Quantum Theory of Many Particle Systems

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Spring semester, 2019

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Preface

Overview

- An introductory course to the quantum theory of many-particle systems.
- A comprehensive understanding of basic principles/language and an overview on the arsenal of many body techniques.
- Applications to real physical systems
- Bridge the gap between the quantum many-body theory and real material calculations.
- Use the functional integral as the foundation because
  - It is economic in developing various many-body techniques (perturbation, effective action)
  - It becomes a language more commonly used in literatures

Contents

- Basic Theory
  - Second quantization and coherent states
  - Path integral formalism
  - Perturbation theory
  - Green's function formalism
  - Effective action theory
- Applications to physical systems
  - Theory of electron liquids
  - Broken symmetry and phase transitions
- Computational methods
  - Density functional theory
  - GW approximation
  - DMFT theory

Resources

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

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

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

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

AS Alexander Altland and Ben D. Simons, *Condensed Matter Field Theory* (Cambridge University Press, 2010).

HJ Hartmut Haug and Antti-Pekka Jauho, *Quantum Kinetics in Transport and Optics of Semiconductors* (Springer, 2008).

Chapter 1

Second quantization and coherent state

1.1 Quantum mechanics

NO§1.1

Basic concepts

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

$$\hat{\boldsymbol{r}}\,|\boldsymbol{r}\rangle = \boldsymbol{r}\,|\boldsymbol{r}\rangle\,, \tag{1.1.1}$$
$$\hat{\boldsymbol{p}}\,|\boldsymbol{p}\rangle = \boldsymbol{p}\,|\boldsymbol{p}\rangle\,. \tag{1.1.2}$$

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

$$\int \mathrm{d}\boldsymbol{r}\,|\boldsymbol{r}\rangle\,\langle\boldsymbol{r}| = 1, \tag{1.1.3}$$
$$\int \mathrm{d}\boldsymbol{p}\,|\boldsymbol{p}\rangle\,\langle\boldsymbol{p}| = 1, \tag{1.1.4}$$
$$|\psi\rangle = \int \mathrm{d}\boldsymbol{r}\,|\boldsymbol{r}\rangle\,\langle\boldsymbol{r}|\,\psi\rangle \equiv \int \mathrm{d}\boldsymbol{r}\,|\boldsymbol{r}\rangle\,\psi(\boldsymbol{r}). \tag{1.1.5}$$

- Overlaps between states:

$$\langle\boldsymbol{r}|\boldsymbol{r}'\rangle = \delta(\boldsymbol{r}-\boldsymbol{r}'), \tag{1.1.6}$$
$$\langle\boldsymbol{p}|\boldsymbol{p}'\rangle = \delta(\boldsymbol{p}-\boldsymbol{p}'), \tag{1.1.7}$$
$$\langle\boldsymbol{r}|\boldsymbol{p}\rangle = \left(\frac{1}{2\pi\hbar}\right)^{3/2} \exp\left(\frac{\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}}{\hbar}\right). \tag{1.1.8}$$

Schrödinger equation

- momentum operator in the position basis:

$$\langle\boldsymbol{r}\,|\hat{\boldsymbol{p}}|\,\psi\rangle = -\mathrm{i}\hbar\frac{\partial}{\partial\boldsymbol{r}}\,\langle\boldsymbol{r}|\,\psi\rangle \equiv -\mathrm{i}\hbar\frac{\partial\psi(\boldsymbol{r})}{\partial\boldsymbol{r}}. \tag{1.1.9}$$

NO(1.11)

- Schrödinger equation:

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left|\psi\right\rangle = \left[\frac{\hat{\boldsymbol{p}}^2}{2m} + V\left(\hat{\boldsymbol{r}}\right)\right]\left|\psi\right\rangle, \tag{1.1.10}$$

$$\mathrm{i}\hbar\frac{\partial\psi(\boldsymbol{r}t)}{\partial t} = \left\langle\boldsymbol{r}\right|\left[\frac{\hat{\boldsymbol{p}}^2}{2m} + V\left(\hat{\boldsymbol{r}}\right)\right]\left|\psi\right\rangle = \left[\frac{1}{2m}\left(-\mathrm{i}\frac{\partial}{\partial\boldsymbol{r}}\right)^2 + V(\boldsymbol{r})\right]\psi(\boldsymbol{r}). \tag{1.1.11}$$

Generalization The concept of *state* can be generalized to:

- Eigenstates of *any* observables/operators.
- Internal degrees of freedom, e.g., spin σ, isospin τ, band index ...

1.2 Identical particles

NO§1.2

Generalization to many-particle systems

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

$$\left|\alpha_1\ldots\alpha_N\right) \equiv \left|\alpha_1\right\rangle\otimes\left|\alpha_2\right\rangle\otimes\cdots\otimes\left|\alpha_N\right\rangle. \tag{1.2.1}$$

- Overlap between product states:

$$\left(\alpha_1\ldots\alpha_N\left|\alpha'_1\ldots\alpha'_N\right.\right) = \left\langle\alpha_1\left|\alpha'_1\right.\right\rangle\left\langle\alpha_2\left|\alpha'_2\right.\right\rangle\ldots\left\langle\alpha_N\left|\alpha'_N\right.\right\rangle, \tag{1.2.2}$$

$$\begin{aligned}\psi_{\alpha_1\ldots\alpha_N}\left(\boldsymbol{r}_1\ldots\boldsymbol{r}_N\right) &\equiv \left(\boldsymbol{r}_1\ldots\boldsymbol{r}_N\left|\alpha_1\ldots\alpha_N\right.\right)\\ &= \psi_{\alpha_1}(\boldsymbol{r}_1)\psi_{\alpha_2}(\boldsymbol{r}_2)\ldots\psi_{\alpha_N}(\boldsymbol{r}_N).\end{aligned} \tag{1.2.3}$$

- Completeness relations:

$$\sum_{\alpha_1\ldots\alpha_N}\left|\alpha_1\ldots\alpha_N\right)\left(\alpha_1\ldots\alpha_N\right| = 1. \tag{1.2.4}$$

Exchange symmetry only totally symmetric (Bosons) and anti-symmetric states (Fermions) are observed in nature:

$$\psi\left(\boldsymbol{r}_{P1},\boldsymbol{r}_{P2},\ldots,\boldsymbol{r}_{PN}\right) = \psi\left(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N\right) \quad \text{(Bosons)}, \tag{1.2.5}$$

$$\psi\left(\boldsymbol{r}_{P1},\boldsymbol{r}_{P2},\ldots,\boldsymbol{r}_{PN}\right) = (-1)^P\psi\left(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N\right) \quad \text{(Fermions)}. \tag{1.2.6}$$

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

$$\hat{\mathcal{P}}\psi\left(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_N\right) = \frac{1}{N!}\sum_P\zeta^P\psi\left(\boldsymbol{r}_{P1},\boldsymbol{r}_{P2},\ldots,\boldsymbol{r}_{PN}\right), \tag{1.2.7}$$

$$\left|\alpha_1\ldots\alpha_N\right\} = \sqrt{N!}\hat{\mathcal{P}}\left|\alpha_1\ldots\alpha_N\right). \tag{1.2.8}$$

  $\zeta = 1$ for Bosons and -1 for Fermions.
  - Pauli exclusion principle due to the anti-symmetry of Fermion states.

– Overlap and orthogonality:

$$\{\,\alpha_1\dots\alpha_N \mid \alpha'_1\dots\alpha'_N\,\} = \begin{cases}(-1)^P & \text{(Fermions)}\\ n_1!n_2!\dots n_p! & \text{(Bosons)}\end{cases}, \tag{1.2.9}$$

NO(1.43a,b)

non-vanishing only when $\alpha'_1\dots\alpha'_N$ is a permutation of $\alpha_1\dots\alpha_N$.

– Closure relation:

$$\sum_{\alpha_1\dots\alpha_N} \hat{\mathcal{P}}\,|\alpha_1\dots\alpha_N)\,(\alpha_1\dots\alpha_N|\,\hat{\mathcal{P}} = \frac{1}{N!}\sum_{\alpha_1\dots\alpha_N} |\alpha_1\dots\alpha_N\}\,\{\alpha_1\dots\alpha_N| = 1. \tag{1.2.10}$$

- Normalized symmetrized states:

$$|\alpha_1\dots\alpha_N\rangle = \frac{1}{\sqrt{\prod_\alpha n_\alpha!}}\,|\alpha_1\dots\alpha_N\}\,. \tag{1.2.11}$$

– Overlap:

$$\langle\beta_1\cdots\beta_N|\alpha_1\cdots\alpha_N\rangle = \frac{1}{\sqrt{\prod_\beta n_\beta!\prod_\alpha n_\alpha!}} S\left(\langle\beta_i|\alpha_j\rangle\right), \tag{1.2.12}$$

NO(1.47)

where S is a permanent (determinant) for Bosons (Fermions).

– Closure relation:

$$\sum_{\alpha_1\dots\alpha_N} \frac{\prod_\alpha n_\alpha!}{N!}\,|\alpha_1\dots\alpha_N\rangle\,\langle\alpha_1\dots\alpha_N| = 1. \tag{1.2.13}$$

1.3 Creation and annihilation operators

1.3.1 Basics

NO§1.3

Creation operator adds one particle to the single-particle state $|\alpha\rangle$

$$a^\dagger_\alpha\,|\alpha_1\dots\alpha_N\rangle = \sqrt{n_\alpha+1}\,|\alpha\alpha_1\dots\alpha_N\rangle\,,\text{(Boson)}, \tag{1.3.1}$$

$$a^\dagger_\alpha\,|\alpha_1\dots\alpha_N\rangle = \begin{cases}|\alpha\alpha_1\dots\alpha_N\rangle & \alpha\notin\{\alpha_1,\dots,\alpha_N\}\\ 0 & \alpha\in\{\alpha_1,\dots,\alpha_N\}\end{cases},\text{(Fermion)}. \tag{1.3.2}$$

- Vacuum state $|0\rangle$: a state with no particle. Note that it is *not* a zero state!
- Fock space: the creation operator changes the number of particles. Therefore, we define

$$\mathcal{B} = \mathcal{B}_0\oplus\mathcal{B}_1\oplus\dots, \tag{1.3.3}$$

$$\mathcal{F} = \mathcal{F}_0\oplus\mathcal{F}_1\oplus\dots. \tag{1.3.4}$$

– Closure relations:

$$|0\rangle\,\langle 0| + \sum_{N=1}^{\infty}\sum_{\alpha_1\dots\alpha_N}\frac{\prod_\alpha n_\alpha!}{N!}\,|\alpha_1\dots\alpha_N\rangle\,\langle\alpha_1\dots\alpha_N| = 1. \tag{1.3.5}$$

- Creating a state:

$$|\alpha_1 \dots \alpha_N\rangle = \frac{1}{\sqrt{\prod_\alpha n_\alpha!}} a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} \dots a^\dagger_{\alpha_N} |0\rangle . \tag{1.3.6}$$

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

$$\hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta - \hat{a}^\dagger_\beta \hat{a}^\dagger_\alpha \equiv [\hat{a}^\dagger_\alpha, \hat{a}^\dagger_\beta]_- = 0 \,(\text{Bosons}) \tag{1.3.7}$$

$$\hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta + \hat{a}^\dagger_\beta \hat{a}^\dagger_\alpha \equiv [\hat{a}^\dagger_\alpha, \hat{a}^\dagger_\beta]_+ = 0 \,(\text{Fermions}) \tag{1.3.8}$$

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

$$a_\alpha |\alpha_1 \dots \alpha_N\rangle = \frac{1}{\sqrt{n_\alpha}} \sum_{i=1}^{N} \zeta^{i-1} \delta_{\alpha,\alpha_i} |\alpha_1 \dots \alpha_{i-1}\alpha_{i+1} \dots \alpha_N\rangle . \tag{1.3.9}$$

- Commutator between the creation and annihilation operators:

$$[a_\alpha, a^\dagger_\beta]_- \equiv a_\alpha a^\dagger_\beta - a^\dagger_\beta a_\alpha = 1, (\text{Bosons}) \tag{1.3.10}$$

$$[a_\alpha, a^\dagger_\beta]_+ \equiv a_\alpha a^\dagger_\beta + a^\dagger_\beta a_\alpha = 1. (\text{Fermions}) \tag{1.3.11}$$

  The proof can be found in NO pp. 14-15.

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

$$|\alpha_1 \dots \alpha_N\rangle \Rightarrow |n_{\alpha_1} n_{\alpha_2} \dots\rangle , \tag{1.3.12}$$

- Bosons:

$$a_{\alpha_i} |n_{\alpha_1} n_{\alpha_2} \dots\rangle = \sqrt{n_{\alpha_i} + 1}\, |n_{\alpha_1} n_{\alpha_2} \dots (n_{\alpha_i} - 1) \dots\rangle , \tag{1.3.13}$$

$$a^\dagger_{\alpha_i} |n_{\alpha_1} n_{\alpha_2} \dots\rangle = \sqrt{n_{\alpha_i}}\, |n_{\alpha_1} n_{\alpha_2} \dots (n_{\alpha_i} + 1) \dots\rangle . \tag{1.3.14}$$

- Fermions

$$a_{\alpha_i} |n_{\alpha_1} n_{\alpha_2} \dots\rangle = \begin{cases} (-1)^{\sum_{j=1}^{i-1} n_{\alpha_j}} |n_{\alpha_1} n_{\alpha_2} \dots (n_{\alpha_i} \to 0) \dots\rangle & n_{\alpha_i} = 1 \\ 0 & n_{\alpha_i} = 0 \end{cases}, \tag{1.3.15}$$

$$a^\dagger_{\alpha_i} |n_{\alpha_1} n_{\alpha_2} \dots\rangle = \begin{cases} (-1)^{\sum_{j=1}^{i-1} n_{\alpha_j}} |n_{\alpha_1} n_{\alpha_2} \dots (n_{\alpha_i} \to 1) \dots\rangle & n_{\alpha_i} = 0 \\ 0 & n_{\alpha_i} = 1 \end{cases}. \tag{1.3.16}$$

Field operators: creation/annihilation operator in the position basis

$$[\hat{\psi}(\boldsymbol{r}), \hat{\psi}(\boldsymbol{r}')]_{-\zeta} = [\hat{\psi}^\dagger(\boldsymbol{r}), \hat{\psi}^\dagger(\boldsymbol{r}')]_{-\zeta} = 0, \tag{1.3.17}$$

$$[\hat{\psi}(\boldsymbol{r}), \hat{\psi}^\dagger(\boldsymbol{r}')]_{-\zeta} = \delta(\boldsymbol{r} - \boldsymbol{r}'). \tag{1.3.18}$$

$$\hat{\psi}(\boldsymbol{r}) = \sum_\alpha \phi_\alpha(\boldsymbol{r}) \hat{a}_\alpha. \tag{1.3.19}$$

Second quantization expresses operators in the creation and annihilation operators:

- Number operator:
$$\hat{n}_\alpha = a_\alpha^\dagger a_\alpha. \tag{1.3.20}$$
- One-body operator $\hat{U} = \sum_i \hat{u}_i$:
$$\hat{U} = \sum_{\alpha\beta} \langle \alpha \,|\, \hat{u} \,|\, \beta \rangle \, a_\alpha^\dagger a_\beta. \tag{1.3.21}$$
  - In the position basis:
$$\hat{T} = -\frac{\hbar^2}{2m} \int \mathrm{d}\boldsymbol{r} \hat{\psi}^\dagger(\boldsymbol{r}) \nabla^2 \hat{\psi}(\boldsymbol{r}), \tag{1.3.22}$$
$$\hat{U} = \int \mathrm{d}\boldsymbol{r} U(\boldsymbol{r}) \, \hat{\psi}^\dagger(\boldsymbol{r}) \hat{\psi}(\boldsymbol{r}). \tag{1.3.23}$$
- Two-body operator $\hat{V} = (1/2) \sum_{ij} \hat{v}_{ij}$:
$$\hat{V} = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} (\alpha\beta \,|\hat{v}|\, \gamma\delta) \, a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma. \tag{1.3.24}$$
  Note the order of the state indexes.
- Proof
  - We assume that a two-body operator $\hat{V}$ may be diagonalized in product states:
$$\hat{v} \, |\alpha\beta) = v_{\alpha\beta} \, |\alpha\beta) \, . \tag{1.3.25}$$
  - We can calculate a general matrix element:
$$\{\alpha_1' \ldots \alpha_N' \,|\hat{v}|\, \alpha_1 \ldots \alpha_N\} = \left(\frac{1}{2} \sum_{i \neq j} v_{\alpha_i \alpha_j} \right) \{\alpha_1' \ldots \alpha_N' | \, \alpha_1 \ldots \alpha_N\} \, . \tag{1.3.26}$$
  - 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:
$$\hat{P}_{\alpha\beta} = \hat{n}_\alpha \hat{n}_\beta - \delta_{\alpha\beta} \hat{n}_\alpha = \hat{a}_\alpha^\dagger \hat{a}_\beta^\dagger \hat{a}_\beta \hat{a}_\alpha. \tag{1.3.27}$$
    and
$$\hat{V} = \frac{1}{2} \sum_{\alpha\beta} v_{\alpha\beta} \hat{P}_{\alpha\beta}. \tag{1.3.28}$$
  - Transform from the diagonal representation to a general basis.
- In the position basis:
$$\hat{V} = \frac{1}{2} \int \mathrm{d}\boldsymbol{r} \mathrm{d}\boldsymbol{r}' v(\boldsymbol{r} - \boldsymbol{r}') \hat{\psi}^\dagger(\boldsymbol{r}) \hat{\psi}^\dagger(\boldsymbol{r}') \hat{\psi}(\boldsymbol{r}') \hat{\psi}(\boldsymbol{r}). \tag{1.3.29}$$

Normal ordering: all $\hat{a}^\dagger$'s are to the left of $\hat{a}$'s.

1.3.2 Second quantized Hamiltonians

Degenerate Electron gas FW§3

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_\sigma \int \mathrm{d}\boldsymbol{r}\hat{\psi}^\dagger_\sigma(\boldsymbol{r})\nabla^2\hat{\psi}_\sigma(\boldsymbol{r}) + \frac{1}{2}\sum_{\sigma\sigma'}\int \mathrm{d}\boldsymbol{r}\mathrm{d}\boldsymbol{r}'\frac{e^2}{|\boldsymbol{r}-\boldsymbol{r}'|}\hat{\psi}^\dagger_\sigma(\boldsymbol{r})\hat{\psi}^\dagger_{\sigma'}(\boldsymbol{r}')\hat{\psi}_{\sigma'}(\boldsymbol{r}')\hat{\psi}_\sigma(\boldsymbol{r}) + \sum_\sigma\int \mathrm{d}\boldsymbol{r}V_b(\boldsymbol{r})\hat{\psi}^\dagger_\sigma(\boldsymbol{r})\hat{\psi}_\sigma(\boldsymbol{r}), \quad (1.3.30)$$

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

$$\hat{H} = \sum_{\boldsymbol{k}\sigma}\frac{\hbar^2k^2}{2m}\hat{a}^\dagger_{\boldsymbol{k}\sigma}\hat{a}_{\boldsymbol{k}\sigma} + \frac{e^2}{2V}\sum_{\boldsymbol{q}\neq 0}\sum_{\boldsymbol{k}\boldsymbol{p}}\frac{4\pi}{q^2}\hat{a}^\dagger_{\boldsymbol{k}+\boldsymbol{q}\sigma}\hat{a}^\dagger_{\boldsymbol{p}-\boldsymbol{q}\sigma'}\hat{a}_{\boldsymbol{p}\sigma'}\hat{a}_{\boldsymbol{k}\sigma}. \quad (1.3.31)$$

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

Electrons in periodic potential are relevant for solids. The natural basis for second quantizing a Hamiltonian is the Bloch basis $\varphi_{n\boldsymbol{k}}$ (the momentum basis counterpart) or the Wannier function basis $w_n(\boldsymbol{R}_i)$ (the position basis counterpart). They are related by:

$$w_n(\boldsymbol{R}_i) = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{k}\in\mathrm{B.Z.}} e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_i}\varphi_{n\boldsymbol{k}}, \quad (1.3.32)$$

$$\varphi_{n\boldsymbol{k}} = \frac{1}{\sqrt{N}}\sum_{\boldsymbol{R}_i} e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_i}w_n(\boldsymbol{R}_i). \quad (1.3.33)$$

Note that in the Bloch basis, the momentum conservation is modified to:

$$\boldsymbol{k}_1 + \boldsymbol{k}_2 = \boldsymbol{k}_1' + \boldsymbol{k}_2' + \boldsymbol{K}, \quad (1.3.34)$$

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

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

$$\hat{H}_{\mathrm{el-ph}} = \sum_{\boldsymbol{q}} M_{\boldsymbol{q}}\hat{a}^\dagger_{\boldsymbol{k}+\boldsymbol{q}}\hat{a}_{\boldsymbol{k}}\hat{c}_{\boldsymbol{q}} + \mathrm{h.c.} \quad (1.3.35)$$

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

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

$$\hat{H} = -\sum_{ij,\sigma} t_{ij}\hat{a}^\dagger_{i\sigma}\hat{a}_{j\sigma} + \sum_{ii'jj'} U_{ii'jj'}\hat{a}^\dagger_{i\sigma}\hat{a}^\dagger_{i'\sigma'}\hat{a}_{j'\sigma'}\hat{a}_{j\sigma}. \quad (1.3.36)$$

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 $\hat{H}_U = -2\sum_{ij} J_{ij}\left(\hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j + \frac{1}{4}\hat{n}_i\hat{n}_j\right)$.

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

$$\hat{H} = -t\sum_{\langle ij\rangle,\sigma}\left[\hat{a}^\dagger_{i\sigma}\hat{a}_{j\sigma} + \text{h.c.}\right] + U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow}, \tag{1.3.37}$$

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

$$\hat{H}_U \equiv U\sum_i \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} = -\frac{2U}{3}\sum_i \left|\hat{\boldsymbol{S}}_i\right|^2 + \frac{N_e U}{2}, \tag{1.3.38}$$

where $\hat{\boldsymbol{S}}_i$ is the "spin operator" :

$$\hat{\boldsymbol{S}}_i = \frac{1}{2}\sum_{\sigma\sigma'}\hat{a}^\dagger_{i\sigma}\boldsymbol{\tau}_{\sigma\sigma'}\hat{a}_{i\sigma'}, \tag{1.3.39}$$

with Pauli matrices

$$\tau_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},\ \tau_y = \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix},\ \tau_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{1.3.40}$$

Anderson impurity model

$$\hat{H} = \sum_\sigma \epsilon_f \hat{f}^\dagger_\sigma \hat{f}_\sigma + U\hat{n}_{f\uparrow}\hat{n}_{f\downarrow} + \sum_{\boldsymbol{k}\sigma}\left[V_{\boldsymbol{k}}\hat{f}^\dagger_\sigma \hat{a}_{\boldsymbol{k}\sigma} + \text{h.c.}\right] + \sum_{\boldsymbol{k}\sigma}\epsilon_{\boldsymbol{k}}\hat{a}^\dagger_{\boldsymbol{k}\sigma}\hat{a}_{\boldsymbol{k}\sigma}. \tag{1.3.41}$$

Kondo model

$$\hat{H} = \sum_{\boldsymbol{k}\sigma}\epsilon_{\boldsymbol{k}}\hat{a}^\dagger_{\boldsymbol{k}\sigma}\hat{a}_{\boldsymbol{k}\sigma} - J\hat{\boldsymbol{S}}^{(i)}\cdot\hat{\boldsymbol{S}}^{(e)}_0, \tag{1.3.42}$$

where $\hat{\boldsymbol{S}}^{(e)}_0$ denotes an electron-spin operator Eq. (1.3.39) at the origin.

1.4 Coherent states

NO§1.4

- Coherent states as eigenstates of the annihilation operator:

$$\hat{a}_\alpha|\phi\rangle = \phi_\alpha|\phi\rangle. \tag{1.4.1}$$ NO(1.112)

  - coherent states must be eigenstates of $\hat{a}_\alpha$ instead of $\hat{a}^\dagger_\alpha$.

- For Fermions, we have to use *Grassmann numbers*, because

$$\phi_\alpha\phi_\beta + \phi_\beta\phi_\alpha = 0. \tag{1.4.2}$$ NO(1.113)

1.4.1 Boson coherent states

Definition

$$|\phi\rangle = e^{\sum_\alpha \phi_\alpha a_\alpha^\dagger}|0\rangle. \tag{1.4.3}$$

Overlap

$$\langle\phi|\phi'\rangle = \exp\left(\phi^* \cdot \phi'\right). \tag{1.4.4}$$

Note that different coherent states are not orthogonal. They form an over-complete basis.

Closure relation

$$\int \mathrm{d}\mu(\phi)|\phi\rangle\langle\phi| = 1. \tag{1.4.5}$$

$$\mathrm{d}\mu(\phi) \equiv \prod_\alpha \frac{\mathrm{d}\phi_\alpha \mathrm{d}\phi_\alpha^*}{2\pi \mathrm{i}} \exp\left[-\sum_\alpha |\phi_\alpha|^2\right] = \prod_\alpha \frac{\mathrm{d}(\mathrm{Re}\phi_\alpha)\mathrm{d}(\mathrm{Im}\phi_\alpha)}{\pi} \exp\left[-\sum_\alpha |\phi_\alpha|^2\right]. \tag{1.4.6}$$

Trace

$$\mathrm{Tr}\hat{A} = \int \mathrm{d}\mu(\phi) \left\langle \phi \middle| \hat{A} \middle| \phi \right\rangle. \tag{1.4.7}$$

Coherent state representation

$$|\psi\rangle = \int \mathrm{d}\mu(\phi)\, |\phi\rangle \langle\phi|\psi\rangle \equiv \int \mathrm{d}\mu(\phi)\psi(\phi^*)\, |\phi\rangle. \tag{1.4.8}$$

- Representations of operators:

$$\hat{a}_\alpha \to \frac{\partial}{\partial \phi_\alpha^*}, \tag{1.4.9}$$

$$\hat{a}_\alpha^\dagger \to \phi_\alpha^*. \tag{1.4.10}$$

- Wave-equation
- Unit-operator:

$$\psi(\phi^*) = \int \mathrm{d}\mu(\phi') e^{\phi^* \cdot \phi'} \psi(\phi'^*). \tag{1.4.11}$$

- Matrix-elements of *normal ordered* operators:

$$\left\langle \phi \middle| \hat{A}\left(\hat{a}^\dagger, \hat{a}\right) \middle| \phi' \right\rangle = A\left(\phi^*, \phi'\right) e^{\phi^* \cdot \phi'}. \tag{1.4.12}$$

Average and variance of the particle number

$$\bar{N} \equiv \frac{\left\langle \phi \middle| \hat{N} \middle| \phi \right\rangle}{\langle \phi | \phi \rangle} = \sum_\alpha |\phi_\alpha|^2, \tag{1.4.13}$$

$$(\Delta N)^2 \equiv \frac{\left\langle \phi \middle| \left(\hat{N} - \bar{N}\right)^2 \middle| \phi \right\rangle}{\langle \phi | \phi \rangle} = \bar{N}. \tag{1.4.14}$$

1.4.2 Grassmann algebra

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

$$\xi_\alpha \xi_\beta + \xi_\beta \xi_\alpha = 0. \tag{1.4.15}$$

A matrix representation of Grassmann numbers requires matrices of dimension at least $2^n \times 2^n$.

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

$$\{1, \xi_\alpha, \xi_{\alpha_1}\xi_{\alpha_2}, \dots, \xi_{\alpha_1}\xi_{\alpha_2}\dots\xi_{\alpha_n}\}. \tag{1.4.16}$$

Conjugate has properties:

$$(\xi_\alpha)^* = \xi^*_\alpha, \tag{1.4.17}$$
$$(\xi^*_\alpha)^* = \xi_\alpha, \tag{1.4.18}$$
$$(\lambda\xi_\alpha)^* = \lambda^*\xi^*_\alpha, \tag{1.4.19}$$
$$(\xi_{\alpha_1}\dots\xi_{\alpha_n})^* = \xi^*_{\alpha_n}\dots\xi^*_{\alpha_1}. \tag{1.4.20}$$

Function

$$f(\xi) = f_0 + f_1\xi, \tag{1.4.21}$$
$$A(\xi^*, \xi) = a_0 + a_1\xi + \bar{a}_1\xi^* + a_{12}\xi^*\xi. \tag{1.4.22}$$

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:

$$\frac{\partial}{\partial\xi}(\xi^*\xi) = -\xi^*. \tag{1.4.23}$$

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

Integral is defined to be a linear mapping with properties mimicking those of ordinary integrals:

$$\int \mathrm{d}\xi\, 1 = \int \mathrm{d}\xi^*\, 1 = 0, \tag{1.4.24}$$
$$\int \mathrm{d}\xi\, \xi = \int \mathrm{d}\xi^*\, \xi^* = 1. \tag{1.4.25}$$

- Note that $\int \mathrm{d}\xi^*\xi$ is not defined!
- Anti-commutation applies.

Reproducing kernel (Dirac function)

$$\delta(\xi, \xi') = -(\xi - \xi'), \tag{1.4.26}$$ NO(1.153)
$$f(\xi) = \int \mathrm{d}\xi' \delta(\xi, \xi') f(\xi'). \tag{1.4.27}$$

Scalar product of Grassmann functions:

$$\langle f \,|\, g\rangle \equiv \int \mathrm{d}\xi^* \mathrm{d}\xi\, e^{-\xi^*\xi} f^*(\xi) g(\xi^*) \tag{1.4.28}$$
$$= f_0^* g_0 + f_1^* g_1. \tag{1.4.29}$$

1.4.3 Fermion coherent states

Definition

$$|\xi\rangle = e^{-\sum_\alpha \xi_\alpha \hat{a}_\alpha^\dagger} |0\rangle = \prod_\alpha \left(1 - \xi_\alpha \hat{a}_\alpha^\dagger\right) |0\rangle . \tag{1.4.30}$$

$$\hat{a}_\alpha |\xi\rangle = \xi_\alpha |\xi\rangle , \tag{1.4.31}$$
$$\langle\xi| \hat{a}_\alpha^\dagger = \langle\xi| \xi_\alpha^*, \tag{1.4.32}$$
$$\hat{a}_\alpha^\dagger |\xi\rangle = -\frac{\partial}{\partial \xi_\alpha} |\xi\rangle , \tag{1.4.33}$$
$$\langle\xi| \hat{a}_\alpha = +\frac{\partial}{\partial \xi_\alpha^*} \langle\xi| . \tag{1.4.34}$$

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

Overlap

$$\langle \xi \,|\, \xi' \rangle = e^{\xi^* \cdot \xi'} \tag{1.4.35}$$

Closure relation

$$\int \prod_\alpha \mathrm{d}\xi_\alpha^* \mathrm{d}\xi_\alpha e^{-\xi^* \cdot \xi} |\xi\rangle \langle\xi| = 1. \tag{1.4.36}$$

Trace of an operator:

$$\mathrm{Tr}\hat{A} \equiv \int \prod_\alpha \mathrm{d}\xi_\alpha^* \mathrm{d}\xi_\alpha e^{-\xi^* \cdot \xi} \left\langle -\xi \right| \hat{A} \left| \xi \right\rangle . \tag{1.4.37}$$

Note that matrix elements do not commute:

$$\langle \psi_i \,|\, \xi \rangle \langle \xi \,|\, \psi_j \rangle = \langle -\xi \,|\, \psi_j \rangle \langle \psi_i \,|\, \xi \rangle . \tag{1.4.38}$$

Coherent state representation

$$|\psi\rangle = \int \prod_\alpha \mathrm{d}\xi_\alpha^* \mathrm{d}\xi_\alpha e^{-\xi^* \cdot \xi} |\xi\rangle \psi(\xi^*). \tag{1.4.39}$$
$$\langle \xi \,|\, \hat{a}_\alpha \,|\, \psi \rangle = \frac{\partial}{\partial \xi_\alpha^*} \psi(\xi^*), \tag{1.4.40}$$
$$\left\langle \xi \right| \hat{a}_\alpha^\dagger \left| \psi \right\rangle = \xi_\alpha^* \psi(\xi^*), \tag{1.4.41}$$

Matrix element of a normal ordered operator

$$\left\langle \xi \right| \hat{A}\left(\hat{a}^\dagger, \hat{a}\right) \left| \xi' \right\rangle = e^{\xi^* \cdot \xi'} A\left(\xi^*, \xi'\right) . \tag{1.4.42}$$

Caveats

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

1.4.4 Gaussian integrals

For complex variables

$$\int \prod_i \frac{\mathrm{d}z_i^* \mathrm{d}z_i}{2\pi \mathrm{i}} e^{-z^\dagger H z + J^\dagger z + z^\dagger J} = [\det H]^{-1} \, e^{J^\dagger H^{-1} J}. \tag{1.4.43}$$

H is a positive-definite Hermitian matrix.

For Grassmann variables

$$\int \prod \mathrm{d}\eta_i^* \mathrm{d}\eta_i e^{-\eta^\dagger H \eta + J^\dagger \eta + \eta^\dagger J} = [\det H] \, e^{-J^\dagger H^{-1} J}. \tag{1.4.44}$$

NO(1.184)

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:

$$\int \prod \mathrm{d}\zeta_i^* \mathrm{d}\zeta_i P(\zeta^*, \zeta) = \left| \frac{\partial(\eta^*, \eta)}{\partial(\zeta^*, \zeta)} \right| \int \prod \mathrm{d}\eta_i^* \mathrm{d}\eta_i P(\zeta^*(\eta^*, \eta), \zeta(\eta^*, \eta)). \tag{1.4.45}$$

  Note the *inverse* of the Jacobian.

- Note that $\det H$ does *not* appear as an inverse. The property is actually exploited when mapping a disordered system into a supersymmetric interacting system. See, K. Efetov, *Supersymmetry in Disorder and Chaos* (Cambridge University Press, 1999).

1.5 Summary

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

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

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

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

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

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

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

Problems

1. A set of N particles are in single-particle states $|\beta_1\rangle \ldots |\beta_N\rangle$. The single-particle states have the coordinate representation $\langle \boldsymbol{r}|\beta_i\rangle = \psi_{\beta_i}(\boldsymbol{r})$. What are the coordinate representations of the normalized symmetrized many-body states for Bosons and Fermions, respectively?

2. Derive Eq. (1.3.31).

   (a) Determine the commutation relations of $\hat{\boldsymbol{S}}_i$ defined in (1.3.39). Are they the same as those for angular momentum operators?

   (b) Prove Eq. (1.3.38) by making use the identity $\boldsymbol{\tau}_{ab} \cdot \boldsymbol{\tau}_{cd} = 2\delta_{ad}\delta_{bc} - \delta_{ab}\delta_{cd}$.

3. Derive the closure relation Eq. (1.4.5) by showing

$$\int \mathrm{d}\mu(\phi) \, |\phi\rangle \langle\phi| = \sum_n |n\rangle \langle n| \,. \tag{1.5.1}$$

4. Boson coherent states are physical states. 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

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2 \tag{1.5.2}$$

   (a) Show

$$\hat{H} = \hbar\omega \left(\hat{a}^\dagger \hat{a} + \frac{1}{2} \right) \tag{1.5.3}$$

   with

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} \left(\hat{a}^\dagger + \hat{a} \right) \tag{1.5.4}$$

$$\hat{p} = \mathrm{i}\sqrt{\frac{\hbar\omega m}{2}} \left(\hat{a}^\dagger - \hat{a} \right) \tag{1.5.5}$$

   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 finite t is

$$|\psi(t)\rangle = e^{-\mathrm{i}\omega t/2} \, |\phi_0 e^{-\mathrm{i}\omega t}\rangle \,. \tag{1.5.6}$$

(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:

$$\int \mathrm{d}\xi \mathrm{d}\xi^* e^{-\xi^* \xi} \left(\xi - \frac{\partial}{\partial \xi^*} \right) A(\xi, \xi^*) = 0, \tag{1.5.7}$$

for ant A.

Chapter 2

Perturbation theory

2.1 Introduction

NO§2.1

2.1.1 Quantum statistical Mechanics

Statistical ensembles

- Micro-canonical ensemble: fixed energy and particle number.
- Canonical ensemble: fixed particle number, exchange energy with a thermal reservoir

$$\rho \propto e^{-\beta E}. \tag{2.1.1}$$

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

$$\rho \propto e^{-\beta(E-\mu N)} \tag{2.1.2}$$

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.

Expectation values

$$\left\langle \hat{R} \right\rangle = \mathrm{Tr}\hat{\rho}\hat{R}, \tag{2.1.3}$$

$$\hat{\rho} = \frac{1}{Z} e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}, \tag{2.1.4}$$

$$Z = \mathrm{Tr} e^{-\beta\left(\hat{H}-\mu\hat{N}\right)}. \tag{2.1.5}$$

Grand canonical potential

$$\Omega = -\frac{1}{\beta} \ln Z. \tag{2.1.6}$$

Observables

$$N = -\frac{\partial \Omega}{\partial \mu}, \tag{2.1.7}$$

$$P = -\frac{\partial \Omega}{\partial V}, \tag{2.1.8}$$

$$S = -\frac{\partial \Omega}{\partial T}. \tag{2.1.9}$$

Gibbs-Duhem relation

$$U = TS - PV + \mu N, \tag{2.1.10}$$

$$\Omega = -PV. \tag{2.1.11}$$

2.1.2 Response functions and Green's function

A wide range of observables of direct experimental interest may be expressed in terms of the average of products of operator at different time.

Response to a time-dependent potential Considering a time-dependent external field:

$$\hat{H}_U(t) = \hat{H} + \hat{O}U(t). \tag{2.1.12}$$

Evolution operator $|\psi(t_f)\rangle = \hat{\mathcal{U}}(t_f, t_i)\,|\psi(t_i)\rangle$:

$$\hat{\mathcal{U}}(t_f, t_i) = T \exp\left[-\frac{\mathrm{i}}{\hbar}\int_{t_i}^{t_f} \hat{H}_U(t)\mathrm{d}t\right]. \tag{2.1.13}$$

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

$$T\left[\hat{O}(t_1)\hat{O}(t_2)\ldots\hat{O}(t_n)\right] = \zeta^P \hat{O}(t_{P1})\hat{O}(t_{P2})\ldots\hat{O}(t_{Pn}). \tag{2.1.14}$$

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

Response of a wave-function

$$\delta\,|\psi(t)\rangle = \int_{t_i}^{t} \mathrm{d}t_1 \delta U(t_1)\,\frac{\delta\hat{\mathcal{U}}(t,t_i)}{\delta U(t_1)}\bigg|_{U\to 0} |\psi(t_i)\rangle = -\frac{\mathrm{i}}{\hbar}\int_{t_i}^{t} \mathrm{d}t_1 \delta U(t_1) e^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\hat{O}^{(H)}(t_1)\left|\psi^{(H)}\right\rangle. \tag{2.1.15}$$

Heisenberg representation

$$\hat{O}^{(H)}(t) = e^{\frac{\mathrm{i}}{\hbar}\hat{H}t}\hat{O}e^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}, \tag{2.1.16}$$

$$\left|\psi^{(H)}\right\rangle = e^{-\frac{\mathrm{i}}{\hbar}\hat{H}t}\,|\psi\rangle\,. \tag{2.1.17}$$

Response of the expectation value of an observable $\hat{R}$

$$\delta\left\langle \hat{R}^{(H)}(t)\right\rangle = -\frac{\mathrm{i}}{\hbar}\int_{-\infty}^{\infty} \mathrm{d}t'\theta(t-t')\left\langle\left[\hat{R}^{(H)}(t), \hat{O}^{(H)}(t')\right]\right\rangle \delta U(t'), \tag{2.1.18}$$

$$D_{RO}(t,t') \equiv \frac{\delta\left\langle \hat{R}^{(H)}(t)\right\rangle}{\delta U(t')} = -\frac{\mathrm{i}}{\hbar}\theta(t-t')\left\langle\left[\hat{R}^{(H)}(t), \hat{O}^{(H)}(t')\right]\right\rangle. \tag{2.1.19}$$

Fluctuation-dissipation theorem dictates that a transport coefficient is specified by the fluctuation/correlation of operators.

Scattering experiments

- An external particle interacts weakly with the constituents of a many-body system through v, Examples include electron energy loss spectroscopy (EELS) and neutron scattering. The scattering cross section is related to correlation function:

$$\sigma(\boldsymbol{q},\omega) = |v(\boldsymbol{q})|^2 \int \mathrm{d}t e^{\mathrm{i}\omega t} \int \mathrm{d}\boldsymbol{r} e^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \left\langle \hat{\rho}^{(H)}\left(\boldsymbol{r}+\boldsymbol{r}_0,t\right)\hat{\rho}^{(H)}(\boldsymbol{r}_0,0)\right\rangle. \tag{2.1.20}$$

- Angle-resolved photoemission spectroscopy (ARPES): a photon excites a photoelectron out of a many-body system [2]:

$$I_{\boldsymbol{k}}(\omega) \propto \int \mathrm{d}t e^{\mathrm{i}\omega t} \left\langle \hat{a}_{\boldsymbol{k}}\left(t\right) a^\dagger_{\boldsymbol{k}}(0)\right\rangle. \tag{2.1.21}$$

Homework: Describe the ARPES technique and derive Eq. (2.1.21).

Real-time Green's function

$$G^{(n)}\left(\alpha_1 t_1,\ldots\alpha_n t_n;\alpha_1' t_1',\ldots\alpha_n' t_n'\right) = (-\mathrm{i})^n \left\langle T\left[\hat{a}_{\alpha_1}(t_1)\ldots\hat{a}_{\alpha_n}(t_n)\hat{a}^\dagger_{\alpha_n'}(t_n')\ldots\hat{a}^\dagger_{\alpha_1'}(t_1')\right]\right\rangle. \tag{2.1.22}$$

It is used for zero-temperature many-body systems.

Thermal Green's function is the Green's function with imaginary time $t=-\mathrm{i}\tau$:[1]

$$\mathcal{G}^{(n)}\left(\alpha_1 \tau_1,\ldots\alpha_n \tau_n;\alpha_1' \tau_1',\ldots\alpha_n' \tau_n'\right) = (-1)^n \left\langle T\left[\hat{a}_{\alpha_1}(\tau_1)\ldots\hat{a}_{\alpha_n}(\tau_n)\hat{a}^\dagger_{\alpha_n'}(\tau_n')\ldots\hat{a}^\dagger_{\alpha_1'}(\tau_1')\right]\right\rangle. \tag{2.1.23}$$

where

$$\hat{a}_\alpha(\tau) \equiv e^{\frac{\hat{H}}{\hbar}\tau}\hat{a}_\alpha e^{-\frac{\hat{H}}{\hbar}\tau}, \tag{2.1.24}$$

$$\hat{a}^\dagger_\alpha(\tau) \equiv e^{\frac{\hat{H}}{\hbar}\tau}\hat{a}^\dagger_\alpha e^{-\frac{\hat{H}}{\hbar}\tau}. \tag{2.1.25}$$

Note that $\hat{a}^\dagger_\alpha(\tau)$ and $\hat{a}_\alpha(\tau)$ are *not* Hermitian adjoints. It is used for finite-temperature equilibrium systems.

2.2 Functional integral formulation

NO§2.2

Functional integral approach a physically intuitive description of the system and a starting point for approximations.

Approximations naturally arise include:

- perturbation expansions
- loop expansions around stationary solutions
- solitons or instantons
- stochastic approximation

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

2.2.1 The Feynman path integral

To evaluate the evolution operator

$$\mathcal{U}(x_f t_f, x_i, t_i) = \left\langle x_f \left| e^{-\frac{i}{\hbar}\hat{H}(t_f - t_i)} \right| x_i \right\rangle, \tag{2.2.1}$$

the path integral approach proceeds as follows:

- Break a finite time interval into infinitesimal steps $\Delta t = \epsilon$:

$$\mathcal{U}(x_f t_f, x_i, t_i) = \int \prod_{k=1}^{M-1} \mathrm{d}x_k \left\langle x_f \left| e^{-\frac{i\epsilon}{\hbar}\hat{H}} \right| x_{M-1} \right\rangle \left\langle x_{M-1} \left| e^{-\frac{i\epsilon}{\hbar}\hat{H}} \right| x_{M-2} \right\rangle \ldots \left\langle x_1 \left| e^{-\frac{i\epsilon}{\hbar}\hat{H}} \right| x_i \right\rangle. \tag{2.2.2}$$

- Evaluate the evolution operator for each step;
  - Insert a complete momentum basis:

$$\left\langle x_n \left| e^{-\mathrm{i}\frac{\epsilon}{\hbar}\hat{H}} \right| x_{n-1} \right\rangle = \int d^3 p_n \left| p_n \right\rangle \left\langle p_n \left| e^{-\mathrm{i}\frac{\epsilon}{\hbar}\hat{H}} \right| x_{n-1} \right\rangle; \tag{2.2.3}$$

  - Express $\hat{H}$ in *normal form*: all the $\hat{p}$'s appear to the left of all the $\hat{x}$'s;
  - $\left\langle p_n \left| e^{-\mathrm{i}\frac{\epsilon}{\hbar}\hat{H}} \right| x_{n-1} \right\rangle = e^{-\mathrm{i}\frac{\epsilon}{\hbar}H(p_n, x_{n-1})} + \mathcal{O}(\epsilon^2)$;
  - Carry out the integral over p_n;
  - 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 $[V(x_{n-1}) + V(x_n)]/2$? It is equivalent in the continuous limit, but $[V(x_{n-1}) + V(x_n)]/2$ yields better precision for a finite ϵ.

- Chain the evolution operator for individual steps together

$$\mathcal{U}(x_f t_f, x_i, t_i) = \lim_{M\to\infty} \int \prod_{k=1}^{M-1} \mathrm{d}x_k \left(\frac{m}{2\pi\mathrm{i}\epsilon\hbar}\right)^{3M/2} e^{\frac{\mathrm{i}}{\hbar}\epsilon\sum_{k=1}^{M}\left[\frac{1}{2}m\left(\frac{x_k - x_{k-1}}{\epsilon}\right)^2 - V(x_{k-1})\right]} \tag{2.2.4}$$

$$\equiv \int_{x_i t_i}^{x_f t_f} \mathcal{D}\left[x(t)\right] e^{\frac{i}{\hbar}\int_{t_i}^{t_f} \mathrm{d}t\left(\frac{1}{2}m\dot{x}^2 - V(x(t))\right)} \equiv \int_{x_i t_i}^{x_f t_f} \mathcal{D}\left[x(t)\right] e^{\frac{i}{\hbar}S[x(t)]}, \tag{2.2.5}$$

  where $x_M = x_f$ and $x_0 = x_i$ are implied.

Hamiltonian form

$$\mathcal{U}(x_f t_f, x_i, t_i) = \lim_{M\to\infty} \int \prod_{k=1}^{M-1} \mathrm{d}x_k \prod_{k=1}^{M} \frac{\mathrm{d}p_k}{2\pi\hbar} e^{\frac{\mathrm{i}}{\hbar}\epsilon\sum_{k=1}^{M}\left[\frac{1}{2}p_k\frac{x_k - x_{k-1}}{\epsilon} - \frac{p_k^2}{2m} - V(x_{k-1})\right]} \tag{2.2.6}$$

$$\equiv \int_{x_i t_i}^{x_f t_f} \mathcal{D}\left[x(t)\right] \mathcal{D}\left[p(t)\right] e^{\frac{i}{\hbar}\int_{t_i}^{t_f} \mathrm{d}t(p(t)\dot{x}(t) - H(p(t), x(t)))} \tag{2.2.7}$$

Expectation value in the path-integrals is automatically *time-ordered*:

$$\int_{x_i t_i}^{x_f t_f} \mathcal{D}\left[x(t)\right] \mathcal{D}\left[p(t)\right] O_1\left(x(t_1)\right) O_2\left(x(t_2)\right) e^{\frac{i}{\hbar} S(p(t),x(t))} = \left\langle x_f \left| T\left[\hat{O}_1(t_1)\hat{O}_2(t_2) e^{-\frac{i}{\hbar}\int_{t_i}^{t_f} \mathrm{d}t \hat{H}(t)}\right] \right| x_i \right\rangle . \quad (2.2.8)$$

2.2.2 Imaginary time path integral and the partition function

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

$$Z = \mathrm{Tr} e^{-\beta \hat{H}} = \int \mathrm{d}x \left\langle x \left| e^{-\beta \hat{H}} \right| x \right\rangle = \int \mathrm{d}x \left\langle x \left| e^{-\frac{i}{\hbar}(-i\hbar\beta)\hat{H}} \right| x \right\rangle \quad (2.2.9)$$

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

$$\mathcal{U}(x_f \tau_f, x_i, \tau_i) = \int_{x_i \tau_i}^{x_f \tau_f} \mathcal{D}\left[x(\tau)\right] e^{-\frac{1}{\hbar}\int_{\tau_i}^{\tau_f} \mathrm{d}\tau \left[\frac{m}{2}(\dot{x}(\tau))^2 + V(x(\tau))\right]} . \quad (2.2.10)$$

- The partition function is a sum over all periodic trajectories of period $\hbar\beta$:

$$Z = \int_{x(\hbar\beta)=x(0)} \mathcal{D}\left[x(t)\right] e^{-\frac{1}{\hbar}\int_{0}^{\hbar\beta} \mathrm{d}\tau \left[\frac{m}{2}(\dot{x}(\tau))^2 + V(x(\tau))\right]} . \quad (2.2.11)$$

- Generalization to many-particle systems:

$$Z = \frac{1}{N!} \sum_P \zeta^P \int_{x_i(\hbar\beta)=x_{Pi}(0)} \prod_i \mathcal{D}\left[x_i(\tau)\right] e^{-\frac{1}{\hbar}\int_{0}^{\hbar\beta} \mathrm{d}\tau H(x(\tau))} . \quad (2.2.12)$$

  There are two choices for intermediate states:

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

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

2.2.3 Coherent state path integral

- Use the coherent states as the intermediate states by inserting:

$$1 = \frac{1}{\mathcal{N}} \int \prod_\alpha d\phi_\alpha^* d\phi_\alpha e^{-\sum_\alpha \phi_\alpha^* \phi_\alpha} \left|\phi_\alpha\right\rangle \left\langle\phi_\alpha\right| \quad (2.2.13)$$

- Normal form of a second quantized Hamiltonian: all creation operators appear to the left of annihilation operators.
- Evolution operator:

$$\mathcal{U}(\phi_f^*, t_f; \phi_i t_i) = \lim_{M\to\infty} \int \prod_{k=1}^{M-1} \frac{\mathrm{d}\phi_k^* \mathrm{d}\phi_k}{\mathcal{N}} e^{\phi_M^* \phi_{M-1} - \mathrm{i}\frac{\epsilon H(\phi_M^*, \phi_{M-1})}{\hbar} + \mathrm{i}\epsilon \sum_{k=1}^{M-1} \left[\mathrm{i}\phi_k^* \frac{\phi_k - \phi_{k-1}}{\epsilon} - \frac{H(\phi_k^*, \phi_{k-1})}{\hbar}\right]} \tag{2.2.14}$$

$$\equiv \lim_{M\to\infty} \int \prod_{k=1}^{M-1} \frac{\mathrm{d}\phi_k^* \mathrm{d}\phi_k}{\mathcal{N}} e^{\phi_f^* \phi_f + \frac{\mathrm{i}}{\hbar}\int_{t_i}^{t_f} \mathrm{d}t \left[\mathrm{i}\hbar\phi^*(t)\frac{\partial\phi(t)}{\partial t} - H(\phi^*(t), \phi(t))\right]}. \tag{2.2.15}$$

The boundary conditions $\phi_M^* = \phi^*(t_f) = \phi_c^*$ and $\phi_0 = \phi(t_i) = \phi_i$ are implied.

2.2.4 Partition function

Boundary conditions are imposed by the trace with coherent states: (1.4.37)

$$\phi_0 = \phi, \tag{2.2.16}$$
$$\phi_M^* = \varsigma\phi^*. \tag{2.2.17}$$

Partition function

$$Z = \lim_{M\to\infty} \int \prod_{k=1}^{M} \frac{\mathrm{d}\phi_k^* \mathrm{d}\phi_k}{\mathcal{N}} e^{-\epsilon \sum_{k=1}^{M} \left[\phi_k^* \left(\frac{\phi_k - \phi_{k-1}}{\epsilon} - \mu\phi_{k-1}/\hbar\right) + H(\phi_k^*, \phi_{k-1})/\hbar\right]} \tag{2.2.18}$$

$$= \int_{\phi(\hbar\beta)=\varsigma\phi(0)} \mathcal{D}\left[\phi^*(\tau)\phi(\tau)\right] e^{-\int_0^{\hbar\beta} \mathrm{d}\tau \left[\sum_\alpha \phi_\alpha^*(\tau)(\partial_\tau - \mu/\hbar)\phi_\alpha(\tau) + H(\phi^*(\tau), \phi(\tau))/\hbar\right]}. \tag{2.2.19}$$

Note that the continuous form *is defined* by the discrete form.

Thermal Green's functions

$$\mathcal{G}^{(n)}\left(\alpha_1\tau_2, \ldots \alpha_n\tau_n; \alpha_1'\tau_1', \ldots \alpha_n'\tau_n'\right) = \frac{(-1)^n}{Z} \int \mathcal{D}\left[\phi^*(\tau)\phi(\tau)\right]$$
$$e^{-\int_0^{\hbar\beta} \mathrm{d}\tau \left[\sum_\alpha \phi_\alpha^*(\tau)(\partial_\tau - \mu/\hbar)\phi_\alpha(\tau) + H(\phi^*(\tau), \phi(\tau))/\hbar\right]} \phi_{\alpha_1}(\tau_1) \ldots \phi_{\alpha_n}(\tau_n) \phi_{\alpha_n'}^*(\tau_n') \ldots \phi_{\alpha_1'}^*(\tau_1'). \tag{2.2.20}$$

Non-interacting system

Partition function for $\hat{H}_0 = \sum_\alpha \epsilon_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha$

$$Z_0 = \lim_{M\to\infty} \prod_\alpha \int \prod_{k=1}^{M} \frac{\mathrm{d}\phi^*_{\alpha,k}\mathrm{d}\phi_{\alpha,k}}{\mathcal{N}} e^{-\epsilon \sum_{k=1}^{M} \left[\phi^*_{\alpha,k}\left(\frac{\phi_{\alpha,k}-\phi_{\alpha,k-1}}{\epsilon}+\frac{\epsilon_\alpha-\mu}{\hbar}\phi_{\alpha,k-1}\right)\right]} \tag{2.2.21}$$ (2.2.18)

$$= \lim_{M\to\infty} \prod_\alpha \left[\det S^{(\alpha)}\right]^{-\zeta} = \prod_\alpha \left(1-\zeta e^{-\beta(\epsilon_\alpha-\mu)}\right)^{-\zeta} = e^{\zeta \mathrm{Tr}\ln \mathcal{G}_0}. \tag{2.2.22}$$ NO(2.69)

$$S^{(\alpha)} = \begin{bmatrix} 1 & 0 & & & 0 & -\zeta a \\ -a & 1 & 0 & & & 0 \\ 0 & -a & 1 & \ddots & & \vdots \\ & 0 & -a & \ddots & & \\ & & 0 & \ddots & 1 & 0 \\ 0 & & & \dots & -a & 1 \end{bmatrix}, a = 1-\frac{\beta(\epsilon_\alpha-\mu)}{M}. \tag{2.2.23}$$

Free Green's function can be obtained by several ways:

Auxiliary fields

$$\mathcal{G}_0(\alpha\tau_q;\alpha'\tau_r) = -\delta_{\alpha\alpha'}\frac{\zeta}{Z_0}\frac{\partial^2}{\partial J^*_q \partial J_r} \int \prod_{k=1}^{M} \frac{\mathrm{d}\phi^*_{\alpha,k}\mathrm{d}\phi_{\alpha,k}}{\mathcal{N}} e^{-\sum_{jk}\phi^*_{\alpha,k}S^{(\alpha)}_{kj}\phi_{\alpha,j}+\sum_i\left(J^*_i\phi_{\alpha,i}+\phi^*_{\alpha,i}J_i\right)}\Big|_{J=J^*=0} \tag{2.2.24}$$

$$= -\delta_{\alpha\alpha'}\left(S^{(\alpha)}\right)^{-1}_{qr} \tag{2.2.25}$$

$$= -\delta_{\alpha\alpha'}e^{-(\epsilon_\alpha-\mu)(\tau_q-\tau_r)/\hbar}\left[\theta(\tau_q-\tau_r)\left(1+\zeta n_\alpha\right)+\zeta\theta(\tau_r-\tau_q)n_\alpha\right], \tag{2.2.26}$$

$$n_\alpha = \frac{1}{e^{\beta(\epsilon_\alpha-\mu)}-\zeta}. \tag{2.2.27}$$ NO(2.75b)

Fourier transform

$$\phi_k = \frac{1}{\sqrt{M}}\sum_{n=0}^{M-1} e^{-\mathrm{i}\omega_n k\epsilon}\tilde{\phi}_n,\ \omega_n = \begin{cases} \frac{(2n+1)\pi}{\hbar\beta} & \zeta=-1 \\ \frac{2n\pi}{\hbar\beta} & \zeta=1 \end{cases}. \tag{2.2.28}$$

It is easy to verify that the boundary conditions Eqs. (2.2.16, 2.2.17) are satisfied.

$$\sum_{jk}\phi^*_{\alpha,k}S^{(\alpha)}_{kj}\phi_{\alpha,j} = \epsilon\sum_n\left(\frac{1-e^{\mathrm{i}\omega_n\epsilon}}{\epsilon}+\frac{\epsilon_\alpha-\mu}{\hbar}e^{\mathrm{i}\omega_n\epsilon}\right)\left|\tilde{\phi}_n\right|^2 \tag{2.2.29}$$

$$\to \epsilon\sum_n\left(-\mathrm{i}\omega_n+\frac{\epsilon_\alpha-\mu}{\hbar}\right)\left|\tilde{\phi}_n\right|^2. \tag{2.2.30}$$

$$\mathcal{G}^{(\alpha)}_0(\omega_n) = -\lim_{\epsilon\to0}\left(\frac{1-e^{\mathrm{i}\omega_n\epsilon}}{\epsilon}+\frac{\epsilon_\alpha-\mu}{\hbar}e^{\mathrm{i}\omega_n\epsilon}\right)^{-1} = \frac{1}{\mathrm{i}\omega_n-\frac{\epsilon_\alpha-\mu}{\hbar}}. \tag{2.2.31}$$

$$\mathcal{G}_0(\alpha\tau;\alpha'\tau') = \delta_{\alpha\alpha'}\frac{1}{\hbar\beta}\sum_{\omega_n}\mathcal{G}^{(\alpha)}_0(\omega_n)e^{-\mathrm{i}\omega_n(\tau-\tau')}. \tag{2.2.32}$$

Frequency sums FW(25.38)

$$\frac{1}{\hbar\beta}\sum_{\omega_n}\frac{e^{\mathrm{i}\omega_n\eta}}{\mathrm{i}\omega_n - x} = -\frac{\zeta e^{\eta x}}{e^{\hbar\beta x}-\zeta}, \text{ for } \eta > 0. \tag{2.2.33}$$

Equation of motion

$$-\left(\frac{\partial}{\partial\tau}+\frac{\epsilon_\alpha-\mu}{\hbar}\right)\mathcal{G}_0^{(\alpha)}(\tau,\tau') = \delta(\tau-\tau'), \tag{2.2.34}$$

$$\mathcal{G}(\hbar\beta,\tau') = \varsigma\mathcal{G}(0,\tau'). \tag{2.2.35}$$

Equal-time Green's function should be interpreted as

$$\mathcal{G}(\tau,\tau) \equiv \mathcal{G}(\tau,\tau+0^+). \tag{2.2.36}$$

Note that the time ordering is the same as the normal ordering at equal times.

2.3 Perturbation theory NO§2.3

2.3.1 General strategy

- Decompose a Hamiltonian into the sum of a one-body operator $\hat{H}_0 = \sum_\alpha \epsilon_\alpha \hat{a}_\alpha^\dagger \hat{a}_\alpha$ and a residual Hamiltonian $\hat{V}$ (in the normal order).
- Express the Grand partition function in terms of averages with respect to $\hat{H}_0$. By applying the time-slicing technique:
  - Operator form

$$Z = \mathrm{Tr}\left[Te^{-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\hat{H}(\tau)}\right] \tag{2.3.1}$$

$$= Z_0\left\langle Te^{-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\hat{V}(\tau)}\right\rangle_0 \tag{2.3.2}$$

$$\left\langle\hat{F}\left(a^\dagger,a\right)\right\rangle_0 \equiv \frac{1}{Z_0}\mathrm{Tr}\left[Te^{-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau\hat{H}_0(\tau)}\hat{F}\left(a^\dagger,a\right)\right] \tag{2.3.3}$$

    Note that
    - τ is the time-slicing index, not the time in the Heisenberg operators.
    - Time-ordering
  - Functional integral form

$$Z = Z_0\left\langle e^{-\frac{1}{\hbar}\int_0^{\hbar\beta}d\tau V\left(\psi_\alpha^*,\psi_\beta^*,\ldots,\psi_\gamma^*,\psi_\delta^*\right)}\right\rangle_0 \tag{2.3.4}$$

$$\left\langle\hat{F}\left(\psi^*,\psi\right)\right\rangle_0 \equiv \frac{1}{Z_0}\int_{\psi(\hbar\beta)=\zeta\psi(0)}\mathcal{D}\left[\psi^*\psi\right]e^{-\int_0^{\hbar\beta}d\tau\left[\partial_\tau+\left(H_0\left(\psi^*,\psi\right)-\mu\right)/\hbar\right]}F\left(\psi^*,\psi\right) \tag{2.3.5}$$

- Expand Eq. (2.3.4) in a power series of V:

$$\frac{Z}{Z_0} = \sum_{n=0}^{\infty}\frac{(-1/\hbar)^n}{n!}\int_0^{\hbar\beta}d\tau_1\ldots d\tau_n\left\langle V(\tau_1)\ldots V(\tau_n)\right\rangle_0 \tag{2.3.6}$$

2.3.2 Convergency

Perturbation theory yields an asymptotic rather than convergent series:

$$Z(g) = \int \frac{\mathrm{d}x}{\sqrt{2\pi}} e^{-\frac{x^2}{2} - \frac{g}{4}x^4} \approx \sum_n g^n Z_n. \tag{2.3.7}$$

- The series is not convergent because $g^n Z_n \sim (4gn/e)^n/\sqrt{n\pi}$ when $n \to \infty$.
  - A finite number of terms sometimes gives a better approximation: minimum $g^n Z_n \sim \sqrt{4g/\pi}\exp(-1/4g)$ occurs at $n \sim 1/4g$.

Alternative methods

- For large g, it is better to expand as a series of $1/g^n$.
- For double-well potential: stationary phase approximation.
- Different strategies complement each other:
  - Perturbative expansion: organize and elucidate
  - Re-summations: focus on different physics
  - Stationary phase approximation: large amplitude collective motion, tunneling

2.3.3 Wick's theorem

- Identity for Gaussian integrals:

$$\frac{\int \mathcal{D}\left[\psi^*\psi\right] \psi_{i_1}\psi_{i_2}\ldots\psi_{i_n}\ldots\psi^*_{j_n}\ldots\psi^*_{j_2}\psi^*_{j_1} e^{-\sum_{ij}\psi^*_i M_{ij}\psi_j}}{\int \mathcal{D}\left[\psi^*\psi\right] e^{-\sum_{ij}\psi^*_i M_{ij}\psi_j}} = \sum_P \zeta^P M^{-1}_{i_{Pn},j_n}\ldots M^{-1}_{i_{P1},j_1} \tag{2.3.8}$$

Proof

- Define a generating function

$$G\left(J^*,J\right) = \frac{\int \mathcal{D}\left[\psi^*\psi\right] \psi^*_{j_1} e^{-\sum_{ij}\psi^*_i M_{ij}\psi_j + \sum_i (J^*_i\psi_i + \psi^* J_i)}}{\int \mathcal{D}\left[\psi^*\psi\right] e^{-\sum_{ij}\psi^*_i M_{ij}\psi_j}} \tag{2.3.9}$$

$$= e^{\zeta \sum_{ij} J^*_i M^{-1}_{ij} J_j} \tag{2.3.10}$$

- Relate the integral with the generating function

$$\cdots = \zeta^n \frac{\delta^{2n} G(J^*,J)}{\delta J^*_{i_1}\ldots\delta J^*_{i_n}\delta J_{j_n}\ldots\delta J_{J_1}}. \tag{2.3.11}$$

- For Eq. (2.3.5), M_{ij} is just the discrete matrix representation of $\partial_\tau - (\hat{H}_0 - \mu)/\hbar$, and $M^{-1}_{ij} = -[\mathcal{G}_0]_{ij}$.

Wick's theorem

- Pair each ψ_i with a ψ^*_j (a complete *contraction*). Each of the pairs contributes a factor M^{-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.

2.3.4 Labeled Feynman diagrams

We consider a two-body interaction:

$$V\left(\psi^*(\tau),\psi(\tau)\right)=\frac{1}{2}\sum_{\alpha\beta\gamma\delta}\langle\alpha\beta|\hat{v}|\gamma\delta\rangle\,\psi^*_\alpha(\tau)\psi^*_\beta(\tau)\psi_\delta(\tau)\psi_\gamma(\tau) \tag{2.3.12}$$

General idea

- A propagator is represented by a directed line.
- Each interaction is represented by a vertex with two incoming and two outgoing lines.
- Connecting interactions with propagators, by all possible ways.
- Drawing all distinct diagrams, determining signs and coefficients.

Distinct labeled diagrams

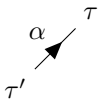
- Labeling each vertex with a time τ and a direction.
- Labeling each propagator with a direction.
- Two labeled diagrams are distinct if they are different in either of the:
  - Connection topology
  - Directions of the vertices and propagation lines

Signs and coefficients

- Each closed loop contributes a sign ζ.
- nth order diagram has an overall factor $(-1/\hbar)^n/2^n n!$.

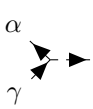
Rules for labeled diagrams

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



$$=g_\alpha(\tau-\tau')=-e^{-(\epsilon_\alpha-\mu)(\tau-\tau')/\hbar}\left[(1+\zeta n_\alpha)\theta(\tau-\tau')+\zeta n_\alpha\theta(\tau'-\tau)\right]. \tag{2.3.13}$$

   - 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



$$=\langle\alpha\beta\,|\,v\,|\,\gamma\delta\rangle \tag{2.3.14}$$

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

$$\frac{(-1/\hbar)^n}{2^n n!}\zeta^{n_L} \tag{2.3.15}$$

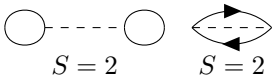
   where n_L is the number of closed loops.

2.3.5 Unlabeled Feynman Diagrams

- The number of the labeled diagrams is huge, and many distinct labeled diagrams yield the same numerical value.
- Simplification: eliminate all τ labels and the directions of the vertices.

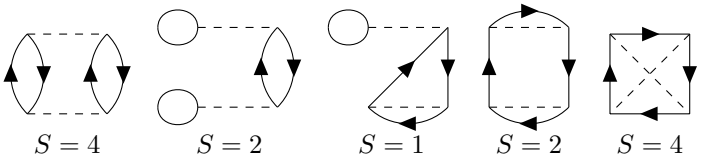
Symmetry factor S

- There are total $2^n n!$ permutations of the time labels and vertex directions.
- For a given *labeled* diagram, there is a subgroup of the permutations that do not change the diagram.
- The symmetry factor S is the rank of the subgroup .
- Examples
  - First order:



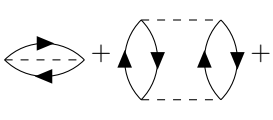
(2.3.16)

  - Second order (connected):



(2.3.17)

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



$$+ \cdots = -\frac{1}{2}\mathrm{Tr}\left[\ln(1-\zeta vgg/\hbar)\right] \tag{2.3.18}$$

- Sum rule:

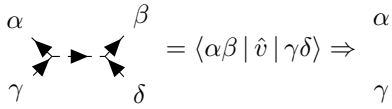
$$\sum \frac{1}{S} = (2n-1)!! \tag{2.3.19}$$

Rules for unlabeled diagrams change the overall functor of a diagram to:

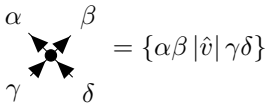
$$\frac{(-1/\hbar)^n \zeta^{n_L}}{S} \tag{2.3.20}$$

2.3.6 Hugenholtz diagrams

- Further simplification: eliminate the interaction lines by using (anti-)symmetrized interaction matrix element:



$$= \langle \alpha\beta \,|\, \hat{v} \,|\, \gamma\delta \rangle \Rightarrow$$



$$= \{\alpha\beta \,|\hat{v}|\, \gamma\delta\} \tag{2.3.21}$$

$$\{\, \alpha\beta \mid \hat{v} | \gamma\delta \,\} \equiv \langle \alpha\beta \,|\, \hat{v} \,|\, \gamma\delta \rangle + \zeta \,\langle \alpha\beta \,|\, \hat{v} \,|\, \delta\gamma \rangle \tag{2.3.22}$$

Symmetry factor

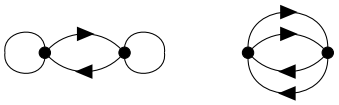
$$S = 2^{n_e} S_D \tag{2.3.23}$$

where S_D is the number of permutations of the *time labels* which yield deformations, and n_e is the number of equivalent pairs of propagator lines. An equivalent pair refers to two propagator lines that begin at the same vertex, end at the same vertex, and point in the same direction.

- Examples
  - First order:

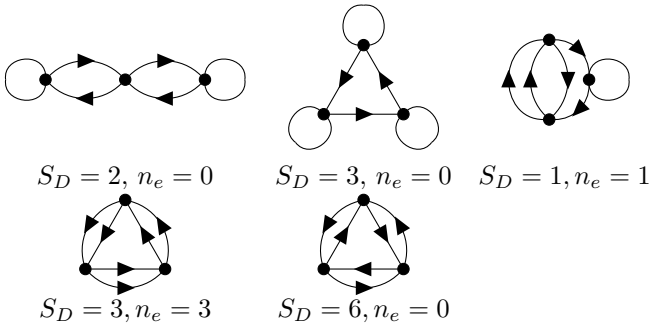
$S_D = 1, n_e = 1$ (2.3.24)

    * Second order (connected):



$S_D = 2,\ n_e = 0 \quad S_D = 2,\ n_e = 2$ (2.3.25)

    * Third order (connected):



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

$S_D = 3, n_e = 3 \quad S_D = 6, n_e = 0$ (2.3.26)

  - Sum rule:

$$\sum \frac{1}{S} = \frac{(2n-1)!!}{2^n} \tag{2.3.27}$$

Number of closed loops n_L is determined by expanding a Hugenholtz diagram to (any) one of corresponding Feynman diagrams, and counting the number of closed loops.

- Overall factor:

$$\frac{(-1/\hbar)^n \zeta^{n_L}}{S} \tag{2.3.28}$$

2.3.7 Frequency and momentum representation

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

- Fourier transform in time:: For a function of time $g(\tau)$ which is periodic/antiperiodic:

$$\tilde{g}(\omega_n) = \int_0^{\hbar\beta} \mathrm{d}\tau e^{\mathrm{i}\omega_n \tau} g(\tau), \tag{2.3.29}$$

$$g(\tau) = \frac{1}{\hbar\beta} \sum_{\omega_n} e^{-\mathrm{i}\omega_n \tau} \tilde{g}(\omega_n), \tag{2.3.30}$$

$$\omega_n = \begin{cases} \frac{2\pi n}{\hbar\beta} & \text{periodic} \\ \frac{(2n+1)\pi}{\hbar\beta} & \text{antiperiodic} \end{cases}. \tag{2.3.31}$$

- Fourier transform in space:

$$\tilde{f}(\boldsymbol{k}) = \int \mathrm{d}\boldsymbol{r} e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} f(\boldsymbol{r}), \tag{2.3.32}$$

$$f(\boldsymbol{r}) = \int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^d} e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} \tilde{f}(\boldsymbol{k}). \tag{2.3.33}$$

- Interaction matrix element in momentum representation:

$$\langle \boldsymbol{k}_1 \boldsymbol{k}_2 \,|\, \hat{v} \,|\, \boldsymbol{k}_3 \boldsymbol{k}_4 \rangle = \frac{1}{\mathcal{V}} \delta_{\boldsymbol{k}_1+\boldsymbol{k}_2, \boldsymbol{k}_3+\boldsymbol{k}_4} \tilde{v}\left(\boldsymbol{k}_1 - \boldsymbol{k}_3\right). \tag{2.3.34}$$

- Green's function in momentum-frequency representation:

$$\tilde{g}\left(\omega_n, \boldsymbol{k}\right) = \frac{1}{\mathrm{i}\omega_n - \left(\epsilon_{\boldsymbol{k}} - \mu\right)/\hbar}. \tag{2.3.35}$$

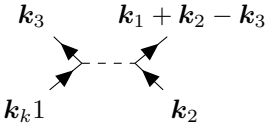
Diagram rules NO(p.94, 96)

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:

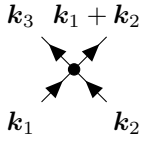
$$= \tilde{g}(\omega_n, \boldsymbol{k}) = \frac{1}{\mathrm{i}\omega_n - \left(\epsilon_{\boldsymbol{k}} - \mu\right)/\hbar}. \tag{2.3.36}$$

   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:



$$= \tilde{v}(\boldsymbol{k}_1 - \boldsymbol{k}_3), \tag{2.3.37}$$



$$= \tilde{v}(\boldsymbol{k}_1 - \boldsymbol{k}_3) + \zeta\tilde{v}(\boldsymbol{k}_2 - \boldsymbol{k}_3). \tag{2.3.38}$$

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

$$\frac{1}{\hbar\beta} \sum_{\omega_n} \int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^d}. \tag{2.3.39}$$

4. Multiply the previous factor by $(\hbar\beta\mathcal{V})^{n_c}$, where n_c is the number of connected part in the diagram.

Loop expansion: the perturbative expansion, in the context of the saddle-point expansion, is also referred as the loop expansion. The "loop" here does not refer to the Fermion loop. It refers to a "momentum loop", i.e., an independent momentum integral performed in a diagram. An nth order diagram has $n+1$ independent momentum integrals. NO(p.126)

2.3.8 The linked cluster theorem

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

$$\Omega = -\frac{1}{\beta}\ln Z = \Omega_0 - \frac{1}{\beta}\sum(\text{all connected graphs}). \tag{2.3.40}$$

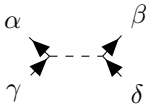
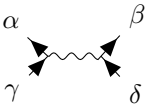
Proof

- Replica approach
  - Exploit the identity:
$$\lim_{n\to 0}\frac{\mathrm{d}}{\mathrm{d}n}Z^n = \ln Z. \tag{2.3.41}$$
  - Z^n can be obtained by calculating the partition function of a system with n replicating fields.
  - The contribution of a graph with n_c connected parts is proportional to n^{n_c}.
  - Z^n terms proportional to n must have $n_c = 1$, i.e., a connected graph.
- Standard approach (Problem 2.10). NO(p.135)

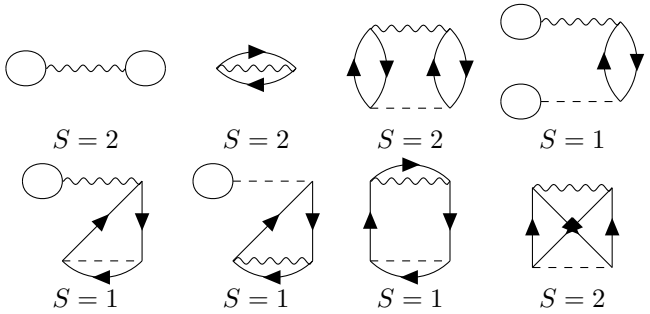
2.3.9 Observables and Green's functions

Observables

$$\left\langle \hat{R}\right\rangle = \frac{\left\langle e^{-\frac{1}{\hbar}\int \mathrm{d}\tau V(\psi^*(\tau),\psi(\tau))} R\left(\psi^*(0),\psi(0)\right)\right\rangle_0}{\left\langle e^{-\frac{1}{\hbar}\int \mathrm{d}\tau V(\psi^*(\tau),\psi(\tau))}\right\rangle_0}. \tag{2.3.42}$$

- For a two-body operator $\hat{R}$: NO(p.100)
  - Starting from the grand potential diagrams, and replacing one of the interaction vertices  with a R-vertex  $= (\alpha\beta|\hat{R}|\gamma\delta)$.
  - The link-cluster theorem still applies: only connected diagrams contribute.
  - Symmetry factors are much simpler:
    - A deformation of diagrams must involve a reversal of the arrow direction of the R-vertex.
      - A diagram is composed of a series of loops.
      - A loop with one time-label fixed has no deformation.

* $S = 2$ if the reverse of the arrow direction of the R-vertex combined with some transformation of the interaction vertices yields a deformation.
* $S = 1$ otherwise.



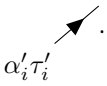
(2.3.43)

- For m-body operators:
  - The symmetry factor S is equal to the number of permutations of the m-joints of R which can be *compensated* by some permutation/direction reversals of the interaction vertices.

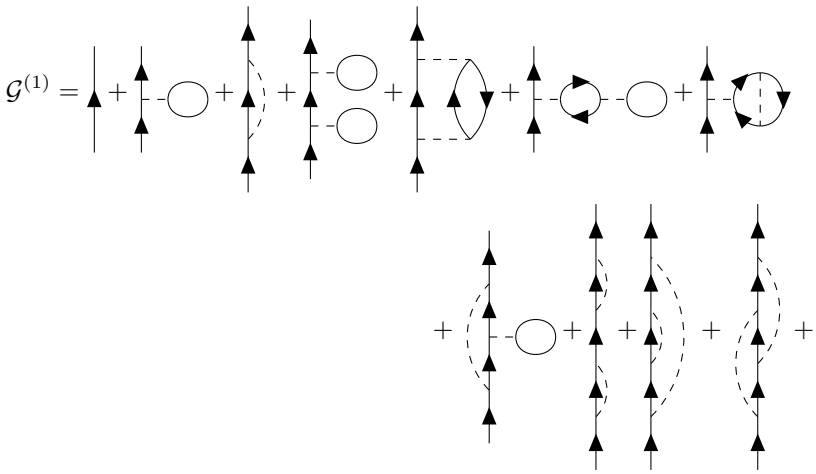
Green's functions

$$\mathcal{G}^{(n)}\left(\alpha_1\tau_2,\dots\alpha_n\tau_n;\alpha_1'\tau_1',\dots\alpha_n'\tau_n'\right) = (-1)^n\left\langle T\left[\hat{a}_{\alpha_1}(\tau_1)\dots\hat{a}_{\alpha_n}(\tau_n)\hat{a}^\dagger_{\alpha_n}(\tau_n)\right]\dots\hat{a}^\dagger_{\alpha_1}(\tau_1)\right\rangle$$
$$= (-1)^n\frac{\left\langle e^{-\frac{1}{\hbar}\int \mathrm{d}\tau V(\psi^*(\tau),\psi(\tau))}\psi_{\alpha_1}(\tau_1)\dots\psi_{\alpha_n}(\tau_n)\psi^*_{\alpha_n'}(\tau_n')\dots\psi^*_{\alpha_1'}(\tau_1')\right\rangle_0}{\left\langle e^{-\frac{1}{\hbar}\int \mathrm{d}\tau V(\psi^*(\tau),\psi(\tau))}\right\rangle_0}. \quad (2.3.44)$$

- The diagram is composed of n external outgoing lines 

and n external incoming lines 

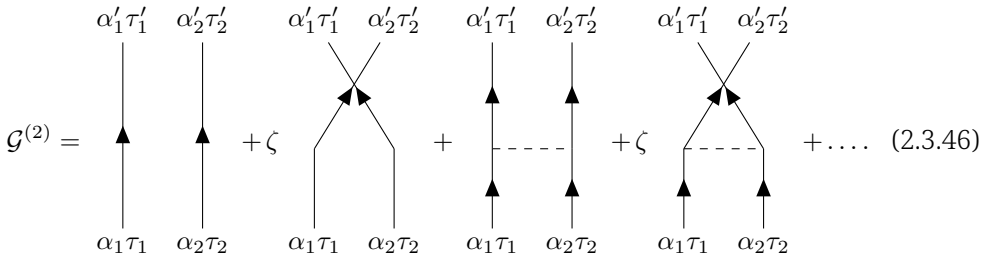
. NO(p.103)



(2.3.45)

- The symmetry factor is always $S = 1$.

- There is an extra sign ζ^P, where P is the permutation of out-going particles with respect to incoming particles.



(2.3.46)

2.4 Zero temperature formalism

NO§3.1

The finite temperature formalism can be applied to the zero temperature by:

- Replacing the trace with the expectation value in a *non-interacting* ground state.
- Rules for Feynman diagram are slightly modified in the propagators and associated factors.

2.4.1 Observables

We seek for analogous expressions for

- ground state energy (2.3.4)
- expectation values of operators (2.3.42)
- Green's function (2.3.44)

Ground state energy

- Basic idea: exploiting the relation

$$\frac{\left\langle \Phi_0 \left| e^{-\frac{\mathrm{i}}{\hbar}\hat{H}T_0} \right| \Phi_0 \right\rangle}{\left\langle \Phi_0 \left| e^{-\frac{\mathrm{i}}{\hbar}\hat{H}_0T_0} \right| \Phi_0 \right\rangle} = \sum_n \left|\langle \Phi_0 \,|\, \Psi_n \rangle\right|^2 e^{-\frac{\mathrm{i}}{\hbar}(E_n - W_0)T_0} \tag{2.4.1}$$

$$\xrightarrow[\mathrm{Im}T_0 \to -\infty]{} \left|\langle \Phi_0 \,|\, \Psi_0 \rangle\right|^2 e^{-\frac{\mathrm{i}}{\hbar}(E_0 - W_0)T_0}, \tag{2.4.2}$$

  where $|\Phi_n\rangle, W_n$ ($|\Psi_n\rangle, E_n$) and the eigenstate and eigen-energy of the non-interacting Hamiltonian $\hat{H}_0$ (full Hamiltonian $\hat{H}$). The relation holds when
  - $|\Phi_0\rangle$is not orthogonal to Ψ_0
  - $|\Psi_0\rangle$is non-degenerate
- Choices of time-contour (Fig. 2.1):
  - C_1: $t = -\mathrm{i}\tau$, choice of the finite temperature formalism.
  - C_2: $t = (1 - \mathrm{i}\eta)\, t_R$ with $\eta = 0^+$, choice of the zero-temperature formalism.

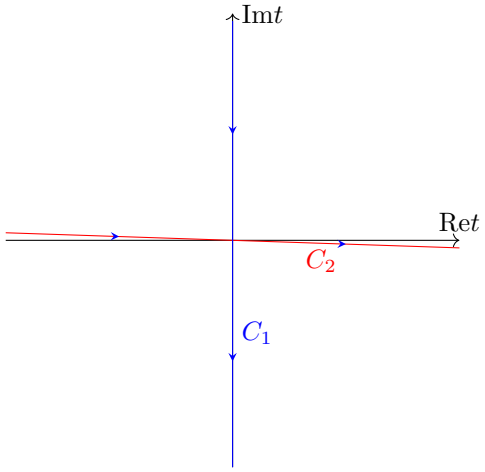


Figure 2.1: Time contours for defining Green's functions.

- Ground state average specified by $\hat{H}_0$: (2.3.3)

$$\left\langle F\left(\hat{a}^\dagger(t_\alpha),\hat{a}(t_\beta)\right)\right\rangle_{H_0} = \frac{\left\langle \Phi_0 \left| Te^{-\frac{\mathrm{i}}{\hbar}\int_{-\frac{T_0}{2}}^{\frac{T_0}{2}} \mathrm{d}t\hat{H}_0\left(\hat{a}^\dagger(t),\hat{a}(t)\right)} F\left(\hat{a}^\dagger(t_\alpha),\hat{a}(t_\beta)\right) \right| \Phi_0 \right\rangle}{\left\langle \Phi_0 \left| Te^{-\frac{\mathrm{i}}{\hbar}\int_{-\frac{T_0}{2}}^{\frac{T_0}{2}} \mathrm{d}t\hat{H}_0(\hat{a}^\dagger(t),\hat{a}(t))} \right| \Phi_0 \right\rangle}. \tag{2.4.3}$$

- Ground state energy (2.3.4)

$$E_0 - W_0 = \lim_{T_0\to(1-\mathrm{i}\eta)\infty} \frac{\mathrm{i}\hbar}{T_0} \ln \left\langle e^{-\frac{\mathrm{i}}{\hbar}\int_{-\frac{T_0}{2}}^{\frac{T_0}{2}} \mathrm{d}t\hat{V}\left(\hat{a}^\dagger(t),\hat{a}(t)\right)} \right\rangle_{H_0}. \tag{2.4.4}$$

Expectation values of operators (2.3.42)

$$\left\langle \Psi_0 \left| \hat{R} \right| \Psi_0 \right\rangle = \lim_{T_0\to(1-\mathrm{i}\eta)\infty} \frac{\left\langle e^{-\frac{\mathrm{i}}{\hbar}\int_{-\frac{T_0}{2}}^{\frac{T_0}{2}} \mathrm{d}t\hat{V}\left(\hat{a}^\dagger(t),\hat{a}(t)\right)} \hat{R}(0) \right\rangle_{H_0}}{\left\langle e^{-\frac{\mathrm{i}}{\hbar}\int_{-\frac{T_0}{2}}^{\frac{T_0}{2}} \mathrm{d}t\hat{V}(\hat{a}^\dagger(t),\hat{a}(t))} \right\rangle_{H_0}}. \tag{2.4.5}$$

Green's function (2.3.44)

$$G^{(n)}\left(\alpha_1 t_1 \ldots \alpha_n t_n; \alpha_1 t_1' \ldots \alpha_n' t_n'\right) = (-\mathrm{i})^n \lim_{T_0 \to (1-\mathrm{i}\eta)\infty} \frac{\left\langle e^{-\frac{\mathrm{i}}{\hbar}\int_{-\frac{T_0}{2}}^{\frac{T_0}{2}} \mathrm{d}t \hat{V}\left(\hat{a}^\dagger(t),\hat{a}(t)\right)} \hat{a}_{\alpha_1}(t_1)\ldots\hat{a}_{\alpha_n}(t_n)\hat{a}^\dagger_{\alpha_n'}(t_n')\ldots\hat{a}^\dagger_{\alpha_1'}(t_1')\right\rangle_{H_0}}{\left\langle T e^{-\frac{\mathrm{i}}{\hbar}\int_{-\frac{T_0}{2}}^{\frac{T_0}{2}} \mathrm{d}t \hat{V}(\hat{a}^\dagger(t),\hat{a}(t))}\right\rangle_{H_0}}. \quad (2.4.6)$$

2.4.2 Zero-temperature Fermion propagators

Particle-hole operators

$$\hat{b}_\alpha = \begin{cases} \hat{a}_\alpha & \epsilon_\alpha > \mu \\ \hat{a}^\dagger_\alpha & \epsilon_\alpha \leq \mu \end{cases}. \quad (2.4.7)$$

$$\hat{K}_0 = \hat{H}_0 - \mu\hat{N} = \sum_{\epsilon_\alpha \leq \mu}(\epsilon_\alpha - \mu) + \sum_\alpha |\epsilon_\alpha - \mu|\, \hat{b}^\dagger_\alpha \hat{b}_\alpha, \quad (2.4.8)$$

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

Generating functional for free Fermion propagator:

$$\mathscr{G}_0[J^*, J] = \left\langle e^{\frac{1}{\hbar}\int \mathrm{d}t\left[J^*_\alpha(t)\hat{a}_\alpha(t) + \hat{a}^\dagger_\alpha(t)J_\alpha(t)\right]}\right\rangle_{K_0}, \quad (2.4.9)$$

$$\mathrm{i}G_0\left(\alpha t; \alpha' t'\right) = -\hbar^2 \left.\frac{\delta^2 \mathscr{G}_0[J^*, J]}{\delta J^*_\alpha(t)\delta J_{\alpha'}(t')}\right|_{J^*=J=0}. \quad (2.4.10)$$

Free Fermion propagator

$$\mathscr{G}_0[J^*, J] = \mathscr{G}_0^{(+)}[J^*, J]\,\mathscr{G}_0^{(-)}[J^*, J], \quad (2.4.11)$$

$$\mathscr{G}_0^{(+)}[J^*, J] = \prod_{\epsilon_\alpha > \mu}\left\langle e^{\frac{1}{\hbar}\int \mathrm{d}t\left[J^*_\alpha(t)\hat{b}_\alpha(t) + \hat{b}^\dagger_\alpha(t)J_\alpha(t)\right]}\right\rangle_{K_0} = \prod_{\epsilon_\alpha > \mu} e^{\sum_{jk} J^*_{\alpha,j} S^{(\alpha)-1}_{ik} J_{\alpha,k}}, \quad (2.4.12)$$

$$\mathscr{G}_0^{(-)}[J^*, J] = \prod_{\epsilon_\alpha \leq \mu}\left\langle e^{\frac{1}{\hbar}\int \mathrm{d}t\left[J^*_\alpha(t)\hat{b}^\dagger_\alpha(t) + \hat{b}_\alpha(t)J_\alpha(t)\right]}\right\rangle_{K_0} = \prod_{\epsilon_\alpha \leq \mu} e^{\sum_{jk} J_{\alpha,j} S^{(\alpha)-1}_{ik} J^*_{\alpha,k}}. \quad (2.4.13)$$

$$S^{(\alpha)} = \begin{bmatrix} 1 & 0 & & & 0 & 0 \\ -a & 1 & 0 & & & 0 \\ 0 & -a & 1 & \ddots & & \vdots \\ & 0 & -a & \ddots & & \\ & & 0 & \ddots & 1 & 0 \\ 0 & & & \ldots & -a & 1 \end{bmatrix}, \; a = 1 - \mathrm{i}\frac{T_0\,|\epsilon_\alpha - \mu|}{\hbar M}. \quad (2.4.14)$$ (2.2.23)

- For $\epsilon_\alpha > \mu$

$$\mathrm{i}G_0(\alpha t_q;\alpha' t_r) = \delta_{\alpha\alpha'}\left(S^{(\alpha)}\right)^{-1}_{qr} = \delta_{\alpha\alpha'}e^{-\frac{\mathrm{i}}{\hbar}(\epsilon_\alpha-\mu)(t_q-t_r)}\theta(t_q-t_r-0^+), \tag{2.4.15}$$

- For $\epsilon_\alpha \le \mu$, do the substitutions $t_q \leftrightarrow t_r$, $\epsilon_\alpha - \mu \to -(\epsilon_\alpha-\mu)$, and append a sign -1 (due to the exchange of J^* and J):

$$\mathrm{i}G_0(\alpha t_q;\alpha' t_r) = -\delta_{\alpha\alpha'}e^{-\frac{\mathrm{i}}{\hbar}(\epsilon_\alpha-\mu)(t_q-t_r)}\theta(t_r-t_q+0^+). \tag{2.4.16}$$

- Complete form: (2.2.26)

$$\mathrm{i}G_0(\alpha t;\alpha' t') = \delta_{\alpha\alpha'}e^{-\frac{\mathrm{i}}{\hbar}(\epsilon_\alpha-\mu)(t_q-t_r)}\left[\theta(t-t'-0^+)\left(1-n_\alpha\right) - \theta(t'-t+0^+)n_\alpha\right], \tag{2.4.17}$$

  where $n_\alpha = \theta(\mu-\epsilon_\alpha)$.
- Fourier transformed form:

$$\tilde{G}_{0\alpha}(\omega) = \int \mathrm{d}t G_0(\alpha t,\alpha 0)e^{\mathrm{i}\omega t} = \frac{1}{\omega-\left(\epsilon_\alpha-\mu\right)/\hbar + \mathrm{i}\eta\mathrm{sgn}\left(\epsilon_\alpha-\mu\right)}. \tag{2.4.18}$$

  – Fourier transforms of $\theta(t)$:

$$\theta(\pm t) = \mp\int \frac{\mathrm{d}\omega}{2\pi\mathrm{i}}\frac{e^{-\mathrm{i}\omega t}}{\omega-\mathrm{i}\eta}. \tag{2.4.19}$$

Homework: Derive Eq. (2.4.17) and (2.4.18) by using the method of equation of motion (see Eq. (2.2.34)):

1. Derive the differential equation of G_0, by using its definition Eq. (2.1.22);
2. Solve the equation to obtain Eq. (2.4.17). Note that a solution must not diverge for $t \to \pm\infty$ in the C_2 contour of Fig. 2.1.
3. Derive the Fourier transformed form Eq. (2.4.18).

2.4.3 Diagram Rules

For Fermion systems, the finite temperature Feynman diagram rules may be adapted for the zero-temperature with replacements:

- $\int_0^{\hbar\beta}\mathrm{d}\tau \to \int_{-T/2}^{T/2}\mathrm{d}t$ or $(1/\hbar\beta)\sum_{\omega_n} \to \int \mathrm{d}\omega/2\pi$, and $\hbar\beta \to T_0$;
- The overall factor $(-1/\hbar)^n\zeta^{n_L}/S \to (-\mathrm{i}/\hbar)^n\zeta^{n_L}/S$;
- $g_\alpha(\tau-\tau') \to -\mathrm{i}G_{0\alpha}(t-t')$ or $\tilde{g}_\alpha(\omega_n) \to -\mathrm{i}\tilde{G}_{0\alpha}(\omega)$. (2.4.17, 2.4.18)

The expectation value of ground state energy can be obtained by

$$E_0 - W_0 = \lim_{T_0\to\infty}\frac{\mathrm{i}}{T_0}\sum \text{all link diagrams}. \tag{2.4.20}$$

A Boson system will have the Bose-Einstein condensation at the zero temperature. It is a *symmetry breaking system*. Its treatment is deferred to a later section.

2.5 Summary

The factor associated a vertex/propagator line is summarized in Table 2.1. An nth order diagram has an overall factor:

$$\begin{cases} \frac{(-1/\hbar)^n}{S}\zeta^{n_L} & T \neq 0 \\ \frac{(-\mathrm{i}/\hbar)^n}{S}\zeta^{n_L} & T = 0 \end{cases}, \tag{2.5.1}$$

where S is the symmetry factor of the diagram, and n_L is the number of loops in the diagram.

In the frequency/momentum representation, there will be an extra factor $\hbar\beta\mathcal{V}$.

For evaluating Green's functions, an extra factor

$$(-1)^P$$

should be incorporated, where P is the permutation of out-going particle lines with respect to incoming particle lines. (2.3.46)

Determining the Symmetry factor

Feynman diagram: assign an index to each vertex and a direction to each interaction line, and count the number of permutations of the vertex indices and directions of the interaction lines that yield deformations.

Hugenholtz diagram: assign an index to each vertex, count the number (S_D) of permutations of the vertex indices that yield deformations and the number (n_e) of equivalent pairs of propagator lines, and $S = 2^{n_e}S_D$.

Observable: count the number of permutations of the joints of the observable that can be compensated by internal symmetry operations to yield deformations.

Green's function: $S = 1$.

In the momentum/frequency representation, the Matsubara frequency is defined to be:

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

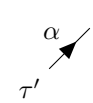
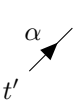
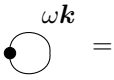
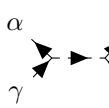
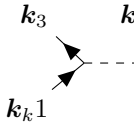
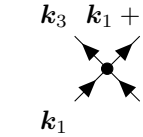
		State/time	Momentum/Frequency
Propagator	$T \neq 0$	 $= g_\alpha(\tau - \tau') =$ $-e^{-(\epsilon_\alpha - \mu)(\tau - \tau')/\hbar}[(1 + \zeta n_\alpha)\theta(\tau - \tau') + \zeta n_\alpha \theta(\tau' - \tau)]$  $= g_\alpha(0^-) = -\zeta n_\alpha$	 $= \tilde{g}(\omega_n, \boldsymbol{k}) = \frac{1}{\mathrm{i}\omega_n - (\epsilon_{\boldsymbol{k}} - \mu)/\hbar}$  $= \frac{1}{\mathrm{i}\omega_n - (\epsilon_{\boldsymbol{k}} - \mu)/\hbar} e^{\mathrm{i}\omega_n \eta}$
	$T = 0$	 $= -\mathrm{i}G_{0\alpha}(t - t') =$ $-e^{-\mathrm{i}(\epsilon_\alpha - \mu)(t - t')/\hbar}[(1 + \zeta n_\alpha)\theta(t - t') + \zeta n_\alpha \theta(t' - t)]$  $= -\mathrm{i}G_{0\alpha}(0^-) = -\zeta n_\alpha$	 $= -\mathrm{i}\tilde{G}_0(\omega, \boldsymbol{k}) =$ $\frac{-\mathrm{i}}{\omega - (\epsilon_{\boldsymbol{k}} - \mu)/\hbar + \mathrm{i}\eta \mathrm{sgn}(\epsilon_{\mathrm{k}} - \mu)}$  $= \frac{-\mathrm{i}}{\omega - (\epsilon_{\boldsymbol{k}} - \mu)/\hbar + \mathrm{i}\eta \mathrm{sgn}(\epsilon_{\mathrm{k}} - \mu)} e^{\mathrm{i}\omega\eta}$
Vertex	Feynman	 $= \langle \alpha\beta \,\vert\, v \,\vert\, \gamma\delta \rangle$	 $=$ $\tilde{v}(\boldsymbol{k}_1 - \boldsymbol{k}_3)$
	Hugenholtz	 $= \{ \alpha\beta \mid \hat{v} \vert \gamma\delta \} \equiv$ $\langle \alpha\beta \,\vert\, \hat{v} \,\vert\, \gamma\delta \rangle + \zeta \langle \alpha\beta \,\vert\, \hat{v} \,\vert\, \delta\gamma \rangle$	 $=$ $\tilde{v}(\boldsymbol{k}_1 - \boldsymbol{k}_3) + \zeta\tilde{v}(\boldsymbol{k}_2 - \boldsymbol{k}_3)$
Internal sums	$T \neq 0$	$\sum_\alpha \int_0^{\hbar\beta} \mathrm{d}\tau$	$\frac{1}{\hbar\beta} \sum_{\omega_n} \int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^d}$
	$T = 0$	$\sum_\alpha \int_{-T/2}^{T/2} \mathrm{d}t$	$\int \frac{\mathrm{d}\omega}{2\pi} \int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^d}$

Table 2.1: Vertex and propagator under different representations.

Chapter 3

Green's functions

3.1 Introduction

3.1.1 Definitions

Real-time (zero temperature) Green's function

$$G^{(n)}\left(\boldsymbol{r}_1 t_1, \ldots \boldsymbol{r}_n t_n; \boldsymbol{r}'_1 t'_1, \ldots \boldsymbol{r}'_n t'_n\right) = (-\mathrm{i})^n \left\langle T\left[\hat{\psi}(\boldsymbol{r}_1 t_1) \ldots \hat{\psi}(\boldsymbol{r}_n t_n)\hat{\psi}^\dagger(\boldsymbol{r}'_n t'_n) \ldots \hat{\psi}^\dagger(\boldsymbol{r}'_1 t'_1)\right]\right\rangle . \tag{3.1.1}$$

Thermal Green's function is the Green's function with imaginary time $t = -\mathrm{i}\tau$:[1]

$$\mathcal{G}^{(n)}\left(\boldsymbol{r}_1 \tau_1, \ldots \boldsymbol{r}_n \tau_n; \boldsymbol{r}'_1 \tau'_1, \ldots \boldsymbol{r}'_n \tau'_n\right) = (-1)^n \left\langle T\left[\hat{\psi}(\boldsymbol{r}_1 \tau_1) \ldots \hat{\psi}(\boldsymbol{r}_n \tau_n)\hat{\psi}^\dagger(\boldsymbol{r}'_n \tau'_n) \ldots \hat{\psi}^\dagger(\boldsymbol{r}'_1 \tau'_1)\right]\right\rangle . \tag{3.1.2}$$

where

$$\hat{\psi}(\boldsymbol{r}\tau) \equiv e^{\frac{\hat{H}}{\hbar}\tau}\hat{\psi}(\boldsymbol{r})e^{-\frac{\hat{H}}{\hbar}\tau}, \tag{3.1.3}$$

$$\hat{\psi}^\dagger(\boldsymbol{r}\tau) \equiv e^{\frac{\hat{H}}{\hbar}\tau}\hat{\psi}^\dagger(\boldsymbol{r})e^{-\frac{\hat{H}}{\hbar}\tau}. \tag{3.1.4}$$

3.1.2 Evaluation of Observables

Green's functions contain sufficient information to evaluate the expectation values of observables:

Kinetic energy:

$$\left\langle \hat{T} \right\rangle = \mathrm{i}\zeta \int \mathrm{d}^3\boldsymbol{r} \left[-\frac{\hbar^2}{2m}\nabla^2_{\boldsymbol{r}} G\left(\boldsymbol{r}t; \boldsymbol{r}'t^+\right)\right]_{\boldsymbol{r}'=\boldsymbol{r}} \tag{3.1.5}$$

$$= \mathrm{i}\zeta\mathcal{V} \int \frac{\mathrm{d}^3\boldsymbol{k}\mathrm{d}\omega}{(2\pi)^4} e^{\mathrm{i}\omega\eta} \frac{\hbar^2 k^2}{2m} \tilde{G}(\boldsymbol{k}, \omega) \tag{3.1.6}$$

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

Interaction energy:

$$\left\langle \hat{V} \right\rangle = \frac{\mathrm{i}\zeta}{2} \int \mathrm{d}^3\boldsymbol{r} \left[\left(\mathrm{i}\hbar \frac{\partial}{\partial t} + \frac{\hbar^2}{2m} \nabla_{\boldsymbol{r}}^2 \right) G\left(\boldsymbol{r}t; \boldsymbol{r}'t'\right) \right]_{\boldsymbol{r}'=\boldsymbol{r}, t'=t^+} \tag{3.1.7}$$

$$= \frac{\mathrm{i}\zeta}{2} \mathcal{V} \int \frac{\mathrm{d}^3\boldsymbol{k}\mathrm{d}\omega}{(2\pi)^4} e^{\mathrm{i}\omega\eta} \left(\hbar\omega - \frac{\hbar^2 k^2}{2m} \right) \tilde{G}(\boldsymbol{k}, \omega) \tag{3.1.8}$$

Ground_state energy:

$$E_0 = \left\langle \hat{T} + \hat{V} \right\rangle = \frac{\mathrm{i}\zeta}{2} \int \mathrm{d}^3\boldsymbol{r} \left[\left(\mathrm{i}\hbar \frac{\partial}{\partial t} - \frac{\hbar^2}{2m} \nabla_{\boldsymbol{r}}^2 \right) G\left(\boldsymbol{r}t; \boldsymbol{r}'t'\right) \right]_{\boldsymbol{r}'=\boldsymbol{r}, t'=t^+} \tag{3.1.9}$$

$$= \frac{\mathrm{i}\zeta}{2} \mathcal{V} \int \frac{\mathrm{d}^3\boldsymbol{k}\mathrm{d}\omega}{(2\pi)^4} e^{\mathrm{i}\omega\eta} \left(\hbar\omega + \frac{\hbar^2 k^2}{2m} \right) \tilde{G}(\boldsymbol{k}, \omega) \tag{3.1.10}$$

3.1.3 Four species of Green's functions

HJ§3.2

Retarded Green's function

$$G^{\mathrm{r}}(\boldsymbol{r}t; \boldsymbol{r}'t') = -\mathrm{i}\theta(t-t') \left\langle \left[\hat{\psi}(\boldsymbol{r}t), \hat{\psi}^\dagger(\boldsymbol{r}'t') \right]_{-\zeta} \right\rangle. \tag{3.1.11}$$

Advanced Green's function

$$G^{\mathrm{a}}(\boldsymbol{r}t; \boldsymbol{r}'t') = -\mathrm{i}\zeta\theta(t'-t) \left\langle \left[\hat{\psi}(\boldsymbol{r}t), \hat{\psi}^\dagger(\boldsymbol{r}'t') \right]_{-\zeta} \right\rangle. \tag{3.1.12}$$

Lesser Green's function

$$G^{<}(\boldsymbol{r}t; \boldsymbol{r}'t') = -\mathrm{i} \left\langle \hat{\psi}^\dagger(\boldsymbol{r}'t') \hat{\psi}(\boldsymbol{r}t) \right\rangle. \tag{3.1.13}$$

Greater Green's function

$$G^{>}(\boldsymbol{r}t; \boldsymbol{r}'t') = -\mathrm{i} \left\langle \hat{\psi}(\boldsymbol{r}t) \hat{\psi}^\dagger(\boldsymbol{r}'t') \right\rangle. \tag{3.1.14}$$

Relations

$$G^{\mathrm{r}} - G^{\mathrm{a}} = G^{>} - G^{<}, \tag{3.1.15}$$

$$G^{\mathrm{r}} = [G^{\mathrm{a}}]^\dagger \tag{3.1.16}$$

$$G(\boldsymbol{r}t; \boldsymbol{r}'t') = \theta(t-t') G^{>}(\boldsymbol{r}t; \boldsymbol{r}'t') + \theta(t'-t) G^{<}(\boldsymbol{r}t; \boldsymbol{r}'t'), \tag{3.1.17}$$

$$G^{\mathrm{r/a}}(\boldsymbol{r}t; \boldsymbol{r}'t') = \pm\theta\left(\pm(t-t')\right) \left[G^{>}(\boldsymbol{r}t; \boldsymbol{r}'t') - G^{<}(\boldsymbol{r}t; \boldsymbol{r}'t') \right]. \tag{3.1.18}$$

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

Merits

- G has a systematic perturbation theory.
- $G^{\mathrm{r/a}}$ have a nicer analytic structure and are directly related to physical responses.
- $G^{<,>}$ are directly related to observables.

3.2 Fluctuation-Dissipation Theorem

HJ§3.3

Spectral function

$$A(\boldsymbol{k},\omega) = \mathrm{i}\left[G^{\mathrm{r}}(\boldsymbol{k},\omega) - G^{\mathrm{a}}(\boldsymbol{k},\omega)\right] = -2\mathrm{Im}G^{\mathrm{r}}(\boldsymbol{k},\omega) \tag{3.2.1}$$

$$= \mathrm{i}\left[G^{>}(\boldsymbol{k},\omega) - G^{<}(\boldsymbol{k},\omega)\right] \tag{3.2.2}$$

- Sum rule:

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} A(\boldsymbol{k},\omega) = 1 \tag{3.2.3}$$

- The density of states can be conveniently computed:

$$\rho(\omega) = \int \frac{\mathrm{d}^3\boldsymbol{k}}{(2\pi)^3} A(\boldsymbol{k},\omega). \tag{3.2.4}$$

- The spectral function can be directly measured by using ARPES technique [2].
- All the Green's functions can be related to the spectral function.

Fluctuation-Dissipation relations

$$G^{<}(\boldsymbol{k},\omega) = -\zeta\frac{\mathrm{i}}{Z}\int \mathrm{d}t\, e^{\mathrm{i}\omega t}\sum_{n,m} e^{-\beta(E_n-\mu N_n)} e^{\mathrm{i}(E_m-E_n)t/\hbar}\left\langle n\left|\,\hat{a}^{\dagger}_{\boldsymbol{k}}\,\right|m\right\rangle\langle m\,|\,\hat{a}_{\boldsymbol{k}}\,|\,n\rangle \tag{3.2.5}$$

$$= -\zeta\frac{\mathrm{i}}{Z}\sum_{n,m} 2\pi\delta\left(\omega - \frac{E_n-E_m}{\hbar}\right)\sum_{n,m} e^{-\beta(E_n-\mu N_n)}\left|\langle m\,|\,\hat{a}_{\boldsymbol{k}}\,|\,n\rangle\right|^2, \tag{3.2.6}$$

$$G^{>}(\boldsymbol{k},\omega) = -\frac{\mathrm{i}}{Z}\sum_{n,m} 2\pi\delta\left(\omega - \frac{E_n-E_m}{\hbar}\right)\sum_{n,m} e^{-\beta(E_m-\mu N_m)}\left|\langle m\,|\,\hat{a}_{\boldsymbol{k}}\,|\,n\rangle\right|^2. \tag{3.2.7}$$

We obtain

$$G^{>}(\boldsymbol{k},\omega) = \zeta e^{\beta(\hbar\omega-\mu)} G^{<}(\boldsymbol{k},\omega) \tag{3.2.8}$$

and

$$G^{<}(\boldsymbol{k},\omega) = -\mathrm{i}\zeta n_{\zeta}(\omega) A(\boldsymbol{k},\omega), \tag{3.2.9}$$

$$G^{>}(\boldsymbol{k},\omega) = -\mathrm{i}\left(1+\zeta n_{\zeta}(\omega)\right) A(\boldsymbol{k},\omega), \tag{3.2.10}$$

$$\begin{Bmatrix} G(\boldsymbol{k},\omega) \\ G^{\mathrm{r}}(\boldsymbol{k},\omega) \\ G^{\mathrm{a}}(\boldsymbol{k},\omega) \end{Bmatrix} = \int \frac{\mathrm{d}\omega_1}{2\pi} A(\boldsymbol{k},\omega_1) \begin{Bmatrix} -\frac{\zeta n_{\zeta}(\omega_1)}{\omega-\omega_1-\mathrm{i}\eta} - \frac{1+\zeta n_{\zeta}(\omega_1)}{\omega_1-\omega-\mathrm{i}\eta} \\ \frac{1}{\omega-\omega_1+\mathrm{i}\eta} \\ \frac{1}{\omega-\omega_1-\mathrm{i}\eta} \end{Bmatrix}, \tag{3.2.11}$$

$$n_{\zeta}(\omega) \equiv \frac{1}{e^{\beta(\hbar\omega-\mu)}-\zeta}. \tag{3.2.12}$$

It follows:

$$\mathrm{Re}\begin{Bmatrix} G(\boldsymbol{k},\omega) \\ G^{\mathrm{r}}(\boldsymbol{k},\omega) \\ G^{\mathrm{a}}(\boldsymbol{k},\omega) \end{Bmatrix} = \mathcal{P}\int \frac{\mathrm{d}\omega_1}{2\pi}\frac{A(\boldsymbol{k},\omega_1)}{\omega-\omega_1}, \tag{3.2.13}$$

$$\mathrm{Im}\begin{Bmatrix} G(\boldsymbol{k},\omega) \\ G^{\mathrm{r}}(\boldsymbol{k},\omega) \\ G^{\mathrm{a}}(\boldsymbol{k},\omega) \end{Bmatrix} = \begin{Bmatrix} -\left[\tanh\frac{\beta(\hbar\omega-\mu)}{2}\right]^{-\zeta} \\ - \\ + \end{Bmatrix}\frac{1}{2}A(\boldsymbol{k},\omega). \tag{3.2.14}$$

3.3 Thermal Green's function and analytic continuation FW§31

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

$$\mathcal{G}(\boldsymbol{k}, \omega_n) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega_1}{2\pi} \frac{A(\boldsymbol{k}, \omega_1)}{\mathrm{i}\omega_n - \omega_1} \tag{3.3.1}$$

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

1. With an analytic form of the thermal Green's function, the spectral function can be determined by

$$A(\boldsymbol{k}, \omega) = \mathrm{i}\left[\mathcal{G}(\boldsymbol{k}, \omega_n)|_{\mathrm{i}\omega_n = \omega + \mathrm{i}\eta} - \mathcal{G}(\boldsymbol{k}, \omega_n)|_{\mathrm{i}\omega_n = \omega - \mathrm{i}\eta}\right]. \tag{3.3.2}$$

2. Various real-time Green's function can be obtained by applying the fluctuation-dissipation relations Eq. (3.2.9–3.2.11).

Homework:

1. Derive Eq. (3.2.9–3.2.14). A useful identity for deriving these equations is:

$$\theta(t) = \int \frac{\mathrm{d}\omega}{2\pi\mathrm{i}} \frac{e^{\mathrm{i}\omega t}}{\omega - \mathrm{i}\eta}. \tag{3.3.3}$$

2. Derive Eq. (3.3.1).

3.4 Non-equilibrium Green's function HJ§4

Necessities for introducing non-equilibrium (Keldysh's) Green's function formalism:

- The real time Green's function are directly related to physical observables.
- Unfortunately, there is no simple perturbation expansion for the real-time Green's function at the finite temperature –perturbative expansion based on the path-integral formalism is only for time-ordered quantities.
- The analytic continuation is only useful when we have an analytic expression for the thermal Green's function. Numerically, the thermal Green's function is only defined for a discrete set of Matsubara frequencies.
- When the system is not an equilibrium one (e.g., a system driven by an external field), there is no guarantee that the system returns to its initial state.

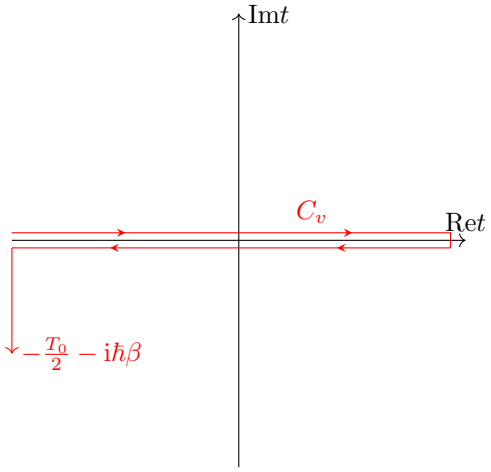


Figure 3.1: Time contour for defining the non-equilibrium Green's functions.

3.4.1 Contour-ordered Green's function

The trick to convert a non-time-order Green's function (e.g., $G^{>}$) to a contour-ordered Green's function:

$$G^{>}(\boldsymbol{r}t;\boldsymbol{r}'t') = -\mathrm{i}\left\langle\hat{\psi}(\boldsymbol{r}t)\hat{\psi}^{\dagger}(\boldsymbol{r}'t')\right\rangle = -\mathrm{i}\frac{\mathrm{Tr}\left[e^{-\beta\hat{H}}\hat{U}\left(-\frac{T_0}{2},t\right)\hat{\psi}(\boldsymbol{r})\hat{U}\left(t,t'\right)\hat{\psi}^{\dagger}(\boldsymbol{r}')\hat{U}\left(t',-\frac{T_0}{2}\right)\right]}{\mathrm{Tr}e^{-\beta\hat{H}}} \tag{3.4.1}$$

$$\to -\mathrm{i}\frac{\mathrm{Tr}\left[\hat{U}\left(-\frac{T_0^-}{2}-\mathrm{i}\hbar\beta,-\frac{T_0^-}{2}\right)\hat{U}\left(-\frac{T_0^-}{2},t^-\right)\hat{\psi}(\boldsymbol{r})\hat{U}\left(t^-,t'^+\right)\hat{\psi}^{\dagger}(\boldsymbol{r}')\hat{U}\left(t'^+,-\frac{T_0^+}{2}\right)\right]}{\mathrm{Tr}e^{-\beta\hat{H}}} \tag{3.4.2}$$

$$= -\mathrm{i}\frac{\mathrm{Tr}\left[T_{C_v}e^{-\frac{\mathrm{i}}{\hbar}\int_{C_v}\mathrm{d}t\hat{H}(t)}\hat{\psi}(\boldsymbol{r}t^-)\hat{\psi}'(\boldsymbol{r}'t'^+)\right]}{\mathrm{Tr}\left[T_{C_v}e^{-\frac{\mathrm{i}}{\hbar}\int_{C_v}dt\hat{H}(t)}\right]} \tag{3.4.3}$$

The contour is defined in Fig. 3.1.

Contour-ordered Green's function is defined as

$$G_{\mathrm{c}}(\boldsymbol{r}t,\boldsymbol{r}'t') = -\mathrm{i}\left\langle T_{c_v}\left[\hat{\psi}(\boldsymbol{r}t)\hat{\psi}^{\dagger}(\boldsymbol{r}'t')\right]\right\rangle. \tag{3.4.4}$$

- There are two-branches of the real time has: $+$ and $-$. The usual Green's functions can be obtained by assigning appropriate branches to the times:

$$G(\boldsymbol{r}t,\boldsymbol{r}'t') = G_c^{++}(\boldsymbol{r}t,\boldsymbol{r}'t'), \tag{3.4.5}$$
$$G^{>}(\boldsymbol{r}t,\boldsymbol{r}'t') = G_c^{-+}(\boldsymbol{r}t,\boldsymbol{r}'t'), \tag{3.4.6}$$
$$G^{<}(\boldsymbol{r}t,\boldsymbol{r}'t') = G_c^{+-}(\boldsymbol{r}t,\boldsymbol{r}'t'). \tag{3.4.7}$$

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

Table 3.1: Langreth rules of contour defined quantities.

- The four components of G_c are not independent:

$$G_c^{++} + G_c^{--} = G^{+-} + G^{-+}. \tag{3.4.8}$$

Perturbation theory of the contour-ordered Green's function is the same as that of the zero-temperature Green's function, albeit time integrals are interpreted as integrals along the contour.

- By assuming that the interaction can be turned on adiabatically, the contribution from the vertical segment of the contour C_v can be ignored. This is valid for (equilibrium or non-equilibrium) steady state problems. However, it may not be valid for transient problems.

Langreth theorem expresses contour defined quantities in the ordinary Green's functions. See Table. 3.1.

Chapter 4

Effective action theory

4.1 Irreducible diagrams and integral equations

NO§2.4

It is possible to derive *exact* integral equations relating connected Green's function and irreducible vertex functions. They are useful for:

- Defining consistent approximations
- Effective action Γ
- Self-energy Σ –effect of a many-body medium to the propagation of a single particle.

4.1.1 Generating function

External sources is introduced into the system by adding a term to the Hamiltonian:

Linear source

$$S = \sum_{\alpha} \int \mathrm{d}\tau \left[J^*_\alpha(\tau)\hat{a}_\alpha(\tau) + \hat{a}^\dagger_\alpha(\tau) J_\alpha(\tau) \right]. \tag{4.1.1}$$

For Fermions, $J(\tau)$ are Grassmann variables.

Bilinear source

$$S = \sum_{\alpha\beta} \int \mathrm{d}\tau_1 \mathrm{d}\tau_2 \left[\hat{a}^\dagger_\alpha(\tau_1)\hat{a}_\beta(\tau_2) V_{\alpha\beta}(\tau_1,\tau_2) + \hat{a}^\dagger_\alpha(\tau_1)\hat{a}^\dagger_\beta(\tau_2)\Delta_{\alpha\beta}(\tau_1,\tau_2) + \text{c.c.} \right]. \tag{4.1.2}$$

- $V_{\alpha\beta}(\tau_1,\tau_2)$: scalar potential.
- $\Delta_{\alpha\beta}(\tau_1,\tau_2)$: pairing potential (superconductivity).

Generating functional

$$\mathscr{G}[V] \equiv \frac{Z[V]}{Z} = \left\langle e^{-\frac{1}{\hbar}\int_0^{\hbar\beta} \mathrm{d}\tau_1 \mathrm{d}\tau_2 \sum_{\alpha\beta} \hat{a}^\dagger_\alpha(\tau_1)\hat{a}_\beta(\tau_2) V_{\alpha\beta}(\tau_1,\tau_2)} \right\rangle. \tag{4.1.3}$$

$$\mathscr{G}[J^*(\tau), J(\tau)] \equiv \frac{Z[J]}{Z} = \left\langle e^{-\frac{1}{\hbar}\int_0^{\hbar\beta} \mathrm{d}\tau \sum_\alpha [J^*_\alpha(\tau)\psi_\alpha(\tau) + \psi^*_\alpha(\tau) J_\alpha(\tau)]} \right\rangle. \tag{4.1.4}$$

The Green's functions can be generated by

$$\mathcal{G}^{(n)}\left(\alpha_1\tau_2,\dots\alpha_n\tau_n;\alpha_1'\tau_1',\dots\alpha_n'\tau_n'\right)=(\zeta\hbar)^n\left.\frac{\delta^n\mathscr{G}[V]}{\delta V_{\alpha_1'\alpha_1}(\tau_1',\tau_1)\dots\delta V_{\alpha_n'\alpha_n}(\tau_1',\tau_1)}\right|_{V\to 0} \tag{4.1.5}$$

$$\mathcal{G}^{(n)}\left(\alpha_1\tau_2,\dots\alpha_n\tau_n;\alpha_1'\tau_1',\dots\alpha_n'\tau_n'\right)=\left(-\zeta\hbar^2\right)^n\left.\frac{\delta^{2n}\mathscr{G}[J^*,J]}{\delta J^*_{\alpha_1}(\tau_1)\dots\delta J^*_{\alpha_n}(\tau_n)\delta J_{\alpha_n'}(\tau_n')\dots J_{\alpha_1'}(\tau_1')}\right|_{J,J^*\to 0}. \tag{4.1.6}$$

Connected generating function

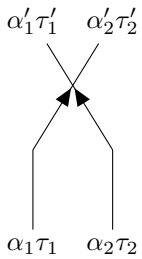
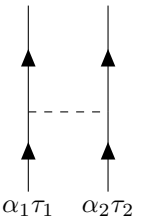
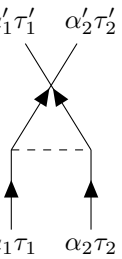
$$W[V]\equiv\ln\mathscr{G}[V]=-\beta\left(\Omega[V]-\Omega[V=0]\right). \tag{4.1.7}$$

$$W[J^*,J]\equiv\ln\mathscr{G}[J^*,J]=-\beta\left(\Omega[J^*,J]-\Omega[J^*=J=0]\right). \tag{4.1.8}$$

It generates *connected Green's functions*:

$$\tilde{\mathcal{G}}_c^{(n)}\left(\alpha_1\tau_2,\dots\alpha_n\tau_n;\alpha_1'\tau_1',\dots\alpha_n'\tau_n'\right)=(\zeta\hbar)^n\left.\frac{\delta^n W[V]}{\delta V_{\alpha_1'\alpha_1}(\tau_1',\tau_1)\dots\delta V_{\alpha_n'\alpha_n}(\tau_1',\tau_1)}\right|_{V\to 0}. \tag{4.1.9}$$

$$\mathcal{G}_c^{(n)}\left(\alpha_1\tau_2,\dots\alpha_n\tau_n;\alpha_1'\tau_1',\dots\alpha_n'\tau_n'\right)=\left(-\zeta\hbar^2\right)^n\left.\frac{\delta^{2n}W[J^*,J]}{\delta J^*_{\alpha_1}(\tau_1)\dots\delta J^*_{\alpha_n}(\tau_n)\delta J_{\alpha_n'}(\tau_n')\dots J_{\alpha_1'}(\tau_1')}\right|_{J,J^*\to 0}. \tag{4.1.10}$$

$\tilde{\mathcal{G}}_c^{(2)}=\zeta$  $+$  $+\zeta$  $+\dots.$ (4.1.11)

$$\mathcal{G}^{(2)}\left(12;1'2'\right)=\tilde{\mathcal{G}}_c^{(2)}\left(12;1'2'\right)+\mathcal{G}(11')\mathcal{G}(22'), \tag{4.1.12}$$

where $\mathcal{G}(11')\equiv\mathcal{G}^{(1)}(1;1')=\tilde{\mathcal{G}}^{(1)}(1;1')$.

$$\mathcal{G}^{(2)}\left(12;1'2'\right)=\mathcal{G}_c^{(2)}\left(12;1'2'\right)+\left[\mathcal{G}(11')\mathcal{G}(22')+\zeta\mathcal{G}(12')\mathcal{G}(21')\right]. \tag{4.1.13}$$

4.1.2 Effective action

Conjugate field

$$\mathcal{G}_{\alpha\alpha'}(\tau,\tau')\equiv-\left\langle T\left[\hat{a}_\alpha(\tau)\hat{a}^\dagger_{\alpha'}(\tau')\right]\right\rangle=\zeta\hbar\frac{\delta W[V]}{\delta V_{\alpha'\alpha}(\tau',\tau)}. \tag{4.1.14}$$

$$\phi_\alpha(\tau) \equiv \langle \hat{a}(\tau) \rangle_{J^*,J} = -\hbar \frac{\delta W[J^*,J]}{\delta J^*_\alpha(\tau)}. \tag{4.1.15}$$

$$\phi^*_\alpha(\tau) \equiv \left\langle \hat{a}^\dagger(\tau) \right\rangle_{J^*,J} = -\zeta\hbar \frac{\delta W[J^*,J]}{\delta J_\alpha(\tau)}. \tag{4.1.16}$$

Effective action (Baym–Kadanoff functional) *is a functional* of the single-particle Green's function $\mathcal{G}$, and related to $W[V]$ by a Legendre transformation:

$$\Gamma[\mathcal{G}] = -W[V] + \frac{\zeta}{\hbar} \sum_{\alpha\alpha'} \int_0^{\hbar\beta} \mathrm{d}\tau \mathrm{d}\tau' \, \mathcal{G}_{\alpha\alpha'}(\tau,\tau') V_{\alpha'\alpha}(\tau',\tau). \tag{4.1.17}$$

$$\equiv -W[V] + \frac{\zeta}{\hbar} \mathrm{Tr}[\mathcal{G}V] \tag{4.1.18}$$

$$\Gamma[\phi^*,\phi] = -W[J^*,J] - \frac{1}{\hbar} \sum_\alpha \int_0^{\hbar\beta} \mathrm{d}\tau \left[\phi^*_\alpha(\tau) J_\alpha(\tau) + J^*_\alpha(\tau) \phi_\alpha(\tau) \right]. \tag{4.1.19}$$

Why?

- It assigns an "energy" to the *physical state/order parameter* of the system, and gives rise to a variational principle.
- It has better analytic properties than $W[V]$ and thus be preferable to approximate.
- It provides a unified foundation for constructing various approximations consistently.
- One may devise non-perturbative approach to construct the functional.

Stationary conditions

$$\frac{\delta\Gamma[\mathcal{G}]}{\delta \mathcal{G}_{\alpha\alpha'}(\tau,\tau')} = \frac{\zeta}{\hbar} V_{\alpha'\alpha}(\tau',\tau). \tag{4.1.20}$$

$$\frac{\delta\Gamma[\phi^*,\phi]}{\delta\phi^*_\alpha(\tau)} = -\frac{1}{\hbar} J_\alpha(\tau), \tag{4.1.21}$$

$$\frac{\delta\Gamma[\phi^*,\phi]}{\delta\phi_\alpha(\tau)} = -\frac{\zeta}{\hbar} J^*_\alpha(\tau). \tag{4.1.22}$$

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

$$\delta\Gamma[\mathcal{G}] = 0. \tag{4.1.23}$$

Vertex functions are generated by

$$\Pi^{(n)}(\alpha_1\tau_2, \ldots \alpha_n\tau_n; \alpha'_1\tau'_1, \ldots \alpha'_n\tau'_n) = \zeta^n \left. \frac{\delta^n\Gamma[\mathcal{G}]}{\delta\mathcal{G}_{\alpha'_1\alpha_1}(\tau'_1,\tau_1) \ldots \delta\mathcal{G}_{\alpha'_n\alpha_n}(\tau'_n,\tau_n)} \right|_{V\to 0}. \tag{4.1.24}$$

$$\Gamma_{m\phi^*,n\phi}(\alpha_1\tau_2, \ldots \alpha_m\tau_m; \alpha'_1\tau'_1, \ldots \alpha'_n\tau'_n) = \left. \frac{\delta^{m+n}\Gamma[\phi^*,\phi]}{\delta\phi^*_{\alpha_1}(\tau_1) \ldots \delta\phi^*_{\alpha_m}(\tau_m) \delta\phi_{\alpha'_n}(\tau'_n) \ldots \delta\phi_{\alpha'_1}(\tau'_1)} \right|_{J^*,J\to 0}. \tag{4.1.25}$$

4.1.3 Self-energy and Dyson's equation

Luttinger-Ward functional $\Phi[\mathcal{G}]$ characterizes the interaction effect in the effective action:

$$\zeta\Gamma[\mathcal{G}] = \zeta\Gamma_0[\mathcal{G}] - \Phi[\mathcal{G}]. \tag{4.1.26}$$

Free effective action for a non-interacting system:

$$W_0[V] = \zeta\left\{\mathrm{Tr}\left[\ln\mathcal{G}\right] - \mathrm{Tr}\left[\ln\mathcal{G}_0\right]\right\}, \tag{4.1.27}$$

$$\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - \frac{V}{\hbar}. \tag{4.1.28}$$

$$\zeta\Gamma_0[\mathcal{G}] = -\mathrm{Tr}\left[\ln\mathcal{G}_0^{-1}\mathcal{G}\right] + \mathrm{Tr}\left[\mathcal{G}_0^{-1}\mathcal{G} - I\right]. \tag{4.1.29}$$

With the decomposition, we have

$$\zeta\Pi^{(1)}(11') \equiv \left.\frac{\delta\Gamma[\mathcal{G}]}{\delta\mathcal{G}(1'1)}\right|_{V\to 0} = [\mathcal{G}_0]^{-1}(11') - [\mathcal{G}]^{-1}(11') - \frac{\delta\Phi[\mathcal{G}]}{\delta\mathcal{G}(1'1)}, \tag{4.1.30}$$

where we adopt the shorthand notation $1 \equiv \{\alpha_1, \tau_1\}$, $1' \equiv \{\alpha_1', \tau_1'\}$.

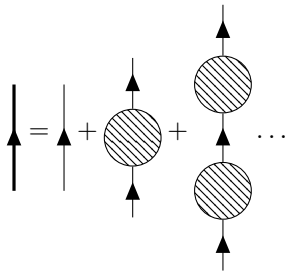
Self energy is defined to be

$$\Sigma(11') = \frac{\delta\Phi[\mathcal{G}]}{\delta\mathcal{G}(1'1)}. \tag{4.1.31}$$

Dyson equation: In the absence of the external source:

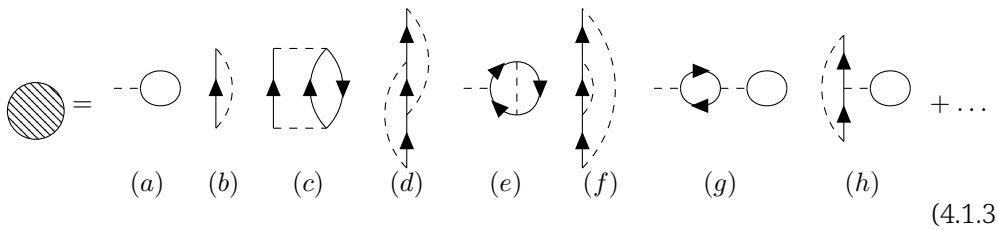
$$[\mathcal{G}]^{-1} = [\mathcal{G}_0]^{-1} - \Sigma, \tag{4.1.32}$$

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0\Sigma\mathcal{G}_0 + \mathcal{G}_0\Sigma\mathcal{G}_0 + \ldots. \tag{4.1.33}$$



(4.1.34)

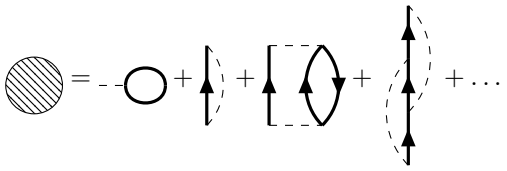
Diagrams of self-energy are one-particle irreducible, i.e., they cannot be separated into two parts by cutting a particle line.



(4.1.35)

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.

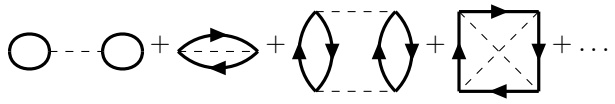
- Alternative definition: all two-particle irreducible diagrams, i.e., the diagrams which cannot be separated by cutting two particle lines.
- With skeleton diagrams, we can construct a *self-consistent equation* for Σ (or $\mathcal{G}$):



(4.1.36)

Diagrams of Luttinger-Ward functional are closed, bold, two-particle irreducible (skeleton) diagrams:

$\Phi[\mathcal{G}] =$



(4.1.37)

- Bold lines represent physical Green's function $\mathcal{G}$.
- Derivative with respect to $\mathcal{G}$ is to remove any of the $2n$ particle lines for a nth order diagrams. It should give rise to the skeleton diagrams of the self-energy. (4.1.31)
- Rules for unlabeled Feynman diagrams should be applied. [1]

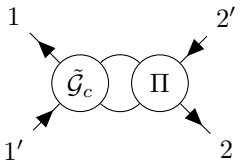
4.1.4 Higher-order vertex functions

Two particle

$$\delta(12)\delta(1'2') = \frac{\delta\mathcal{G}(11')}{\delta\mathcal{G}(22')} = \int \mathrm{d}3 \frac{\delta\mathcal{G}(11')}{\delta V(3'3)} \frac{\delta V(3'3)}{\delta\mathcal{G}(22')}, \tag{4.1.38}$$

$$= \hbar^2 \int \mathrm{d}3\mathrm{d}3' \frac{\delta^2 W[V]}{\delta V(3'3)\delta V(1'1)} \frac{\delta^2\Gamma[\mathcal{G}]}{\delta\mathcal{G}(22')\delta\mathcal{G}(33')}, \tag{4.1.39}$$ (4.1.14,4.1.24)

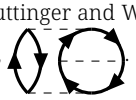
$$\equiv \int \mathrm{d}3\mathrm{d}3' \, \tilde{\mathcal{G}}_c^{(2)}(13;1'3') \, \Pi^{(2)}(3'2',32) \, . \tag{4.1.40}$$ (4.1.14, 4.1.20)



$= \delta(12)\delta(1'2'),$ (4.1.41) NO(2.196a)

Irreducible electron-hole interaction

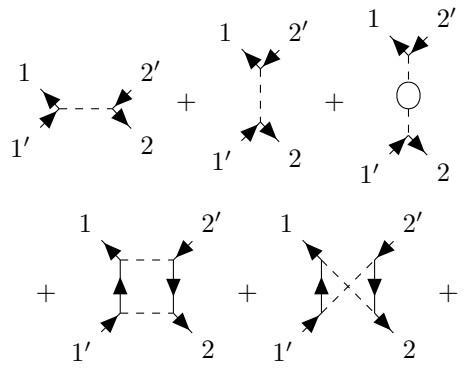
$$\zeta\Pi^{(2)}(3'2',32) = \frac{\delta\zeta\Pi^{(1)}(3'3)}{\delta\mathcal{G}(22')} = \left[\mathcal{G}^{-1}\right](3'2)\left[\mathcal{G}^{-1}\right](2'3) - \frac{\delta^2\Phi[\mathcal{G}]}{\delta\mathcal{G}(33')\delta\mathcal{G}(22')} \tag{4.1.42}$$

[1] The symmetry factor suggested by Luttinger and Ward is $S = 2n$ [3]. This may not be true for certain higher order diagrams with $n > 2$, for instance, 

We define the irreducible interaction I in the direct particle-hole channel:

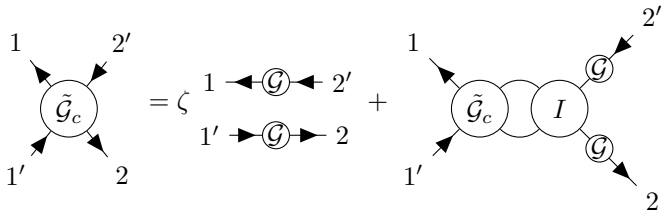
$$I(12;1'2') = \frac{\delta^2 \Phi\left[\mathcal{G}\right]}{\delta \mathcal{G}(1'1)\delta \mathcal{G}(2'2)} = \frac{\delta \Sigma\left(11'\right)}{\delta \mathcal{G}(2'2)}. \tag{4.1.43}$$

It includes all scattering diagrams that are irreducible in the direct electron-hole channel:

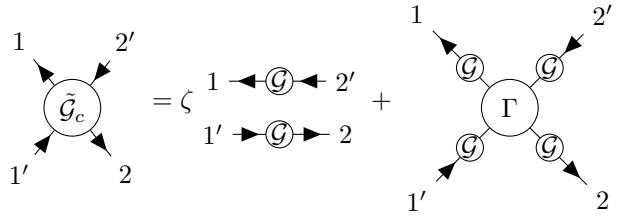
$I(12;1'2') =$  (4.1.44)

Dyson Equation

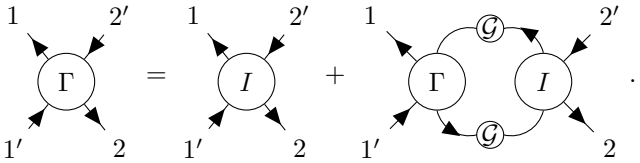
$$\tilde{\mathcal{G}}_c^{(2)}(12;1'2') = \zeta \mathcal{G}(12')\mathcal{G}(21') + \int \mathrm{d}3\mathrm{d}3'\mathrm{d}4\mathrm{d}4' \tilde{\mathcal{G}}_c^{(2)}(13;1'3') I(3'4';34)\mathcal{G}(24')\mathcal{G}(42'). \tag{4.1.45}$$

 (4.1.46)

Scattering amplitude Γ between a pair of electron and hole is defined by:

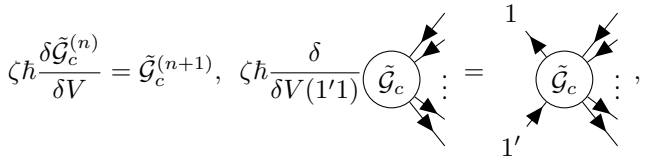
 (4.1.47) NO(2.188a)

Bethe-Salpeter equation relates the scattering amplitude with the irreducible interaction I:

 (4.1.48)

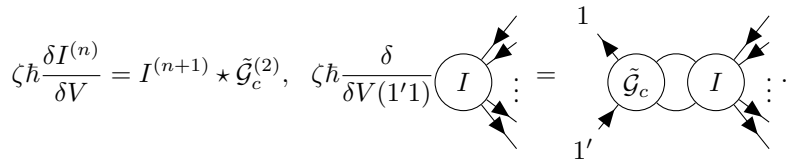
Higher order equations can be obtained by successively applying the derivative $\delta/\delta V$ to Eq. (4.1.45) or (4.1.46). Useful identities:

$$\zeta\hbar\frac{\delta\tilde{\mathcal{G}}_c^{(n)}}{\delta V} = \tilde{\mathcal{G}}_c^{(n+1)}, \quad \zeta\hbar\frac{\delta}{\delta V(1'1)}$$



(4.1.49) (4.1.14)

$$\zeta\hbar\frac{\delta I^{(n)}}{\delta V} = I^{(n+1)} \star \tilde{\mathcal{G}}_c^{(2)}, \quad \zeta\hbar\frac{\delta}{\delta V(1'1)}$$



(4.1.50) (4.1.43)

where $I^{(n)} \equiv \delta^n \Phi[\mathcal{G}]/\delta V(1'1)\ldots\delta V(n'n)$ denotes n-body effective interaction.

Homework: Derive an equation for $\tilde{G}_c^{(4)}$:

1. Derive the equation graphically by applying Eqs. (4.1.49, 4.1.50);
2. Write down the equation in text form from the graphical form.

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.

Conserving approximation: A self-consistent approximation with its self-energy and high order vertices derived from a thermodynamic functional via derivatives (e.g., the Luttinger-Ward functional) is automatically consistent with conservation laws on particle number, momentum, and energy [1].

Chapter 5

Theory of electron liquid

Chapter 6

Broken symmetry and collective phenomena

Bibliography

[1] Gordon Baym and Leo P. Kadanoff. Conservation Laws and Correlation Functions. *Phys. Rev.*, 124(2):287–299, October 1961.

[2] Andrea Damascelli, Zahid Hussain, and Zhi-Xun Shen. Angle-resolved photoemission studies of the cuprate superconductors. *Rev. Mod. Phys.*, 75(2):473–541, April 2003.

[3] J. M. Luttinger and J. C. Ward. Ground-State Energy of a Many-Fermion System. II. *Phys. Rev.*, 118(5):1417–1427, June 1960.