{k}}}{\omega-(\epsilon_{\boldsymbol{k}}-\mu)/\hbar+\mathrm{i}\eta} + \frac{\mathcal{N}_{\boldsymbol{k}}}{\omega-(\epsilon_{\boldsymbol{k}}-\mu)/\hbar-\mathrm{i}\eta}, \tag{5.62}$$

  (4.90)

  where $\{\mathcal{N}_{\boldsymbol{k}}\}$ is the momentum occupation number of a low excited state of the *non-interacting* system. It is *not* the momentum occupation number $n_{\boldsymbol{k}} = \left\langle \hat{a}^\dagger_{\boldsymbol{k}} \hat{a}_{\boldsymbol{k}} \right\rangle$ of the interacting system.
- G is a functional of G_0, provided that the perturbative expansion converges. As a result, the energy is a functional of $\mathcal{N}_{\boldsymbol{k}}$.

5.3.1 Phenomenological approach

GV§8.3

For small deviation from the ground state configuration $\mathcal{N}^{(0)}_{\boldsymbol{k}\sigma} = \theta(k_F-k)$, we can always expand the energy functional to the second order of $\delta\mathcal{N}_{\boldsymbol{k}\sigma} = \mathcal{N}_{\boldsymbol{k}\sigma} - \mathcal{N}^{(0)}_{\boldsymbol{k}\sigma}$:

$$E[\mathcal{N}] = E_0 + \sum_{\boldsymbol{k}\sigma} \mathcal{E}_{\boldsymbol{k}\sigma}\delta\mathcal{N}_{\boldsymbol{k}\sigma} + \frac{1}{2}\sum_{\boldsymbol{k}\sigma,\boldsymbol{k}'\sigma'} f_{\boldsymbol{k}\sigma,\boldsymbol{k}'\sigma'}\delta\mathcal{N}_{\boldsymbol{k}\sigma}\delta\mathcal{N}_{\boldsymbol{k}'\sigma'}. \tag{5.63}$$

Effective mass: $\mathcal{E}_{\boldsymbol{k}\sigma}$ is the quasiparticle energy, the energy required to add/remove a particle into/from the ground state of the system. Near the Fermi surface:

$$\mathcal{E}_{\boldsymbol{k}\sigma} \approx \mu + \hbar v_F^*(k-k_F), \tag{5.64}$$

where v_F^* is the effective Fermi velocity, and defines the effective mass by:

$$v_F^* = \frac{\hbar k_F}{m^*}. \tag{5.65}$$

Note that the effective mass could be *very different* from the bare electron mass.

Quasiparticle density of states is modified by the effective mass:

$$N^*(0) = \frac{m^*}{m}N(0). \tag{5.66}$$

It can be determined by measuring the low-temperature heat capacity:

GV§8.3.2

$$c_v(T) = \frac{\pi^2}{3}N^*(0)k_{\mathrm{B}}^2 T. \tag{5.67}$$

Proof

1. One first needs to generalize the theory to the finite temperature. The entropy of the non-interacting system is

$$S = -k_{\mathrm{B}} \sum_{\boldsymbol{k}\sigma} \left[\mathcal{N}_{\boldsymbol{k}\sigma} \ln \mathcal{N}_{\boldsymbol{k}\sigma} + (1 - \mathcal{N}_{\boldsymbol{k}\sigma}) \ln (1 - \mathcal{N}_{\boldsymbol{k}\sigma}) \right], \tag{5.68}$$

   which is *not* changed when adiabatically switching on the interaction. By minimizing the grand potential

$$\Omega \left[\mathcal{N} \right] = E \left[\mathcal{N} \right] - TS - \mu \sum_{\boldsymbol{k}\sigma} \mathcal{N}_{\boldsymbol{k}\sigma}, \tag{5.69}$$

   we obtain

$$\mathcal{N}_{\boldsymbol{k}\sigma} = \left\{ \exp \left[\beta \left(\tilde{\mathcal{E}}_{\boldsymbol{k}\sigma} - \mu \right) \right] + 1 \right\}^{-1}. \tag{5.70}$$

   Note that it is determined by $\tilde{\mathcal{E}}_{\boldsymbol{k}}$ instead of $\mathcal{E}_{\boldsymbol{k}}$, and $\tilde{\mathcal{E}}_{\boldsymbol{k}}$ has the correction due to $\delta \mathcal{N}_{\boldsymbol{k}\sigma} = \mathcal{N}_{\boldsymbol{k}\sigma} - \mathcal{N}^{(0)}_{\boldsymbol{k}\sigma}$.
2. One can show that the interaction correction to the total energy is of the order of T^4:

$$E \left[\mathcal{N} \right] \approx E_0 + \sum_{\boldsymbol{k}\sigma} \mathcal{E}_{\boldsymbol{k}\sigma} \delta \mathcal{N}_{\boldsymbol{k}\sigma} + \mathcal{O} \left(T^4 \right). \tag{5.71}$$

   It is thus negligible.

3. Thus, when determining the heat capacity, the system can be treated as if it is non-interacting.

Local quasiparticle energy is the energy required to add/remove a particle in the presence of other excitations

$$\tilde{\mathcal{E}}_{\boldsymbol{k}\sigma} = \frac{\delta E}{\delta \mathcal{N}_{\boldsymbol{k}\sigma}} = \mathcal{E}_{\boldsymbol{k}\sigma} + \sum_{\boldsymbol{k}'\sigma'} f_{\boldsymbol{k}\sigma,\boldsymbol{k}'\sigma'} \delta \mathcal{N}_{\boldsymbol{k}'\sigma'}. \tag{5.72}$$

The energy of a quasiparticle is modified by its interaction with quasi-particles.

Landau Fermi-liquid parameters: For isotropic systems, $f_{\boldsymbol{k}\sigma,\boldsymbol{k}'\sigma'} = f_{\sigma\sigma'}(\cos\theta)$, where θ is the angle between $\boldsymbol{k}$ and $\boldsymbol{k}'$ ($|\boldsymbol{k}| \approx |\boldsymbol{k}'| \approx k_F$). The system can be characterized by a set of parameters:

$$F_l^{\mathrm{s,a}} = \frac{\mathcal{V} N^*(0)}{4} \int_{-1}^{1} \mathrm{d}x \, \left[f_{\uparrow\uparrow}(x) \pm f_{\uparrow\downarrow}(x) \right] P_l(x), \tag{5.73}$$

where $P_l(x)$ is the Legendre function.

Compressibility

$$\frac{1}{K} = \rho^2 \frac{\partial \mu}{\partial \rho} = \frac{\rho k_F}{3} \frac{\partial \mu}{\partial k_F},$$

and

$$\delta\mu = \tilde{\mathcal{E}}_{k_F + \delta k_F, \sigma} - \tilde{\mathcal{E}}_{k_F, \sigma} = v_F^* \hbar \delta k_F + \sum_{\boldsymbol{k}'\sigma'} f_{\boldsymbol{k}\sigma,\boldsymbol{k}'\sigma'} \delta \mathcal{N}_{\boldsymbol{k}'\sigma'}, \tag{5.74}$$

where $\delta \mathcal{N}_{\boldsymbol{k}\sigma} = 1$ in a thin shell between k_F and $k_F + \delta k_F$. It results in:

$$\frac{K}{K_0} = \frac{m^*/m}{1 + F_0^{\mathrm{s}}}. \tag{5.75}$$

The compressibility can be determined by measuring the sound velocity $v_s = 1/\sqrt{nmK}$.

Spin susceptibility

$$\frac{\chi}{\chi_0} = \frac{m^*/m}{1 + F_0^{\mathrm{a}}}. \tag{5.76}$$

Mass renormalization for a system with the translational symmetry: GV§8.3.6

$$\frac{m^*}{m} = 1 + F_1^{\mathrm{s}}. \tag{5.77}$$

Proof:

- Look at the system from a reference frame in which the system has an infinitesimal velocity $\boldsymbol{v}$. The quasiparticle now has the energy

$$\mathcal{E}_{\boldsymbol{k}\sigma} + \hbar \boldsymbol{v} \cdot \boldsymbol{k}. \tag{5.78}$$

- It can also be regarded as a system with the Fermi-sea shifted by a wave vector $m\boldsymbol{v}/\hbar$. The change of the quasi-particle energy includes:
  1. The change of $\mathcal{E}_{\boldsymbol{k}\sigma}$ for $\boldsymbol{k} \to \boldsymbol{k} + m\boldsymbol{v}/\hbar$;
  2. The shifted distribution induces $\delta\mathcal{N}_{\boldsymbol{k}\sigma}$, which gives rise to the interaction correction.
- Equate the changes of the quasiparticle energy from the two different considerations.

5.3.2 Microscopic underpinning

GV§8.5

Spectral function A quasi-particle in an interacting system does not have a definite energy-momentum relation. Instead, it is described by the spectral function

$$A_\sigma(\boldsymbol{k},\omega) = -2\mathrm{Im}G^{\mathrm{r}}(\boldsymbol{k},\omega) = -2\hbar \frac{\mathrm{Im}\Sigma^{\mathrm{r}}_\sigma(\boldsymbol{k},\omega)}{\left[\hbar\omega - \epsilon_{\boldsymbol{k}} - \mathrm{Re}\Sigma^{\mathrm{r}}_\sigma(\boldsymbol{k},\omega)\right]^2 + \left[\mathrm{Im}\Sigma^{\mathrm{r}}_\sigma(\boldsymbol{k},\omega)\right]^2}, \tag{5.79}$$ (2.64)

which can be interpreted as the probability that the energy of the system changes $\hbar\omega$ after adding an electron/hole with a momentum $\hbar\boldsymbol{k}$:

$$A_\sigma(\boldsymbol{k},\omega) = A^{>}_\sigma(\boldsymbol{k},\omega) + A^{<}_\sigma(\boldsymbol{k},\omega) \tag{5.80}$$ (2.65)

$$A^{>}_\sigma(\boldsymbol{k},\omega) \equiv \mathrm{i}G^{>}_\sigma(\boldsymbol{k},\omega) = \frac{1}{Z}\sum_{n,m} 2\pi\delta\left(\omega - \frac{E_m - E_n}{\hbar}\right) e^{-\beta K_n} \left|\left\langle m, N+1 \middle| \hat{a}^\dagger_{\boldsymbol{k}\sigma} \middle| n, N\right\rangle\right|^2 \tag{5.81}$$ (2.72)

$$A^{<}_\sigma(\boldsymbol{k},\omega) \equiv -\mathrm{i}G^{<}_\sigma(\boldsymbol{k},\omega) = \frac{1}{Z}\sum_{n,m} 2\pi\delta\left(\omega + \frac{E_m - E_n}{\hbar}\right) e^{-\beta K_n} \left|\langle m, N-1 | \hat{a}_{\boldsymbol{k}\sigma} | n, N\rangle\right|^2 \tag{5.82}$$ (2.70)

For a non-interacting system, it is reduced to a Dirac function.

Quasiparticle energy is determined by the equation

$$\mathcal{E}_{\boldsymbol{k}\sigma} = \epsilon_{\boldsymbol{k}\sigma} + \mathrm{Re}\Sigma^{\mathrm{r}}_\sigma\left(\boldsymbol{k}, \frac{\mathcal{E}_{\boldsymbol{k}\sigma}}{\hbar}\right). \tag{5.83}$$

Coherent peak: the spectral function has a sharp peak (coherent peak) near the quasiparticle energy:

$$A_\sigma(\boldsymbol{k},\omega) = Z_{\boldsymbol{k}\sigma} \frac{\frac{1}{\tau_{\boldsymbol{k}\sigma}}}{\left(\omega - \frac{\mathcal{E}_{\boldsymbol{k}\sigma}}{\hbar}\right)^2 + \left(\frac{1}{2\tau_{\boldsymbol{k}\sigma}}\right)^2} + A_{\mathrm{incoh.}}(\boldsymbol{k},\omega), \tag{5.84}$$

$$\frac{1}{Z_{\boldsymbol{k}\sigma}} = 1 - \frac{1}{\hbar}\left.\frac{\partial \mathrm{Re}\Sigma^{\mathrm{r}}_\sigma(\boldsymbol{k},\omega)}{\partial\omega}\right|_{\hbar\omega=\mathcal{E}_{\boldsymbol{k}\sigma}}, \tag{5.85}$$

$$\frac{\hbar}{2\tau_{\boldsymbol{k}\sigma}} = Z_{\boldsymbol{k}\sigma}\left|\mathrm{Im}\Sigma^{\mathrm{r}}\left(\boldsymbol{k}, \mathcal{E}_{\boldsymbol{k}\sigma}/\hbar\right)\right|. \tag{5.86}$$

$Z_{\boldsymbol{k}\sigma}$ is called the quasi-particle weight. Near the Fermi surface, we have

$$\mathrm{Im}\Sigma^{\mathrm{r}}_\sigma\left(\boldsymbol{k}, \frac{\mathcal{E}_{\boldsymbol{k}\sigma}}{\hbar}\right) \propto \left(\mathcal{E}_{\boldsymbol{k}\sigma} - \mu\right)^2 \tag{5.87}$$

Fermi surface: A Fermi-liquid has the property that there exists a Fermi surface defined by the equations:

$$\mu - \epsilon_{\boldsymbol{k}_{F\sigma}} - \mathrm{Re}\Sigma^{\mathrm{r}}_\sigma\left(\boldsymbol{k}_{F\sigma}, \frac{\mu}{\hbar}\right) = 0, \tag{5.88}$$

$$\mathrm{Im}\Sigma^{\mathrm{r}}_\sigma\left(\boldsymbol{k}_{F\sigma}, \frac{\mu}{\hbar}\right) = 0. \tag{5.89}$$

The equations define a $d-1$ surface in the momentum space as well as the Fermi energy $\mathcal{E}_F = \mu$.

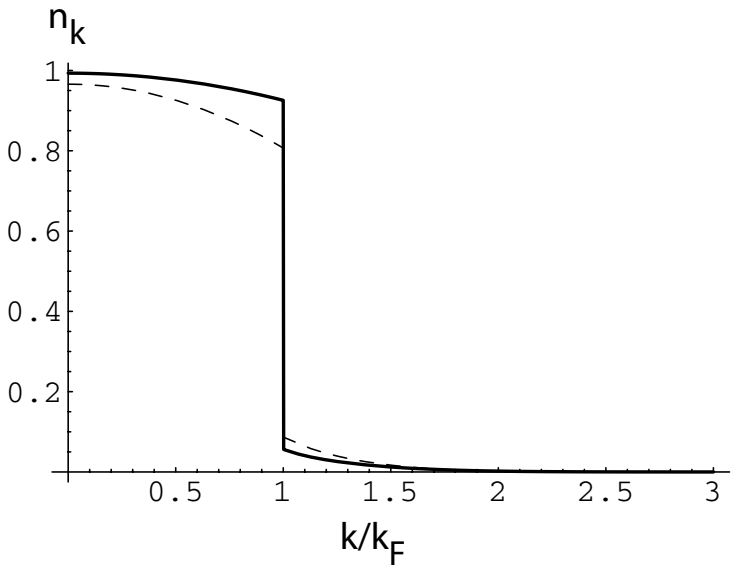


Figure 5.1: Momentum occupation number for an electron gas with $r_s = 2$ (solid line) and $r_s = 5$ (dashed line). GV Fig. 8.14

Luttinger theorem: The volume enclosed by the Fermi surface (Fermi sea) coincides with that of a non-interaction Fermi liquid of *the same density* [5]. GV§8.5.4

Effective mass:

$$\frac{\hbar^2 k_{F\sigma}}{m^*} = \left.\frac{\mathrm{d}\mathcal{E}_{k\sigma}}{\mathrm{d}k}\right|_{k=k_{F\sigma}}, \tag{5.90}$$

$$\frac{m}{m^*} = Z_{\boldsymbol{k}_F\sigma}\left(1 + \frac{m}{\hbar^2 k_{F\sigma}}\left.\frac{\partial \mathrm{Re}\Sigma^{\mathrm{r}}_\sigma(k,\mu/\hbar)}{\partial k}\right|_{k=k_{F\sigma}}\right). \tag{5.91}$$

Momentum occupation number $n_{\boldsymbol{k}\sigma}$ has a discontinuous jump at $k = k_F$ by an amount $Z_{\boldsymbol{k}_F\sigma}$. See Fig. 5.1. GV§8.5.2

Proof: Near the Fermi surface, $\mathrm{Im}\Sigma^{\mathrm{r}} \to 0$, we have

$$A_\sigma(\boldsymbol{k},\omega) \to 2\pi\delta\left[\omega - \frac{\epsilon_{\boldsymbol{k}} + \mathrm{Re}\Sigma^{\mathrm{r}}_\sigma(\boldsymbol{k},\omega)}{\hbar}\right] + A_{\mathrm{incoh.}}(\boldsymbol{k},\omega) \tag{5.92}$$

$$= 2\pi Z_{\boldsymbol{k}_F\sigma}\delta\left[\omega - \frac{\mathcal{E}_{\boldsymbol{k}\sigma}}{\hbar}\right] + A_{\mathrm{incoh.}}(\boldsymbol{k},\omega) \tag{5.93}$$

The momentum occupation number is determined by

$$n_{\boldsymbol{k}\sigma} = \mathrm{i}\int\frac{\mathrm{d}\omega}{2\pi}G^<_\sigma(\boldsymbol{k},\omega) = \int_{-\infty}^{\mu/\hbar}\frac{\mathrm{d}\omega}{2\pi}A_\sigma(\boldsymbol{k},\omega). \tag{5.94}$$ (2.74)

For two $\boldsymbol{k}$'s located in ($\mathcal{E}_{\boldsymbol{k}} \le \mu$) and out ($\mathcal{E}_{\boldsymbol{k}} > \mu$) of the Fermi-sea, the difference of $A_{\mathrm{incoh.}}(\boldsymbol{k},\omega)$ is negligible, and the difference of the integral is $Z_{\boldsymbol{k}_F\sigma}$.

Landau energy functional: The ground state energy functional Eq. (5.26) can be rewritten as (5.32)

$$E[\mathcal{N}_{\boldsymbol{k}}] - E_0 = \mathrm{i}\hbar\sum_{\boldsymbol{k}}\int\frac{\mathrm{d}\omega}{2\pi}\left[\ln\left[1 - \frac{1}{\hbar}G_0(\boldsymbol{k},\omega)\Sigma(\boldsymbol{k},\omega)\right] + \frac{1}{\hbar}\Sigma(\boldsymbol{k},\omega)G(\boldsymbol{k},\omega)\right] + \frac{\mathrm{i}\hbar}{T_0}\Phi[G], \tag{5.95}$$

where Σ is a functional of G, and $G = G[G_0]$ is regarded as a functional of G_0. G_0 is determined by $\mathcal{N}_{\boldsymbol{k}}$ through Eq. (5.62).

[5] The Luttinger theorem is valid only for systems with the time-reversal symmetry. For magnetic systems with the spin-orbit coupling, there exists a *Berry curvature correction* to the measure of the phase space. The Fermi sea volume will depend on the external magnetic field, and the theorem breaks down [29].

Quasiparticle energy We can prove that the quasiparticle energy defined in Eq. (5.83) is indeed the quasiparticle energy appeared in the energy functional Eq. (5.63):

- We consider $\mathcal{N}_{\boldsymbol{k}}$ is changed from 0 to 1 for a $\boldsymbol{k}$ near the Fermi surface. It induces a change of the Green's function $G_0(\boldsymbol{k},\omega)$

$$\frac{1}{\hbar\omega-\epsilon_{\boldsymbol{k}}+\mathrm{i}\eta}\longrightarrow\frac{1}{\hbar\omega-\epsilon_{\boldsymbol{k}}-\mathrm{i}\eta}. \tag{5.96}$$

- The change of the energy:

$$\delta E=\delta E_0-\hbar\sum_{\boldsymbol{k}}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi\mathrm{i}}\delta\ln\left[1-\frac{1}{\hbar}G_0\left(\boldsymbol{k},\omega\right)\Sigma\left(\boldsymbol{k},\omega\right)\right] \tag{5.97}$$

$$=\epsilon_{\boldsymbol{k}}-\hbar\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{\pi}\mathrm{Im}\left[\ln\frac{\hbar\omega-\epsilon_{\boldsymbol{k}}-\Sigma\left(\boldsymbol{k},\omega\right)-\mathrm{i}\eta}{\hbar\omega-\epsilon_{\boldsymbol{k}}-\mathrm{i}\eta}\right] \tag{5.98}$$

  where the variation is only acted on G_0 because $\delta E[G]/\delta G=0$.
- Near the Fermi surface, Σ is approximately real [Eq. (5.87)]. Note that $\mathrm{Im}\ln(x-\mathrm{i}\eta)=-\pi\theta(-x)$, we have

$$\delta E=\epsilon_{\boldsymbol{k}}+\hbar\int_{-\infty}^{\infty}\mathrm{d}\omega\left[\theta\left(\frac{\mathcal{E}_{\boldsymbol{k}}}{\hbar}-\omega\right)-\theta\left(\frac{\epsilon_{\boldsymbol{k}}}{\hbar}-\omega\right)\right]=\mathcal{E}_{\boldsymbol{k}}. \tag{5.99}$$ (5.83)

Interaction parameters $f_{\boldsymbol{k}\sigma,\boldsymbol{k}'\sigma'}$ can be determined by inspecting how the local quasi-particle energy changes when $\mathcal{N}_{\boldsymbol{k}\sigma}$ is varied:

$$\tilde{\mathcal{E}}_{\boldsymbol{k}\sigma}=\mathcal{E}_{\boldsymbol{k}\sigma}+\delta\mathcal{E}_{\boldsymbol{k}\sigma}=\epsilon_{\boldsymbol{k}\sigma}+\Sigma_\sigma\left(\boldsymbol{k},\frac{\mathcal{E}_{\boldsymbol{k}\sigma}+\delta\mathcal{E}_{\boldsymbol{k}\sigma}}{\hbar}\right)+\delta\Sigma_\sigma\left(\boldsymbol{k},\mathcal{E}_{\boldsymbol{k}\sigma}/\hbar\right). \tag{5.100}$$

- It leads to:

$$\delta\mathcal{E}_{\boldsymbol{k}\sigma}=Z_{\boldsymbol{k}\sigma}\delta\Sigma_\sigma\left(\boldsymbol{k},\mathcal{E}_{\boldsymbol{k}\sigma}/\hbar\right). \tag{5.101}$$

- By comparing to Eq. (5.72), we obtain

$$f_{\boldsymbol{k}\sigma,\boldsymbol{k}'\sigma'}=Z_{\boldsymbol{k}\sigma}\frac{\delta\Sigma_\sigma\left(\boldsymbol{k},\mathcal{E}_{\boldsymbol{k}\sigma}/\hbar\right)}{\delta\mathcal{N}_{\boldsymbol{k}'\sigma'}}. \tag{5.102}$$

- The interaction parameters can be related to the scattering amplitude Eq. (5.50) by

$$f_{\boldsymbol{k}\sigma,\boldsymbol{k}'\sigma'}=\frac{1}{\mathcal{V}}Z_{\boldsymbol{k}\sigma}Z_{\boldsymbol{k}'\sigma'}\mathcal{T}(11',11') \tag{5.103}$$

  with $1\equiv(\boldsymbol{k},\mathcal{E}_{\boldsymbol{k}\sigma},\sigma)$ and $1'\equiv(\boldsymbol{k}',\mathcal{E}_{\boldsymbol{k}'\sigma'},\sigma')$. See GV§8.5.5 for a derivation [6].

5.4 Generalizations

- In principle, as long as we know the energy functional (e.g., $\Phi[G]$), we solve the many-particle problem.
- Unfortunately, there is no easy way to determine the exact form of the functional. Even worse, its existence is not always guaranteed [14]:
  - The Legendre transformation Eq. (5.14) is well defined only when the map from ϕ to $\mathcal{G}$ is invertible.
  - The physical solutions of the stationary condition $\delta\Gamma[\mathcal{G}]=0$ may be saddle points and not extrema [5].
- It is often more useful and practical to define functionals which are less general.

[6] There are a number of sign errors in relevant equations of GV: (8.170), the first term of (8.172), the second term of (8.173) and (8.175). There is also a factor $1/\hbar$ for the second term of (8.175). (8.175) is actually the Bethe-Salpeter equation (5.50).

Density functional theory: one can introduce a bilinear source

$$S = \int \mathrm{d}\tau \mathrm{d}\boldsymbol{r} \hat{\rho}(\boldsymbol{r}\tau)\phi(\boldsymbol{r}) = \hbar\beta \int \mathrm{d}\boldsymbol{r} \hat{\rho}(\boldsymbol{r})\phi(\boldsymbol{r}). \tag{5.104}$$

After the Legendre transformation, we can define an energy function of the local density $\rho(\boldsymbol{r}) \equiv \langle \hat{\rho}(\boldsymbol{r}) \rangle$.

- Kohn-Hohenberg theorem: the map from ϕ to ρ is invertible.
- The functional can be constructed empirically.

Dynamic mean field theory: For a tight-binding (lattice) model, one can introduce a bilinear source [13]

$$S = \sum_i \int \mathrm{d}\tau \mathrm{d}\tau' \psi^*_{i\sigma}(\tau)\psi_{i\sigma'}(\tau')M_{i,\sigma\sigma'}(\tau - \tau'). \tag{5.105}$$

It results in an energy functional of $\mathcal{G}_{\mathrm{loc}}(\tau - \tau') \equiv -\langle \psi_{i\sigma}(\tau)\psi^*_{i\sigma'}(\tau') \rangle$.

- The functional can be obtained by solving the Anderson impurity model Eq. (1.92) in an effective medium.
- All local correlation effects are included in the approach.

Problems

1. Derive Eq. (5.36) and (5.43) by starting from the Luttinger-Ward functional Eq. (5.37) and applying the definitions Eq. (5.31) and (5.42).
2. Determine the self-energy and the irreducible interaction with respect to $\Phi_{\mathrm{GW}}[\mathcal{G}]$ (Eq. 5.38).
3. Determine the Bethe-Salpeter equation Eq. (5.50) in the frequency/momentum domain.
4. Derive the spin susceptibility formula Eq. (5.76).

Chapter 6

Theory of electron liquid

6.1 Energy

FW§12

The second quantized Hamiltonian of a homogeneous electron gas (jellium model) reads:

$$\hat{H} = \sum_{\boldsymbol{k}\sigma} \frac{\hbar^2 k^2}{2m} \hat{a}^\dagger_{\boldsymbol{k}\sigma} \hat{a}_{\boldsymbol{k}\sigma} + \frac{e^2}{2\mathcal{V}} \sum_{\boldsymbol{q}\neq 0} \sum_{\boldsymbol{k}\sigma,\boldsymbol{p}\sigma'} \frac{4\pi}{q^2} \hat{a}^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma} \hat{a}^\dagger_{\boldsymbol{p}-\boldsymbol{q}\sigma'} \hat{a}_{\boldsymbol{p}\sigma'} \hat{a}_{\boldsymbol{k}\sigma}. \tag{6.1}$$

(1.82)

Dimensionless form: we choose the unit of the length as the average distance between electrons r_0:

$$\frac{4\pi}{3} r_0^3 N = \mathcal{V}. \tag{6.2}$$

Dimensionless density parameter

$$r_s = \frac{r_0}{a_0}, \tag{6.3}$$

where $a_0 = \hbar^2/me^2$ is the Bohr radius.

The dimensionless form of the Hamiltonian is

$$\hat{H} = \frac{e^2}{2a_0} \left(\frac{1}{r_s^2} \sum_{\boldsymbol{k}\sigma} k^2 \hat{a}^\dagger_{\boldsymbol{k}\sigma} \hat{a}_{\boldsymbol{k}\sigma} + \frac{1}{r_s} \frac{1}{\mathcal{V}} \sum_{\boldsymbol{q}\neq 0} \sum_{\boldsymbol{k}\sigma,\boldsymbol{p}\sigma'} \frac{4\pi}{q^2} \hat{a}^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma} \hat{a}^\dagger_{\boldsymbol{p}-\boldsymbol{q}\sigma'} \hat{a}_{\boldsymbol{p}\sigma'} \hat{a}_{\boldsymbol{k}\sigma} \right), \tag{6.4}$$

where the volume and momenta have been scaled by the new length unit: $\mathcal{V} \to \mathcal{V}/r_0^3 = 4\pi N/3$, $\boldsymbol{k}, \boldsymbol{p}, \boldsymbol{q} \to \boldsymbol{k}r_0, \boldsymbol{p}r_0, \boldsymbol{q}r_0$.

Counter-intuitively, the high-density limit $r_s \to 0$ is the *non-interacting* limit.

6.1.1 Hartree-Fock approximation

We calculate the expectation value of the Hamiltonian with respect to the ground state of an ideal *non-interacting* electron gas, i. e., a filled Fermi sea with

$$k_F r_0 = \frac{1}{\alpha}, \ \alpha = \left(\frac{4}{9\pi} \right)^{1/3}. \tag{6.5}$$

Kinetic energy: we have $n^0_{\boldsymbol{k}\sigma} = \left\langle \hat{a}^\dagger_{\boldsymbol{k}\sigma} \hat{a}_{\boldsymbol{k}\sigma} \right\rangle_0 = \theta(k_F - |\boldsymbol{k}|)$, and

$$E_0 = \frac{e^2}{2a_0 r_s^2} \sum_{\boldsymbol{k}\sigma} k^2 n^0_{\boldsymbol{k}\sigma} = 2 \times \frac{e^2}{2a_0 r_s^2} \mathcal{V} \int_0^{1/\alpha} \frac{4\pi k^2 \mathrm{d}k}{(2\pi)^3} k^2 = \frac{3N}{5\alpha^2 r_s^2} \,\mathrm{Ry}. \tag{6.6}$$

where $\mathrm{Ry} \equiv e^2/2a_0$. The average electron kinetic energy is

$$\epsilon_0 = \frac{E_0}{N} \approx \frac{2.21}{r_s^2} \,\mathrm{Ry}. \tag{6.7}$$

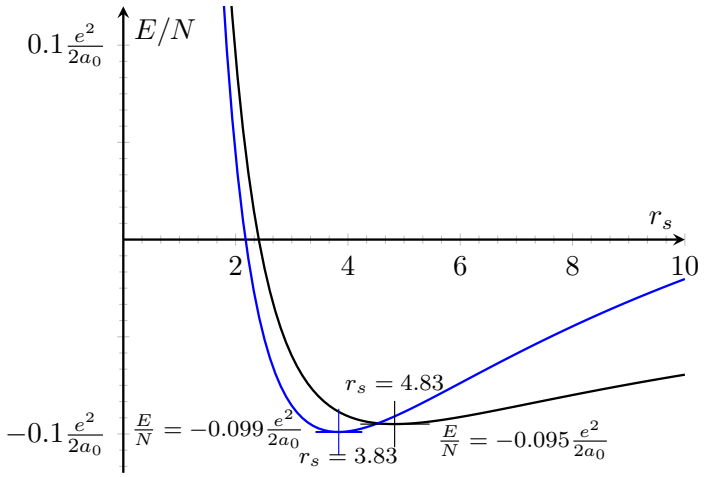


Figure 6.1: Approximate ground state energy of an electron gas. Black: Hartree-Fock approximation Eq. (6.7)+Eq. (6.11); Blue: Eq. (6.31).

Exchange energy: to calculate the expectation value of the second term, we apply Wick's theorem

$$\left\langle \hat{a}^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma}\hat{a}^\dagger_{\boldsymbol{p}-\boldsymbol{q}\sigma'}\hat{a}_{\boldsymbol{p}\sigma'}\hat{a}_{\boldsymbol{k}\sigma}\right\rangle_0 = \left\langle \hat{a}^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma}\hat{a}_{\boldsymbol{k}\sigma}\right\rangle_0 \left\langle \hat{a}^\dagger_{\boldsymbol{p}-\boldsymbol{q}\sigma'}\hat{a}_{\boldsymbol{p}\sigma'}\right\rangle_0 - \left\langle \hat{a}^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma}\hat{a}_{\boldsymbol{p}\sigma'}\right\rangle_0 \left\langle \hat{a}^\dagger_{\boldsymbol{p}-\boldsymbol{q}\sigma'}\hat{a}_{\boldsymbol{k}\sigma}\right\rangle_0 \tag{6.8}$$

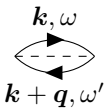
$$= \delta_{\boldsymbol{q},0} n^0_{\boldsymbol{k}\sigma} n^0_{\boldsymbol{p}\sigma'} - \delta_{\boldsymbol{q},\boldsymbol{p}-\boldsymbol{k}}\delta_{\sigma\sigma'} n^0_{\boldsymbol{k}\sigma} n^0_{\boldsymbol{k}+\boldsymbol{q},\sigma}. \tag{6.9}$$

We have

$$E_{\mathrm{x}} = -\frac{e^2}{2a_0}\frac{1}{r_s}\frac{1}{\mathcal{V}}\sum_{\boldsymbol{q}\neq 0}\frac{4\pi}{q^2}\sum_{\boldsymbol{k}\sigma} n^0_{\boldsymbol{k}\sigma} n^0_{\boldsymbol{k}+\boldsymbol{q},\sigma} = -\frac{3}{2\pi\alpha r_s} N\,\mathrm{Ry}, \tag{6.10}$$

$$\epsilon_{\mathrm{x}} = \frac{E_{\mathrm{x}}}{N} \approx -\frac{0.916}{r_s}\,\mathrm{Ry}. \tag{6.11}$$

Perturbative approach: the exchange energy can also be obtained from the diagram



$$= \mathrm{i}\hbar\mathcal{V}\left(\frac{\mathrm{i}}{\hbar}\right)\frac{1}{2}(-1)\sum_{\sigma\sigma'}\int\frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3}v(q)\int\frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^3}$$

$$\times\,\delta_{\sigma\sigma'}\int\frac{\mathrm{d}\omega}{2\pi}G_0(\boldsymbol{k},\omega)e^{\mathrm{i}\omega\eta}\int\frac{\mathrm{d}\omega'}{2\pi}G_0(\boldsymbol{k}+\boldsymbol{q},\omega')e^{\mathrm{i}\omega'\eta}. \tag{6.12}$$

Note that $\int\frac{\mathrm{d}\omega}{2\pi}G_0(\boldsymbol{k},\omega)e^{\mathrm{i}\omega\eta} = \mathrm{i}n^0_{\boldsymbol{k}}$.

Self energy (5.35)

$$= 0, \tag{6.13}$$

$$\Sigma(\boldsymbol{k},\omega) = \hbar = \delta_{\sigma\sigma'}\mathrm{i}\int\frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3}v(q)\int\frac{\mathrm{d}\nu}{2\pi}G_0(\boldsymbol{k}+\boldsymbol{q},\nu)e^{\mathrm{i}\nu\eta} \tag{6.14}$$

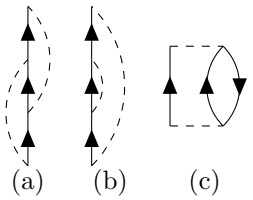
$$= -\delta_{\sigma\sigma'}\int\frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3}v(q)n^0_{\boldsymbol{k}+\boldsymbol{q}} = \frac{e^2k_F}{\pi}S\left(\frac{k}{k_F}\right), \tag{6.15}$$ MH(5.19)

$$S(x) = -\left(1+\frac{1-x^2}{x}\ln\left|\frac{1+x}{1-x}\right|\right). \tag{6.16}$$

The singularity at $k = k_F$ results in a vanishing effective mass, which is actually unphysical. (5.91)

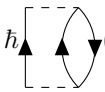
6.1.2 High order contributions

The second order diagrams of the self energy are evaluated in MH §5.1.5–5.1.7:



(6.17)

- (a) is convergent and has an on-shell value independent of the density.
- (b) can be interpreted as a self-energy correction to the propagator line of Eq. (6.14). The correction is ω-independent. It has no effect because of Luttinger's theorem.
- (c) diverges:

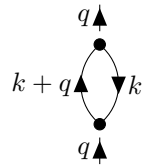


$$\hbar(\boldsymbol{k},\omega) = \mathrm{i}\delta_{\sigma\sigma'}\int\frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3}\int\frac{\mathrm{d}\nu}{2\pi}\left[v(q)\right]^2\chi_0(\boldsymbol{q},\nu)G_0(\boldsymbol{k}+\boldsymbol{q},\omega+\nu) \tag{6.18}$$

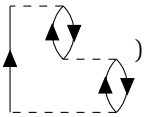
$$\sim\int\frac{\mathrm{d}q}{q^2}\to\infty, \tag{6.19}$$

where $\chi_0(\boldsymbol{q},\nu)$ denotes the polarization bubble:

$$\chi_0(\boldsymbol{q},\nu) =$$

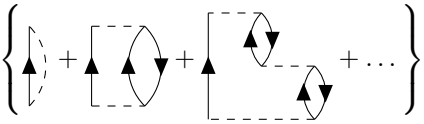


$$= -\frac{\mathrm{i}}{\hbar}\sum_{\sigma\sigma'}\delta_{\sigma\sigma'}\int\frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^3}\int\frac{\mathrm{d}\omega}{2\pi}G_0(\boldsymbol{k}+\boldsymbol{q},\omega+\nu)G_0(\boldsymbol{k},\omega). \tag{6.20}$$

Higher order diagrams with more bubbles (e.g., ) diverge even worse.

Re-summation The divergence can be removed by summing all direct ring diagrams:

$$\Sigma^{\mathrm{RPA}}(\boldsymbol{k},\omega) = \hbar\left\{\quad+\quad+\quad+\ldots\right\} \tag{6.21}$$



$$= \mathrm{i}\int\frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3}\int\frac{\mathrm{d}\nu}{2\pi}v(\boldsymbol{q})\left\{1+v(\boldsymbol{q})\chi_0(\boldsymbol{q},\nu)+\left[v(\boldsymbol{q})\chi_0(\boldsymbol{q},\nu)\right]^2+\cdots\right\}G_0(\boldsymbol{k}+\boldsymbol{q},\omega+\nu) \tag{6.22}$$

$$= \mathrm{i}\int\frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3}\int\frac{\mathrm{d}\nu}{2\pi}\frac{v(\boldsymbol{q})}{1-v(q)\chi_0(\boldsymbol{q},\nu)}G_0(\boldsymbol{k}+\boldsymbol{q},\omega+\nu) \tag{6.23}$$

$$\equiv \mathrm{i}\int\frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3}\int\frac{\mathrm{d}\nu}{2\pi}W(\boldsymbol{q},\nu)G_0(\boldsymbol{k}+\boldsymbol{q},\omega+\nu), \tag{6.24}$$

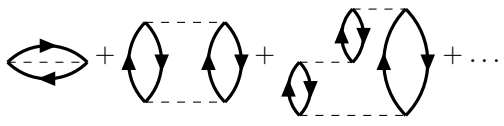
where $W(\boldsymbol{q},\nu)\equiv v(\boldsymbol{q})/\varepsilon_{\mathrm{RPA}}(\boldsymbol{q},\nu)$ can be interpreted as a *screened* e-e interaction by the dielectric function

$$\varepsilon_{\mathrm{RPA}}(\boldsymbol{q},\nu) = 1-v(\boldsymbol{q})\chi_0(\boldsymbol{q},\nu). \tag{6.25}$$

The effective mass becomes finite.

Ground state energy The GW approximation for the Luttinger-Ward functional

$$\Phi_{\mathrm{GW}}[G] =$$



(6.26) (5.38)

$$= -\frac{1}{2}\mathcal{V}T_0\int\frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3}\int\frac{\mathrm{d}\nu}{2\pi}\ln\left\{1-v(\boldsymbol{q})\chi_0[G](\boldsymbol{q},\nu)\right\} \tag{6.27}$$

can now be justified: It is a re-summation of the most diverging diagrams of the perturbative expansion.

The ground state energy can be calculated by the G_0W_0 approximation:

$$E[G] - E_0 = \mathrm{i}\hbar \left\{ \sum_{\boldsymbol{k}} \int \frac{\mathrm{d}\omega}{2\pi} \left\{ \ln\left[G_0(\boldsymbol{k},\omega) G^{-1}(\boldsymbol{k},\omega) \right] + G_0^{-1}(\boldsymbol{k},\omega) G(\boldsymbol{k},\omega) - 1 \right\} + \frac{1}{T_0}\Phi[G] \right\} \tag{6.28}$$ (5.26)

$$\approx \frac{\mathrm{i}\hbar}{T_0}\Phi_{\mathrm{GW}}[G_0] + \mathcal{O}\left(\delta G^2\right) \tag{6.29}$$

$$= -\frac{\mathrm{i}\hbar}{2}\mathcal{V}\int \frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3}\int \frac{\mathrm{d}\nu}{2\pi} \ln\left[1 - v(\boldsymbol{q})\chi_0(\boldsymbol{q},\nu)\right] + \mathcal{O}\left(\delta G^2\right) \tag{6.30}$$

The correction due to $\delta G \equiv G - G_0$ is of the second order because $\delta E[G]/\delta G = 0$. The evaluation of the integral can be found in FW Eq. (12.53-12.61). Note that the energy includes the exchange energy Eq. (6.10). The total ground state energy can be written as (in Ry):

$$\epsilon(r_s) = \frac{E}{N} \approx \frac{2.21}{r_s^2} - \frac{0.916}{r_s} + 0.0622\ln r_s - 0.094 + \mathcal{O}\left(r_s \ln r_s\right)\ldots \tag{6.31}$$ FW(12.62)

The correction to the kinetic energy and the exchange energy is called the correlation energy. The constant term includes the contribution of Eq. (6.17a). The singular expansion (i.e., $\propto \ln r_s$) is a result of the divergence observed in Eq. (6.17c).

Further improvement requires quantum Monte Carlo (QMC) simulations. An interpolation formula for the ground state energy of the electron gas is presented in GV §1.7.2.

Wigner crystal phase becomes more stable (lower energy) than the electron liquid phase when r_s is sufficiently large. The phase transition occurs at $r_s \sim 100$ in 3D. There could be more phase transitions before the transition to the Wigner crystal (e.g., to a ferromagnetic electron liquid). The issue is yet to be fully clarified. See GV §1.7.2.

6.1.3 General structure of the self-energy

The Green's function satisfies the equation:

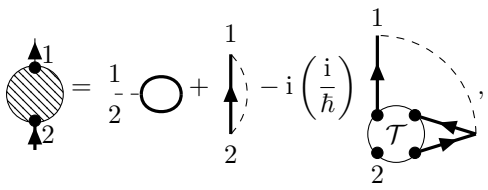
$$\hat{G}_0^{-1}G(1,1') = \delta(1-1') - \frac{\mathrm{i}}{\hbar}\int \mathrm{d}2\, v(1-2)\left\langle T\left[\hat{\psi}^\dagger(2)\hat{\psi}(2)\hat{\psi}(1)\hat{\psi}^\dagger(1')\right]\right\rangle \tag{6.32}$$

$$= \delta(1-1') - \frac{\mathrm{i}}{\hbar}\int \mathrm{d}2\, v(1-2)G^{(2)}(12,1'2)\,. \tag{6.33}$$

It suggests:

$$\int \mathrm{d}2\,\Sigma(1,2)G(2,1') = -\mathrm{i}\int \mathrm{d}2\, v(1-2)G^{(2)}(12,1'2)\,. \tag{6.34}$$

Substituting Eq. (5.12) and (5.49) into the equation, we obtain an *exact* relation for Σ:



(6.35)

$$\Sigma(k) = \Sigma_{\mathrm{HF}}(k) + \frac{1}{\hbar}\int \mathrm{d}p\mathrm{d}q\, v(q)\mathcal{T}(k+q, p-q; k, p)\, G(p)\, G(p-q)\, G(k+q)\,. \tag{6.36}$$

where the first two terms are nothing but the Hartree-Fock contribution.

$\mathcal{T}$ can be obtained from the irreducible interaction I by solving the Bethe-Salpeter equation Eq. (5.50). By choosing a proper set of diagrams in Eq. (5.43) or assuming an approximated form for I (see §6.2.3), one could close Eq. (6.35).

For certain systems (e.g., Fermions with hard-core interaction), re-summation is needed for obtaining I. An example can be found in FW §11.

6.2 Density response function

6.2.1 Basic properties

GV §3.3

Density response function describes how the density changes in response to an infinitesimal external scalar potential:

$$\delta\rho(\boldsymbol{r}t) = \int \mathrm{d}\boldsymbol{r}' \int \mathrm{d}t' \chi^{\mathrm{r}}(\boldsymbol{r}t, \boldsymbol{r}'t')\phi(\boldsymbol{r}'t'), \tag{6.37}$$

$$\chi^{\mathrm{r}}(\boldsymbol{r}t, \boldsymbol{r}'t') = -\frac{\mathrm{i}}{\hbar}\theta(t-t') \left\langle [\hat{\rho}(\boldsymbol{r}t), \hat{\rho}(\boldsymbol{r}'t')] \right\rangle . \tag{6.38}$$

(2.44)

For spatially-temporally uniform systems, it is more convenient to use the Fourier transformed form

$$\delta\rho(\boldsymbol{q},\omega) = \chi^{\mathrm{r}}(\boldsymbol{q},\omega)\phi_{\mathrm{ext}}(\boldsymbol{q},\omega), \tag{6.39}$$

$$\chi^{\mathrm{r}}(\boldsymbol{q},\omega) = -\frac{\mathrm{i}}{\hbar\mathcal{V}} \int_0^\infty \mathrm{d}t\, e^{\mathrm{i}\omega t} \left\langle [\hat{\rho}_{\boldsymbol{q}}(t), \hat{\rho}_{-\boldsymbol{q}}] \right\rangle , \tag{6.40}$$

where $\hat{\rho}_{\boldsymbol{q}}(t) \equiv \sum_i e^{-\mathrm{i}\boldsymbol{q}\cdot\hat{\boldsymbol{r}}_i(t)} = \sum_{\boldsymbol{k}\sigma} \hat{a}^\dagger_{\boldsymbol{k}-\boldsymbol{q},\sigma}(t)\hat{a}_{\boldsymbol{k}\sigma}(t)$.

Time ordered density correlation function is defined as

$$\chi(\boldsymbol{r}t, \boldsymbol{r}'t') = -\frac{\mathrm{i}}{\hbar} \left\langle \hat{T} \left[\Delta\hat{\rho}(\boldsymbol{r}t)\Delta\hat{\rho}(\boldsymbol{r}'t')\right] \right\rangle = \frac{\mathrm{i}}{\hbar} G^{(2)}_{\mathrm{c}} \left(\boldsymbol{r}t, \boldsymbol{r}'t'; \boldsymbol{r}t^+, \boldsymbol{r}'t'^+\right), \tag{6.41}$$

where $\Delta\hat{\rho}(\boldsymbol{r}t) \equiv \hat{\rho}(\boldsymbol{r}t) - \rho_0$. The thermal (imaginary time) version of the correlation function is defined as

$$\chi^{\mathrm{T}}(\boldsymbol{r}\tau, \boldsymbol{r}'\tau') = -\frac{1}{\hbar} \left\langle \hat{T} \left[\Delta\hat{\rho}(\boldsymbol{r}\tau)\Delta\hat{\rho}(\boldsymbol{r}'\tau')\right] \right\rangle . \tag{6.42}$$

Fluctuation-dissipation theorem can be established for the density correlation/response functions.

§2.2.1

Density structure factor is defined as

$$S(\boldsymbol{q},\omega) = \mathrm{i}\hbar\rho_0^{-1}\chi^{>}(\boldsymbol{q},\omega) = \frac{1}{N}\int_{-\infty}^{\infty} \mathrm{d}t\, e^{\mathrm{i}\omega t} \left\langle \Delta\hat{\rho}_{\boldsymbol{q}}(t)\Delta\hat{\rho}_{-\boldsymbol{q}} \right\rangle \tag{6.43}$$

$$= \frac{1}{ZN}\sum_{m,n} 2\pi\delta\left(\omega - \frac{K_n - K_m}{\hbar}\right) e^{-\beta K_m} \left|\langle m \left| \Delta\hat{\rho}_{\boldsymbol{q}} \right| n\rangle\right|^2 , \tag{6.44}$$

Eq. (2.72)

which is related to the PAIR CORRELATION FUNCTION OR RADIAL DISTRIBUTION FUNCTION.

GV §A4

Fluctuation-dissipation relations The spectral function is defined by

(2.74–2.79)

$$B(\boldsymbol{q},\omega) = -2\mathrm{Im}\chi^{\mathrm{r}}(\boldsymbol{q},\omega) = \mathrm{i}\left[\chi^{>}(\boldsymbol{q},\omega) - \chi^{<}(\boldsymbol{q},\omega)\right] \tag{6.45}$$

$$= \frac{\rho_0}{\hbar}\left(1 - e^{-\beta\hbar\omega}\right) S(\boldsymbol{q},\omega), \tag{6.46}$$

(2.75)

$$B(\boldsymbol{q},\omega) = -B(-\boldsymbol{q},-\omega). \tag{6.47}$$

The density response functions are related to the spectral function by:

$$\begin{Bmatrix} \chi(\boldsymbol{q},\omega) \\ \chi^{\mathrm{r}}(\boldsymbol{q},\omega) \\ \chi^{\mathrm{a}}(\boldsymbol{q},\omega) \end{Bmatrix} = \int \frac{\mathrm{d}\omega_1}{2\pi} B(\boldsymbol{q},\omega_1) \begin{Bmatrix} -\frac{n_{\mathrm{B}}(\omega_1)}{\omega-\omega_1-\mathrm{i}\eta} + \frac{1+n_{\mathrm{B}}(\omega_1)}{\omega-\omega_1+\mathrm{i}\eta} \\ \frac{1}{\omega-\omega_1+\mathrm{i}\eta} \\ \frac{1}{\omega-\omega_1-\mathrm{i}\eta} \end{Bmatrix}, \tag{6.48}$$

(2.77)

$$\mathrm{Re}\begin{Bmatrix} \chi(\boldsymbol{q},\omega) \\ \chi^{\mathrm{r}}(\boldsymbol{q},\omega) \\ \chi^{\mathrm{a}}(\boldsymbol{q},\omega) \end{Bmatrix} = \mathcal{P}\int \frac{\mathrm{d}\omega_1}{2\pi} \frac{B(\boldsymbol{q},\omega_1)}{\omega-\omega_1}, \tag{6.49}$$

$$\mathrm{Im}\begin{Bmatrix} \chi(\boldsymbol{q},\omega) \\ \chi^{\mathrm{r}}(\boldsymbol{q},\omega) \\ \chi^{\mathrm{a}}(\boldsymbol{q},\omega) \end{Bmatrix} = \begin{Bmatrix} -\coth\frac{\beta\hbar\omega}{2} \\ - \\ + \end{Bmatrix} \frac{1}{2} B(\boldsymbol{q},\omega). \tag{6.50}$$

$$\chi^{\mathrm{T}}(\boldsymbol{q},\omega_n)=\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega_1}{2\pi}\frac{B(\boldsymbol{q},\omega_1)}{\mathrm{i}\omega_n-\omega_1} \tag{6.51}$$

where $n_{\mathrm{B}}(\omega)=1/(e^{\beta\hbar\omega}-1)$ is the Bose distribution function.

f-sum rules

$$\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\omega B(\boldsymbol{q},\omega)=\frac{\rho_0 q^2}{m}. \tag{6.52}$$

To derive the sum rule, we make use of the continuity equation and the commutation relation

$$\left[\hat{\boldsymbol{j}}_{\boldsymbol{q}},\hat{\rho}_{-\boldsymbol{q}'}\right]=\frac{\hbar\boldsymbol{q}}{m}\hat{\rho}_{\boldsymbol{q}-\boldsymbol{q}'}, \tag{6.53}$$

where $\hat{\boldsymbol{j}}_{\boldsymbol{q}}$ is the current density operator.

Higher order sum rules could also be established. See GV §3.3.3.

Stiffness theorem The energy/grand potential of a system with an inhomogeneous density is

$$E\left[\rho_{\boldsymbol{q}}\right]=E_0-\frac{1}{\mathcal{V}}\sum_{\boldsymbol{q}}\frac{\left|\delta\rho_{\boldsymbol{q}}\right|^2}{2\chi^{\mathrm{r}}(\boldsymbol{q})}, \tag{6.54}$$

where $\chi^{\mathrm{r}}(\boldsymbol{q})\equiv\chi^{\mathrm{r}}(\boldsymbol{q},\omega=0)$.

Proof GV §3.2.9

- Consider a system perturbed by an external potential

$$\hat{H}_\phi=\hat{H}+\frac{1}{\mathcal{V}}\sum_{\boldsymbol{q}}\delta\hat{\rho}_{-\boldsymbol{q}}\phi_{\boldsymbol{q}}. \tag{6.55}$$

- The perturbation induces a density change $\delta\rho_{\boldsymbol{q}}$. Conversely, to create a given density distribution,

$$\phi_{\boldsymbol{q}}=\frac{\delta\rho_{\boldsymbol{q}}}{\chi^{\mathrm{r}}(\boldsymbol{q})}, \tag{6.56}$$

- We scale the perturbation with a factor λ: $\hat{H}_\phi(\lambda)=\hat{H}+\lambda\frac{1}{\mathcal{V}}\sum_{\boldsymbol{q}}\delta\hat{\rho}_{-\boldsymbol{q}}\phi_{\boldsymbol{q}}$. By applying the Hellman-Feynman theorem, we have

$$E_\phi=\left\langle\hat{H}_\phi\right\rangle=E_0+\int_0^1\mathrm{d}\lambda\left\langle\frac{\partial\hat{H}_\phi(\lambda)}{\partial\lambda}\right\rangle \tag{6.57}$$

$$\approx E_0+\int_0^1\mathrm{d}\lambda\,\lambda\frac{1}{\mathcal{V}}\sum_{\boldsymbol{q}}\chi^{\mathrm{r}}(\boldsymbol{q})\left|\phi_{\boldsymbol{q}}\right|^2=E_0+\frac{1}{2}\frac{1}{\mathcal{V}}\sum_{\boldsymbol{q}}\chi^{\mathrm{r}}(\boldsymbol{q})\left|\phi_{\boldsymbol{q}}\right|^2. \tag{6.58}$$

- The internal energy of the system is

$$E\left[\rho_{\boldsymbol{q}}\right]=\left\langle\hat{H}\right\rangle=E_\phi-\frac{1}{\mathcal{V}}\sum_{\boldsymbol{q}}\chi^{\mathrm{r}}(\boldsymbol{q})\left|\phi_{\boldsymbol{q}}\right|^2. \tag{6.59}$$

Note that the stiffness theorem can be generalized for arbitrary observables.

Compressibility sum rule

$$\lim_{\boldsymbol{q}\to0}\left[\frac{1}{\chi^{\mathrm{r}}(\boldsymbol{q})}+v(\boldsymbol{q})\right]=-\frac{\partial^2\left[\rho_0\epsilon\left(\rho_0\right)\right]}{\partial\rho_0^2}=-\frac{1}{\rho_0^2K}, \tag{6.60}$$

where K is the compressibility. The compressibility of a two-dimensional electron gas can be measured by QUANTUM CAPACITANCE experiments. It can be negative. GV§5.2.3

Proof GV §3.3.4

- Introduce a long-wavelength density modulation $\delta\rho_{\boldsymbol{q}}$.

- Determine the change of the energy by
  - applying the stiffness theorem: $\delta E = -\left|\delta\rho_{\boldsymbol{q}}\right|^2 / 2\mathcal{V}\chi^{\mathrm{r}}(\boldsymbol{q})$;
  - calculating the energy directly, including the electrostatic energy and the local energy

$$\delta E = \delta \int \mathrm{d}\boldsymbol{r}\rho(\boldsymbol{r})\epsilon\left[\rho(\boldsymbol{r})\right] + \frac{1}{2\mathcal{V}} v(\boldsymbol{q})\left|\delta\rho_{\boldsymbol{q}}\right|^2 . \tag{6.61}$$

- Equate the results from the two approaches and set $\boldsymbol{q} \to 0$.

Proper density response function is defined by

$$\frac{1}{\tilde{\chi}^{\mathrm{r}}(\boldsymbol{q},\omega)} = \frac{1}{\chi^{\mathrm{r}}(\boldsymbol{q},\omega)} + v(\boldsymbol{q}). \tag{6.62}$$

It is the density response function of a fictitious system in which the positive charge background always compensates the change of the electron density.

Dielectric function is defined as the ratio between the applied external potential and the total (screened) potential:

$$\phi_{\mathrm{sc}}(\boldsymbol{q},\omega) \equiv \phi(\boldsymbol{q},\omega) + \phi_{\mathrm{ind}}(\boldsymbol{q},\omega) = \frac{\phi(\boldsymbol{q},\omega)}{\epsilon(\boldsymbol{q},\omega)}, \tag{6.63}$$

where $\phi_{\mathrm{ind}}(\boldsymbol{q}) = v(\boldsymbol{q})\delta\rho(\boldsymbol{q},\omega)$ is the Coulomb potential induced by the perturbed electron density.

$$\frac{1}{\epsilon(\boldsymbol{q},\omega)} = 1 + v(\boldsymbol{q})\chi^{\mathrm{r}}(\boldsymbol{q},\omega), \tag{6.64}$$

$$\epsilon(\boldsymbol{q},\omega) = 1 - v(\boldsymbol{q})\tilde{\chi}^{\mathrm{r}}(\boldsymbol{q},\omega), \tag{6.65}$$

$$\chi^{\mathrm{r}}(\boldsymbol{q},\omega) = \frac{\tilde{\chi}^{\mathrm{r}}(\boldsymbol{q},\omega)}{\epsilon(\boldsymbol{q},\omega)}. \tag{6.66}$$

6.2.2 Random phase approximation (RPA)

GV §5.3

The random phase approximation assumes

$$\tilde{\chi}^{\mathrm{r}}(\boldsymbol{q},\omega) \approx \chi_0^{\mathrm{r}}(\boldsymbol{q},\omega), \tag{6.67}$$

where $\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega)$ is the density response function of an ideal (non-interacting) electron gas.

Intuitive picture We treat electrons as independent particles, and approximate the effect of the e-e interaction to the average potential ϕ_{ind} (Hartree approximation):

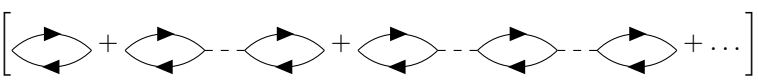
$$\delta\rho(\boldsymbol{q},\omega) = \chi_0^{\mathrm{r}}(\boldsymbol{q},\omega)\left[\phi(\boldsymbol{q},\omega) + v(\boldsymbol{q})\delta\rho(\boldsymbol{q},\omega)\right], \tag{6.68}$$

where $\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega)$ is the density response function of independent electrons. The full density response function is

$$\epsilon_{\mathrm{RPA}}(\boldsymbol{q},\omega) = 1 - v(\boldsymbol{q})\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega), \tag{6.69}$$ (6.65)

$$\chi^{\mathrm{r}}_{\mathrm{RPA}}(\boldsymbol{q},\omega) = \frac{\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega)}{\epsilon_{\mathrm{RPA}}(\boldsymbol{q},\omega)} = \frac{\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega)}{1 - v(\boldsymbol{q})\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega)}. \tag{6.70}$$ (6.66)

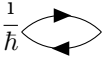
Diagrams corresponding to RPA are

$\chi_{\mathrm{RPA}}(\boldsymbol{q},\omega) = \frac{\mathrm{i}}{\hbar}\Big[$  $\Big]$ (6.71)

$= \dfrac{\frac{\mathrm{i}}{\hbar}$  $}{1 - v(\boldsymbol{q})\Big[\frac{\mathrm{i}}{\hbar}$  $\Big]}$. (6.72) (6.25)

Lindhard function is the density response function of a non-interacting electron gas: GV §4.4

$$\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega) = \frac{\mathrm{i}}{\hbar} \tag{6.73}$$



$$= -\frac{\mathrm{i}}{\hbar}\sum_\sigma \int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^3}\int \frac{\mathrm{d}\nu}{2\pi}\left[G_\sigma^<(\boldsymbol{k}+\boldsymbol{q},\nu+\omega)G_\sigma^{\mathrm{a}}(\boldsymbol{k},\nu) + G_\sigma^{\mathrm{r}}(\boldsymbol{k}+\boldsymbol{q},\omega+\nu)G_\sigma^<(\boldsymbol{k},\nu)\right] \quad \text{Tab. 4.1} \tag{6.74}$$

$$= 2\int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^3}\frac{f(\epsilon_{\boldsymbol{k}}) - f(\epsilon_{\boldsymbol{k}+\boldsymbol{q}})}{\hbar\omega + \epsilon_{\boldsymbol{k}} - \epsilon_{\boldsymbol{k}+\boldsymbol{q}} + \mathrm{i}\eta}, \tag{6.75}$$ (2.74, 2.77)

where $f(\epsilon) = n_+(\epsilon) = 1/(e^{\beta(\epsilon-\mu)}+1)$ is the Fermi-Dirac distribution function.

Zero temperature The function can be determined analytically :

$$\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega) = N(0)\frac{k_F}{q}\left[\Psi_3\left(\frac{\omega+\mathrm{i}\eta}{qv_F} - \frac{q}{2k_F}\right) - \Psi_3\left(\frac{\omega+\mathrm{i}\eta}{qv_F} + \frac{q}{2k_F}\right)\right], \tag{6.76}$$

$$\Psi_3(z) = \frac{z}{2} + \frac{1-z^2}{4}\ln\frac{z+1}{z-1} \overset{|z|\to\infty}{\longrightarrow} \frac{1}{3z} + \frac{1}{15z^3}, \tag{6.77}$$

where $N(0) = mk_F/(\pi\hbar)^2$ is the density of states at the Fermi surface, and $v_F = \hbar k_F/m$ is the Fermi velocity. More explicitly,

$$\frac{\mathrm{Re}\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega)}{N(0)} = -\frac{1}{2} + \frac{1-\nu_-^2}{4\tilde{q}}\ln\left|\frac{\nu_- - 1}{\nu_- + 1}\right| - \frac{1-\nu_+^2}{4\tilde{q}}\ln\left|\frac{\nu_+ - 1}{\nu_+ + 1}\right|, \tag{6.78}$$

$$\frac{\mathrm{Im}\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega)}{N(0)} = \frac{\pi}{4\tilde{q}}\left[\theta\left(1-\nu_+^2\right)\left(1-\nu_+^2\right) - \theta\left(1-\nu_-^2\right)\left(1-\nu_-^2\right)\right], \tag{6.79}$$

$$\tilde{q} \equiv \frac{q}{k_F},\quad \nu_\pm \equiv \frac{\omega}{qv_F} \pm \frac{q}{2k_F}. \tag{6.80}$$

Finite temperature The function can be determined by

$$\frac{\mathrm{Re}\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega)}{N(0)} = -\int_0^\infty \mathrm{d}x \frac{F(x,T)}{2\tilde{q}}\left(\ln\left|\frac{x-\nu_-}{x+\nu_-}\right| - \ln\left|\frac{x-\nu_+}{x+\nu_+}\right|\right), \tag{6.81}$$

$$\frac{\mathrm{Im}\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega)}{N(0)} = -\frac{\pi\omega}{4\epsilon_F\tilde{q}} - \frac{k_BT}{4\epsilon_F\tilde{q}}\ln\frac{1+\exp\left[\beta\left(\nu_-^2\epsilon_F - \mu\right)\right]}{1+\exp\left[\beta\left(\nu_+^2\epsilon_F - \mu\right)\right]}, \tag{6.82}$$

$$F(x,T) = \frac{x}{\exp\left[\beta\left(x^2\epsilon_F - \mu\right)\right] + 1}, \tag{6.83}$$

where $\epsilon_F \equiv \hbar^2k_F^2/2m$, and μ is the chemical potential at finite temperature.

See Fig. 6.2 for the Lindhard function, and Fig. 6.3 for a comparison between χ_0^{r} and $\chi_{\mathrm{RPA}}^{\mathrm{r}}$. See GV §4 for a thorough discussion on the Lindhard function.

Long-wavelength and static limit: The Lindhard function has a singularity at $q \to 0$ and $\omega \to 0$. The limit depends on the ratio ω/v_Fq. Depending on the order of taking the limits, we have:

$$\lim_{\boldsymbol{q}\to 0}\lim_{\omega\to 0}\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega) = -N(0), \tag{6.84}$$

$$\lim_{\omega\to 0}\lim_{\boldsymbol{q}\to 0}\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega) \to \frac{\rho_0q^2}{m\omega^2}\left[1 + \frac{3}{5}\frac{q^2v_F^2}{\omega^2}\right] \quad (\text{for } v_Fq \ll \omega), \tag{6.85}$$ (6.77)

corresponding to the static limit and dynamic limit, respectively.

It is common to see the behavior in response functions:

- When calculating non-equilibrium responses (e.g., conductivity), one should use the dynamic limit.
- The static limit of a response function could be different from usual thermodynamic susceptibilities. There are three different kinds of static susceptibilities:
  - isolated susceptibility $\chi^{\mathrm{iso}} = \lim_{\omega\to 0}\chi^{\mathrm{r}}(\omega)$;

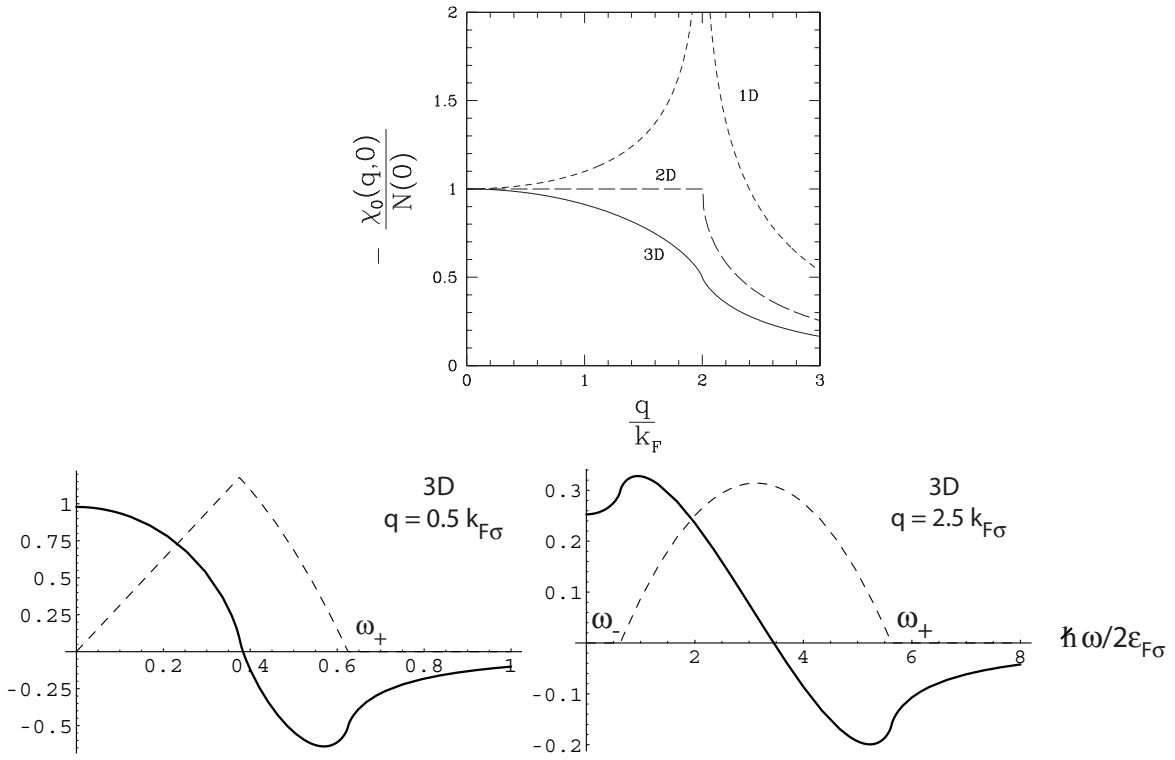


Figure 6.2: Lindhard function at zero temperature in different parameter regimes, shown as $-\chi_0(\boldsymbol{q},\omega)/N(0)$. Top: static response function for $\omega = 0$; Bottom left: $q < 2k_F$; Bottom right: $q > 2k_F$. The dashed lines show the imaginary part of the response function. GV Fig. 4.1, .4, .5

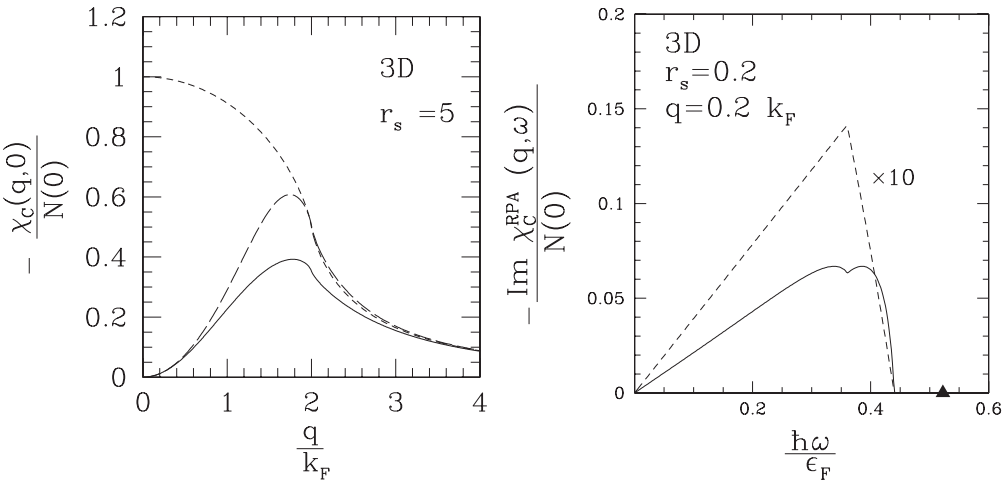


Figure 6.3: Comparison between the RPA density response function and the Lindhard function. Left: static response functions, the solid line for the RPA, the short dashed line for the Lindhard, and the long dashed line for the one with the local field correction (see §6.2.3); Right: imaginary part of the RPA (solid line) and the Lindhard function (short dashed line). The solid triangle indicates a δ-function peak associated with a plasmon resonance (see §6.3). GV Fig. 5.9, 5.10

– isothermal static susceptibility $\chi^{\mathrm{T}} \equiv -(\partial\rho/\partial\mu)_T$;
– adiabatic static susceptibility $\chi^{\mathrm{ad}} \equiv -(\partial\rho/\partial\mu)_S$.

There exist inequalities:

$$\chi^{\mathrm{T}} \geq \chi^{\mathrm{ad}} \geq \chi^{\mathrm{iso}}. \tag{6.86}$$

See Eq. (4.2.32–34) of Ref. [15].

Friedel oscillation: electrons screening an external potential are restricted in $|\boldsymbol{k}| > k_F$. The sharp restriction in the momentum space results in an oscillation in the real space. FW §14

The RPA response function is shown in Fig. 6.3. The static density response function can be written as

$$\chi^{\mathrm{r}}_{\mathrm{RPA}}(\boldsymbol{q}) = -\frac{N(0)\,(q/k_F)^2\, g\,(q/k_F)}{(q/k_F)^2 + [4\pi e^2 N(0)/k_F^2]\, g\,(q/k_F)}, \tag{6.87}$$

$$g(x) \equiv \frac{1}{2} - \frac{1}{2x}\left(1 - \frac{x^2}{4}\right) \ln\left|\frac{1-\frac{x}{2}}{1+\frac{x}{2}}\right|. \tag{6.88}$$

In the presence of a test charge $-Ze$, $\phi_{\boldsymbol{q}} = Ze^2/q^2$, the induced density is $\delta\rho_{\boldsymbol{q}} = \chi^{\mathrm{r}}_{\mathrm{RPA}}(\boldsymbol{q})\phi_{\boldsymbol{q}}$, and

$$\delta\rho(\boldsymbol{r}) = -Z\int \frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3}\, e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \frac{(q_{\mathrm{TF}}/k_F)^2\, g\,(q/k_F)}{(q/k_F)^2 + (q_{\mathrm{TF}}/k_F)^2\, g\,(q/k_F)} \underset{r\to\infty}{\sim} -\frac{Z}{\pi}\frac{2\xi}{(4+\xi)^2}\frac{\cos(2k_F r)}{r^3}, \tag{6.89}$$

where $q_{\mathrm{TF}} \equiv \sqrt{4\pi e^2 N(0)} = (4\alpha r_s/\pi)^{1/2}\, k_F$ is the Thomas-Fermi wave number, $\xi \equiv q_{\mathrm{TF}}^2/2k_{\mathrm{F}}^2$. It is different from what would be expected from a pure hydrostatic (long-wavelength limit) consideration, i.e., the Thomas-Fermi approximation. The latter predicts $\delta\rho(\boldsymbol{r}) = -Zq_{\mathrm{TF}}^2 e^{-q_{\mathrm{TF}}r}/(4\pi r)$.

At finite temperature, the Fermi surface is smeared. $\delta\rho(\boldsymbol{r})$ eventually becomes $\delta\rho(\boldsymbol{r}) \to -Zq_{\mathrm{D}}^2 e^{-q_{\mathrm{D}}r}/(4\pi r)$ at $r \to \infty$, where $q_{\mathrm{D}} \equiv \sqrt{4\pi\rho_0 e^2\beta}$ is the Debye screening length. See FW §33.

Caveats of the RPA:

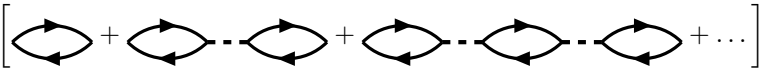
- It completely ignores exchange-correlation effects by assuming that electrons just feel a mean-field electrostatic potential (Hartree approximation).
- It violates the compressibility sum rule Eq. (6.60) –the RPA predicts a compressibility always the same as that of a non-interacting electron gas:

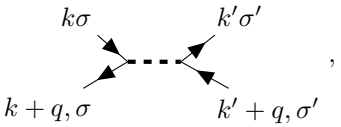
$$\frac{1}{\rho_0^2 K} = -\lim_{\boldsymbol{q}\to 0}\frac{1}{\tilde{\chi}^{\mathrm{r}}(\boldsymbol{q})} \approx -\lim_{\boldsymbol{q}\to 0}\frac{1}{\chi^{\mathrm{r}}_0(\boldsymbol{q})} = \frac{1}{N(0)}. \tag{6.90}$$ (6.60)

6.2.3 Local field correction

GV §5.4

Exact series of diagrams of the density response function can be obtained from Eq. (5.49) and the Bethe-Salpeter equation Eq. (5.50): (6.41)

$$\chi(\boldsymbol{q},\omega) = \frac{\mathrm{i}}{\hbar}\Big[$$  $$\Big], \tag{6.91}$$

$$I_{\boldsymbol{k}\omega\sigma,\boldsymbol{k}'\omega'\sigma'}(\boldsymbol{q},\nu) \equiv$$  $$, \tag{6.92}$$

where we denote the irreducible electron-hole interaction I as a bold vertex. Compared to the RPA:

- The exact (bold) Green's function assumes the places of the free Green's function;
- The irreducible interaction I assumes the places of the bare interaction $v(\boldsymbol{q})$.

Note that $I_{\boldsymbol{k}\omega\sigma,\boldsymbol{k}'\omega'\sigma'}(\boldsymbol{q},\nu)$ is in general *not* a local interaction, i.e., it cannot be written as a form $I(\boldsymbol{r}-\boldsymbol{r}')$.

Local field approximation involves two drastic approximations:

1. Approximate the irreducible electron-hole interaction as

$$I_{\boldsymbol{k}\omega\sigma,\boldsymbol{k}'\omega'\sigma'}(\boldsymbol{q},\nu) \approx [1 - G_{\sigma\sigma'}(\boldsymbol{q})]\, v(\boldsymbol{q}). \tag{6.93}$$

   The dependences on $\boldsymbol{k}$ and $\boldsymbol{k}'$ are ignored. It basically assumes that the irreducible effective interaction is a *local* interaction $I(\boldsymbol{r}_1 - \boldsymbol{r}_2)$. The dependence on frequencies is also ignored –It is a static approximation.

2. Replace the electron-hole bubble with the non-interacting counterpart, i.e., the Lindhard function. This is justified by the fact that the exact Green's function is close to the non-interacting one except for small renormalization effects. §5.3.2

As a result, we have

$$\chi^{\mathrm{r}}(\boldsymbol{q},\omega) \approx \frac{\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega)}{1 - v(\boldsymbol{q})\,[1 - G_+(q)]\,\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega)}, \tag{6.94}$$

where

$$G_{\pm}(q) \equiv \frac{G_{\uparrow\uparrow}(q) \pm G_{\uparrow\downarrow}(q)}{2}. \tag{6.95}$$

Physical interpretation: The effective potential seen by an electron is different from the mean-field potential of the Hartree approximation because:

- The electrostatic field seen by an electron must not include the contribution from itself;
- Because of the antisymmetry of the wave function, an electron at a give position excludes the presence in its proximity of another electron with the same spin orientation –exchange holes;
- Coulomb repulsion prevents two electrons staying too close –correlation holes.

To take account of these corrections, we introduce the local effective potential felt by an electron:

$$\phi_{\mathrm{eff},\sigma}(\boldsymbol{q},\omega) = \phi_\sigma(\boldsymbol{q},\omega) + \sum_{\sigma'} v(\boldsymbol{q})\,[1 - G_{\sigma\sigma'}(q)]\,\delta\rho_{\sigma'}(\boldsymbol{q},\omega). \tag{6.96}$$

The term proportional to $-v(\boldsymbol{q})G_{\sigma\sigma'}(q)$ is the correction due to the aforementioned effects.

Determination of $G(q)$: various approaches have been developed for determining the local field correction factor.

- Asymptotic behaviors of $G(q)$ are known. GV §5.6
- One of most successful approaches is developed by Singwi, Tosi, Land, and Sjölander, usually referred as "STLS" scheme. GV §5.4.4
- Ichimaru and Utsumi develop an interpolation formula [12]. See Fig. 6.4 for $G(q)$ from the Ichimaru-Utsumi interpolation formula. Further developments are reviewed in Ref. [11].

Effective interactions The local field correction introduces vertex corrections to RPA. In the RPA, the effective interaction between two particles is always $W(\boldsymbol{q},\nu) \equiv v(\boldsymbol{q})/\varepsilon_{\mathrm{RPA}}(\boldsymbol{q},\nu)$, no matter what the particles are. With the local field correction, the effective interaction will be different for different circumstances: GV §5.5

Test charge-test charge interaction A test charge (not an electron) just sees the electrostatic potential. Therefore, the interaction between two test charges is screened by the dielectric function defined in Eq. (6.63):

$$W_{\mathrm{tt}} = \frac{v(\boldsymbol{q})}{\epsilon(\boldsymbol{q},\omega)}, \tag{6.97}$$

$$\frac{1}{\tilde{\chi}^{\mathrm{r}}(\boldsymbol{q},\omega)} = \frac{1}{\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega)} + v(\boldsymbol{q})\,G_+(q), \tag{6.98}$$ (6.94,6.62)

$$\epsilon(\boldsymbol{q},\omega) = 1 - v(\boldsymbol{q})\tilde{\chi}^{\mathrm{r}}(\boldsymbol{q},\omega) = 1 - \frac{v(\boldsymbol{q})\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega)}{1 + v(\boldsymbol{q})G_+(q)\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega)} \tag{6.99}$$ (6.65)

Electron-test charge interaction A test charge density $\rho_{\rm t}(\boldsymbol{q},\omega)$ induces a perturbing potential $\phi(\boldsymbol{q},\omega) = v(\boldsymbol{q})\rho_{\rm t}(\boldsymbol{q},\omega)$ and an electron density change $\delta\rho(\boldsymbol{q},\omega) = \chi^{\rm r}(\boldsymbol{q},\omega)\phi(\boldsymbol{q},\omega)$. The potential seen by an electron has the exchange-correlation correction:

$$\phi_{\rm eff}(\boldsymbol{q},\omega) = \phi(\boldsymbol{q},\omega) + v(\boldsymbol{q})\left[1 - G_+(q)\right]\delta\rho(\boldsymbol{q},\omega) \tag{6.100}$$ (6.96)

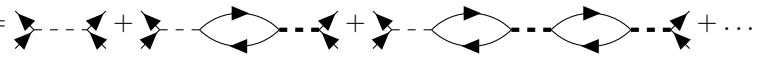
$$= \frac{\phi(\boldsymbol{q},\omega)}{1 - v(\boldsymbol{q})\left[1 - G_+(q)\right]\chi_0^{\rm r}(\boldsymbol{q},\omega)}. \tag{6.101}$$

As a result,

$$W_{\rm et} = \frac{v(\boldsymbol{q})}{\epsilon_{\rm et}(\boldsymbol{q},\omega)}, \tag{6.102}$$

$$\epsilon_{\rm et}(\boldsymbol{q},\omega) = 1 - v(\boldsymbol{q})\left[1 - G_+(q)\right]\chi_0^{\rm r}(\boldsymbol{q},\omega). \tag{6.103}$$

It corresponds to the diagrams:

$W_{\rm et} =$  (6.104)

By applying Eq. (6.35) and (5.50), we can determine the self-energy:

$$\Sigma_{\rm LFA}\left(\boldsymbol{k},\omega\right) = \mathrm{i}\int\frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^3}\int\frac{\mathrm{d}\nu}{2\pi}W_{\rm et}(\boldsymbol{q},\nu)G(\boldsymbol{k}+\boldsymbol{q},\omega+\nu). \tag{6.105}$$

Electron-electron interaction is defined to be the IRREDUCIBLE ELECTRON-ELECTRON INTERACTION, which includes all diagrams irreducible in the *particle-particle channel*. GV §6.3.6

- An electron density $\rho_\uparrow$ with spin $\uparrow$ exerts effective *external* potentials to the system:

$$\phi_\uparrow(\boldsymbol{q},\omega) = v(\boldsymbol{q})\left[1 - G_{\uparrow\uparrow}(q)\right]\rho_\uparrow(\boldsymbol{q},\omega), \tag{6.106}$$

$$\phi_\downarrow(\boldsymbol{q},\omega) = v(\boldsymbol{q})\left[1 - G_{\downarrow\uparrow}(q)\right]\rho_\uparrow(\boldsymbol{q},\omega). \tag{6.107}$$

- They result in effective local potentials

$$\phi_{{\rm eff},\downarrow} = \left[\frac{1}{1 - v(1-G_+)\chi_0^{\rm r}} - \frac{1}{1 + vG_-\chi_0^{\rm r}}\right]\frac{\rho_\uparrow}{\chi_0^{\rm r}}, \tag{6.108}$$

$$\phi_{{\rm eff},\uparrow} = \phi_{{\rm eff},\downarrow} - \frac{2vG_-}{1 + vG_-\chi_0^{\rm r}}\rho_\uparrow. \tag{6.109}$$

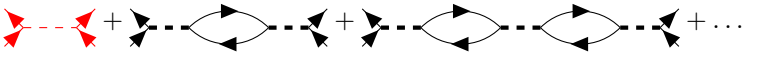
- The effective external potentials Eqs (6.106, 6.107) include the exchange-correlation corrections, which are contributions from the effective many-body medium consisting of all other electrons. They should be excluded from the effective interaction. It amounts to subtract from $\phi_{{\rm eff},\uparrow}$ and $\phi_{{\rm eff},\downarrow}$ the contributions $-vG_{\uparrow\uparrow}\rho_\uparrow$ and $-vG_{\downarrow\uparrow}\rho_\uparrow$, respectively.
- The effective interaction can be obtained by dividing the resulting effective potentials by $\rho_\uparrow$:

$$W_{\uparrow\uparrow} = v + \left[v\left(1 - G_+\right)\right]^2\chi^{\rm r} + \left(vG_-\right)^2\chi_{\rm s}^{\rm r}, \tag{6.110}$$

$$W_{\uparrow\downarrow} = v + \left[v\left(1 - G_+\right)\right]^2\chi^{\rm r} - \left(vG_-\right)^2\chi_{\rm s}^{\rm r}, \tag{6.111}$$

where $\chi_{\rm S}^{\rm r}$ is the spin density response function with respect to the spin density operator $\hat{S}_z = \hat{\rho}_\uparrow - \hat{\rho}_\downarrow$.

The formula is known as the Kukkonen-Overhauser electron-electron effective interaction formula. It corresponds to the diagrams:

$W =$  (6.112)

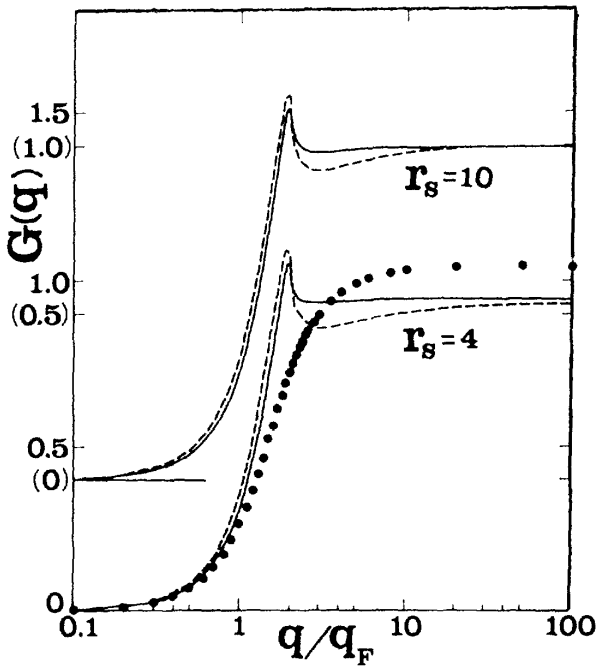


Figure 6.4: Local-field correction $G_+(q)$ for $r_s = 4$ and 10. The solid lines show $G(q)$ from the Ichimaru-Utsumi interpolation formula. Ref. [12]

6.3 Plasmon

6.3.1 Collective excitation

GV §5.3.3

In the absence of the external potential, we have the equation

$$\epsilon(\boldsymbol{q},\omega)\phi_{\rm sc}(\boldsymbol{q},\omega) = 0. \tag{6.113}$$

(6.63)

The equation could be Fourier transformed to the real space and becomes an equation governing the propagation of a potential/density wave. The dispersion of the wave is determined by the equation

$$\epsilon(\boldsymbol{q},\Omega_{\boldsymbol{q}}) = 0. \tag{6.114}$$

Note that a zero of the dielectric function is also a pole of the density response function. (6.66)

Applying Eq. (6.65) and the the RPA approximation $\tilde{\chi}^{\rm r} \approx \chi_0^{\rm r}$ as well as the long-wavelength limit Eq. (6.85), we obtain

$$\Omega_{\boldsymbol{q}} \approx \sqrt{\omega_{\rm p}^2 + \frac{3}{5}q^2 v_{\rm F}^2}, \tag{6.115}$$

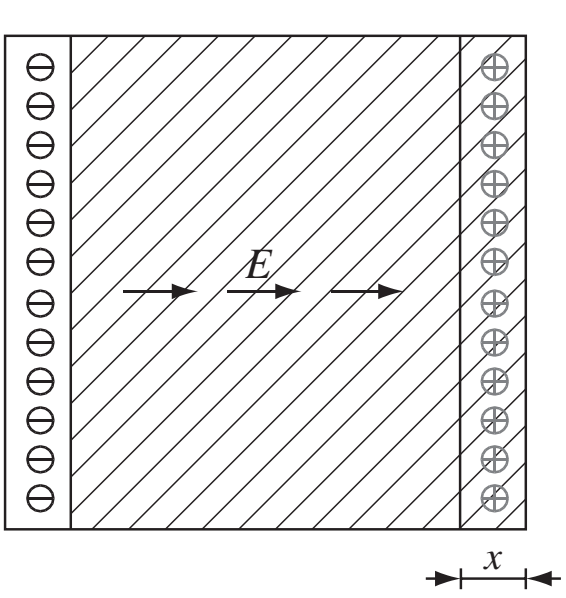
where

$$\omega_{\rm p} = \sqrt{\frac{4\pi\rho_0 e^2}{m}} \tag{6.116}$$

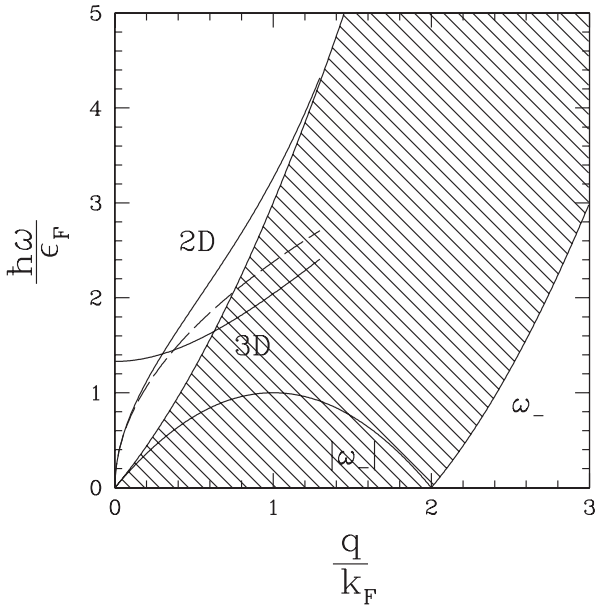
is the *plasma* frequency.

Classical picture: The plasma mode at $\boldsymbol{q} = 0$ is the oscillation of an electron gas as a whole relative to its fix positive charge background (see Fig. 6.5a):

- A displacement x results in two parallel layers of opposite charges at the two ends of the system: $\rho_{\rm layer} = \rho_0 x$.
- The charge layers give rise to an electric field in the bulk $E = 4\pi e\rho_0 x$, which exerts a restoring force to electrons.
- The equation of motion: $m\ddot{x} = -eE = -4\pi e^2\rho_0 x$. It predicts an oscillating frequency $\omega_{\rm p}$.



(a) Illustration of the plasma oscillation.



(b) The electron-hole continuum (shaded area) and the dispersion of plasmons. When the dispersion enters into the continuum, the plasmon is heavily damped and ceases to exist in practice.

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GV Fig. 5.8

Electron-hole continuum and damping: A plasmon has an infinite lifetime only when the dielectric function has a vanishing imaginary part at the frequency of the plasmon. This is true when the Lindhard function has a vanishing imaginary part at the frequency. It depends on whether or not an plasmon (or any other collective excitations) could excite an electron out of the Fermi sea to create an electron-hole pair: (6.79)

- The process of exciting one electron from $\boldsymbol{k}$ to $\boldsymbol{k}+\boldsymbol{q}$ is constraint by the conservations of the energy and momentum:

$$\hbar\Omega_{\boldsymbol{q}} = \frac{\hbar^2 |\boldsymbol{k}+\boldsymbol{q}|^2}{2m} - \frac{\hbar^2 |\boldsymbol{k}|^2}{2m} = \frac{\hbar^2 q^2}{2m} + \frac{\hbar^2}{m}\boldsymbol{k}\cdot\boldsymbol{q}. \tag{6.117}$$

- Because the maximum $|\boldsymbol{k}|$ of occupied states is k_F, the excitation is possible only when

$$\max\left(0, \omega_-(q)\right) \leq \Omega_{\boldsymbol{q}} \leq \omega_+(q), \tag{6.118}$$

$$\omega_\pm(q) = \frac{\hbar q^2}{2m} \pm v_{\mathrm{F}} q. \tag{6.119}$$

The region constrained by Eq. (6.118) is called the electron-hole continuum. We note that it is exactly the region for $\mathrm{Im}\chi_0^{\mathrm{r}}(\boldsymbol{q},\omega) \neq 0$. When the wavevector-energy of a plasmon enters into the continuum, it will be damped. See Fig. 6.5b.

Oscillator strength: the density response function $\chi^{\mathrm{r}}(\boldsymbol{q},\omega)$ could be regarded as the propagator of a plasmon, just like $G^{\mathrm{r}}(\boldsymbol{k},\omega)$ for an electron. The counterpart of the quasi-particle weight for a plasmon is defined as

$$\frac{1}{Z'_{\boldsymbol{q}}} = \left.\frac{\partial \mathrm{Re}\epsilon(\boldsymbol{q},\omega)}{\partial\omega}\right|_{\omega=\Omega_{\boldsymbol{q}}} \approx \frac{2}{\Omega_{\boldsymbol{q}}}. \tag{6.120}$$ (5.85)

As a result:

$$\mathrm{Im}\chi^{\mathrm{r}}_{\mathrm{RPA}}(\boldsymbol{q},\omega) \approx -\frac{\Omega_{\boldsymbol{q}}}{2v(\boldsymbol{q})}\pi\left[\delta\left(\omega-\Omega_{\boldsymbol{q}}\right) - \delta\left(\omega+\Omega_{\boldsymbol{q}}\right)\right]. \tag{6.121}$$

Note that it satisfies the f-sum rule Eq. (6.52).

6.3.2 Functional integrals of plasmons

AS §6.2

By using functional integral formalism, one can obtain an effective action for plasmons directly from an action for interacting electrons. It demonstrates how quasi-particles/collective excitations emerge in an interacting electron system.

Action of electrons We start from the action for interacting electrons. The action can be written as (3.34)

$$S\left[\psi,\psi^*\right]=\sum_{k\sigma}\psi^*_{k\sigma}\left(-\mathrm{i}\hbar\omega_n+\frac{\hbar^2\left|\boldsymbol{k}\right|^2}{2m}-\mu\right)\psi_{k\sigma}+\frac{1}{2\hbar\beta\mathcal{V}}\sum_{kk'q\sigma\sigma'}v(\boldsymbol{q})\psi^*_{k+q,\sigma}\psi^*_{k'-q,\sigma'}\psi_{k'\sigma'}\psi_{k\sigma}, \tag{6.122}$$

where we adopt the short-hand notation $k\equiv(\omega_n,\boldsymbol{k})$, $\sum_k\equiv\sum_{\omega_n}\sum_{\boldsymbol{k}}$, and

$$\psi_{k\sigma}\equiv(\hbar\beta\mathcal{V})^{-1/2}\int\mathrm{d}\tau\int\mathrm{d}\boldsymbol{r}\,e^{\mathrm{i}\omega_n\tau-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\psi_\sigma(\boldsymbol{r},\tau). \tag{6.123}$$

Note that ψ is a Grassmann variable, not a field operator.

The interaction part of the action can be re-organized as

$$S_{\mathrm{int}}\left[\psi,\psi^*\right]=\frac{1}{2\mathcal{V}\hbar\beta}\sum_q v(\boldsymbol{q})\rho_{-q}\rho_q, \tag{6.124}$$

where $\rho_q\equiv\sum_{k\sigma}\psi^*_{k\sigma}\psi_{k+q,\sigma}$. Note that $\rho^*_q=\rho_{-q}$.

Hubbard-Stratonovich transformation is a trick to convert an interacting system to an equivalent system in which particles are non-interacting but coupled to fluctuating auxiliary fields.

We exploit the Gaussian integral identity

$$\exp\left(-\frac{1}{2}\rho^\dagger V\rho\right)=\left[\det\left(2V\right)\right]^{-1}\int\prod_i\frac{\mathrm{d}\phi^*_i\mathrm{d}\phi_i}{2\pi\mathrm{i}}\exp\left[-\frac{1}{2}\phi^\dagger V^{-1}\phi-\frac{\mathrm{i}}{2}\left(\rho^\dagger\phi+\phi^\dagger\rho\right)\right], \tag{6.125}$$

(1.146)

where V is a *positive-definite* Hermitian matrix (repulsive interaction). Note that i factor on the right hand side is needed to give rise to the minus sign (repulsive interaction) on the left hand side.

- In case of an attractive interaction, i.e., V is *negative-definite*, the identity

$$\exp\left(-\frac{1}{2}\rho^\dagger V\rho\right)=\left[\det\left(-2V\right)\right]^{-1}\int\prod_i\frac{\mathrm{d}\phi^*_i\mathrm{d}\phi_i}{2\pi\mathrm{i}}\exp\left[\frac{1}{2}\phi^\dagger V^{-1}\phi-\frac{1}{2}\left(\rho^\dagger\phi+\phi^\dagger\rho\right)\right] \tag{6.126}$$

  should be used. Now ρ is coupled to a *real* potential ϕ.
- The real-time counterpart of the transformation:

$$e^{-\frac{\mathrm{i}}{2}\rho^\dagger V\rho}=\left[\det\left(2V\right)\right]^{-1}\int\prod_i\frac{\mathrm{d}\phi^*_i\mathrm{d}\phi_i}{2\pi}\exp\left\{\frac{\mathrm{i}}{2}\left[\phi^\dagger V^{-1}\phi-\left(\rho^\dagger\phi+\phi^\dagger\rho\right)\right]\right\}. \tag{6.127}$$

Transformed action: By applying the Hubbard-Stratonovich transformation, we obtain:

$$e^{-S_{\mathrm{int}}/\hbar}=\frac{1}{Z_{\phi0}}\int\mathrm{D}\phi\,\exp\left\{-\frac{1}{\hbar^2\beta\mathcal{V}}\sum_q\left[\frac{1}{2}\phi_{-q}v^{-1}(\boldsymbol{q})\phi_q+\mathrm{i}\rho_{-q}\phi_q\right]\right\}, \tag{6.128}$$

$$Z_{\phi0}\equiv\int\mathrm{D}\phi e^{-S_{\phi0}[\phi]/\hbar}, \tag{6.129}$$

$$S_{\phi0}\left[\phi\right]\equiv\frac{1}{8\pi e^2\hbar\beta\mathcal{V}}\sum_q\left|\boldsymbol{q}\right|^2\left|\phi_q\right|^2=\frac{1}{8\pi e^2}\int\mathrm{d}\boldsymbol{r}\int_0^{\hbar\beta}\mathrm{d}\tau\left|\boldsymbol{\nabla}\phi\left(\boldsymbol{r}\tau\right)\right|^2, \tag{6.130}$$

where $\phi(\boldsymbol{r}\tau)\equiv(\hbar\beta\mathcal{V})^{-1}\sum_q\phi_q e^{-\mathrm{i}\nu_m\tau+\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}$ with $q\equiv(\nu_m,\boldsymbol{q})$. We assume that ϕ is a real field, therefore $\phi_{-q}=\phi^*_q$.

- The action is transformed to

$$S\left[\psi,\psi^*,\phi\right]=\frac{1}{8\pi e^2\hbar\beta\mathcal{V}}\sum_q|\boldsymbol{q}|^2\left|\phi_q\right|^2+\sum_{kk'\sigma}\psi^*_{k\sigma}\left[\left(-\mathrm{i}\hbar\omega_n+\frac{\hbar^2|\boldsymbol{k}|^2}{2m}-\mu\right)\delta_{kk'}+\frac{\mathrm{i}}{\hbar\beta\mathcal{V}}\phi_{k-k'}\right]\psi_{k'\sigma} \tag{6.131}$$

$$=\int\mathrm{d}\boldsymbol{r}\int_0^{\hbar\beta}\mathrm{d}\tau\left\{\frac{1}{8\pi e^2}\left|\boldsymbol{\nabla}\phi\left(\boldsymbol{r}\tau\right)\right|^2+\sum_\sigma\psi^*_\sigma(\boldsymbol{r}\tau)\left[\hbar\partial_\tau-\frac{\hbar^2\nabla^2}{2m}-\mu+\mathrm{i}\phi\right]\psi_\sigma(\boldsymbol{r}\tau)\right\}. \tag{6.132}$$

  The first term is the energy associated with the fluctuating potential, while the second term describes a non-interacting electron system coupled to an *imaginary* potential $\mathrm{i}\phi$.

- After completing the integrals over ψ and ψ^*, we can express the partition function as

$$\frac{Z}{Z_0}=\frac{1}{Z_{\phi0}}\int\mathrm{D}\phi\,\exp\left(-\frac{S_{\phi0}\left[\phi\right]-\hbar W_0\left[\mathrm{i}\phi\right]}{\hbar}\right), \tag{6.133}$$

  where

$$W_0\left[\mathrm{i}\phi\right]\equiv\ln\left\langle\exp\left[-\frac{\mathrm{i}}{\hbar}\int\mathrm{d}\tau\int\mathrm{d}\boldsymbol{r}\rho(\boldsymbol{r}\tau)\phi(\boldsymbol{r}\tau)\right]\right\rangle_0=\mathrm{Tr}\ln\left[1-\mathrm{i}\hat{\mathcal{G}}_0\frac{\hat{\phi}}{\hbar}\right] \tag{6.134}$$ (5.19)

  is exactly the connected generating functional for a free electron system, albeit with an imaginary potential. One can interpret $-\beta^{-1}W_0\left[\mathrm{i}\phi\right]$ as the grand potential of a non-interacting system in the presence of a potential $\mathrm{i}\phi$. (5.8)

- We can expand $W_0\left[\mathrm{i}\phi\right]$ as a series around $\phi=0$:

$$W_0\left[\mathrm{i}\phi\right]=\sum_{n=1}^{\infty}\frac{1}{n!}\left(-\frac{\mathrm{i}}{\hbar}\right)^n\int\mathrm{d}1\ldots\mathrm{d}n\,\mathcal{G}^{(n)}_{\mathrm{c}0}\left(1\ldots n;1^+\ldots n^+\right)\phi(1)\ldots\phi(n)\,. \tag{6.135}$$ (5.10)

  where $\mathcal{G}^{(n)}_{\mathrm{c}0}$ is the n-particle connected Green's function of a *non-interacting* system.

  First order: $\mathcal{G}^{(1)}_{\mathrm{c}0}=\rho_0$ is a constant. As a result, only $\phi_{q=0}$ component is contributing. However, there is no $\phi_{q=0}$ component because of the charge neutrality. (6.1)

  Second order:

$$\hbar W^{(2)}_0\left[\mathrm{i}\phi\right]=-\frac{1}{2\hbar}\int\mathrm{d}1\mathrm{d}2\mathcal{G}^{(2)}_{\mathrm{c}0}\left(12;1^+2^+\right)\phi(1)\phi(2) \tag{6.136}$$

$$=\frac{1}{2}\int\mathrm{d}1\mathrm{d}2\chi^{\mathrm{T}}_0\left(1,2\right)\phi(1)\phi(2). \tag{6.137}$$ (6.41)

Action of plasmons: to the second order of ϕ, we have

$$S_{\mathrm{p}}\equiv S_{\phi0}\left[\phi\right]-\hbar W_0\left[\mathrm{i}\phi\right]=\frac{1}{8\pi e^2\hbar\beta\mathcal{V}}\sum_q|\boldsymbol{q}|^2\left[1-v(\boldsymbol{q})\chi^{\mathrm{T}}_0(q)\right]\left|\phi_q\right|^2+\ldots \tag{6.138}$$

It corresponds to the RPA.

- We observe the emergence of a bosonic field theory out of a Fermion system. By substituting ω with $\mathrm{i}\nu_m$ in Eq. (6.85), we obtain $\chi^{\mathrm{T}}_0(\boldsymbol{q},\nu_m)\to-\rho_0q^2/m\nu_m^2$ for the dynamic limit. We have

$$S_{\mathrm{p}}=\frac{1}{2\hbar\beta\mathcal{V}}\sum_q\frac{1}{v(q)\nu_m^2}\left[\nu_m^2+\omega_{\mathrm{p}}^2\right]\left|\phi_q\right|^2. \tag{6.139}$$

- We could have the full knowledge of the field, not limited to a low energy effective one.
- Higher order terms will introduce corrections. They represent the effects of fluctuations. The corrections could sometimes become so significant that the RPA (mean-field) result is qualitatively wrong – *be cautious*. In principle, one can directly calculate $W\left[\mathrm{i}\phi\right]$ numerically.

6.3.3 Collective excitations

AS §6.2

There are many possible ways to decompose the interaction:

Direct channel is the decomposition shown in Eq. (6.124).

Exchange channel decomposes the interaction as

$$S_{\text{int}}[\psi,\psi^*] = -\frac{1}{2\mathcal{V}\hbar\beta}\sum_{qkk'\sigma\sigma'} v(\boldsymbol{k}-\boldsymbol{k}')\rho^\dagger_{k'q,\sigma\sigma'}\rho_{kq,\sigma\sigma'}, \tag{6.140}$$

with $\rho_{kq,\sigma\sigma'} \equiv \psi^*_{k\sigma'}\psi_{k+q,\sigma}$.

Pairing channel decomposes the interaction as

$$S_{\text{int}}[\psi,\psi^*] = \frac{1}{2\mathcal{V}\hbar\beta}\sum_{qkk'\sigma\sigma'} v(\boldsymbol{k}-\boldsymbol{k}')\Phi^\dagger_{k'q,\sigma\sigma'}\Phi_{kq,\sigma\sigma'}, \tag{6.141}$$

with $\Phi_{kq,\sigma\sigma'} \equiv \psi_{k+q\sigma}\psi_{-k\sigma'}$.

The arbitrariness can only be eliminated by physical reasoning:

- Had effective actions been treated exactly, different decompositions would be equivalent.
- An incorrect decomposition usually leads to difficulty in getting a meaningful low energy (long-wavelength) effective theory.
- When $|\boldsymbol{q}|$ is assumed to be small (long-wavelength limit), the different decompositions are actually non-overlapping. Therefore, one can introduce several decoupling auxiliary fields simultaneously in the long-wavelength limit.

Second quantization approach The approximation like Eq. (6.138) in the functional integral approach is equivalent to approximating the interaction part of the second quantized Hamiltonian as

$$\begin{aligned}\hat{H}_{\text{int}} \approx\ & \frac{e^2}{2\mathcal{V}}\sum_{\boldsymbol{q}\neq 0}\sum_{\boldsymbol{k}\sigma,\boldsymbol{p}\sigma'}\frac{4\pi}{q^2}\left\{\left\langle\hat{a}^\dagger_{\boldsymbol{p}-\boldsymbol{q}\sigma'}\hat{a}_{\boldsymbol{p}\sigma'}\right\rangle\hat{a}^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma}\hat{a}_{\boldsymbol{k}\sigma} + \left\langle\hat{a}^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma}\hat{a}_{\boldsymbol{k}\sigma}\right\rangle\hat{a}^\dagger_{\boldsymbol{p}-\boldsymbol{q}\sigma'}\hat{a}_{\boldsymbol{p}\sigma'}\right. && (6.142)\\ & \left. - \left\langle\hat{a}^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma}\hat{a}_{\boldsymbol{p}\sigma'}\right\rangle\hat{a}^\dagger_{\boldsymbol{p}-\boldsymbol{q}\sigma'}\hat{a}_{\boldsymbol{k}\sigma} - \left\langle\hat{a}^\dagger_{\boldsymbol{p}-\boldsymbol{q}\sigma'}\hat{a}_{\boldsymbol{k}\sigma}\right\rangle\hat{a}^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma}\hat{a}_{\boldsymbol{p}\sigma'} + \ldots\right\}, && (6.143)\end{aligned}$$

i.e., applying Wick's theorem to *contract* part of $\hat{H}_{\text{int}}$ to yield a *bilinear* form. The many possible ways of the contractions correspond to the different channels of the decompositions –the first and second lines correspond to the direct and the exchange channels respectively.

It is difficult to go beyond the mean-field approximation to consider fluctuation effects in the second quantization approach. In contrast, it is straightforward for the functional integral approach to consider the fluctuation effects –they are corrections due to the high order terms of $W[\mathrm{i}\phi]$.

Problems

1. Hartree-Fock approximation: consider an interacting electron system subject to a single body potential $u(\boldsymbol{r})$. In this case, system is not uniform and the plane-wave states are not eigenstates. We assume that Green's function can still be diagonalized in a basis $\varphi_a(\boldsymbol{r})$.

FW §10

   (a) Determine the ground state energy to the first order of the interaction $v(\boldsymbol{r}-\boldsymbol{r}')$ by using the rules of the unlabeled Feynman diagrams or the Hugenholtz diagrams. What is the matrix element for an interaction vertex?

   (b) The resulting ground state energy could be regarded as a functional of the single-particle basis wave function $\varphi_a(\boldsymbol{r})$. $\varphi_a(\boldsymbol{r})$ should be chosen such that the ground state energy is *minimized*. Determine the equation satisfied by $\varphi_a(\boldsymbol{r})$.

2. Determine the expression for Eq. (6.17a), and show that it is independent of the density. MH §5.1.5

3. Alternative proof of the stiffness theorem:

   (a) Construct an effective action $\Gamma[\rho]$ by coupling the system to a local potential $\phi(\boldsymbol{r})$;

   (b) Expand the functional to the second order of $\delta\rho$

$$\Delta\Omega[\rho] = \frac{1}{\beta}\Gamma[\rho] \approx \frac{1}{\beta}\left(\Gamma[\rho_0] + \frac{1}{2}\sum_{\boldsymbol{q}} \left.\frac{\delta^2\Gamma[\rho]}{\delta\rho_{\boldsymbol{q}}\delta\rho_{-\boldsymbol{q}}}\right|_{\rho\to\rho_0} \delta\rho_{\boldsymbol{q}}\delta\rho_{-\boldsymbol{q}}\right) + \ldots, \tag{6.144}$$

   and relate the expansion coefficient with the response function $\chi \equiv \delta\rho/\delta\phi$. Hint: Eq. (5.44).

4. Re-derive Eq. (6.75) by using the standard perturbative technique of the thermal Green's function: FW §30

   (a) Determine χ_0^{T}. See Eq. (6.42).

   (b) Carry out the summation over the Matsubara frequency. Hint: apply Eq. (3.51).

   (c) Get an expression of χ_0^{r} by applying the analytic continuation.

5. Substitute Eq. (6.138) into (6.133) and complete the integral to obtain an expression for the grand potential of the system. How is the expression compared to Eq. (6.30)?

Chapter 7

Phase transitions and spontaneous symmetry breaking

7.1 General theory

7.1.1 Phase transitions

NO §4.1

Equation of state is defined in the space of three variables:

1. temperature T;
2. external field;
3. the thermodynamic variable conjugate to the external field.

Ferromagnetic phase transition external field – magnetic field H; conjugate thermodynamic variable – magnetization M. See Fig. 7.1a.

- $T > T_c$: paramagnetic phase. $M - H$ curves are continuous.
- $T < T_c$: ferromagnetic phase. $M - H$ curves are non-analytic. $\uparrow$ and $\downarrow$ phases coexist between A and B.
- $T = T_c$: critical point. The coexistence region is reduced to a *single* point. The phase transition becomes *continuous*.

Liquid-gas transition external field – pressure P; conjugate thermodynamic variable – volume V or the density $\rho \equiv N/V$. See Fig. 7.1b.

- Liquid, gas and fluid phases are analogous to the ferromagnetic $\uparrow$, ferromagnetic $\downarrow$ and the paramagnetic phases, respectively.
- The transition becomes continuous at the critical point C.
- Liquid-gas coexistence region is a curved surface instead of a plane in the ferromagnetic case.

7.1.2 Landau theory

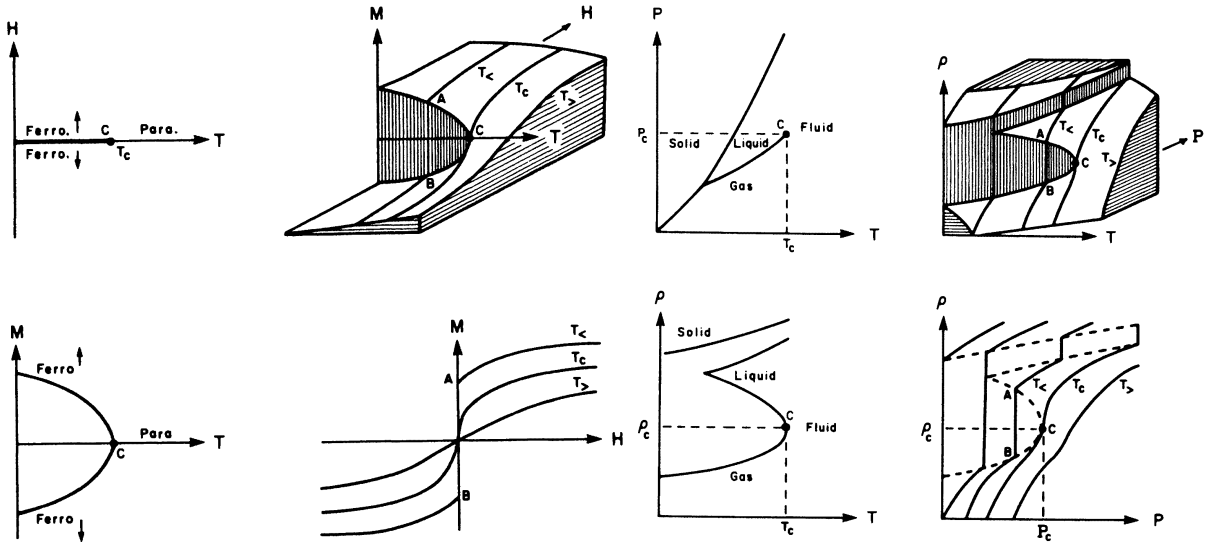
NO §4.1, 4.2

Paradigm

- There exists an order parameter (e.g., the magnetization M) which is zero in one phase (disordered phase) and is non-zero in the other phase (ordered phase).
- There exists a Landau functional $\mathcal{L}[m(\boldsymbol{r}), H, T]$ which is a *continuous* function(al) of its arguments and gives rise to the partition function of the system by

$$Z = \int \mathrm{D}\,[m(\boldsymbol{r})]\, e^{-\beta \mathcal{L}[m(\boldsymbol{r}), H, T]}. \tag{7.1}$$

  This is the definition of the Landau functional.



(a) Phase diagrams for the ferromagnetism. (b) Phase diagrams for gas-liquid-solid phase transitions. NO Fig. 4.2

Figure 7.1

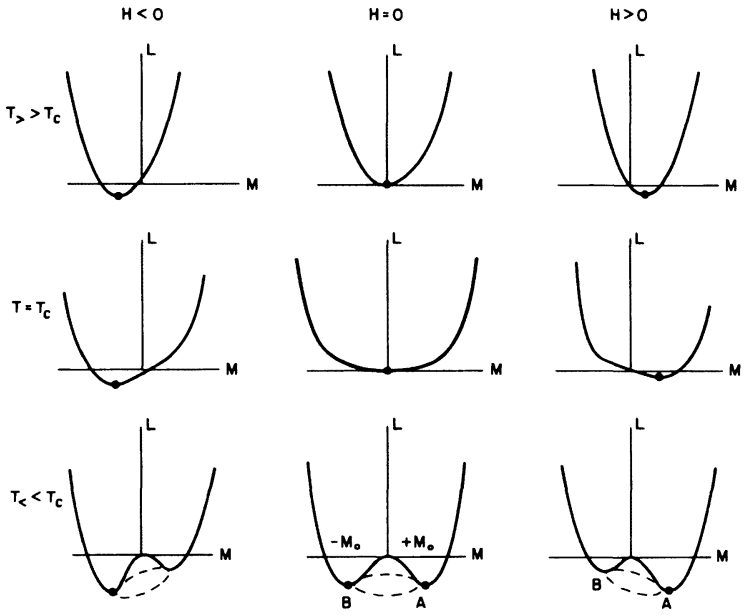


Figure 7.2: The Landau function for various parameter regimes. NO Fig. 4.3

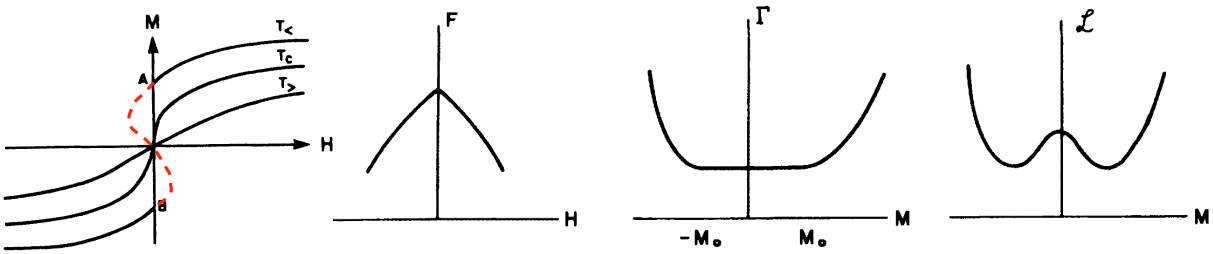


Figure 7.3: From left to right: H-M relation, $F \equiv -W$, Γ function, and the desirable form of $\mathcal{L}$. The red dashed line indicates the H-M relation which could give rise to the double well in $\mathcal{L}$. NO Fig. 4.4

  - The functional can be identified/derived from microscopic Hamiltonians/actions (see §7.2, 7.3, NO §4.2).
  - The functional can be constructed phenomenologically:
    * The form of $\mathcal{L}$ is constrained by the *symmetries* of the system.
    * Phase transition occurs when $\mathcal{L}$ has multiple degenerate minima. See Fig. 7.2.
    * Near the critical point, one could expand the functional as a power series in m. For example:

$$\mathcal{L}\left[m(\boldsymbol{r}), H, T\right] \approx \int \mathrm{d}^D \boldsymbol{r} \left[\frac{a}{2}\left|\boldsymbol{\nabla} m(\boldsymbol{r})\right|^2 + c_1 h m + d_2 t m^2 + c_3 h m^3 + b_4 m^4\right], \tag{7.2}$$

      with

$$t \equiv T - T_c \tag{7.3}$$
$$h \equiv H - H_c \tag{7.4}$$

    * The order parameter may have multiple components.
    * UNIVERSALITY, i.e., universal behavior shared by classes of diverse physical systems, is expected because only a few terms of the expansion are *relevant* and the form is constrained by symmetry. §7.1.4

- A quantum system could be regarded as a classical system in $D = d + 1$ dimensions (d spatial dimensions and one dimensional imaginary time). (3.34)
  - The span of the time dimension is finite at finite temperatures. As a result, it becomes irrelevant at the critical point because of the diverging correlation length. (7.18)
  - At zero temperature, the time becomes a true dimension. Phase transitions which are impossible at finite temperature could become possible –QUANTUM CRITICALITY.

Effective action and Landau functional One could construct an effective action as a functional of $m(\boldsymbol{r})$ by using the procedure shown in §5.1:

$$\Gamma\left[m(\boldsymbol{r})\right] = -W\left[H(\boldsymbol{r})\right] - \beta \int \mathrm{d}\boldsymbol{r} m(\boldsymbol{r}) H(\boldsymbol{r}). \tag{7.5}$$

It is tempted to interpret the Landau functional as

$$\beta\tilde{\mathcal{L}}\left[m(\boldsymbol{r})\right] = \Gamma\left[m(\boldsymbol{r})\right] + \beta M H. \tag{7.6}$$

where $M \equiv \int \mathrm{d}\boldsymbol{r} m(\boldsymbol{r})$, and H is the spatial average of $H(\boldsymbol{r})$. Unfortunately, the association is *not* correct in general:

- $\tilde{\mathcal{L}}$ is the free energy of a system with a given configuration of the order parameter, not the Landau functional that determines the partition function and free energy. (7.1)
- $\delta\tilde{\mathcal{L}}/\delta m = 0$ does give rise to the correct equilibrium state. The association has no problem when $T > T_c$.

Figure 7.4: A Mexican hat showing the energy landscape of a symmetry breaking system.

- When $T < T_c$, however, because
$$\frac{\partial \tilde{\mathcal{L}}}{\partial M} = 0, \tag{7.7}$$
$\tilde{\mathcal{L}}$ is a constant in the coexistence region instead of the double well. See Fig. 7.3.
- The effective action is useful in determining the critical point of the phase transition because the susceptibility $\chi \equiv \partial M/\partial H$ diverges at the point:
$$\frac{\partial^2 \tilde{\mathcal{L}}}{\partial M^2} = -\frac{1}{\chi} \to 0, \tag{7.8}$$ (6.54)

Symmetry breaking Although the Landau functional $\mathcal{L}$ for $T < T_c$ has all symmetries, its minima break (part of) the symmetries.

- The symmetry group of the minima is a *subgroup* of the symmetry group of the system:
$$G' \subset G. \tag{7.9}$$
The degenerate states of the minima are connected by the elements of $G'' = G/G'$.
- The symmetry breaking is a result of the thermodynamic limit:
$$M = \lim_{H\to 0}\lim_{N\to\infty} M(H) \neq \lim_{N\to\infty}\lim_{H\to 0} M(H) = 0. \tag{7.10}$$
The order of the two limits matters.
- For discrete G'', the system is trapped in one of the minima, the probability tunneling to other minima goes to zero in the thermodynamic limit. The system becomes *non-ergodic*.
- For continuous G'', fluctuations (via collective Goldstone modes) may or may not destroy the order. It depends on the dimensionality of the space and tensorial character of the order parameter.

Order parameters and conjugate fields for a variety of phase transitions are shown in Table 7.1.

7.1.3 Mean field theory

NO §4.3

The mean field approximation is just the *stationary-phase* approximation for evaluating Eq.. (7.1):
$$\left.\frac{\delta \mathcal{L}}{\delta m(\boldsymbol{r})}\right|_{m(\boldsymbol{r})\to \bar{m}} = 0, \tag{7.11}$$

Phase transition	Order parameter	Conjugate field	Broken symmetry
Ferromagnetic	magnetization $\boldsymbol{m}_i = \left\langle \hat{\boldsymbol{S}}_i \right\rangle$	Zeeman field $\boldsymbol{H} \cdot \sum_i \hat{\boldsymbol{S}}_i$	Time-reversal
Anti-ferromagnetic	staggered magnetization $\boldsymbol{m}_i = \begin{cases} \hat{\boldsymbol{S}}_i & i \in A \\ -\hat{\boldsymbol{S}}_i & i \in B \end{cases}$	staggered Zeeman field $\boldsymbol{H}_{\mathrm{S}} \cdot \left(\sum_{i \in A} \hat{\boldsymbol{S}}_i - \sum_{i \in B} \hat{\boldsymbol{S}}_i \right)$	Time-reversal
Ferroelectric	polarization $\boldsymbol{d}_i$	electric field $\boldsymbol{E} \cdot \sum_i \hat{\boldsymbol{d}}_i$	Spatial inversion
Liquid-gas	density difference	pressure P	None
Charge density wave (CDW)	density $\rho(\boldsymbol{r})$	potential $\hat{\rho}(\boldsymbol{r})\phi(\boldsymbol{r})$	Translation
Spin density wave (SDW)	spin density $\boldsymbol{S}(\boldsymbol{r}) = \sum_{\sigma\sigma'} \left\langle \hat{\psi}^\dagger_\sigma(\boldsymbol{r}) \hat{\boldsymbol{\tau}}_{\sigma\sigma'} \psi_{\sigma'}(\boldsymbol{r}) \right\rangle$	spin potential $\hat{\boldsymbol{S}}(\boldsymbol{r}) \cdot \boldsymbol{h}(\boldsymbol{r})$	Translation and time reversal
Superfluity (Bosons)	condensate amplitude $\phi = \left\langle \hat{\psi}(\boldsymbol{r}) \right\rangle$	condensate source $J\hat{\psi}^\dagger + \mathrm{h.c.}$	$U(1)$ gauge
Superconductivity	pairing amplitude $\Phi(\boldsymbol{r} - \boldsymbol{r}') = \left\langle \hat{\psi}_\uparrow(\boldsymbol{r}) \hat{\psi}_\downarrow(\boldsymbol{r}') \right\rangle$	pairing potential $\Delta(\boldsymbol{r} - \boldsymbol{r}') \hat{\psi}^\dagger_\downarrow(\boldsymbol{r}') \hat{\psi}^\dagger_\uparrow(\boldsymbol{r}) + \mathrm{h.c.}$	$U(1)$ gauge

Table 7.1: Order parameters and conjugate fields.

$$Z \sim e^{-\beta \mathcal{L}[\bar{m}, H, T]}. \tag{7.12}$$

By assuming a spatially uniform stationary solution, we have

$$\bar{m} \propto \begin{cases} \pm(-t)^{1/2} & T < T_c,\ H = H_c \\ h^{1/3} & T = T_c \end{cases}. \tag{7.13}$$

Correlation function The Landau functional can be expanded as a quadratic form around the stationary solution:

$$\mathcal{L}[m(\boldsymbol{r}), H = H_c, T] \approx \int \mathrm{d}^D \boldsymbol{r} \left\{ \frac{a}{2} |\boldsymbol{\nabla} \delta m(\boldsymbol{r})|^2 + b|t| [\delta m(\boldsymbol{r})]^2 \right\}, \tag{7.14}$$

$$b = \begin{cases} d_2 & T > T_c \\ 2d_2 & T < T_c \end{cases}. \tag{7.15}$$

The correlation function can be determined:

$$\chi_{mm}(\boldsymbol{r} - \boldsymbol{r}') = -\beta \langle \delta m(\boldsymbol{r}) \delta m(\boldsymbol{r}') \rangle \sim e^{-|\boldsymbol{r} - \boldsymbol{r}'|/\xi}, \tag{7.16}$$

$$\chi_{mm}(\boldsymbol{q}) \sim \frac{1}{q^2 + \xi^{-2}}, \tag{7.17}$$

$$\xi = \sqrt{\frac{a}{2b}} |t|^{-1/2}. \tag{7.18}$$

At the critical point, the correlation length diverges , and

$$\chi_{mm}(r) \sim \int \frac{\mathrm{d}^D \boldsymbol{q}}{(2\pi)^D} \frac{e^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}}{q^2} \sim \frac{1}{r^{D-2}}. \tag{7.19}$$

7.1.4 Fluctuations

NO §4.4

The validity of the mean field approximation depends critically on the dimension D:

- $D > D_{\mathrm{c}}$: the mean field theory is valid and predicts correct critical exponents.
- $D_{\mathrm{c}} \geq D > D_\ell$: the mean field theory still works but predicts incorrect critical exponents.

- $D \leq D_\ell$: the mean field theory is invalid and qualitatively wrong.

D_c and D_ℓ are called UPPER CRITICAL DIMENSION and LOWER CRITICAL DIMENSION, respectively.

Upper critical dimension We examine the relative importance of different terms of $\mathcal{L}$ by dimensional analysis. We rescale the Landau functional Eq. (7.2) to

$$\beta\mathcal{L}\left[\phi\right] = \int \mathrm{d}^D\boldsymbol{r}\left[\frac{1}{2}\left|\boldsymbol{\nabla}\phi(\boldsymbol{r})\right|^2 + \frac{r_0}{2}\left|\phi(\boldsymbol{r})\right|^2 + \frac{u_0}{4}\left|\phi(\boldsymbol{r})\right|^4\right], \tag{7.20}$$

where r_0 *vanishes* at the critical point. From $\beta\mathcal{L} \sim 1$, we have

$$[\phi] = L^{-\frac{D-2}{2}}, \tag{7.21}$$
$$[r_0] = L^{-2}, \tag{7.22}$$
$$[u_0] = L^{D-4}. \tag{7.23}$$

We can then recast the functional into a dimensionless form by the transformation (for $T > T_c$)

$$\boldsymbol{r} = \boldsymbol{x} r_0^{-1/2}, \tag{7.24}$$
$$\phi = \tilde{\phi} r_0^{\frac{D-2}{4}}, \tag{7.25}$$
$$\beta\mathcal{L}\left[\phi\right] \to \beta\mathcal{L}\left[\tilde{\phi}\right] = \int \mathrm{d}^D\boldsymbol{x}\left[\frac{1}{2}\left|\boldsymbol{\nabla}\tilde{\phi}(\boldsymbol{x})\right|^2 + \frac{1}{2}\tilde{\phi}^2(\boldsymbol{x}) + \frac{g}{4}\tilde{\phi}^4(\boldsymbol{x})\right], \tag{7.26}$$

with

$$g = u_0 r_0^{\frac{D-4}{2}}. \tag{7.27}$$

When the system approaches the critical point, $r_0 \to 0$:

- $D > 4$: $g \to 0$. The $\tilde{\phi}^4$ term is *irrelevant*. The mean field theory describes accurately the critical behavior.
- $D < 4$: $g \to \infty$. The $\tilde{\phi}^4$ term is *relevant*. The mean field theory will give the wrong critical behavior.
- $D = 4$: The case is marginal and corrections should be expected.

It indicates that for ϕ^4 term, $D_\mathrm{c} = 4$.

For other possible terms:

- ϕ^n:
$$D_\mathrm{c} = \frac{2n}{n-2}. \tag{7.28}$$
It turns out all orders of the expansion are relevant in *two-dimensions*.
- $(\nabla\phi)^n$ and $\phi\nabla^n\phi$ are irrelevant when $n > 2$.

Lower critical dimension The mean field approximation may completely break down in low dimensions due to fluctuations generated by GOLDSTONE MODES.

Mermin-Wagner theorem: continuous symmetries cannot be spontaneously broken for $D \leq 2$, i.e., $D_\ell = 2$ [19].

An example is the systems described by Eq. (7.20) with a 2-component ϕ field, i.e., ϕ is a complex field and for $T < T_c$:

$$\phi(\boldsymbol{r}) \approx \left|\bar{\phi}\right| e^{\mathrm{i}\varphi(\boldsymbol{r})}, \tag{7.29}$$

where $|\bar{\phi}| \equiv \sqrt{r_0/u_0}$ is the magnitude of the order parameter. We ignore its spatial variation because its collective mode is gapped [1]. The functional becomes (7.14)

$$\beta \mathcal{L}[\varphi] = \frac{|\bar{\phi}|^2}{2} \int \mathrm{d}^D \boldsymbol{r} \, |\boldsymbol{\nabla} \varphi(\boldsymbol{r})|^2 + \text{constant}, \tag{7.30}$$

i.e., the excitation of $\varphi(\boldsymbol{r})$ is *gapless*. The corresponding collective mode has a dispersion $\omega_{\boldsymbol{q}} \propto q$ with a vanishing energy at $\boldsymbol{q} \to 0$. It is the characteristic of the Goldstone mode.

The fluctuations of φ is

$$\chi_{\varphi\varphi}(\boldsymbol{r} - \boldsymbol{r}') \sim \int \frac{\mathrm{d}^D \boldsymbol{q}}{(2\pi)^D} \frac{e^{\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}-\boldsymbol{r}')}}{q^2}. \tag{7.31}$$ (7.19)

It diverges for $D \leq 2$.

Topological defect The two-component model admits a special form of excitation because φ is only defined modulo 2π. In 2D, one can have a distribution of $\varphi(\boldsymbol{r})$ like

$$\varphi(r, \theta) = \theta, \tag{7.32}$$

where θ is the polar angle of $\boldsymbol{r}$. Because $\phi(\boldsymbol{r})$ is single-valued, $|\phi(\boldsymbol{r})|$ must vanish at $r = 0$. To minimize the energy cost, $|\phi(\boldsymbol{r})| = |\bar{\phi}|$ except for a small core area with $r \lesssim a$, where a is a length scale set by an underlying microscopic model. The excitation is called a vortex, which is a TOPOLOGICAL DEFECT.

The nature and classification of topological defects are determined by the *homotopy* group of the degenerate state space. See Ref. [18] for a comprehensive review or reprints in Topology section of Ref. [2].

Kosterlitz–Thouless transition It turns out the particular 2-component system has a phase transition in 2D. However, the transition is a TOPOLOGICAL PHASE TRANSITION: it has *no* order parameter, and both phases before and after the transition are disordered phases. They are different in correlation functions –either the usual exponential decay or the one that decreases with the distance like a power. Microscopically, they are different in whether or not topological vortex excitations proliferate in the system:

- The cost of the energy to create a vortex is

$$E_{\mathrm{v}} = \pi J \ln \frac{L}{a}, \tag{7.33}$$

where $J \equiv |\bar{\phi}|^2 / \beta$, and L is the size of the system.

- The vortex can be created anywhere in the system. It results in a prefactor for the partition function, or equivalently, an entropy

$$S = 2k_B \ln \frac{L}{a}. \tag{7.34}$$

- The cost of the free energy to create a vortex is

$$F_{\mathrm{v}} = E_{\mathrm{v}} - TS = (\pi J - 2k_B T) \ln \frac{L}{a}. \tag{7.35}$$

As a result, when $T > T_{\mathrm{KT}} \equiv \pi J / 2k_B$, the vortex excitations will proliferate.

7.2 Bose-Einstein condensation and superfluidity

AS §6.3

7.2.1 Phase transition

Non-interacting Boson system The Bose-Einstein condensation (BEC) occurs when the states with $\epsilon_a > 0$ cannot accommodate all particles even one sets $\mu = 0$ (maximally allowed value):

$$\sum_{\epsilon_a > 0} n_{\mathrm{B}}(\epsilon_a) = N_1 < N. \tag{7.36}$$

[1] One can view Eq. (7.20) as the classical energy of an elastic media. The collective mode is just the sound wave.

A macroscopic number of particles will accumulate in the state with $\epsilon_a = 0$. We have the condensate density

$$\rho_{\mathrm{c}}(T) = \rho\left[1 - \left(\frac{T}{T_{\mathrm{c}}}\right)^{3/2}\right]. \tag{7.37}$$

Interacting Boson system We consider a Boson system with a repulsive contact interaction $v(\boldsymbol{r} - \boldsymbol{r}') = g\delta(\boldsymbol{r} - \boldsymbol{r}')$ and $g > 0$.

$$S[\psi, \psi^*] = \int \mathrm{d}\boldsymbol{r} \int \mathrm{d}\tau \left\{\psi^*(\boldsymbol{r}\tau)\left(\hbar\partial_\tau - \frac{\hbar^2\nabla^2}{2m} - \mu\right)\psi(\boldsymbol{r}\tau) + \frac{g}{2}\left[\psi^*(\boldsymbol{r}\tau)\psi(\boldsymbol{r}\tau)\right]^2\right\} \tag{7.38}$$

$$= \sum_k \psi_k^*\left(-\mathrm{i}\hbar\omega_n + \frac{\hbar^2|\boldsymbol{k}|^2}{2m} - \mu\right)\psi_k + \frac{g}{2\mathcal{V}\hbar\beta}\sum_{kk'q}\psi_{k+q}^*\psi_{k'-q}^*\psi_{k'}\psi_k. \tag{7.39}$$ (6.122)

Phase transition We can interpret the action Eq. (7.38) as a Landau functional defined in $D = d+1$ dimensional $(\boldsymbol{r}, \tau)$-space. For a uniform field $\psi(\boldsymbol{r}) = \phi$, the action is reduced to

$$S[\phi, \phi^*] = \hbar\beta\mathcal{V}\left[-\mu|\phi|^2 + \frac{g}{2}|\phi|^4\right]. \tag{7.40}$$

It predicts a *mean-field* critical point at $\mu = 0$, and $|\bar{\phi}|^2 = \mu/g$ for $\mu > 0$.

We note that the condition Eq. (7.8) that the susceptibility diverges is nothing but the requirement that the occupation number of the zero energy state is a macroscopic number:

$$\chi_{\psi_0\psi_0^*} = -\frac{1}{\hbar}\langle\psi_0\psi_0^*\rangle = -N_{\mathrm{c}}/\hbar \to -\infty. \tag{7.41}$$

7.2.2 Superfluidity

Goldstone mode The BEC state breaks the gauge symmetry, i.e., the invariance under the transformation of $\psi \to \psi e^{\mathrm{i}\varphi}$. The Goldstone mode is the spatial-modulation of the phase φ. We introduce the transformation of the field [2]

$$\psi(\boldsymbol{r}, \tau) = [\rho_{\mathrm{c}} + \rho_1(\boldsymbol{r}, \tau)]^{1/2} e^{\mathrm{i}\varphi(\boldsymbol{r},\tau)}, \tag{7.42}$$

where $\rho_{\mathrm{c}} \equiv |\bar{\phi}|^2$. The action is transformed to

$$S[\rho_1, \varphi] = \int \mathrm{d}\boldsymbol{r} \int \mathrm{d}\tau \left\{-\mu\rho + \frac{g}{2}\rho^2 + \frac{\hbar^2}{8m\rho}|\boldsymbol{\nabla}\rho_1|^2 + \mathrm{i}\hbar\rho\partial_\tau\varphi + \frac{\hbar^2\rho}{2m}|\boldsymbol{\nabla}\varphi|^2\right\} \tag{7.43}$$

$$\approx \int \mathrm{d}\boldsymbol{r} \int \mathrm{d}\tau \left\{\frac{g}{2}\rho_1^2 + \frac{\hbar^2}{8m\rho_{\mathrm{c}}}|\boldsymbol{\nabla}\rho_1|^2 + \mathrm{i}\hbar\rho_1\partial_\tau\varphi + \frac{\hbar^2\rho_{\mathrm{c}}}{2m}|\boldsymbol{\nabla}\varphi|^2\right\} - \frac{1}{2}\hbar\beta\mu N_{\mathrm{c}} + 2\pi\mathrm{i}\hbar N_{\mathrm{c}} n_\tau, \tag{7.44}$$

where n_τ is the winding number of φ-field along the time direction: $\varphi(\boldsymbol{r}, \hbar\beta) = \varphi(\boldsymbol{r}, 0) + 2\pi n_\tau$. Summing n_τ enforces the quantization of N_{c}.

After completing the integral over ρ_1, the action is transformed to

$$S[\varphi] = \frac{1}{2}\sum_{\boldsymbol{k}}\int \mathrm{d}\tau \left[\left(g + \frac{\hbar^2k^2}{4m\rho_{\mathrm{c}}}\right)^{-1}|\hbar\partial_\tau\varphi_{\boldsymbol{k}}(\tau)|^2 + \frac{\hbar^2k^2}{m}\rho_{\mathrm{c}}|\varphi_{\boldsymbol{k}}(\tau)|^2\right]. \tag{7.45}$$

It describes a collective excitation with the dispersion

$$\omega_{\boldsymbol{k}} = \sqrt{\frac{g\rho_{\mathrm{c}}}{m}k^2 + \left(\frac{\hbar k^2}{2m}\right)^2}. \tag{7.46}$$

[2] While the transformation looks innocent, it is actually non-trivial. This is because a functional integral is defined by its discrete time form. A direct change of variables in the functional integral leads to a complicated discrete form. To establish the transformation, one needs to first apply the operator transformation $\hat{a} = e^{-\mathrm{i}\hat{\varphi}}\hat{\rho}^{1/2}$ with the commutation relation $[\hat{\varphi}, \hat{\rho}] = \mathrm{i}$ to the second quantized Hamiltonian of the system. The functional integral is constructed by using the Fock state $\hat{\rho}|n\rangle = n|n\rangle$ and its conjugate $|\varphi\rangle$ with $\langle\varphi|n\rangle = (2\pi)^{-1/2}e^{\mathrm{i}n\varphi}$, which could be regarded as the analogues of $|x\rangle$ and $|p\rangle$ respectively. It is then straightforward to follow the procedure shown in §3.1 and apply the identity $\sum_n \int_0^{2\pi}\mathrm{d}\varphi f(\varphi)e^{\mathrm{i}n\varphi} = \int_0^\infty \mathrm{d}\rho \int_{-\infty}^{\infty}\mathrm{d}\varphi f(\varphi)e^{\mathrm{i}\rho\varphi}$.

Superfluidity If the condensate maintains a spatial gradient of $\bar{\varphi}(\boldsymbol{r})$, the current density is

$$\boldsymbol{j}_{\mathrm{s}}(\boldsymbol{r}) = \frac{1}{\hbar\beta}\int_0^{\hbar\beta} \mathrm{d}\tau \left(-\frac{\mathrm{i}\hbar}{2m}\right) \langle \psi^*(\boldsymbol{r}\tau)\boldsymbol{\nabla}\psi(\boldsymbol{r},\tau) - [\boldsymbol{\nabla}\psi^*(\boldsymbol{r}\tau)]\,\psi(\boldsymbol{r},\tau)\rangle \tag{7.47}$$

$$= \frac{1}{\hbar\beta}\int_0^{\hbar\beta} \mathrm{d}\tau \left\langle \left(\frac{\hbar\rho}{m}\right)\boldsymbol{\nabla}\varphi(\boldsymbol{r})\right\rangle \approx \frac{\hbar\rho}{m}\boldsymbol{\nabla}\bar{\varphi}(\boldsymbol{r}), \tag{7.48}$$

where we neglect the effect of fluctuations ($T \to 0$). The current density is induced by a *deformation* of the field configuration. It is analogous to the elastic force, i.e., a "momentum current," induced by the deformation of a solid. The current is *dissipationless*, and is therefore called as SUPERCURRENT. Note that the supercurrent is proportional to the total density instead of the condensate density in the limit of $T \to 0$ [24].

Critical velocity When a BEC flows through a pipe at a uniform velocity $\boldsymbol{V}$, an excitation in the fluid with a wave-vector $\boldsymbol{k}$ and frequency $\omega_{\boldsymbol{k}}$ has the frequency

$$\omega'_{\boldsymbol{k}} = \omega_{\boldsymbol{k}} + \boldsymbol{k}\cdot\boldsymbol{V}, \tag{7.49}$$

when observed in the laboratory frame in which the pipe is stationary. Note that the system reaches equilibrium by exchanging energy with the environment through the wall of the pipe. As long as $\omega'_{\boldsymbol{k}} > 0$, the BEC can reach an equilibrium and keep flowing. When $\omega'_{\boldsymbol{k}}$ becomes negative, however, excitations will be spontaneously and continuously generated, until the system is fully dissipated. This is the LANDAU CRITERION. The consideration suggests a critical velocity

$$V_c = \min\left(\frac{\omega_{\boldsymbol{k}}}{|\boldsymbol{k}|}\right). \tag{7.50}$$

For the dispersion Eq. (7.46), the critical velocity $V_c = \sqrt{g\rho_{\mathrm{c}}/m}$.

The critical velocity suggested by the Landau criterion should be regarded as an upper limit. The experimentally observed critical velocity is usually much lower. It is believed that the superfluidity is destroyed due to the excitations of vortex rings [24].

7.2.3 Bogoliubov transformation

The problem can also be treated by using the original field variables. The action Eq. (7.39) is approximated as a bilinear form of ψ_k and ψ_k^* for $k \neq 0$:

$$S[\psi,\psi^*] \approx -\mu\psi_0^*\psi_0 + \frac{g}{2\mathcal{V}\hbar\beta}|\psi_0^*\psi_0|^2 + \sum_{k\neq 0}\psi_k^*\left(-\mathrm{i}\hbar\omega_n + \frac{\hbar^2|\boldsymbol{k}|^2}{2m} - \mu\right)\psi_k$$
$$+ \frac{g}{2\mathcal{V}\hbar\beta}\sum_{k\neq 0}\left[\psi_k^*\psi_{-k}^*\psi_0^2 + \psi_k\psi_{-k}\psi_0^{*2} + 4\psi_k^*\psi_k|\psi_0|^2\right]. \tag{7.51}$$

The mean-field approximation sets

$$\rho_{\mathrm{c}} \equiv \frac{1}{\mathcal{V}\hbar\beta}\psi_0^*\psi_0 = \frac{\mu}{g}. \tag{7.52}$$

While it is straightforward to apply the Gaussian integral formula Eq. (1.146), we can do it explicitly:

- Rewrite the action as:

$$S[\psi,\psi^*] \approx S_0 + \frac{1}{2}\sum_{k\neq 0}\Psi_k^\dagger\begin{bmatrix} -\mathrm{i}\hbar\omega_n + \frac{\hbar^2|\boldsymbol{k}|^2}{2m} + g\rho_{\mathrm{c}} & g\rho_{\mathrm{c}}e^{\mathrm{i}\varphi} \\ g\rho_{\mathrm{c}}e^{-\mathrm{i}\varphi} & \mathrm{i}\hbar\omega_n + \frac{\hbar^2|\boldsymbol{k}|^2}{2m} + g\rho_{\mathrm{c}}\end{bmatrix}\Psi_k, \tag{7.53}$$

where we set $\psi_0 = \sqrt{\mathcal{V}\hbar\beta}\rho_{\mathrm{c}}^{1/2}e^{-\mathrm{i}\varphi/2}$, $S_0 \equiv -\hbar\beta g N_{\mathrm{c}}\rho_{\mathrm{c}}/2$, and

$$\Psi_k \equiv \begin{bmatrix}\psi_k \\ \psi_{-k}^*\end{bmatrix}. \tag{7.54}$$

- Apply the BOGOLIUBOV TRANSFORMATION

$$\Psi_k = \begin{bmatrix} u_k & v_k^* \\ v_k & u_k^* \end{bmatrix} \Phi_k \equiv \begin{bmatrix} u_k & v_k^* \\ v_k & u_k^* \end{bmatrix} \begin{bmatrix} \phi_k \\ \phi_{-k}^* \end{bmatrix}, \tag{7.55}$$

$$|u_k|^2 - |v_k|^2 = 1 \tag{7.56}$$

to diagonalize the matrix in Eq. (7.53). The second condition ensures that $\psi^* \partial_\tau \psi$ is transformed to $\phi^* \partial_\tau \phi$, i.e., the canonical structure is *not* changed. In the second quantization language, the transformation preserves the commutation relations of the Boson creation and annihilation operators. The coefficients are obtained by solving the *generalized* eigenvalue problem:

$$\begin{bmatrix} \frac{\hbar^2 |\boldsymbol{k}|^2}{2m} + g\rho_c & g\rho_c e^{i\varphi} \\ g\rho_c e^{-i\varphi} & \frac{\hbar^2 |\boldsymbol{k}|^2}{2m} + g\rho_c \end{bmatrix} \begin{bmatrix} u_k \\ v_k \end{bmatrix} = E_{\boldsymbol{k}} \tau_z \begin{bmatrix} u_k \\ v_k \end{bmatrix}. \tag{7.57}$$

It yields:

$$E_{\boldsymbol{k}} = \hbar\omega_{\boldsymbol{k}} = \hbar \sqrt{\frac{g\rho_c}{m} k^2 + \left(\frac{\hbar k^2}{2m}\right)^2}, \tag{7.58}$$ (7.46)

$$\begin{bmatrix} u_k \\ v_k \end{bmatrix} = \begin{bmatrix} \sqrt{\frac{\hbar^2 k^2/2m + g\rho_c}{2E_{\boldsymbol{k}}} + \frac{1}{2}} \\ -e^{-i\varphi} \sqrt{\frac{\hbar^2 k^2/2m + g\rho_c}{2E_{\boldsymbol{k}}} - \frac{1}{2}} \end{bmatrix}. \tag{7.59}$$

- The action is diagonalized to

$$S[\psi, \psi^*] \approx S_0 + \sum_{k \neq 0} \left(-i\hbar\omega_n + E_{\boldsymbol{k}}\right) |\phi_k|^2. \tag{7.60}$$

For an equivalent treatment in the second quantization form, see §4.2 of Ref. [25].

7.3 Superconductivity

AS §6.4

7.3.1 Introduction

Superconducting state is an ordered state of conducting electrons, which shows *dissipationless conduction* and *perfect diamagnetism* (Meissner effect). A comprehensive survey of the superconductivity can be found in Ref. [27]. The superfluidity of He^3 can be regarded as the "superconductivity" of charge-neutral particles [28].

Bardeen-Cooper-Schrieffer (BCS) theory reveals that the superconductivity is induced by the formation of COOPER PAIRS – bound pairs of electrons. Electrons pair because of the presence of an *attractive interaction* at the Fermi surface.

Attractive interaction in conventional superconductors is mediated by *phonons* (lattice vibrations):

- The action of an electron-phonon coupled system is

$$S[\psi, \psi^*, c, c^*] = \sum_q c_q^* \left(-i\hbar\nu_m + \hbar\omega_{\boldsymbol{q}}\right) c_q + \frac{1}{\sqrt{\hbar\beta\mathcal{V}}} \sum_q \left(M_{\boldsymbol{q}} \rho_{-q} c_q + M_{\boldsymbol{q}}^* \rho_q c_q^*\right) + S_e[\psi, \psi^*], \tag{7.61}$$ (1.83)

where $\omega_{\boldsymbol{q}}$ is the dispersion of phonons, $q \equiv (\boldsymbol{q}, \nu_m)$, $\rho_q \equiv \sum_{k\sigma} \psi_{k\sigma}^* \psi_{k+q,\sigma}$, and S_e denote the action of electrons.

- Complete the functional integrals over c_q and c_q^*:

$$S[\psi, \psi^*] = \frac{1}{2\hbar\beta\mathcal{V}} \sum_q |M_{\boldsymbol{q}}|^2 D_q \rho_{-q} \rho_q + S_e[\psi, \psi^*], \tag{7.62}$$ (1.146)

$$D_q = \frac{1}{i\hbar\nu_n - \hbar\omega_{\boldsymbol{q}}} + \frac{1}{-i\hbar\nu_n - \hbar\omega_{\boldsymbol{q}}} = -\frac{1}{\hbar} \frac{2\omega_{\boldsymbol{q}}}{\omega_{\boldsymbol{q}}^2 + \nu_n^2}. \tag{7.63}$$

It indicates an effective e-e interaction mediated by phonons

$$V_{\text{eff}}(\boldsymbol{q},\nu_n) = -\frac{|M_{\boldsymbol{q}}|^2}{\hbar}\frac{2\omega_{\boldsymbol{q}}}{\omega_{\boldsymbol{q}}^2+\nu_n^2} \overset{\mathrm{i}\nu_n\to\nu}{\longrightarrow} \frac{|M_{\boldsymbol{q}}|^2}{\hbar}\frac{2\omega_{\boldsymbol{q}}}{\nu^2-\omega_{\boldsymbol{q}}^2}, \tag{7.64}$$

which is *attractive* when

$$\omega_{\boldsymbol{q}} > |\nu| \backsimeq |\epsilon_{\boldsymbol{k}+\boldsymbol{q}} - \epsilon_{\boldsymbol{k}}|/\hbar, \tag{7.65}$$

i.e., within a thin shell of states around the Fermi surface.

- The attractive interaction mediated by phonons prevails over the repulsive Coulomb interaction within the thin shell of states with an energy width $\sim \hbar\omega_D$, where ω_D is the Debye frequency of phonons.
- The attractive interaction mediated by phonons is regarded as a "weak" interaction because $\hbar\omega_D \ll \mu$. Migdal's theorem states that vertex corrections are negligible. FW §47
- The BCS theory can be demonstrated by a simplified effective model:

$$\hat{H} = \sum_{\boldsymbol{k}\sigma}\epsilon_{\boldsymbol{k}}\hat{a}^\dagger_{\boldsymbol{k}\sigma}\hat{a}_{\boldsymbol{k}\sigma} - \frac{g}{\mathcal{V}}\sum_{\boldsymbol{k}\boldsymbol{k}'\boldsymbol{q}}\hat{a}^\dagger_{\boldsymbol{k}+\boldsymbol{q}\uparrow}\hat{a}^\dagger_{-\boldsymbol{k}\downarrow}\hat{a}_{-\boldsymbol{k}'\downarrow}\hat{a}_{\boldsymbol{k}'+\boldsymbol{q}\uparrow} \tag{7.66}$$

$$\equiv \sum_{\boldsymbol{k}\sigma}\epsilon_{\boldsymbol{k}}\hat{a}^\dagger_{\boldsymbol{k}\sigma}\hat{a}_{\boldsymbol{k}\sigma} - \frac{g}{\mathcal{V}}\sum_{\boldsymbol{q}}\hat{\Phi}^\dagger_{\boldsymbol{q}}\Phi_{\boldsymbol{q}}, \tag{7.67}$$

where

$$\hat{\Phi}_{\boldsymbol{q}} \equiv \sum_{\boldsymbol{k}}\hat{a}_{\boldsymbol{k}+\boldsymbol{q}\uparrow}\hat{a}_{-\boldsymbol{k}\downarrow} \tag{7.68}$$

annihilates a pair of electrons (Cooper pair), and the summation over $\boldsymbol{k}$ is implicitly limited in the thin shell of states near the Fermi surface.

- The more realistic treatment, which is called the strong coupling theory, can be found in §10 of Ref. [22].
- Unconventional superconductivity in such as high-T_c cuprates is also induced by the formation of Cooper pairs. However, many believe that in these systems the attractive interaction arises directly out of the electron-electron interaction instead of the electron-phonon coupling.

7.3.2 Cooper instability

It is natural to expect that the Cooper pairs, which are composite Bosons, condense in the low temperature. This is exactly the origin of the superconductivity. In the condensate phase, one expects that the pair amplitude [3]

$$\Phi(\boldsymbol{r}) \equiv \left\langle\hat{\Phi}(\boldsymbol{r})\right\rangle \equiv \langle\psi_\uparrow(\boldsymbol{r})\psi_\downarrow(\boldsymbol{r})\rangle \neq 0. \tag{7.69}$$

At the critical point, the PAIR CORRELATION FUNCTION (7.8)

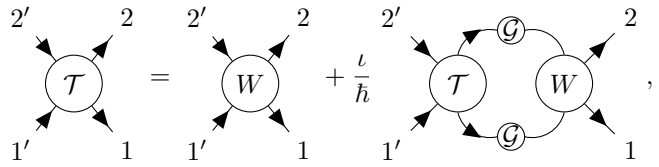
$$\chi_{\Phi\Phi^*}(q) = -\frac{1}{\hbar^2\beta\mathcal{V}}\left\langle\Delta\Phi_q\Delta\Phi_q^*\right\rangle \tag{7.70}$$

$$= -\frac{1}{\hbar^2\beta\mathcal{V}}\sum_{\boldsymbol{k}\boldsymbol{k}'}\left[\left\langle\psi_{k+q\uparrow}\psi_{-k\downarrow}\psi^*_{-k'\downarrow}\psi^*_{k'+q\uparrow}\right\rangle - \left\langle\psi_{k+q\uparrow}\psi_{-k\downarrow}\right\rangle\left\langle\psi^*_{-k'\downarrow}\psi^*_{k'+q\uparrow}\right\rangle\right] \tag{7.71}$$

diverges at $q=0$. The correlation function is proportional to the two-particle Green's function, and in turn to the two-particle scattering amplitude $\mathcal{T}$ by Eq. (5.49). It implies that $\mathcal{T}$ diverges at the critical point.

[3] More generally, the two electrons of a Cooper pair need not to be at the exactly same position. As a result, the order parameter should be defined as $\Phi(\boldsymbol{r},\boldsymbol{r}') = \langle\psi_\uparrow(\boldsymbol{r})\psi_\downarrow(\boldsymbol{r}')\rangle$ with $\Phi_{\boldsymbol{k},\boldsymbol{q}} = \int \mathrm{d}\boldsymbol{r}\int \mathrm{d}\boldsymbol{r}'\Phi(\boldsymbol{r},\boldsymbol{r}')\exp[-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')-\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}+\boldsymbol{r}')/2]$. A spatially uniform order parameter ($\boldsymbol{q}=0$) still has a $\boldsymbol{k}$ dependence. The rotational symmetry of the $\boldsymbol{k}$ dependence is referred as the PAIRING SYMMETRY. The special case we study here has the s-wave symmetry. High-T_c cuprate superconductors have the d-wave symmetry $\Phi_{\boldsymbol{k},\boldsymbol{0}} \propto \cos k_x a - \cos k_y a$. More exotic pairing symmetries are possible. See *p.* 287 of Ref. [2] or Ref. [28].

Bethe-Salpeter equation can be constructed in the *particle-particle* channel [4]:



(7.72)

where W denotes the irreducible electron-electron interaction. For Eq. (7.70): §6.2.3

$$1 \equiv (k+q,\uparrow),\ 2 \equiv (-k,\downarrow),\ 1' \equiv (k'+q,\uparrow),\ 2' \equiv (-k',\downarrow). \tag{7.73}$$

$$\mathcal{T}_{kk'}(q) = W_{kk'}(q) - \frac{1}{\hbar^2\beta\mathcal{V}}\sum_{k''} W_{kk''}(q)\mathcal{G}(k''+q)\mathcal{G}(-k'')\mathcal{T}_{k''k'}(q). \tag{7.74}$$

To the lowest order, we approximate:

$$W_{kk'}(q) \approx -g,\ \mathcal{G} \approx \mathcal{G}_0. \tag{7.75}$$

The BS equation can be solved:

$$\mathcal{T}(q) = -\frac{g}{1+g\chi^0_{\Phi\Phi^*}(q)}, \tag{7.76}$$

$$\chi^0_{\Phi\Phi^*}(q) \equiv -\frac{1}{\hbar^2\beta\mathcal{V}}\left\langle \Delta\Phi_q \Delta\Phi^*_q \right\rangle_0 = -\frac{1}{\hbar^2\beta\mathcal{V}}\sum_{k''}\mathcal{G}_0(k''+q)\mathcal{G}_0(-k''). \tag{7.77}$$

Pair correlation function $\chi^0_{\Phi\Phi^*}(q)$ describes how the pair amplitude of *a non-interacting system* responses to an external pairing potential which couples to the system by the action

$$S_\Delta = \int \mathrm{d}\tau \int \mathrm{d}\boldsymbol{r}\left[\Phi^*(\boldsymbol{r}\tau)\Delta(\boldsymbol{r}\tau) + \Phi(\boldsymbol{r}\tau)\Delta^*(\boldsymbol{r}\tau)\right]. \tag{7.78}$$

It is the "Lindhard function" for the pair correlation function.

$$\chi^0_{\Phi\Phi^*}(\boldsymbol{q},\nu_m) = \frac{1}{\hbar\mathcal{V}}\sum_{\boldsymbol{k}}\frac{1-f\left(\xi_{\boldsymbol{k}+\boldsymbol{q}/2}\right)-f\left(\xi_{\boldsymbol{k}-\boldsymbol{q}/2}\right)}{\mathrm{i}\nu_m - \xi_{\boldsymbol{k}+\boldsymbol{q}/2}-\xi_{\boldsymbol{k}-\boldsymbol{q}/2}}, \tag{7.79}$$ (4.109)

where $\xi_{\boldsymbol{k}} \equiv (\epsilon_{\boldsymbol{k}}-\mu)/\hbar$. Note that ν_m is the bosonic Matsubara frequency.

$$\chi^0_{\Phi\Phi^*}(\boldsymbol{0},0) \approx -N_1(0)\int_{-\hbar\omega_D}^{\hbar\omega_D}\mathrm{d}\epsilon\,\frac{\tanh\frac{\beta\epsilon}{2}}{2\epsilon} \approx -N_1(0)\ln\left(\frac{2e^\gamma}{\pi}\hbar\beta\omega_D\right), \tag{7.80}$$ FW (51.42)

where $N_1(0) = N(0)/2$ is the density of states at the Fermi surface *per spin specie*.

Long-wavelength expansion For small $|\boldsymbol{q}|$, AS §6.7.3

$$\chi^0_{\Phi\Phi^*}(\boldsymbol{q},0) \approx \chi^0_{\Phi\Phi^*}(\boldsymbol{0},0) + \left[\frac{7\zeta(3)}{48\pi^2}\right]N_1(0)(\hbar\beta v_{\mathrm{F}})^2\left|\boldsymbol{q}\right|^2. \tag{7.81}$$

Cooper instability The scattering amplitude diverges when

$$\frac{1}{gN_1(0)} = \ln\left(\frac{2e^\gamma}{\pi}\hbar\beta\omega_D\right). \tag{7.82}$$ (7.76)

It predicts a phase transition at

$$k_B T_c = \frac{2e^\gamma}{\pi}\hbar\omega_D e^{-1/N_1(0)g} \approx 1.13\hbar\omega_D e^{-1/N_1(0)g}. \tag{7.83}$$

T_c is the SUPERCONDUCTING TRANSITION TEMPERATURE.

[4] The equation can be established by defining the effective action as a functional of the anomalous Green's function $\mathcal{F}(1,1') = -\left\langle \psi_\uparrow(1)\psi_\downarrow(1')\right\rangle$. See §5.2.6 and Ref. [16].

7.3.3 Mean field theory

Action corresponding to Eq. (7.67) is

$$S\left[\psi,\psi^*\right]=\sum_{k\sigma}\psi^*_{k\sigma}\left(-\mathrm{i}\hbar\omega_n+\hbar\xi_{\boldsymbol{k}}\right)\psi_{k\sigma}-\frac{g}{\hbar\beta\mathcal{V}}\sum_q\Phi^*_q\Phi_q. \tag{7.84}$$

Hubbard-Stratonovich transformation For an *attractive interaction*, we apply Eq. (6.126). The action is transformed to

$$S\left[\psi,\psi^*,\Delta,\Delta^*\right]=\sum_{k\sigma}\psi^*_{k\sigma}\left(-\mathrm{i}\hbar\omega_n+\hbar\xi_{\boldsymbol{k}}\right)\psi_{k\sigma}+\frac{1}{\hbar\beta\mathcal{V}}\sum_q\left(\Phi^*_q\Delta_q+\Phi_q\Delta^*_q\right)+\frac{1}{\hbar\beta\mathcal{V}}\sum_q\frac{1}{g}\left|\Delta_q\right|^2. \tag{7.85}$$

It is converted to a non-interacting electron system coupled to a random pairing field.

Nambu representation For the case of a uniform $\Delta(\boldsymbol{r}\tau)=\Delta\equiv|\Delta|\exp(\mathrm{i}\varphi)$, we introduce a spinor

$$\Psi_{\boldsymbol{k}}=\begin{bmatrix}\psi_{k\uparrow}\\ \psi^*_{-k\downarrow}\end{bmatrix}. \tag{7.86}$$

The action can be rewritten as

$$S_\Delta\left[\psi,\psi^*\right]=-\hbar\sum_k\Psi^\dagger_k\mathscr{G}^{-1}_k\Psi_k+\hbar\beta\mathcal{V}\frac{|\Delta|^2}{g}, \tag{7.87}$$

$$\mathscr{G}^{-1}_k\equiv\begin{bmatrix}\mathrm{i}\omega_n-\xi_{\boldsymbol{k}} & \Delta/\hbar\\ \Delta^*/\hbar & \mathrm{i}\omega_n+\xi_{\boldsymbol{k}}\end{bmatrix}, \tag{7.88}$$

$$\mathscr{G}_k=-\left\langle\Psi_{\boldsymbol{k}}\Psi^*_{\boldsymbol{k}}\right\rangle=-\frac{1}{\omega_n^2+\xi^2_{\boldsymbol{k}}+|\Delta/\hbar|^2}\begin{bmatrix}\mathrm{i}\omega_n+\xi_{\boldsymbol{k}} & -\Delta/\hbar\\ -\Delta^*/\hbar & \mathrm{i}\omega_n-\xi_{\boldsymbol{k}}\end{bmatrix}. \tag{7.89}$$

Anomalous Green's function is the off-diagonal component of the generalized Green's function in the Nambu representation:

$$\mathscr{G}\left(\boldsymbol{x}\tau,\boldsymbol{x}'\tau'\right)=-\left\langle\hat{T}_\tau\left[\hat{\Psi}\left(\boldsymbol{x}\tau\right)\hat{\Psi}^\dagger\left(\boldsymbol{x}'\tau'\right)\right]\right\rangle \tag{7.90}$$

$$=\begin{bmatrix}-\left\langle\hat{T}_\tau\left[\hat{\psi}_\uparrow\left(\boldsymbol{x}\tau\right)\hat{\psi}^\dagger_\uparrow\left(\boldsymbol{x}'\tau'\right)\right]\right\rangle & -\left\langle\hat{T}_\tau\left[\hat{\psi}_\uparrow\left(\boldsymbol{x}\tau\right)\hat{\psi}_\downarrow\left(\boldsymbol{x}'\tau'\right)\right]\right\rangle\\ -\left\langle\hat{T}_\tau\left[\hat{\psi}^\dagger_\downarrow\left(\boldsymbol{x}\tau\right)\hat{\psi}^\dagger_\uparrow\left(\boldsymbol{x}'\tau'\right)\right]\right\rangle & -\left\langle\hat{T}_\tau\left[\hat{\psi}^\dagger_\downarrow\left(\boldsymbol{x}\tau\right)\hat{\psi}_\downarrow\left(\boldsymbol{x}'\tau'\right)\right]\right\rangle\end{bmatrix}. \tag{7.91}$$

Bogoliubov transformation $\mathscr{G}^{-1}_k$ can be diagonalized by a *unitary* transformation

$$\Psi_{\boldsymbol{k}}=\begin{bmatrix}u_{\boldsymbol{k}} & v^*_{\boldsymbol{k}}\\ v_{\boldsymbol{k}} & -u_{\boldsymbol{k}}\end{bmatrix}\tilde{\Psi}_{\boldsymbol{k}}, \tag{7.92}$$

$$|u_{\boldsymbol{k}}|^2+|v_{\boldsymbol{k}}|^2=1.$$

It is equivalent to the eigenvalue problem

$$\begin{bmatrix}\hbar\xi_{\boldsymbol{k}} & -\Delta\\ -\Delta^* & -\hbar\xi_{\boldsymbol{k}}\end{bmatrix}\begin{bmatrix}u_{\boldsymbol{k}}\\ v_{\boldsymbol{k}}\end{bmatrix}=E_{\boldsymbol{k}}\begin{bmatrix}u_{\boldsymbol{k}}\\ v_{\boldsymbol{k}}\end{bmatrix}. \tag{7.93}$$

$$E_{\boldsymbol{k}}=\sqrt{\left(\hbar\xi_{\boldsymbol{k}}\right)^2+|\Delta|^2}, \tag{7.94}$$

$$u_{\boldsymbol{k}}=\sqrt{\frac{1}{2}\left(1+\frac{\hbar\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right)}, \tag{7.95}$$

$$v_{\boldsymbol{k}}=-\sqrt{\frac{1}{2}\left(1-\frac{\hbar\xi_{\boldsymbol{k}}}{E_{\boldsymbol{k}}}\right)}e^{-\mathrm{i}\varphi}. \tag{7.96}$$

With the transformation, the action becomes

$$S_\Delta\left[\psi,\psi^*\right]=\sum_{k\sigma}\tilde{\psi}^*_{k\sigma}\left(-\mathrm{i}\hbar\omega_n+E_{\boldsymbol{k}}\right)\tilde{\psi}_{k\sigma}+\hbar\beta\mathcal{V}\frac{|\Delta|^2}{g}. \tag{7.97}$$

It describes Fermionic quasi-particles with gapped spectrums $E_{\boldsymbol{k}}$. $|\Delta|$ is called the SUPERCONDUCTING GAP.

Partition function can be written as

$$Z=\frac{1}{Z_{\Delta 0}}\int \mathrm{D}\left[\psi,\psi^*,\Delta,\Delta^*\right]\exp\left\{-\frac{1}{\hbar^2\beta\mathcal{V}}\sum_q\frac{1}{g}\left|\Delta_q\right|^2-\frac{1}{\hbar}S_\mathrm{e}\left[\psi,\psi^*,\Delta,\Delta^*\right]\right\}, \tag{7.98}$$

$$S_\mathrm{e}\left[\psi,\psi^*,\Delta,\Delta^*\right]\equiv\sum_{k\sigma}\psi^*_{k\sigma}\left(-\mathrm{i}\hbar\omega_n+\hbar\xi_{\boldsymbol{k}}\right)\psi_{k\sigma}+\frac{1}{\hbar\beta\mathcal{V}}\sum_q\left(\Phi^*_q\Delta_q+\Phi_q\Delta^*_q\right), \tag{7.99}$$

$$Z_{\Delta 0}\equiv\int \mathrm{D}\left[\Delta,\Delta^*\right]\exp\left[-\frac{1}{\hbar^2\beta\mathcal{V}}\sum_q\frac{1}{g}\left|\Delta_q\right|^2\right]. \tag{7.100}$$

- We can integrate out ψ,ψ^*:

$$Z=\frac{1}{Z_{\Delta 0}}\int \mathrm{D}\left[\Delta,\Delta^*\right]\exp\left[-\frac{1}{\hbar^2\beta\mathcal{V}}\sum_q\frac{1}{g}\left|\Delta_q\right|^2\right]\int \mathrm{D}\left[\psi,\psi^*\right]\exp\left\{-\frac{1}{\hbar}S_\mathrm{e}\left[\psi,\psi^*,\Delta,\Delta^*\right]\right\} \tag{7.101}$$

$$\equiv\frac{1}{Z_{\Delta 0}}\int \mathrm{D}\left[\Delta,\Delta^*\right]\exp\left\{-\frac{1}{\hbar^2\beta\mathcal{V}}\sum_q\frac{1}{g}\left|\Delta_q\right|^2+W\left[\Delta,\Delta^*\right]\right\}, \tag{7.102}$$

$$W\left[\Delta,\Delta^*\right]\equiv\ln Z_\mathrm{e}, \tag{7.103}$$ (5.7)

$$Z_\mathrm{e}=\int \mathrm{D}\left[\psi,\psi^*\right]\exp\left\{-\frac{1}{\hbar}S_\mathrm{e}\left[\psi,\psi^*,\Delta,\Delta^*\right]\right\}. \tag{7.104}$$

- The Landau functional can be defined as

$$\mathcal{L}=\frac{1}{\hbar^2\beta^2\mathcal{V}}\sum_q\frac{1}{g}\left|\Delta_q\right|^2-\frac{1}{\beta}W\left[\Delta,\Delta^*\right]. \tag{7.105}$$

Mean-field approximation is the stationary phase approximation: $\delta\mathcal{L}/\delta\Delta^*_q=0$. Differentiating the Landau functional with respect to a uniform $\Delta=\Delta_{q=0}/\hbar\beta\mathcal{V}$, we have

$$\frac{1}{g}\Delta=\frac{1}{\beta\mathcal{V}}\frac{\partial W\left[\Delta,\Delta^*\right]}{\partial\Delta^*}, \tag{7.106}$$

$$\frac{\partial W\left[\Delta,\Delta^*\right]}{\partial\Delta^*}=-\frac{1}{Z_\mathrm{e}}\int \mathrm{D}\left[\psi,\psi^*\right]\frac{\Phi_{q=0}}{\hbar}\exp\left\{-\frac{1}{\hbar}S_\mathrm{e}\left[\psi,\psi^*,\Delta,\Delta^*\right]\right\} \tag{7.107}$$

$$\equiv-\frac{1}{\hbar}\left\langle\Phi_{q=0}\right\rangle_\mathrm{e}=\frac{1}{\hbar}\sum_k\left[\mathscr{G}_k\right]_{12}, \tag{7.108}$$ (7.89)

Therefore, the self-consistent equation for determining Δ is

$$\frac{1}{g}=\frac{1}{\hbar^2\beta\mathcal{V}}\sum_k\frac{1}{\omega_n^2+\xi^2_{\boldsymbol{k}}+\left|\Delta/\hbar\right|^2}\approx N_1(0)\int_0^{\hbar\omega_D}\mathrm{d}\epsilon\,\frac{\tanh\frac{\beta\sqrt{\epsilon^2+\Delta^2}}{2}}{\sqrt{\epsilon^2+|\Delta|^2}}. \tag{7.109}$$

- The equation is reduced to Eq. (7.80) when $T=T_c$, $\Delta=0$.

- It can also determine the temperature dependence of the superconducting gap:

$$|\Delta(T)| \approx \begin{cases} \Delta(0) - \sqrt{2\pi\Delta(0)k_BT}e^{-\Delta(0)/k_BT} & T \ll T_c \\ \pi\left[\frac{8}{7\zeta(3)}\right]^{1/2} k_BT_c\left(1-\frac{T}{T_c}\right)^{1/2} & T_c - T \ll T_c \end{cases}. \tag{7.110}$$ FW (51.46)

$$\frac{\Delta(0)}{k_BT_c} = \pi e^{-\gamma} \approx 1.76. \tag{7.111}$$ FW (51.44)

Note that the ratio between the zero-temperature gap and the critical temperature is a *universal* constant –a unique prediction of the *weak-coupling* BCS theory.

Thermodynamic properties The Landau functional with respect to the mean-field uniform Δ is the *mean-field* grand potential Ω_s of a superconducting system. According to Eq. (7.97), a superconducting system is equivalent to a non-interacting Fermion system with the dispersion Eq. (7.94). We thus have :

$$\frac{\Omega_\mathrm{s}(|\Delta|)-\Omega_0}{\mathcal{V}} = \frac{|\Delta|^2}{g} - \frac{4N_1(0)}{\beta}\int_0^{\hbar\omega_D} \mathrm{d}\epsilon \left[\ln\frac{1+e^{-\beta E}}{1+e^{-\beta\epsilon}} + \frac{1}{2}\beta(E-\epsilon)\right], \tag{7.112}$$ (3.43)

$$= -N_1(0)\left[\frac{1}{2}|\Delta|^2\left(1+\ln\left|\frac{\Delta(0)}{\Delta}\right|^2\right) + \frac{4}{\beta}\int_0^{\hbar\omega_D}\mathrm{d}\epsilon\ln\left(1+e^{-\beta E}\right) - \frac{\pi^2}{3\beta^2}\right], \tag{7.113}$$ FW (51.53)

$$\approx \begin{cases} -\frac{N_1(0)}{2}\Delta^2(0) + \frac{1}{3}\pi^2 N_1(0)\left(k_\mathrm{B}T\right)^2 & T\to 0 \\ -\frac{8}{7\zeta(3)}N_1(0)\left(\pi k_\mathrm{B}T_c\right)^2\frac{1}{2}\left(1-\frac{T}{T_c}\right)^2 & T\to T_c \end{cases}, \tag{7.114}$$ FW (51.54, 63)

where $E \equiv \sqrt{\epsilon^2+|\Delta|^2}$.

- The CRITICAL FIELD of a superconductor is determined by

$$\frac{H_c^2}{8\pi} = -\frac{\Omega_\mathrm{s}-\Omega_0}{\mathcal{V}}. \tag{7.115}$$

- The specific heat has a jump at the critical point: FW (51.66)

$$\left[\frac{C_\mathrm{s}-C_\mathrm{n}}{C_\mathrm{n}}\right]_{T_c} = \frac{12}{7\zeta(3)} \approx 1.43. \tag{7.116}$$

7.3.4 Effective field theory and Anderson-Higgs mechanism

Landau-Ginzburg theory One can construct an effective Landau functional from the microscopic action. It can then be fitted into the general phase-transition theory presented in §7.1.

We seek for a *classical* Landau functional in the limit of $T \to T_c$, $\Delta_q \to 0$:

Local density approximation The zeroth order approximation to the functional is the local density approximation:

$$S_\mathrm{LDA}[\Delta,\Delta^*] \approx \hbar\beta\int \mathrm{d}\boldsymbol{r}\left[\frac{\Omega_\mathrm{s}(|\Delta(\boldsymbol{r})|)-\Omega_0}{\mathcal{V}}\right]. \tag{7.117}$$ (7.113)

One can then expand the functional to arbitrary orders of $|\Delta(\boldsymbol{r})|^2$.

Gradient correction To obtain the gradient correction, we expand $W[\Delta,\Delta^*]$ as a power series of $|\Delta_q|^2$. To the second order:

$$\hbar W[\Delta,\Delta^*] \approx -\frac{1}{\hbar\beta\mathcal{V}}\sum_q \chi^0_{\Phi\Phi^*}(q)|\Delta_q|^2. \tag{7.118}$$ (7.77)

In the static limit $\Delta_q = \hbar\beta\Delta_{\boldsymbol{q}}\delta_{\nu_m,0}$, we apply Eq. (7.81) and obtain

$$\hbar W[\Delta,\Delta^*] \approx \frac{N_1(0)}{\mathcal{V}}\sum_{\boldsymbol{q}}\left\{\ln\left(\frac{2e^\gamma}{\pi}\hbar\beta\omega_D\right) - \left[\frac{7\zeta(3)}{48\pi^2}\right](\hbar\beta v_\mathrm{F})^2|\boldsymbol{q}|^2\right\}|\Delta_{\boldsymbol{q}}|^2. \tag{7.119}$$

The gradient correction can then be identified.
Adding the gradient correction to S_{LDA}, we obtain

$$S\left[\Delta,\Delta^*\right] \approx \frac{\hbar\beta N_1(0)}{\mathcal{V}} \sum_{\boldsymbol{q}} \left\{ \ln\frac{T}{T_c} + \left[\frac{7\zeta(3)}{48\pi^2}\right] (\hbar\beta v_{\mathrm{F}})^2 \left|\boldsymbol{q}\right|^2 \right\} \left|\Delta_{\boldsymbol{q}}\right|^2 + \ldots \tag{7.120}$$

$$\approx \hbar\beta N_1(0) \int \mathrm{d}\boldsymbol{r} \left\{ \left(\ln\frac{T}{T_c}\right) \left|\Delta(\boldsymbol{r})\right|^2 + \left[\frac{7\zeta(3)}{48\pi^2}\right] (\hbar\beta v_{\mathrm{F}})^2 \left|\boldsymbol{\nabla}\Delta(\boldsymbol{r})\right|^2 + b\left|\Delta(\boldsymbol{r})\right|^4 \right\}, \tag{7.121}$$

where S_{LDA} is expanded to the order of $|\Delta(\boldsymbol{r})|^4$, and b can be fixed by Eq. (7.110):

$$b = \left[\frac{7\zeta(3)}{16\pi^2}\right] \beta^2. \tag{7.122}$$

Landau-Ginzburg functional One defines a "wave function"

$$F(\boldsymbol{r}) \equiv \left[\frac{7\zeta(3)\rho_0}{8\pi^2}\right]^{1/2} \frac{\Delta(\boldsymbol{r})}{k_{\mathrm{B}}T_c}. \tag{7.123}$$

The Landau-Ginzburg functional is defined by

$$\mathcal{L}\left[F,F^*\right] \equiv \frac{S\left[\Delta,\Delta^*\right]}{\hbar\beta} \tag{7.124}$$

$$\approx \int \mathrm{d}\boldsymbol{r} \left\{ \frac{\hbar^2}{4m} \left|\boldsymbol{\nabla}F(\boldsymbol{r})\right|^2 + a\frac{\left(k_{\mathrm{B}}T_c\right)^2}{\epsilon_{F0}} \left[\left(\frac{T}{T_c}-1\right) \left|F(\boldsymbol{r})\right|^2 + \frac{1}{2\rho_0}\left|F(\boldsymbol{r})\right|^4 \right] \right\}, \tag{7.125}$$

$$a \equiv \frac{6\pi^2}{7\zeta(3)} \approx 7.04. \tag{7.126}$$

In the presence of a magnetic field, the gradient operator should be replaced with $\boldsymbol{\nabla} \to \boldsymbol{\nabla} + (\mathrm{i}2e/\hbar c)\boldsymbol{A}$ because of the gauge symmetry (see next).

Quantum effect *is suppressed* when $T \to T_c$. This is a result of the diverging coefficients of the expansion of $\chi^0_{\Phi\Phi^*}(\boldsymbol{q},\nu_m)$ with respect to ν_m.

Gauge symmetry With the Nambu representation, the action Eq. (7.85) can be written as

$$S\left[\psi,\psi^*,\Delta,\Delta^*,\boldsymbol{A},\phi\right] = \int_0^{\hbar\beta} \mathrm{d}\tau \int \mathrm{d}\boldsymbol{r} \left[-\hbar\Psi^\dagger(\boldsymbol{r}\tau)\hat{\mathscr{G}}^{-1}\Psi(\boldsymbol{r}\tau) + \frac{\left|\Delta(\boldsymbol{r}\tau)\right|^2}{g} \right], \tag{7.127}$$

$$\hat{\mathscr{G}}^{-1} = \frac{1}{\hbar} \begin{bmatrix} -\hbar\partial_\tau - \frac{1}{2m}\left(-\mathrm{i}\hbar\boldsymbol{\nabla} + \frac{e}{c}\boldsymbol{A}\right)^2 - \mathrm{i}e\phi + \mu & \Delta(\boldsymbol{r}\tau) \\ \Delta^*(\boldsymbol{r}\tau) & -\hbar\partial_\tau + \frac{1}{2m}\left(-\mathrm{i}\hbar\boldsymbol{\nabla} - \frac{e}{c}\boldsymbol{A}\right)^2 + \mathrm{i}e\phi - \mu \end{bmatrix}, \tag{7.128}$$

where we couple the system to an Euclidean electromagnetic (EM) field $(\mathrm{i}\phi, \boldsymbol{A})$ [5].

- The action is invariant under a global $U(1)$ gauge transformation

$$\Delta\left(\boldsymbol{r}\tau\right) \to \Delta\left(\boldsymbol{r}\tau\right) e^{\mathrm{i}\varphi}, \tag{7.129}$$

$$\Psi(\boldsymbol{r}\tau) \to \exp\left(\mathrm{i}\frac{\varphi}{2}\hat{\tau}_3\right)\Psi(\boldsymbol{r}\tau). \tag{7.130}$$

As a result, the degenerate states of a superconductor are defined by the $U(1)$ phase angles of the order parameter. A Goldstone mode is expected.

[5] Note that in the Euclidean space-time, the scalar component of the electromagnetic field is imaginary.

- It is also invariant under the *local* $U(1)$ gauge transformation

$$\Delta(\boldsymbol{r}\tau) \to \Delta(\boldsymbol{r}\tau)\, e^{\mathrm{i}\varphi(\boldsymbol{r}\tau)}, \tag{7.131}$$

$$\Psi(\boldsymbol{r}\tau) \to \exp\left[\mathrm{i}\frac{\varphi(\boldsymbol{r}\tau)}{2}\hat{\tau}_3\right]\Psi(\boldsymbol{r}\tau), \tag{7.132}$$

$$\phi(\boldsymbol{r}\tau) \to \phi(\boldsymbol{r}\tau) - \frac{\hbar}{2e}\partial_\tau\varphi(\boldsymbol{r}\tau), \tag{7.133}$$

$$\boldsymbol{A}(\boldsymbol{r}\tau) \to \boldsymbol{A}(\boldsymbol{r}\tau) - \frac{\hbar c}{2e}\boldsymbol{\nabla}\varphi(\boldsymbol{r}\tau). \tag{7.134}$$

- As a result, a superconductor couples to the EM field only through

$$\tilde{\phi}(\boldsymbol{r}\tau) = \phi(\boldsymbol{r}\tau) + \frac{\hbar}{2e}\partial_\tau\varphi(\boldsymbol{r}\tau), \tag{7.135}$$

$$\tilde{\boldsymbol{A}}(\boldsymbol{r}\tau) = \boldsymbol{A}(\boldsymbol{r}\tau) + \frac{\hbar c}{2e}\boldsymbol{\nabla}\varphi(\boldsymbol{r}\tau). \tag{7.136}$$

Supercurrent The electric current density is defined by [6]

$$\boldsymbol{j}(\boldsymbol{r}\tau) = -c\left.\frac{\delta S}{\delta \boldsymbol{A}(\boldsymbol{r}\tau)}\right|_{\boldsymbol{A}\to\tilde{\boldsymbol{A}}} = \frac{\mathrm{i}e\hbar}{2m}\Psi^\dagger(\boldsymbol{r}\tau)\left(\overrightarrow{\boldsymbol{\nabla}} - \overleftarrow{\boldsymbol{\nabla}}\right)\Psi(\boldsymbol{r}\tau) - \frac{e^2}{mc}\rho(\boldsymbol{r}\tau)\tilde{\boldsymbol{A}}(\boldsymbol{r}\tau), \tag{7.137}$$ (7.127)

$$\boldsymbol{j}_q = -\frac{e\hbar}{m}\sum_k\left(\boldsymbol{k}+\frac{\boldsymbol{q}}{2}\right)\Psi_k^\dagger e^{\mathrm{i}\omega_n\eta\hat{\tau}_3}\Psi_{k+q} - \frac{e^2\rho_0}{mc}\delta_{q,0}\tilde{\boldsymbol{A}}_q. \tag{7.138}$$

The response of the electric current density *to* $\tilde{\boldsymbol{A}}$ is

$$\boldsymbol{j}_\mathrm{s}(\boldsymbol{r}) \equiv \langle\boldsymbol{j}(\boldsymbol{r})\rangle_{\tilde{\boldsymbol{A}}} \approx \int \mathrm{d}\boldsymbol{r}K(\boldsymbol{r}-\boldsymbol{r}')\tilde{\boldsymbol{A}}(\boldsymbol{r}') \tag{7.139}$$

$$K(\boldsymbol{r}-\boldsymbol{r}') \equiv \frac{\delta}{\delta\tilde{\boldsymbol{A}}(\boldsymbol{r}'\tau)}\left(\frac{1}{Z}\int \mathrm{D}\left[\psi,\psi^*\right]\boldsymbol{j}(\boldsymbol{r}\tau)e^{-S/\hbar}\right)\Big|_{\tilde{\boldsymbol{A}}\to 0} \tag{7.140}$$

$$= \left(\frac{1}{Z}\int \mathrm{D}\left[\psi,\psi^*\right]\left[\frac{\delta\boldsymbol{j}}{\delta\tilde{\boldsymbol{A}}} + \frac{1}{\hbar c}\langle\boldsymbol{j}(\boldsymbol{r}\tau)\boldsymbol{j}(\boldsymbol{r}'\tau)\rangle - \frac{1}{\hbar c}\langle\boldsymbol{j}(\boldsymbol{r}\tau)\rangle\langle\boldsymbol{j}(\boldsymbol{r}'\tau)\rangle\right]e^{-S/\hbar}\right)\Big|_{\tilde{\boldsymbol{A}}\to 0} \tag{7.141}$$

$$K_{\boldsymbol{q}} = \left[-\frac{e^2\langle\rho\rangle}{mc}\delta_{\boldsymbol{q},0} + \frac{1}{\hbar^2 c\beta\mathcal{V}}\langle(\Delta\boldsymbol{j}_{\boldsymbol{q}})(\Delta\boldsymbol{j}_{-\boldsymbol{q}})\rangle_{\tilde{\boldsymbol{A}}=0}\cdot\right], \tag{7.142}$$

Superfluid density is defined by the response function at $\boldsymbol{q}\to 0$. By applying Wick's theorem, we have

$$K_{\boldsymbol{q}\to 0} = -\frac{e^2}{mc}\rho_\mathrm{s} \tag{7.143}$$

$$\rho_\mathrm{s} = \rho_0 + \frac{2}{3}\frac{1}{\hbar^2\beta\mathcal{V}}\sum_k\frac{\hbar^2|\boldsymbol{k}|^2}{2m}\mathrm{Tr}\left[\mathscr{G}_k\mathscr{G}_k\right] = \rho_0 - \frac{4}{3}\frac{1}{\beta\mathcal{V}}\sum_k(\mu+\hbar\xi_{\boldsymbol{k}})\frac{(\hbar\omega_n)^2 - E_{\boldsymbol{k}}^2}{\left[(\hbar\omega_n)^2+E_{\boldsymbol{k}}^2\right]^2} \tag{7.144}$$

$$= \rho_0 - \frac{\beta\mu N(0)}{3}\int_0^\infty \mathrm{d}\epsilon\,\frac{1}{\cosh^2(\beta E/2)} \approx \rho_0\begin{cases}1-\sqrt{2\pi\beta\Delta(0)}e^{-\beta\Delta(0)} & T\to 0\\ 2\left(1-\frac{T}{T_c}\right) & T\to T_c\end{cases}. \tag{7.145}$$ FW (52.34)

The supercurrent response at $\boldsymbol{q}\to 0$ is

$$\boldsymbol{j}_\mathrm{s} = -\frac{e\hbar}{2m}\rho_\mathrm{s}\left(\boldsymbol{\nabla}\varphi + \frac{2e}{\hbar c}\boldsymbol{A}\right). \tag{7.146}$$

It is analogous to Eq. (7.48). The response is called the JOSEPHSON EFFECT. See §5.2 of Ref. [21] for a treatment of the effect.

[6] Note that the equal-time production like $\Psi^\dagger(\boldsymbol{r}\tau)\Psi(\boldsymbol{r}\tau)$ should be properly interpreted: to define the physical current, $\psi^*_{\uparrow(\downarrow)}$ should always have a time infinitesimally ahead that of $\psi_{\uparrow(\downarrow)}$.

Effective action of the Goldstone mode must have a form consistent with all the symmetries of the original microscopic model, including the local gauge symmetry. In the long-wavelength limit, we have

$$S_{\mathrm{G}}\left[\varphi, \boldsymbol{A}, \phi\right] = \frac{1}{2}\int \mathrm{d}\tau \int \mathrm{d}\boldsymbol{r}\left[c_1\left(\frac{1}{2}\partial_\tau\varphi + \frac{e}{\hbar}\phi\right)^2 + c_2\left|\frac{1}{2}\boldsymbol{\nabla}\varphi + \frac{e}{\hbar c}\boldsymbol{A}\right|^2\right] + \ldots \tag{7.147}$$

$$= \frac{1}{2\hbar\beta\mathcal{V}}\sum_q\left[c_1\left|-\frac{\mathrm{i}\nu_m}{2}\varphi_q + \frac{e}{\hbar}\phi_q\right|^2 + c_2\left|\frac{\mathrm{i}}{2}\boldsymbol{q}\varphi_q + \frac{e}{\hbar c}\boldsymbol{A}_q\right|^2\right] + \ldots \tag{7.148}$$

S_{G} can be obtained from S by integrating out all unwanted variables:

$$S_{\mathrm{G}}\left[\varphi, \boldsymbol{A}, \phi\right] = -\hbar\ln\int \mathrm{D}\left[\left|\Delta\right|, \psi, \psi^*\right]\exp\left\{-\frac{S\left[\psi, \psi^*, \Delta, \Delta^*, \boldsymbol{A}, \phi\right]}{\hbar}\right\}. \tag{7.149}$$

The coefficients can be related to correlation functions:

- From Eq. (7.149), we have

$$c_1(q) = (\hbar\beta\mathcal{V})\left(\frac{\hbar}{e}\right)^2\frac{\delta^2 S_{\mathrm{G}}}{\delta\phi_q\delta\phi_{-q}} = \mathrm{i}\frac{\hbar^2}{e}\frac{\delta\rho_q}{\delta\phi_q} = \frac{1}{\beta\mathcal{V}}\left\langle\left(\Delta\rho_q\right)\left(\Delta\rho_{-q}\right)\right\rangle_0 \equiv -\hbar^2\chi_{\rho\rho}(q), \tag{7.150}$$

  where $\chi_{\rho\rho}(q)$ is the density correlation function for the superconducting system, and $\rho_q \equiv \sum_k \Psi_k^\dagger e^{\mathrm{i}\omega_n\eta\hat{\tau}_3}\hat{\tau}_3\Psi_{k+q}$. In the long-wavelength limit, $\chi_{\rho\rho}(0) \approx -N(0)$, we have

$$c_1 \equiv \lim_{q\to 0} c_q(q) = \hbar^2 N(0). \tag{7.151}$$

- Similarly:

$$c_2(q) = (\hbar\beta\mathcal{V})\left(\frac{\hbar c}{e}\right)^2\frac{\delta^2 S_{\mathrm{G}}}{\delta\boldsymbol{A}_q\delta\boldsymbol{A}_{-q}} = -\left(\frac{\hbar}{e}\right)^2 c\frac{\delta\boldsymbol{j}_q}{\delta\boldsymbol{A}_q} \tag{7.152}$$

  We have already obtained its long-wavelength limit in Eq. (7.146). Therefore,

$$c_2 \equiv \lim_{q\to 0} c_2(q) = \frac{\hbar^2}{m}\rho_{\mathrm{s}}. \tag{7.153}$$

Anderson-Higgs mechanism When the Goldstone mode is coupled to a massless (long-range) gauge field (e.g., the EM field), it disappears and gives rise to a finite mass (short range) to the gauge field.

- The total action for a superconductor coupled to the EM field is

$$S\left[\varphi, \boldsymbol{A}, \phi\right] = S_{\mathrm{G}}\left[\varphi, \boldsymbol{A}, \phi\right] + \frac{1}{8\pi}\int \mathrm{d}\tau \int \mathrm{d}\boldsymbol{r}\left[\left(\boldsymbol{\nabla}\phi - \frac{1}{c}\partial_\tau\boldsymbol{A}\right)^2 + \left|\boldsymbol{\nabla}\times\boldsymbol{A}\right|^2\right]. \tag{7.154}$$

- Since the action of the EM field is gauge-invariant, one can preform the gauge transformation Eq. (7.135,7.136). The resulting action does not depend on φ –the Goldstone mode disappears!

$$S\left[\tilde{\boldsymbol{A}}, \tilde{\phi}\right] = \frac{1}{8\pi}\int \mathrm{d}\tau \int \mathrm{d}\boldsymbol{r}\left[\left(\boldsymbol{\nabla}\tilde{\phi} - \frac{1}{c}\partial_\tau\tilde{\boldsymbol{A}}\right)^2 + \left|\boldsymbol{\nabla}\times\tilde{\boldsymbol{A}}\right|^2 + \frac{4\pi e^2}{mc^2}\rho_{\mathrm{s}}\left|\tilde{\boldsymbol{A}}\right|^2 + 4\pi e^2 N(0)\left|\tilde{\phi}\right|^2\right]. \tag{7.155}$$

- We can decompose $\tilde{\boldsymbol{A}}$ to the transverse and longitudinal components: $\tilde{\boldsymbol{A}} = \tilde{\boldsymbol{A}}^{\mathrm{T}} + \tilde{\boldsymbol{A}}^{\mathrm{L}}$ with $\boldsymbol{\nabla}\cdot\tilde{\boldsymbol{A}}^{\mathrm{T}} = 0$ and $\boldsymbol{\nabla}\times\tilde{\boldsymbol{A}}^{\mathrm{L}} = 0$.

$$S\left[\tilde{\boldsymbol{A}}, \tilde{\phi}\right] = \frac{1}{8\pi}\int \mathrm{d}\tau \int \mathrm{d}\boldsymbol{r}\left[c^{-2}\left(\partial_\tau\tilde{\boldsymbol{A}}^{\mathrm{T}}\right)^2 + \left|\boldsymbol{\nabla}\times\tilde{\boldsymbol{A}}^{\mathrm{T}}\right|^2 + \frac{4\pi e^2}{mc^2}\rho_{\mathrm{s}}\left|\tilde{\boldsymbol{A}}^{\mathrm{T}}\right|^2\right]$$
$$+ \frac{1}{8\pi}\int \mathrm{d}\tau \int \mathrm{d}\boldsymbol{r}\left[\left(\boldsymbol{\nabla}\tilde{\phi} - c^{-1}\partial_\tau\tilde{\boldsymbol{A}}^{\mathrm{L}}\right)^2 + \frac{4\pi e^2}{mc^2}\rho_{\mathrm{s}}\left|\tilde{\boldsymbol{A}}^{\mathrm{L}}\right|^2 + 4\pi e^2 N(0)\left|\tilde{\phi}\right|^2\right]. \tag{7.156}$$

– The transverse component $\tilde{\boldsymbol{A}}^{\mathrm{T}}$ gains a mass. It will be screened – MEISSNER EFFECT;
– The longitudinal component of $\tilde{\boldsymbol{A}}^{\mathrm{L}}$ is coupled to the scalar field. After integrating out $\tilde{\boldsymbol{A}}^{\mathrm{L}}$, it gives rise a plasmon-like mode – This is what the Goldstone mode finally becomes.

Meissner effect The magnetic field must vanish inside the bulk of a superconductor – the perfect diamagnetism. Differentiating the action with respect to $\boldsymbol{A}^T$, we obtain

$$\boldsymbol{\nabla}\times\boldsymbol{B}\equiv-\nabla^2\boldsymbol{A}^T=\frac{4\pi}{c}\boldsymbol{j}_{\mathrm{s}}=-\frac{4\pi e^2\rho_{\mathrm{s}}}{mc^2}\boldsymbol{A}^T\implies\left(\frac{4\pi e^2\rho_{\mathrm{s}}}{mc^2}-\nabla^2\right)\boldsymbol{B}(\boldsymbol{r})=0. \tag{7.157}$$

It predicts a PENETRATION DEPTH that is $\lambda=c\left(4\pi e^2\rho_{\mathrm{s}}/m\right)^{-1/2}$.

Problems

1. Determine the upper critical dimensions of ϕ^n, $(\boldsymbol{\nabla}\phi)^n$, and $\phi\boldsymbol{\nabla}^n\phi$ terms in a Landau functional.

2. Determine an expression for the density-correlation function of superconductors [see Eq. (7.150)]. To simplify the calculation, one can assume $\beta\Delta\gg1$.

   (a) Determine the long-wavelength limit $\chi_{\rho\rho}(\boldsymbol{q}=0,\nu_m)$.

   (b) Determine the expansion of $\chi_{\rho\rho}(\boldsymbol{q}=0,\nu_m)$ in the limits of $\hbar\nu_m\ll\Delta$ and $\hbar\nu_m\gg\Delta$, respectively.

   (c) Compare the result with the density response function of a normal system [Eq. (6.85)].

   Hint: Mathematica is actually very good in carrying out frequency summations. Use "Sum" for the summation and "Series" for the expansion.

3. Integrating out either $\tilde{\phi}$ or $\tilde{\boldsymbol{A}}^{\mathrm{L}}$ from the action Eq. (7.155). What is the dispersion of the resulting plasmon-like mode? What is the regime of validity of the result?

4. Stoner magnetism: consider the Hubbard model Eq. (1.90). The interaction term can be rewritten as

$$\hat{H}_U=\frac{U}{4}\sum_i(n_{i\uparrow}+n_{i\downarrow})^2-U\sum_i\left(S_i^z\right)^2, \tag{7.158}$$

   where $S_i^z\equiv(n_{i\uparrow}-n_{i\downarrow})/2$. One can neglect the first term. With the remaining term, develop a mean field theory and obtain its effective Landau-Ginzburg functional. AS §6.7.8

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