Condensed matter quantum many-body theory

Björn Sbierski
B.Sbierski@uni-tuebingen.de

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Organization

- Lecture: Thursdays 10:15 - 12:00 (room D8H33), start on Oct. 19, 2023 (blackboard lecture, English language)
- Tutorial session: Wednesdays 12:15 - 14:00 (room D7H33), start on Oct. 25, 2023.
  - Tutor: Wilson Santana Martins (wilson.santana-martins@uni-tuebingen.de)
  - Weekly homework will be assigned in the lecture on Thursday, each homework contains two exercises. Solutions are to be handed in via eMail to the tutor or on paper in the tutor's mailbox on the 8th floor. Deadline: **Tuesday** 18:00. The homework will be graded according to a coarse grading scheme with 0, 1 or 2 points per exercise. In the tutorial session, the graded homework will be handed back and the solutions will be discussed.
- Requirements to pass the course: (i) at least 50% of all available homework points and (ii) present at least two exercises on the board in the tutorial session.
- ILIAS: Lecture notes + problem sets in single PDF, please "join" the course.
- Hint: If you electronically annotate the PDF of the lecture notes, the program "PDF Arranger" (for linux) allows you to merge the newly added sections with your annotated pages.

Prerequisites

- Quantum Mechanics (QM), Solid State Theory, Statistical Physics

Philosophy

- Course time is rather short for the course topic → formalism first, applications second.
- Goal: Learn tools and concepts that can be applied to various condensed matter settings → exercises

Contents

1. Second quantization and applications
2. Mean-field theory
3. Time dependence in quantum theory
4. Green functions (real time)

5. Equilibrium GF: Imaginary time and Matsubara formalism
6. Measurement: Linear response theory
7. Perturbation theory and Feynman diagrams
8. Interacting electron gas: Random-phase approximation and screening
9. Disordered metals and their conductivity

Literature

[Altland] Alexander Altland and Ben Simons, *Condensed Matter Field Theory*, Cambridge University Press, 2nd Ed.

[Brouwer] Piet Brouwer, Quantum Field Theory and Many Body Physics (online PDF notes, not published)

[Bruus] Henrik Bruus, Karsten Flensberg, *Many-Body Quantum Theory in Condensed Matter Physics*, Oxford Graduate Texts

[Coleman] Piers Coleman, *Introduction to Many-Body Physics*, Cambridge University Press

[Tremblay] André-Marie Tremblay, Refresher in many-body theory (online PDF notes, not published)

Thanks

- I acknowledge Georg Rohringer for sharing unpublished lecture notes that helped to shape this course.

1 Second quantization and applications

Idea:

- Find *convenient formulation* of the formalism of *many-body* QM beyond symmetrized wavefunctions.
- Despite the name, there is *no* additional "quantization" step beyond the one of elementary QM: $x, p \to \hat{x}, \hat{p}$ with $[\hat{x}, \hat{p}] = i\hbar$.
- Application to elementary problems.

1.1 First quantization

Single-particle systems

- Single particle (say electron with charge $-e$) moving in external fields [potentials $U(\mathbf{r}, t)$ and $\mathbf{A}(\mathbf{r}, t)$]:

$$H = \frac{1}{2m}\left(-i\hbar\nabla_{\mathbf{r}} + e\mathbf{A}(r,t)\right)^2 + U(\mathbf{r}, t) \tag{1}$$

  Examples and eigenstates (from elementary QM):

  1. No potentials [$U = 0$, $\mathbf{A} = 0$]: Plane-wave eigenstates $|\mathbf{k}\rangle$, labeled by momentum, wavefunction $\psi_{\mathbf{k}}(\mathbf{r}) = \langle \mathbf{r}|\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}/\sqrt{V}$), energy $E_{\mathbf{k}} = \hbar^2 k^2/(2m)$.
  2. Harmonic oscillator in d=1 [$\mathbf{A} = 0$, $U(x) = m\omega^2 x^2/2$]: Hermite polynomials with Gaussian envelope $|n\rangle$, $n \in \mathbb{N}$, $\psi_n(x) = \langle x|n\rangle \propto H_n(x/l)e^{-x^2/l^2}$ with $l = \sqrt{\hbar/(m\omega)}$, energy $E_n = \hbar\omega(n + 1/2)$.
  3. Electrons in d=2 with B-field in z-direction [Landau gauge $\mathbf{A} = xB\mathbf{e}_y$, $U = 0$]: Landau level eigenstates $|n, k_y\rangle$ with $\langle \mathbf{r}|n, k_y\rangle \propto H_n(x/l - k_y l)e^{-(x/l-k_y l)^2}\frac{1}{\sqrt{L_y}}e^{ik_y y}$, energy $E_{n,k_y} = \hbar\omega(n + 1/2)$.

- Setup:
  - Assume $\{|\nu\rangle\}_\nu$ is the known and complete set of eigenstates of *single*-particle Hamiltonian H, ν is the set of quantum numbers $\nu = (k_x, k_y, k_z)$ or (n) or (n, k_y).
  - Recall: Completeness relation $\sum_\nu |\nu\rangle\langle\nu| = 1$ in single particle Hilbert space $\mathcal{H}$, wavefunction $\psi_\nu(\mathbf{r}) = \langle \mathbf{r}|\nu\rangle$, probability density to find the particle in state ν at position $\mathbf{r}$ is $|\psi_\nu(\mathbf{r})|^2$.

Systems with N *identical* particles

- Many body wavefunction $\psi(\mathbf{r}_1, ..., \mathbf{r}_N)$: Probability density $|\psi(\mathbf{r}_1, ..., \mathbf{r}_N)|^2$ to find N particles around points $\mathbf{r}_{1,2,...,N}$ in configuration space.
- Symmetrization requirement: Exchanging identical particles (say $1 \leftrightarrow 2$) yields sign $\psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = \pm\psi(\mathbf{r}_2, \mathbf{r}_1, ..., \mathbf{r}_N)$ with + for bosons and - for fermions.
- For $N = 1$: Expand wavefunction in eigenstates (or any basis): $\psi(\mathbf{r}) = \sum_\nu A_\nu \psi_\nu(\mathbf{r})$. Similar: Any N-particle state can be written as superposition of **product states** where particle j is placed in single particle state $|\nu_j\rangle$:

$$\psi(\mathbf{r}_1, ..., \mathbf{r}_N) = \sum_{\nu_1,...,\nu_N} A_{\nu_1,...,\nu_N} \underbrace{\psi_{\nu_1}(\mathbf{r}_1)\cdots\psi_{\nu_N}(\mathbf{r}_N)}_{\text{product state}} \tag{2}$$

- Note: Product states from Eq. (2) form a basis, but they do *not* respect symmetrization requirement (needs to be encoded in $A_{\nu_1,...,\nu_N}$).

- Physical basis: For efficiency, change to **symmetrized product states** as basis (S_N is the permutation group with $N!$ elements p)

$$\boxed{S_\pm \prod_{j=1}^{N} \psi_{\nu_j}(\mathbf{r}_j) = \mathcal{N} \sum_{p\in S_N} \begin{cases} \prod_{j=1}^{N} \psi_{\nu_j}(\mathbf{r}_{p(j)}) & : \text{bosons} \\ \text{sgn}(p) \prod_{j=1}^{N} \psi_{\nu_j}(\mathbf{r}_{p(j)}) & : \text{fermions} \end{cases}} \tag{3}$$

  For fermions:

  - sign of a permutation, $\text{sgn}(p) = \pm 1$ is the parity of the number of transpositions of two elements that is required to build p from identity, e.g. $\text{sgn}(321) = -\text{sgn}(123) = -1$.
  - the state is known as "Slater determinant", it is the determinant of the matrix a with entries $a_{nm} = \psi_{\nu_n}(\mathbf{r}_m)$.
  - For $N = 2$ fermions $S_\pm \psi_{\nu_1}(\mathbf{r}_1)\psi_{\nu_2}(\mathbf{r}_2) \propto \psi_{\nu_1}(\mathbf{r}_1)\psi_{\nu_2}(\mathbf{r}_2) - \psi_{\nu_1}(\mathbf{r}_2)\psi_{\nu_2}(\mathbf{r}_1)$. If $\nu_1 = \nu_2$, we find zero. We cannot put two (or more) fermions in the same single-particle state $\rightarrow$ Pauli-principle.

- Use Eq. (3) as basis: Expansion coefficient $B_{\nu_1,\nu_2,,...,\nu_N}$ (fully symmetric in indices, only specify *which* ν are involved):

$$\psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = \sum_{\nu_1,\nu_2,...,\nu_N} B_{\nu_1,\nu_2,...,\nu_N} \left[S_\pm \psi_{\nu_1}(\mathbf{r}_1)\psi_{\nu_2}(\mathbf{r}_2)\cdots\psi_{\nu_N}(\mathbf{r}_N)\right] \tag{4}$$

One- and two-particle operators T and V

- Use position basis, say, to express local one-particle operator $T = T(\mathbf{r}, \nabla_\mathbf{r})$ e.g. $T = U(\mathbf{r})$ or $T = -\hbar^2\nabla^2_\mathbf{r}/(2m)$.

- Action of T in single-particle basis $|\nu\rangle$:

$$T = \sum_{a,b} |\nu_b\rangle\, T_{\nu_b\nu_a}\, \langle\nu_a| \tag{5}$$

  with the matrix element $T_{\nu_b\nu_a} = \int_\mathbf{r} \psi^\star_{\nu_b}(\mathbf{r}) T(\mathbf{r}, \nabla_\mathbf{r}) \psi_{\nu_a}(\mathbf{r})$.

- $N > 1$: All particle coordinates must appear symmetrically, thus $T(\mathbf{r}, \nabla_\mathbf{r}) \rightarrow T(\mathbf{r}_j, \nabla_{\mathbf{r}_j}) \equiv T_j$ and $T_{tot} = \sum_{j=1}^{N} T_j$.

- Action of T_{tot} on product state (ket at j-th position gives state of j-th particle):

$$T_{tot}\,|\nu_{n_1}\rangle\,|\nu_{n_2}\rangle\,...\,|\nu_{n_N}\rangle = \sum_b \left(T_{\nu_b\nu_{n_1}}\,|\nu_b\rangle\,|\nu_{n_2}\rangle\,...\,|\nu_{n_N}\rangle + T_{\nu_b\nu_{n_2}}\,|\nu_{n_1}\rangle\,|\nu_b\rangle...\,|\nu_{n_N}\rangle + ... + T_{\nu_b\nu_{n_N}}\,|\nu_{n_1}\rangle\,|\nu_{n_2}\rangle\,...|\nu_b\rangle\right) \tag{6}$$

- Two-particle operator V, e.g. Coulomb interaction $V_{jk} = V(\mathbf{r}_j - \mathbf{r}_k) = e^2/(4\pi\varepsilon_0|\mathbf{r}_j - \mathbf{r}_k|)$. In general:

$$V_{jk} = \sum_{\nu_a,\nu_b,\nu_c,\nu_d} \left|\nu_c^{(j)}\right\rangle \left|\nu_d^{(k)}\right\rangle V_{\nu_c\nu_d,\nu_a\nu_b} \left\langle\nu_a^{(j)}\right| \left\langle\nu_b^{(k)}\right| \tag{7}$$

  where $V_{\nu_c\nu_d,\nu_a\nu_b}$ is the matrix element and $V_{tot} = \sum_{j>k} V_{jk}$ (the $j > k$ avoids double-counting!).

- Typical N-particle Hamiltonian: $H_{tot} = T_{tot} + V_{tot} = \sum_{j=1}^{N} T_j + \sum_{j>k} V_{jk}$, e.g. helium atom with two electrons:

$$H^{\text{He}}_{tot} = \sum_{j=1,2} \left(-\hbar^2\nabla^2_{\mathbf{r}_j}/(2m) - \frac{2e^2}{4\pi\varepsilon_0|\mathbf{r}_j|}\right) + \frac{e^2}{4\pi\varepsilon_0|\mathbf{r}_1 - \mathbf{r}_2|} \tag{8}$$

- Note: Even if $|\nu\rangle$ are single-particle eigenstates, Eq. (3) is not an eigenstate of a general interacting many-body Hamiltonian (with $V_{tot} \neq 0$).

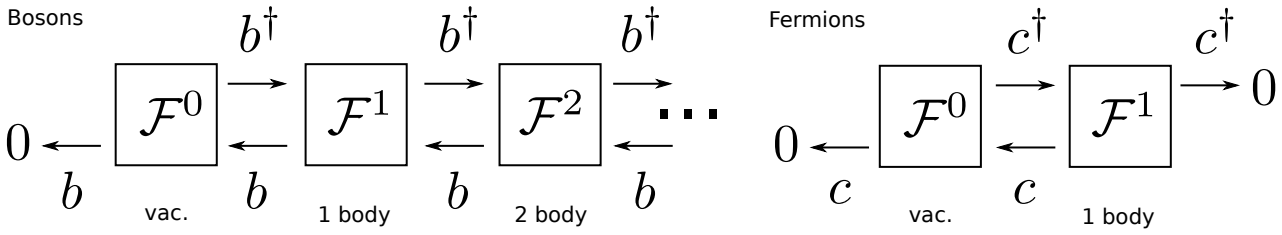

Figure 1: Action of creation and annihilation operators in Fock space, for bosons and fermions. For simplicity only one single-particle basis state is assumed.

1.2 Second quantization

Occupation number basis

- Consider sym. product state in Eq. (3), $S_\pm |\nu_{j_1}\rangle |\nu_{j_2}\rangle \cdots |\nu_{j_N}\rangle$ with N single-particle states occupied.
- Sym. product states are inconvenient:
  - computations are cumbersome, e.g. overlap of two states requires calculation of $(N!)^2$ terms.
  - N is fixed, but grand-canonical formulation of statistical mechanics requires fluctuating N
- All information needed for this state is the number of appearances n_j ("occupation") of single-particle state $|\nu_j\rangle$. Recall: $n_j = 0, 1$ for fermions, and $0, 1, 2, ...$ bosons.
- Definition of occupation number representation of N-particle basis state:

$$S_\pm |\nu_{j_1}\rangle |\nu_{j_2}\rangle \cdots |\nu_{j_N}\rangle \equiv |n_1, n_2, ...\rangle \tag{9}$$

  with $N = n_1 + n_2 + ...$ and occupation number operator $\hat{n}_j$ with $\hat{n}_j |n_1, n_2, ..., n_j, ...\rangle = n_j |n_1, n_2, ..., n_j, ...\rangle$.
- Important for fermionic case: For Eq. (9) we must fix an ordering of single-particle basis $\{|\nu_1\rangle, |\nu_2\rangle, ...\}$ and request $j_1 \leq j_2 \leq ... \leq j_N$.
- **Fock space**: Consider $\mathcal{F}^N = \text{span}\{|n_1, n_2, ...\rangle\}_{n_1+n_2+...=N}$ and combine via direct product for $N = 0, 1, 2, ...$:

$$\mathcal{F} = \mathcal{F}^0 \oplus \mathcal{F}^1 \oplus \mathcal{F}^2 \oplus ... \tag{10}$$

  Remarks:
  - Due to direct sum ($\oplus$) states with unequal N are orthogonal.
  - $\mathcal{F}^0$ is spanned by **vacuum state** $|0, 0, ...\rangle \equiv |0\rangle$ (proper normalized quantum state without particles $\neq 0$).
  - General **many-body state** $|\psi\rangle \in \mathcal{F}$ may consist of contributions with different particle number N ($\rightarrow$ theory of superconductivity).
- Next: Define operators acting on Fock space that can be used to do calculations in a simplified manner.

Bosonic creation and annihilation operators

- Define creation operator $b_j^\dagger : \mathcal{F} \rightarrow \mathcal{F}$ by its action to increase occupation number in single-particle state $|\nu_j\rangle$ by one (Fig. 1):

$$b_j^\dagger |n_1, ..., n_j, ...\rangle \equiv \sqrt{n_j + 1} |n_1, ..., n_j + 1, ...\rangle \tag{11}$$

- What is hermitian adjoint b_j? Use

$$\sqrt{n_j+1} = \left\langle n_1, ..., n_j+1, ... | b_j^\dagger | n_1, ..., n_j, ... \right\rangle^\star = \left\langle n_1, ..., n_j, ... | \left(b_j^\dagger\right)^\dagger | n_1, ..., n_j+1, ... \right\rangle \tag{12}$$

  so that $\left(b_j^\dagger\right)^\dagger = b_j$ acts as an annihilation operator:

$$b_j | n_1, ..., n_j, ... \rangle = \sqrt{n_j} | n_1, ..., n_j - 1, ... \rangle \tag{13}$$

  For the case $n_j = 0$, we have $b_j | n_1, ..., n_j = 0, ... \rangle = 0$ by the prefactor.

- From the definition follows: $b_j^\dagger b_j = \hat{n}_j$ is the occupation number operator.

- Further properties of $b_j, b_j^\dagger$:

  - Since $b_i^\dagger b_j^\dagger | n_1, ...n_i, ..., n_j, ... \rangle = b_j^\dagger b_i^\dagger | n_1, ...n_i, ..., n_j, ... \rangle$ by definition and this holds for all states $|n_1, n_2, ...\rangle$, we have $\left[b_j^\dagger, b_i^\dagger\right] = 0$. By hermitian conjugation also $[b_j, b_i] = 0$. Similar for $i < j$: $\left[b_i, b_j^\dagger\right] = 0$.
  - Careful with $b_i, b_i^\dagger$: We see this from application to vacuum state $b_i b_i^\dagger |0\rangle = |0\rangle$ but $b_i^\dagger b_i |0\rangle = 0$. This is consistent with $\left[b_i, b_i^\dagger\right] = 1$. Ex. 1.1 shows that this holds as operator identity in general.

- Represent the sym. product state by running over all single-particle states ν_j and insert n_j bosons:

$$\boxed{S_+ | \nu_{j_1} \rangle | \nu_{j_2} \rangle \cdots | \nu_{j_N} \rangle = | n_1, n_2, ... \rangle = \left[\prod_{j=1}^{\infty} \frac{1}{\sqrt{n_j!}}\right] b_{j_1}^\dagger b_{j_2}^\dagger ... b_{j_N}^\dagger |0\rangle = \prod_{j=1}^{\infty} \frac{1}{\sqrt{n_j!}} \left(b_j^\dagger\right)^{n_j} |0\rangle} \tag{14}$$

Fermionic creation and annihilation operators

- Analogous to bosonic case, define $c_j^\dagger : \mathcal{F} \to \mathcal{F}$

$$c_j^\dagger | n_1, ..., n_j, ... \rangle \equiv \begin{cases} (-1)^{s_j} | n_1, ..., 1, ... \rangle & : n_j = 0 \\ 0 & : n_j = 1 \end{cases} \tag{15}$$

  where $s_j = \sum_{i=1}^{j-1} n_i$ depends on the occupation of the single-particle states "below" j.

- Example $c_2^\dagger | 1, 1 \rangle = 0$ and $c_2^\dagger | 0, 0 \rangle = | 0, 1 \rangle$ and $c_2^\dagger | 1, 0 \rangle = - | 1, 1 \rangle$.

- Hermitian adjoint of $c_j^\dagger$ is found as above for bosons:

$$c_j | n_1, ..., n_j, ... \rangle = \begin{cases} 0 & : n_j = 0 \\ (-1)^{s_j} | n_1, ..., 0, ... \rangle & : n_j = 1 \end{cases} \tag{16}$$

- We can generate any basis state of $\mathcal{F}$ by repeated application of the $c_j^\dagger$ to the vacuum state $|0\rangle$ (note the order!):

$$\boxed{S_- | \nu_{j_1} \rangle | \nu_{j_2} \rangle \cdots | \nu_{j_N} \rangle = | n_1, n_2, ... \rangle = c_{j_1}^\dagger c_{j_2}^\dagger ... c_{j_N}^\dagger |0\rangle = \prod_{j=1}^{\infty} \left(c_j^\dagger\right)^{n_j} |0\rangle} \tag{17}$$

- Repeated application of $c_i^\dagger$ and $c_j^\dagger$, for $i = j$ it is clear that $c_i^\dagger c_i^\dagger = 0$. For $i \neq j$: From the definition in Eq. (15), we have $c_i^\dagger c_j^\dagger | n_1, n_2, ... \rangle = -c_j^\dagger c_i^\dagger | n_1, n_2, ... \rangle$. Since this holds for every basis vector $|n_1, n_2, ...\rangle$, we have $0 = c_i^\dagger c_j^\dagger + c_j^\dagger c_i^\dagger = \left\{c_i^\dagger, c_j^\dagger\right\}$, the hermitian adjoint yields $\{c_i, c_j\} = 0$. In Ex. 1.1 one shows that $\left\{c_i, c_j^\dagger\right\} = \delta_{ij} \, \forall i, j$. We have the occupation number operator $\hat{n}_i = c_i^\dagger c_i$.

Intermediate summary

- The creation and annihilation operators on Fock space fulfill basic (anti-)commutation relations. Bosons:
$$[b_i, b_j] = 0 = \left[b_i^\dagger, b_j^\dagger\right], \ \left[b_i, b_j^\dagger\right] = \delta_{ij}, \tag{18}$$
Fermions:
$$\{c_i, c_j\} = 0 = \left\{c_i^\dagger, c_j^\dagger\right\}, \ \left\{c_i, c_j^\dagger\right\} = \delta_{ij}. \tag{19}$$
- Achievement: Complicated "permutation-entanglement" of the symmetrized product state in Eq. (3) is generated by applying N **creation operators** to a single reference state $|0\rangle$.
- Notation: $a_j^\dagger$ and a_j denote either bosonic or fermionic creation and annihilation operators, with respect to ordered basis $\{|\nu_1\rangle, |\nu_2\rangle, ...\}$. Next: Express all operators using $a_j^\dagger$, a_j.

One- and two-body operators via $a, a^\dagger$

- Task: Represent one-body (=single-particle) operators using the $a, a^\dagger$-operators. First consider bosons.
- Recall $T = \sum_{k,k'} |\nu_{k'}\rangle T_{k'k} \langle\nu_k|$ where $T_{k'k} = \langle\nu_{k'}|T|\nu_k\rangle$ and $T_{tot} = \sum_{i=1}^N T_i$.
- Apply T_{tot} to $S_+ |\nu_{j_1}\rangle |\nu_{j_2}\rangle \cdots |\nu_{j_N}\rangle = |n_1, n_2, ...\rangle = \mathcal{N} b_{j_1}^\dagger b_{j_2}^\dagger ... b_{j_N}^\dagger |0\rangle$, it is clear how it acts on the lhs (T_{tot} commutes with S_+)
$$T_{tot} |n_1, n_2, ...\rangle = \sum_{i=1}^N \sum_{k,k'} T_{k'k} \delta_{k,j_i} S_+ |\nu_{j_1}\rangle |\nu_{j_2}\rangle \cdots \underbrace{|\nu_{k'}\rangle}_{pos.\, i} \cdots |\nu_{j_N}\rangle = \mathcal{N} \sum_{i=1}^N \sum_{k,k'} T_{k'k} \delta_{k,j_i} b_{j_1}^\dagger b_{j_2}^\dagger ... \underbrace{b_{k'}^\dagger}_{pos.\, i} ... b_{j_N}^\dagger |0\rangle \tag{20}$$
- Goal: Re-express rhs with the original string $b_{j_1}^\dagger b_{j_2}^\dagger ... b_{j_i} ... b_{j_N}^\dagger$ appearing in $|n_1, n_2, ...\rangle$ and read off modifying operator in front. Denote $j_i \equiv j$ and assume $b_j^\dagger$ appears $p > 0$ times in total (for $p = 0$ the δ_{k,j_i} yields zero). Use $b_j b_j^\dagger = b_j^\dagger b_j + 1 = \hat{n}_j + 1$, then
$$b_{k'}^\dagger \left(b_j^\dagger\right)^{p-1} |0\rangle = b_{k'}^\dagger \frac{\hat{n}_j + 1}{(p-1)+1} \left(b_j^\dagger\right)^{p-1} |0\rangle = b_{k'}^\dagger \frac{b_j b_j^\dagger}{p} \left(b_j^\dagger\right)^{p-1} |0\rangle = \frac{1}{p} b_{k'}^\dagger b_j \left(b_j^\dagger\right)^p |0\rangle \tag{21}$$
The sum $\sum_{i=1}^N$ yields p identical contributions. We find the operator identity: $T_{tot} = \sum_{k,k'} b_{k'}^\dagger T_{k'k} b_k$.
- Generalize to fermions and to two-body operators (note the order!):
$$T_{tot} = \sum_{k,k'} a_{k'}^\dagger T_{k'k} a_k \tag{22}$$
$$V_{tot} = \sum_{k,k',j,j'} a_{k'}^\dagger a_{j'}^\dagger V_{k'j',kj} a_j a_k \tag{23}$$
with $V_{k'j',kj} = \langle\nu_{k'}| \langle\nu_{j'}| V |\nu_k\rangle |\nu_j\rangle$.

Change of single-particle basis

- Consider a different basis, $\{|\tilde{\nu}_1\rangle, |\tilde{\nu}_2\rangle, ...\}$ with operators $\tilde{a}_{\tilde{j}}^\dagger$ and $\tilde{a}_{\tilde{j}}$. From insertion of completeness relation, we find $\left|\tilde{\nu}_{\tilde{j}}\right\rangle = \sum_j |\nu_j\rangle \left\langle\nu_j|\tilde{\nu}_{\tilde{j}}\right\rangle$. Further, by definition $|\nu_j\rangle = a_j^\dagger |0\rangle$ and $\left|\tilde{\nu}_{\tilde{j}}\right\rangle = \tilde{a}_{\tilde{j}}^\dagger |0\rangle$.
- Then we have $\tilde{a}_{\tilde{j}}^\dagger |0\rangle = \sum_j \left\langle\nu_j|\tilde{\nu}_{\tilde{j}}\right\rangle a_j^\dagger |0\rangle$ and this can be extended to N-particle Fock space basis states, leading to the operator identity:
$$\boxed{\tilde{a}_{\tilde{j}}^\dagger = \sum_j \left\langle\tilde{\nu}_{\tilde{j}}|\nu_j\right\rangle^\star a_j^\dagger} \tag{24}$$
Upon taking hermitian adjoint, we find $\tilde{a}_{\tilde{j}} = \sum_j \left\langle\tilde{\nu}_{\tilde{j}}|\nu_j\right\rangle a_j$.

- Simple facts:
  - $\tilde{a}_{\tilde{j}}^{(\dagger)}$ also fulfill (anti-)commutation relations
  - total particle number operator remains unchanged $\hat{N} = \sum_j a_j^\dagger a_j = \sum_{\tilde{j}} \tilde{a}_{\tilde{j}}^\dagger \tilde{a}_{\tilde{j}}$
- Example: Change basis to real-space $\{|\tilde{\nu}_1\rangle, |\tilde{\nu}_2\rangle, ...\} = \{|\mathbf{r}\rangle\}_\mathbf{r}$, the corresponding creation (and annihilation) operators

$$\tilde{a}_\mathbf{r}^\dagger \equiv \Psi^\dagger(\mathbf{r}) = \sum_j \langle \mathbf{r}|\nu_j\rangle^\star a_j^\dagger = \sum_j \psi_j^\star(\mathbf{r}) a_j^\dagger, \qquad \Psi(\mathbf{r}) = \sum_j \psi_j(\mathbf{r}) a_j, \tag{25}$$

  are called **quantum-field operators**. Remarks:
  - $\psi_j(\mathbf{r}) \in \mathbb{C}$ is 1st quantized wavefunction, $\Psi(\mathbf{r})$ is 2nd quantized annihilation operator
  - (anti-)commutator for $a_j, a_j^\dagger \Rightarrow \left[\Psi(\mathbf{r}), \Psi^\dagger(\mathbf{r}')\right] = \delta(\mathbf{r}-\mathbf{r}')$ (bos.) or $\{\Psi(\mathbf{r}), \Psi^\dagger(\mathbf{r}')\} = \delta(\mathbf{r}-\mathbf{r}')$ (ferm.)
  - If initial basis is momentum eigenstates $\{|\mathbf{k}\rangle\}$: $\Psi(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_\mathbf{k} e^{i\mathbf{k}\cdot\mathbf{r}} a_\mathbf{k}$.

Solution of non-interacting many-particle systems

- Consider many-particle system where H is only comprised of one-body operators (="non-interacting"),

$$H = T_{tot} = \sum_{\tilde{k},\tilde{k}'} \tilde{a}_{\tilde{k}'}^\dagger T_{\tilde{k}'\tilde{k}} \tilde{a}_{\tilde{k}} = \sum_l \underbrace{a_l^\dagger a_l}_{\hat{n}_l} \varepsilon_l \tag{26}$$

  where we diagonalized the hermitian matrix $T = U \mathrm{diag}(\varepsilon_1, \varepsilon_2, ...) U^\dagger$ where the $\varepsilon_l \in \mathbb{R}$ are the real eigenvalues on the diagonal.
- All symmetrized product states $|n_1, n_2, ...\rangle$ are eigenstates of H,

$$H\,|n_1, n_2, ...\rangle = \left(\sum_l n_l \varepsilon_l\right) |n_1, n_2, ...\rangle \equiv E_{n_1,n_2,...}\,|n_1, n_2, ...\rangle \tag{27}$$

  and the $E_{n_1,n_2,...}$ are the eigenenergies of the many-body problem. For an N-particle system, we select those with $n_1 + n_2 + ... = N$.
- Remark: In a similar way, we can solve non-interacting systems in which the total particle number $\hat{N}$ is not conserved, $H = \sum_{k,k'} \tilde{a}_{\tilde{k}'}^\dagger T_{\tilde{k}'\tilde{k}} \tilde{a}_{\tilde{k}} + (\tilde{a}_{\tilde{k}'} X_{\tilde{k}'\tilde{k}} \tilde{a}_{\tilde{k}} + h.c.) \rightarrow$ Bogoliubov transform to $H = \sum_l a_l^\dagger a_l \varepsilon_l$, see Ex. 1.2.

Specific operators in second quantization

- Kinetic energy T: In first quantization $\langle \mathbf{r}|T|\mathbf{r}'\rangle = -\frac{\hbar^2}{2m}\delta(\mathbf{r}-\mathbf{r}')\nabla_\mathbf{r}^2$ or $\langle \mathbf{k}|T|\mathbf{k}'\rangle = \frac{\hbar^2 k^2}{2m}\delta_{\mathbf{k},\mathbf{k}'}$. In 2nd quantization, in these two bases, we have from Eq. (22):

$$T_{tot} = \sum_\mathbf{k} \frac{\hbar^2 k^2}{2m} a_\mathbf{k}^\dagger a_\mathbf{k} = -\frac{\hbar^2}{2m} \int_\mathbf{r} \Psi^\dagger(\mathbf{r}) \left(\nabla_\mathbf{r}^2 \Psi(\mathbf{r})\right) \tag{28}$$

- Spin of electron $\mathbf{S}$: Use basis $\{|\nu_j, \sigma\rangle\}_{j,\sigma=\uparrow,\downarrow}$. In 1st quantization, the spin operator is $\mathbf{S} = (S^x, S^y, S^z) = \frac{\hbar}{2}\boldsymbol{\tau}$, with $\boldsymbol{\tau} = (\tau_x, \tau_y, \tau_y) = (\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix})$ the vector of Pauli matrices. It acts as an identity in the non-spin part of the Hilbert-space. In second quantization:

$$S_{tot}^x = \sum_{j,\sigma,j',\tau'} \langle \nu_j, \sigma|S_x|\nu_{j'}, \sigma'\rangle\, c_{j,\sigma}^\dagger c_{j',\sigma'} = \frac{\hbar}{2} \sum_{j,\sigma,\sigma'} \langle \sigma|\tau_x|\sigma'\rangle\, c_{j,\sigma}^\dagger c_{j,\sigma'} = \frac{\hbar}{2} \sum_j \left(c_{j,\uparrow}^\dagger c_{j,\downarrow} + c_{j,\downarrow}^\dagger c_{j,\uparrow}\right). \tag{29}$$

- Particle density $\rho(\mathbf{r})$: In 1st quantization $\langle \mathbf{r}'|\rho(\mathbf{r})|\mathbf{r}''\rangle = \delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{r}'-\mathbf{r}'')$, then

$$\rho_{tot}(\mathbf{r}) = \int_{\mathbf{r}'} \int_{\mathbf{r}''} \Psi^\dagger(\mathbf{r}')\delta(\mathbf{r}-\mathbf{r}')\delta(\mathbf{r}'-\mathbf{r}'')\Psi(\mathbf{r}'') = \Psi^\dagger(\mathbf{r})\Psi(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{k},\mathbf{k}'} e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}} a_\mathbf{k}^\dagger a_{\mathbf{k}'} = \frac{1}{V} \sum_\mathbf{q} \left[\sum_\mathbf{k} a_\mathbf{k}^\dagger a_{\mathbf{k}+\mathbf{q}}\right] e^{i\mathbf{q}\cdot\mathbf{r}} \tag{30}$$

  Fourier transform $\rho_{tot}(\mathbf{q}) \equiv \int_\mathbf{r} e^{-i\mathbf{q}\cdot\mathbf{r}} \rho_{tot}(\mathbf{r}) = \sum_\mathbf{k} a_\mathbf{k}^\dagger a_{\mathbf{k}+\mathbf{q}}$.

1.3 Second quantization and statistical mechanics

- Assume all eigenstates of isolated many-body quantum system are known: $H|\psi\rangle = E_\psi|\psi\rangle$
- Couple system to thermal bath (allow energy exchange) → system state given by thermal density matrix (=Gibbs state, canonical ensemble) at temperature $\beta = 1/(k_B T)$:

$$\rho = \frac{e^{-\beta H}}{Z} = \frac{1}{Z}\sum_\psi |\psi\rangle\, e^{-\beta E_\psi}\, \langle\psi| \tag{31}$$

- The normalization factor Z is the **partition function**:

$$Z = \mathrm{Tr} e^{-\beta H} = \sum_\psi \left\langle \psi | e^{-\beta H} | \psi \right\rangle = \sum_\psi e^{-\beta E_\psi} \tag{32}$$

  → link to thermodynamics, free energy $F = -\beta^{-1}\ln Z = U - TS$ is minimized, here $U = \langle H\rangle$ and $S = -k_B \mathrm{Tr}\,[\rho\,\ln\rho]$.

- Thermal average of quantum mechanical operator A:

$$\langle A\rangle = \mathrm{Tr}\,[A\rho] = \frac{1}{Z}\sum_\psi \langle\psi|A|\psi\rangle\, e^{-\beta E_\psi} \tag{33}$$

  Do not confuse this with the quantum expectation value of A in pure many-body state $|\psi\rangle$, denoted by $\langle\psi|A|\psi\rangle$.

- Bath with particle exchange → grand canonical ensemble, replace $H \to H - \mu\hat{N}$ with μ chemical potential and $\hat{N}$ particle number *operator* in system.

- Example: Distribution function = thermal average of occupation number operator $\hat{n}_\nu$ in single-particle eigenstate $|\nu\rangle$ at energy ε_ν in non-interacting system $H = \sum_\nu \varepsilon_\nu a_\nu^\dagger a_\nu - \mu\hat{N}$
  - Fermions:

$$\left\langle c_\nu^\dagger c_\nu \right\rangle = \frac{\sum_{n_\nu=0,1} n_\nu e^{-n_\nu\beta(\varepsilon_\nu-\mu)}}{\sum_{n_\nu=0,1} e^{-n_\nu\beta(\varepsilon_\nu-\mu)}} = \frac{0 + e^{-\beta\xi_\nu}}{1+e^{-\beta\xi_\nu}} = \frac{1}{e^{\beta\xi_\nu}+1} \equiv n_F(\xi_\nu) \tag{34}$$

    where $\xi_\nu \equiv \varepsilon_\nu - \mu$ is the energy measured relative to chemical potential.
  - Bosons: A similar calculation (→ Ex. 1.3) yields

$$\left\langle b_\nu^\dagger b_\nu \right\rangle = \frac{1}{e^{\beta\xi_\nu}-1} \equiv n_B(\xi_\nu) \tag{35}$$

  - At small occupation numbers (when $\beta\xi_\nu \gg 1$) the ± 1 can be neglected against $e^{\beta\xi_\nu}$. Then for both fermions and bosons $n(\xi_\nu) \simeq e^{-\beta\xi_\nu}$ (classical Maxwell-Boltzmann result).

1.4 Application: Non-interacting quantum particles

- Consider identical particles of mass m in $d = 3$ dimensions at temperature T. Classical viewpoint: Thermal momentum per particle from $T_{kin} = \frac{1}{2m}p^2 = 3k_BT$ where $p = \sqrt{\langle p^2\rangle}$ is the classical root-mean-square momentum.
- At which T can we expect quantum effects (see differences between bosons/fermions)? Thermal de-Broglie wavelength

$$\lambda_T = h/p = h/\sqrt{3mk_BT} \tag{36}$$

  → Quantum effects to matter when particle-particle distance $r = \rho^{-1/3} \lesssim \lambda_T$ where ρ is the particle density.
- Next: Full quantum treatment, approximate particles as non-interacting.

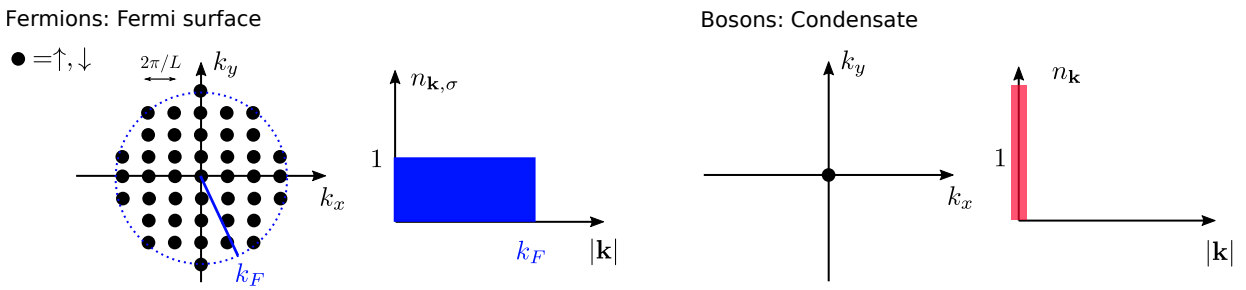

Figure 2: Non-interacting ground state of non-interacting (spinful) fermions and bosons confined in a box of linear size L with periodic boundary conditions. A cut through momentum space in the $k_z = 0$ plane is shown.

Non-interacting fermions (Fermi surface)

- Examples: Conduction electron gas in metals, ^{3}He, neutron star
- Hamiltonian $H = \sum_{\mathbf{k},\sigma}(\varepsilon_{\mathbf{k}} - \mu)c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}$ with isotropic $\varepsilon_{\mathbf{k}} = \hbar^2k^2/(2m)$ in free space where $|\mathbf{k},\sigma\rangle$ is plane-wave eigenstate in box of linear size L, $k_{x,y,z} = 2\pi n_{x,y,z}/L$.
- Alternative: Lattice potentials, lattice constant a. Then $\varepsilon_{\mathbf{k}}$ is a band structure, could still be approximately parabolic $m \to m^\star$ or more strongly deformed, e.g. from tight-binding model on cubic lattice $\varepsilon_{\mathbf{k}} = -2t\sum_\alpha \cos k_\alpha a$, then we have Brillouin zone $k_\alpha \in [-\frac{\pi}{a}, \frac{\pi}{a})$.
- Occupation of single-particle eigenstate $|\mathbf{k},\sigma\rangle$ from Eq. (34): $n_{\mathbf{k},\sigma} = \frac{1}{e^{\beta(\varepsilon_{\mathbf{k}}-\mu)}+1} \overset{T=0}{\to} \Theta(\mu - \varepsilon_{\mathbf{k}})$. At $T = 0$ this is a step-function, all states with energies below μ (also called Fermi-energy ε_F) are occupied. The largest occupied wavevector $k = |\mathbf{k}|$ is the Fermi wavevector k_F with $\varepsilon_F = \hbar^2k_F^2/(2m)$ (k_F generalizes to Fermi *surface* for anisotropic case).
- Ground state = Fermi sea (FS): All single-particle levels with $k < k_F$ occupied, $|FS\rangle = \prod_{k<k_F,\sigma} c^\dagger_{\mathbf{k},\sigma}|0\rangle$, see Fig. 2.
- Excitations with spin σ and momentum $\mathbf{k}$: Adding electrons above Fermi surface or create hole below Fermi surface by removing electron of opposite spin and momentum

$$f^\dagger_{\mathbf{k}\sigma} = \begin{cases} c^\dagger_{\mathbf{k}\sigma} & : k > k_F \\ c_{-\mathbf{k}\bar{\sigma}} & : k < k_F \end{cases} \tag{37}$$

  For $k < k_F$, use $c^\dagger_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma} = 1 - f^\dagger_{-\mathbf{k}\bar{\sigma}}f_{-\mathbf{k}\bar{\sigma}}$, then

$$H = \sum_{\mathbf{k},\sigma} \underbrace{|\varepsilon_{\mathbf{k}} - \mu|}_{\geq 0\,(\text{exc.})} f^\dagger_{\mathbf{k}\sigma}f_{\mathbf{k}\sigma} + E_{FS} \tag{38}$$

  where $E_{FS} = 2V\int_{k<k_F}(\varepsilon_{\mathbf{k}} - \mu) = -\frac{2}{5}N\varepsilon_F$ is the ground-state energy (factor 2 for spin) and the Fermi sea $|FS\rangle$ is the vacuum of f-excitations ($f_{\mathbf{k}\sigma}|FS\rangle = 0$).
- Ground-state density:

$$\rho = \left\langle \hat{N} \right\rangle / V = \frac{2}{V}\sum_{k<k_F} = \frac{2}{(2\pi)^3}\int_0^{k=k_F} \mathrm{d}\mathbf{k} = \frac{2}{(2\pi)^3} \times \frac{4}{3}\pi k_F^3 = \frac{1}{3\pi^2}\left(\frac{2m\varepsilon_F}{\hbar^2}\right)^{3/2} \tag{39}$$

  Example: Gas of conduction electrons in Cu: $\rho \sim 10^{29}m^{-3}$, $\varepsilon_F \sim 7eV \sim k_B \times 80000K$. $\to$ Electrons in metals are strongly "quantum" even at room temperature and their behavior is dominated by fermionic statistics.

- Finite T: Free energy

$$F = -k_B T \ln Z = -k_B T \sum_{\mathbf{k},\sigma} \ln\left[1 + e^{-\beta(\varepsilon_{\mathbf{k}}-\mu)}\right] = -2k_B T V \int_{\mathbf{k}} \ln\left[1 + e^{-\beta(\varepsilon_{\mathbf{k}}-\mu)}\right] \tag{40}$$

where $\frac{1}{V}\sum_{\mathbf{k}} \to \int_{\mathbf{k}} = \frac{1}{(2\pi)^d}\int \mathrm{d}\mathbf{k}$ and the factor 2 is for spin. From this, obtain pressure and particle number

$$P = -\partial F/\partial V = -F/V = f = 2k_B T \int_{\mathbf{k}} \ln\left[1 + e^{-\beta(\varepsilon_{\mathbf{k}}-\mu)}\right]$$
$$N = -\partial F/\partial \mu = 2\int_{\mathbf{k}} n_F(\varepsilon_{\mathbf{k}} - \mu)$$

which means that for given N the value of μ is to be adapted ($\to$ Sommerfeld expansion).

- Combine to get equation of state $PV = ...$:
  - at high T: $n_F(\varepsilon_{\mathbf{k}} - \mu) \simeq e^{-\beta(\varepsilon_{\mathbf{k}}-\mu)} \simeq \ln\left[1 + e^{-\beta(\varepsilon_{\mathbf{k}}-\mu)}\right]$ and we find the ideal gas law: $PV = Nk_B T$
  - at low T: $P \simeq 2k_B T \int_{|\mathbf{k}|<k_F} [-\beta(\varepsilon_{\mathbf{k}} - \mu)] = 2N\varepsilon_F/(5V)$ which means $PV = 2N\varepsilon_F/5$ is independent of T.

Non-interacting bosons (Bose-Einstein condensation [BEC])

- Assume spinless bosons (e.g. ^{4}He or potassium atoms), otherwise same Hamiltonian as for fermionic gas in a box above. Note: $\mu \leq \min\{\varepsilon_{\mathbf{k}}\}$ for convergent density integral,

$$\rho = \left\langle \hat{N} \right\rangle / V = \frac{1}{V}\sum_{\mathbf{k}} n_B(\varepsilon_{\mathbf{k}} - \mu) = \int_{\mathbf{k}} \frac{1}{e^{\beta(\varepsilon_{\mathbf{k}}-\mu)} - 1} \tag{41}$$

- Define $x = \beta\varepsilon_{\mathbf{k}} = \beta\hbar^2 k^2/(2m)$ and $\bar{\lambda}_T = \sqrt{2\pi\hbar^2/(mk_B T)}$ the thermal de-Broglie wavelength [the bar is for changed prefactor as compared with Eq. (36)]. Then

$$\rho = \frac{1}{\bar{\lambda}_T^3}\int_0^\infty \mathrm{d}x\, \frac{2\sqrt{x/\pi}}{e^{x-\beta\mu} - 1} \tag{42}$$

which implicitly determines $\mu\beta$ as $\rho = N/V$ is fixed. As T is decreased, μ increases towards zero.

- At $\mu = 0$, the integral is $\zeta(3/2) = 2.61$ and we obtain with $a = \rho^{-1/3}$ the particle spacing $(\bar{\lambda}_T/a)^3 = 2.61$ which corresponds to temperature $k_B T_0 = 3.31\frac{\hbar^2}{ma^2}$.

- What happens at $T < T_0$? In Eq. (41), need to split off the $k = 0$ singe-particle level before taking thermodynamic limit $V \to \infty$:

$$N = N_0 + \sum_{\mathbf{k}\neq 0} n_B(\varepsilon_{\mathbf{k}} - \mu) \longrightarrow \rho = N/V = \rho_0(T) + \frac{1}{\bar{\lambda}_T^3}\int_0^\infty \mathrm{d}x\, \frac{2\sqrt{x/\pi}}{e^x - 1} \tag{43}$$

As the temperature lowers, the second term decreases as $\sim T^{3/2}$ but N/V must stay fixed.

- This is compensated by an increase of the particle density in the condensate which is $\rho_0 = \rho\left[1 - (T/T_0)^{3/2}\right]$ $\to N_0 \sim N$, a macroscopic number of particles sit in a single lowest energy level! This can be seen as a condensation (droplet formation) in momentum space.

- Experiment: BEC of cold bosonic atoms (Rb) in magnetic trap, first seen in 1995 by Eric Cornell, Carl Wiemann and Wolfgang Ketterle groups. $\to$ Nobel prize 2001.

Exercises

Exercise 1.1. Creation and annihilation operators

(a) Using equations (11) and (13) for the bosonic Fock space operators show that $\left[b_i, b_j^\dagger\right] = \delta_{ij}$ holds for all i, j as an operator identity.

(b) For fermions, from the equations (15) and (16) show analogously $\left\{c_i, c_j^\dagger\right\} = \delta_{ij}$.

(c) The harmonic oscillator in d=1, see Eq. (1) case 2, was treated algebraically in your elementary quantum mechanics course. Recall that this Hamiltonian can be written as $H = \hbar\omega(\bar{a}^\dagger\bar{a} + 1/2)$. Discuss similarities and differences between the operators $\bar{a}, \bar{a}^\dagger$ and the operators $a, a^\dagger$ discussed in this lecture.

Exercise 1.2. Transverse field Ising model (TFIM) in 1D

Here we are interested in finding the exact eigenenergies of the 1D TFIM, $H = -\sum_i \sigma_i^z\sigma_{i+1}^z - \Gamma\sum_i \sigma_i^x$ where σ_i^x, σ_i^z are Pauli matrices acting in the spin-1/2 Hilbert space at site $i = 1, 2, .., L$ and we assume periodic boundary conditions, i.e. $\sigma_{L+1}^z \equiv \sigma_1^z$. We will find the excitation spectrum, in particular the gap Δ between the ground- and lowest excited state. This is done as a function of the transverse field Γ and we determine the critical value Γ_c at which a quantum phase transition between a paramagnetic ground state (for large Γ approximated by a product state of spins pointing in x-direction, $|\rightarrow, \rightarrow, \rightarrow, ...\rangle$) and the two degenerate ground states (for $\Gamma = 0$ exactly given by $|\uparrow, \uparrow, ...\rangle$ and $|\downarrow, \downarrow, ...\rangle$) occurs.

1. Consider the Jordan-Wigner transformation in 1D that maps spin-1/2 to fermionic operators $c_i, c_i^\dagger$:

$$\begin{aligned} \sigma_i^x &= \left(1 - 2c_i^\dagger c_i\right) \\ \sigma_i^z &= -\left[\prod_{j<i}\left(1 - 2c_j^\dagger c_j\right)\right]\left(c_i + c_i^\dagger\right) \end{aligned}$$

   Confirm that σ_i^x and σ_i^z indeed fulfills the spin algebra by computing $\sigma_i^\alpha\sigma_i^\alpha = 1$, $\sigma_i^\alpha\sigma_{i'}^\alpha = \sigma_{i'}^\alpha\sigma_i^\alpha$ for $i \neq i'$ and $\alpha \in \{x, z\}$ and $\sigma_i^x\sigma_i^z = -\sigma_i^z\sigma_i^x$ as well as $\sigma_i^x\sigma_{i'}^z = \sigma_{i'}^z\sigma_i^x$ and for $i \neq i'$.

2. Insert the Jordan-Wigner transformation in the 1D TFIM Hamiltonian and use a Fourier-transformation $c_k = \frac{1}{\sqrt{L}}\sum_j c_j e^{-ikj}$ to obtain

$$H = \sum_k \left(2\left[\Gamma - \cos k\right] c_k^\dagger c_k + i\sin k\left[c_{-k}^\dagger c_k^\dagger + c_{-k}c_k\right] - \Gamma\right) \tag{44}$$

3. Solve this c-particle number *non-conserving* Hamiltonian using a Bogoliubov transformation, $c_k = u_k\gamma_k + iv_k\gamma_{-k}^\dagger$ where $\gamma_k^{(\dagger)}$ again fulfill fermionic anti-commutation relations if u_k, v_k are real numbers satisfying $u_k^2 + v_k^2 = 1$, $u_{-k} = u_k$ and $v_{-k} = -v_k$. They can be parameterized by an angle, $u_k = \cos(\theta_k/2)$ and $v_k = \sin(\theta_k/2)$. Find (k-dependent!) θ_k such that

$$H = \sum_k \varepsilon_k\gamma_k^\dagger\gamma_k + const. \tag{45}$$

   and show that the single-particle energy is $\varepsilon_k = 2\sqrt{1 - 2\Gamma\cos k + \Gamma^2}$. What is the critical value of Γ at which ε_k becomes gapless (at which k, Γ do we find $\varepsilon_k = 0$?).

Exercise 1.3. Non-interacting bosons in equilibrium

Consider non-interacting bosons with Hamiltonian $H = \sum_\nu \varepsilon_\nu b_\nu^\dagger b_\nu - \mu\hat{N}$ in equilibrium at temperature T and chemical potential μ.

1. Derive the equilibrium bosonic occupation number formula (35). Use the explicit formula for the thermal expectation value, Eq. (33), and evaluate the geometrical sum. What condition must be fulfilled for μ?

2. We are now interested in the total particle number, $N = n_B(\xi_1) + n_B(\xi_2) + ...$ As an alternative to just summing Eq. (35) found in 1., consider the following:
For a *general* many-body Hamiltonian $H = H_0 - \mu\hat{N}$ with possibly fermionic or interacting H_0 but known partition function Z (Eq. 32) show that the *total* particle number can be calculated as $N \equiv \left\langle \hat{N} \right\rangle = -\partial F/\partial\mu$ where $F = -\beta^{-1} \ln Z$ is the free energy. Specialize to the non-interacting bosonic case, find a closed expression for F and, by taking a μ-derivative, confirm $N = n_B(\xi_1) + n_B(\xi_2) + ...$

Exercise 1.4. Effective low energy Hamiltonians: From Anderson's impurity model to the Kondo model

It is often useful to simplify Hamiltonians to effective models which are only valid below a certain energy scale. Here we explore such a procedure for the example of the Anderson impurity model which describes a localized electronic level of an impurity atom (at energy ε_d, operators $d_\sigma^{(\dagger)}$, $\sigma \in \{\uparrow, \downarrow\}$) embedded in a host metal described by a Fermi gas of non-interacting conduction ($c_{\mathbf{k}\sigma}$) with an extended Fermi surface.

$$H = H_0 + \sum_\sigma \varepsilon_d d_\sigma^\dagger d_\sigma + U n_{d,\uparrow} n_{d,\downarrow} + \sum_{\mathbf{k},\sigma} V_{\mathbf{k}} d_\sigma^\dagger c_{\mathbf{k}\sigma} + h.c., \qquad H_0 = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}. \tag{46}$$

Here, $n_{d,\sigma} = d_\sigma^\dagger d_\sigma$ and the spin-preserving hopping of electrons on (or off) the impurity level is described by the matrix element $V_{\mathbf{k}}$ ($V_{\mathbf{k}}^\star$). The chemical potential has been set to zero. The difficulty in this Hamiltonian sits in the interaction term $\sim U > 0$ that models the effective Coulomb repulsion felt by two electrons (of opposite spin) simultaneously occupying the impurity site.

1. Consider the atomic limit $V_{\mathbf{k}} \to 0$ for which the impurity atom decouples from the metal. What are the eigenstates of the latter? What are the conditions on ε_d and U so that in the ground state the impurity level is occupied by a single electron? Assume that these conditions hold in the following. What is the energetic distance ("gap") ΔE to the lowest excited impurity state?

2. Denote the ground state energy of H_0 by E_0 (Fermi sea energy). We now want to switch back on a small $V_{\mathbf{k}}$ (with $|V_{\mathbf{k}}|$ smaller than all other energy scales) and derive a low energy effective Hamiltonian valid for excitations at energies E close to the ground state energy of the decoupled system, $E \simeq E_0 + \varepsilon_d$. Start with the (many-body) Schrödinger equation $H|\psi\rangle = E|\psi\rangle$, multiply with projection operators $P_n (= P_n^\dagger = P_n^2)$ which project to the Hilbert space with impurity occupation number $n_d = 0, 1, 2$:

$$P_0 = (1 - n_{d,\uparrow})(1 - n_{d,\downarrow}), \quad P_1 = (1 - n_{d,\uparrow}) n_{d,\downarrow} + (1 - n_{d,\downarrow}) n_{d,\uparrow}, \quad P_2 = n_{d,\uparrow} n_{d,\downarrow}, \tag{47}$$

and define $|\psi\rangle_n \equiv P_n |\psi\rangle$ and $H_{nn'} \equiv P_n H P_{n'} = H_{n'n}^\dagger$. Show that the Schrödinger equation can then be decomposed in block form as

$$\begin{pmatrix} H_{00} & H_{01} & 0 \\ H_{10} & H_{11} & H_{12} \\ 0 & H_{21} & H_{22} \end{pmatrix} \begin{pmatrix} |\psi\rangle_0 \\ |\psi\rangle_1 \\ |\psi\rangle_2 \end{pmatrix} = E \begin{pmatrix} |\psi\rangle_0 \\ |\psi\rangle_1 \\ |\psi\rangle_2 \end{pmatrix} \tag{48}$$

What are H_{00}, H_{11}, H_{22}, H_{10}, H_{21} in the language of 2nd quantization? Show that upon elimination of $|\psi\rangle_0$ and $|\psi\rangle_2$ one has:

$$E|\psi\rangle_1 = \left[H_{11} + H_{12} (E - H_{22})^{-1} H_{21} + H_{10} (E - H_{00})^{-1} H_{01} \right] |\psi\rangle_1 . \tag{49}$$

3. If the term [...] on the rhs of Eq. (49) would not depend on E, we could interpret it as the effective Hamiltonian H_{eff} for the physics of the low-E subspace in which the impurity level is singly occupied. Show that

$$\begin{aligned} H_{12} (E - H_{22})^{-1} H_{21} &= \sum_{\mathbf{k},\sigma} \sum_{\mathbf{k}',\sigma'} V_{\mathbf{k}'}^\star c_{\mathbf{k}'\sigma'}^\dagger n_{d\bar{\sigma}'} d_{\sigma'} (E - H_0 - 2\varepsilon_d - U)^{-1} V_{\mathbf{k}} d_\sigma^\dagger n_{d\bar{\sigma}} c_{\mathbf{k}\sigma} \\ &\simeq \sum_{\mathbf{k},\sigma} \sum_{\mathbf{k}',\sigma'} \frac{-V_{\mathbf{k}'}^\star V_{\mathbf{k}}}{U + \varepsilon_d - \varepsilon_{\mathbf{k}'}} c_{\mathbf{k}'\sigma'}^\dagger c_{\mathbf{k}\sigma} n_{d\bar{\sigma}'} c_{d\sigma'} c_{d\sigma}^\dagger n_{d\bar{\sigma}} \end{aligned}$$

and approximate $V_{\mathbf{k}} = V$ as $\mathbf{k}$-independent for momenta $\mathbf{k}$ close to the Fermi surface, for which $U + \varepsilon_d - \varepsilon_{\mathbf{k}'} \simeq U + \varepsilon_d$. Use d-electron spin operators $S^+ = d^\dagger_\uparrow d_\downarrow$, $S^- = d^\dagger_\downarrow d_\uparrow$ and $S^z = \frac{1}{2}\left(d^\dagger_\uparrow d_\uparrow - d^\dagger_\downarrow d_\downarrow\right)$ (c.f. Eq. (29) with $\hbar = 1$) to show that

$$H_{12}\left(E - H_{22}\right)^{-1} H_{21} \simeq \frac{|V|^2}{U + \varepsilon_d} \sum_{\mathbf{k},\mathbf{k}'} \left(S^+ c^\dagger_{\mathbf{k}',\downarrow} c_{\mathbf{k}\uparrow} + S^- c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}',\downarrow} + S^z \left[c^\dagger_{\mathbf{k}'\uparrow} c_{\mathbf{k}\uparrow} - c^\dagger_{\mathbf{k}'\downarrow} c_{\mathbf{k}\downarrow} \right] \right) + \text{pot. scat.} \quad (50)$$

where the rightmost term describes (spin-independent) potential scattering $\sum_{\mathbf{k},\mathbf{k}',\sigma} K_{\mathbf{k},\mathbf{k}'} c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k}',\sigma}$. The $K_{\mathbf{k},\mathbf{k}'}$ does not need to be determined as it could be removed by a redefinition of $c_{\mathbf{k},\sigma}$.

4. Argue that the term $H_{10}\left(E - H_{00}\right)^{-1} H_{01}$ in (49) yields a similar contribution as in 3. where only the prefactor is changed to $|V|^2/(-\varepsilon_d)$, no detailed calculation is necessary. Show that the effective Hamiltonian takes the form (up to pot. scattering)

$$H_{\text{eff}} \simeq H_0 + \varepsilon_d + \sum_{\mathbf{k},\mathbf{k}'} \frac{J}{\mathcal{V}} \left(S^+ c^\dagger_{\mathbf{k}',\downarrow} c_{\mathbf{k}\uparrow} + S^- c^\dagger_{\mathbf{k}\uparrow} c_{\mathbf{k}',\downarrow} + S^z \left[c^\dagger_{\mathbf{k}'\uparrow} c_{\mathbf{k}\uparrow} - c^\dagger_{\mathbf{k}'\downarrow} c_{\mathbf{k}\downarrow} \right] \right) = H_0 + \varepsilon_d + 2J \mathbf{S} \cdot \mathbf{S}_c(\mathbf{r} = 0) \quad (51)$$

with $J = \mathcal{V}|V|^2 \frac{U}{(U+\varepsilon_d)(-\varepsilon_d)} > 0$ known as the Kondo model and $\mathcal{V}$ the volume. Discuss in words the physical content of this model.

Exercise 1.5. Coulomb interactions in first-order perturbation theory

Consider electrons in a metal at $T = 0$ in their Fermi sea ground-state $|FS\rangle = \prod_{k \le k_F, \sigma} c^\dagger_{\mathbf{k},\sigma} |0\rangle$. The Coulomb interaction can be written as

$$V'_{el-el} = \frac{1}{2V} {\sum_{\mathbf{k}_{1,2},\mathbf{q}}}' \sum_{\sigma_{1,2}} \frac{4\pi e_0^2}{q^2} c^\dagger_{\mathbf{k}_1+\mathbf{q},\sigma_1} c^\dagger_{\mathbf{k}_2-\mathbf{q},\sigma_2} c_{\mathbf{k}_2,\sigma_2} c_{\mathbf{k}_1,\sigma_1} \quad (52)$$

and the prime at the sum excludes the $q = 0$ term which cancels the positive background charge of the ions. We have seen that the non-interacting (FS) ground state energy per electron depends on density ρ as $E_0/N \sim \varepsilon_F \sim \rho^{2/3}$. What about the typical potential energy? It depends inversely on the mean electron-electron distance $a = \rho^{-1/3}$, thus $E_{pot}/N \sim e_0^2/a \sim \rho^{1/3}$. It follows that $E_{pot}/E_0 \sim \rho^{-1/3}$ and we read off the (possibly counter-intuitive) fact that interactions are negligible at *high* densities where the kinetic energy in E_0 due to Pauli exclusion dominates. Thus at high densities, perturbation theory should be a good starting point to treat interactions. We introduce the Bohr radius $a_0 = \hbar^2/(m e_0^2) = 0.053nm$ as our unit of length and the Rydberg $1\text{Ry} = e_0^2/(2a_0) = 13.6\text{eV}$ as the unit of energy. (In this problem, do not include the chemical potential in E_0.)

1. Define the dimensionless quantity r_s as the radius (in units of a_0) of a sphere containing exactly one electron and express r_s in terms of a_0 and k_F. Confirm that for the ground-state energy per particle, we have $E_0/N \simeq \frac{2.21}{r_S^2}\text{Ry}$.

2. Find the first-order perturbative correction to the ground-state energy, $E_0^{(1)}/N = \left\langle FS | V'_{el-el} | FS \right\rangle / N$. Confirm $E_0^{(1)}/N \simeq -\frac{0.916}{r_s}\text{Ry}$.

3. Plot the final result for the total energy per particle $\left(E_0 + E_0^{(1)}\right)/N$ as a function of r_s. According to 1st order perturbation theory, is the electron gas stable under Coulomb interactions? If yes, what $r_s^\star$ minimizes the energy $E^\star/N$?

2 Mean-field theory

Idea:

- Approximate interacting problems as "non-interacting problem + self-consistency condition" (non-perturbative method!)
- Concept of spontaneous symmetry breaking (for more extensive discussion → course on stat. mech.)

From now on, we will work in units such that $\hbar = 1$ and $k_B = 1$.

2.1 Basic concepts

Setup

- Consider many-body problem with one- and two-body interactions, c.f. Eq. (22) and (23) ($a_j^{(\dagger)}$ are bosonic or fermionic Fock-space operators):

$$H = \sum_i \xi_i a_i^\dagger a_i + \frac{1}{4} \sum_{i,i',j,j'} V_{ij,i'j'} a_i^\dagger a_j^\dagger a_{j'} a_{i'} \tag{53}$$

  Remarks:

  - The factor 1/4 is a convention. For fermions, it ensures that the interaction term $V_{12,34} a_1^\dagger a_2^\dagger a_4 a_3$ only appears one time after the sum is written out. Alternatively, we could replace $\frac{1}{4}\sum_{i,i',j,j'} \to \sum_{i<i',j<j'}$.
  - To treat bosons and fermions alike, introduce $\zeta = \pm 1$ for bosons/fermions. Then $a_i^\dagger a_j^\dagger = \zeta a_j^\dagger a_i^\dagger$ and $a_i a_j = \zeta a_j a_i$. It follows that $V_{ij,i'j'} = \zeta V_{ji,i'j'} = \zeta V_{ij,j'i'} = V_{ji,j'i'}$.

- Goal: Approximate *unknown thermal state* ρ of the system as a thermal state of a *non-interacting* "trial" Hamiltonian $\rho \overset{!}{=} \rho_0 = e^{-\beta H_0}/Z_0$.
  This state is characterized by H_0, which has the non-interacting part of H and a part that should capture the effect of interactions.

$$\boxed{H_0 = \sum_i \xi_i a_i^\dagger a_i + \sum_{i,i'} a_i^\dagger h_{ii'}^{(0)} a_{i'}} \tag{54}$$

- Physical picture:
  - $h_{ii'}^{(0)}$ is a potential generated by the effect of all other particles and their interactions in H → "mean-field theory (MFT)", see Fig. 3(a)
  - the Hamiltonian H_0 is called the mean-field Hamiltonian

- Note:
  - We can in principle always solve H_0, see Sec. 1.2, the eigenstates will be number states $|n_{\tilde{\nu}_1}, n_{\tilde{\nu}_2}, ...\rangle$ which are properly symmetrized product states (Slater determinants / permanents).
  - The used orbitals $|\tilde{\nu}_j\rangle$ will in general differ from the orbitals $|\nu_j\rangle$ that $a_i^{(\dagger)}$ refer to.
  - Rephrase goal of mean-field theory (for $T = 0$): Find a set of orbitals $|\tilde{\nu}_j\rangle$ such that a product state using these orbitals best represents the true ground state of H.

- Question: What is $h_{ij}^{(0)}$? → Via variational principle using minimization of free energy.

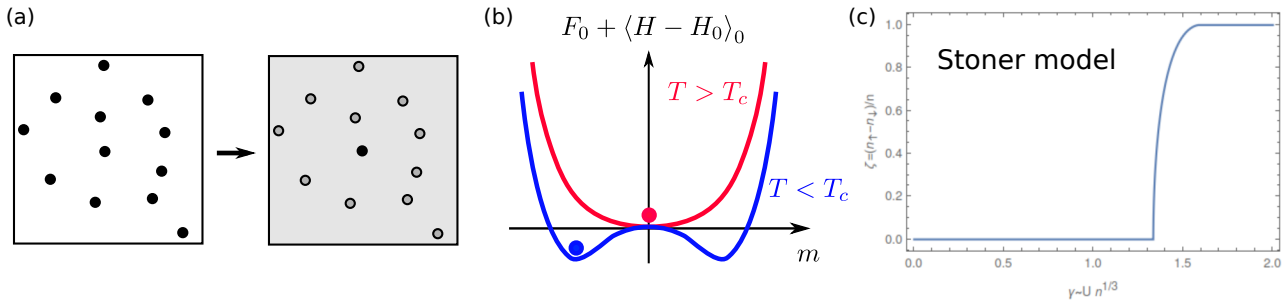

Figure 3: (a) Mean-field idea: Instead of treating the full correlations between individual particles, a single particle (centered) is considered in the averaged field (grey background) exerted by all other particles. (b) MFT free energy landscape for a system undergoing spontaneous symmetry breaking below T_c. (c) Spin density inbalance in the ground state of the Stoner model according to MFT as a function of the paramter γ, see Eq. (70).

Gibbs-Bogoliubov-Feynman inequality

- Consider two general Hamiltonians, we call them H and H_0 (although H_0 could also be interacting). It holds:

$$\boxed{F \leq F_0 + \langle H - H_0 \rangle_0} \tag{55}$$

  where $F_{(0)} = -T \ln Z_{(0)} = -T \ln \mathrm{Tr} e^{-\beta H_{(0)}}$ are the free energies of the systems associated to H, H_0 (both in contact with thermal bath) and $\langle A \rangle_0 \equiv \frac{1}{Z_0} \mathrm{Tr}\left[A e^{-\beta H_0}\right]$ the thermal average with respect to state $\rho_0 = e^{-\beta H_0}/Z_0$.

- Proof: TODO

Variational approach to $h^{(0)}_{ii'}$

- Associate the H_0 in the Eq. (55) with the trial Hamiltonian in Eq. (54).
  Determine $h^{(0)}_{ii'}$ such that the rhs of Eq. (55) is minimized.

- Search for extrema of the rhs of Eq. (55). For all k, l demand:

$$0 \stackrel{!}{=} \frac{\partial}{\partial h^{(0)}_{kl}} \left(F_0 + \langle H - H_0 \rangle_0\right) \tag{56}$$

- Prepare:

$$\frac{\partial F_0}{\partial h^{(0)}_{kl}} = -T \frac{1}{Z_0} \mathrm{Tr}\left[-\beta a^\dagger_k a_l e^{-\beta H_0}\right] = \left\langle a^\dagger_k a_l \right\rangle_0,$$
$$\frac{\partial (Z_0^{-1})}{\partial h^{(0)}_{kl}} = -\frac{\partial Z_0}{\partial h^{(0)}_{kl}} \frac{1}{Z_0^2} = \frac{\beta \left\langle a^\dagger_k a_l \right\rangle_0}{Z_0},$$

  and for any operator A we use the product rule and the above to obtain

$$\frac{\partial \langle A \rangle_0}{\partial h^{(0)}_{kl}} = \frac{\partial}{\partial h^{(0)}_{kl}} \left(\frac{1}{Z_0} \mathrm{Tr}\left[A e^{-\beta H_0}\right]\right) = \beta \left\langle a^\dagger_k a_l \right\rangle_0 \langle A \rangle_0 + \left\langle \frac{\partial A}{\partial h^{(0)}_{kl}} \right\rangle_0 - \beta \left\langle A a^\dagger_k a_l \right\rangle_0 \tag{57}$$

- We insert these preparations in Eq. (56), use $A = H - H_0 = \sum_{i,i'} a^\dagger_i \left(\sum_{j,j'} V_{ij,i'j'} a^\dagger_j a_{j'} - h^{(0)}_{ii'}\right) a_{i'}$:

$$\begin{aligned} 0 &\stackrel{!}{=} \left\langle a^\dagger_k a_l \right\rangle_0 + \beta \left\langle a^\dagger_k a_l \right\rangle_0 \langle H - H_0 \rangle_0 - \left\langle a^\dagger_k a_l \right\rangle_0 + \left\langle -\beta \left(H - H_0\right) a^\dagger_k a_l \right\rangle_0 \\ 0 &\stackrel{!}{=} \left\langle \left(H - H_0\right) a^\dagger_k a_l \right\rangle_0 - \langle H - H_0 \rangle_0 \left\langle a^\dagger_k a_l \right\rangle_0 \end{aligned} \tag{58}$$

- **Wick's theorem (simplified form)**: For *any* non-interacting Hamiltonian H_0 with thermal state $\rho_0 = e^{-\beta H_0}/Z_0$, the following holds for a *normal ordered* ($= a^\dagger$ left of a) string of n creation and n annihilation operators (with respect to a fixed basis):

$$\left\langle a_1^\dagger a_2^\dagger ... a_n^\dagger a_{n'} ... a_{2'} a_{1'} \right\rangle_0 = \sum_{p \in S_n} \zeta^{P(p)} \left\langle a_1^\dagger a_{p(1')} \right\rangle_0 \left\langle a_2^\dagger a_{p(2')} \right\rangle_0 \cdots \left\langle a_n^\dagger a_{p(n')} \right\rangle_0 \tag{59}$$

  with $P(p) \equiv [1 - \mathrm{sgn}(p)]/2$ which is zero for an even permutation p [$\mathrm{sgn}(p) = +1$] and unity for and odd one [$\mathrm{sgn}(p) = -1$] so that $\zeta^{P(p)}$ is unity except for an odd permutation of fermions where it is -1. As an example

$$\left\langle a_1^\dagger a_2^\dagger a_{2'} a_{1'} \right\rangle_0 = \left\langle a_1^\dagger a_{1'} \right\rangle_0 \left\langle a_2^\dagger a_{2'} \right\rangle_0 + \zeta \left\langle a_1^\dagger a_{2'} \right\rangle_0 \left\langle a_2^\dagger a_{1'} \right\rangle_0 \tag{60}$$

  We will prove a more general version later, but in Ex. 2.1 you will show that Eq. (60) holds.

- Continue in Eq. (58), insert $H - H_0$ and normal order the term $\left\langle (H - H_0)\, a_k^\dagger a_l \right\rangle_0$ by using the (anti-) commutation relations ($a_p a_{p'}^\dagger = \delta_{p,p'} + \zeta a_{p'}^\dagger a_p$). Then apply Wick's theorem.

- After straightforward algebra ($\rightarrow$ Ex. 2.2) and remembering that Eq. (58) should hold for all k, l, we find the condition:

$$\boxed{h_{ii'}^{(0)} = \sum_{j,j'} V_{ij,i'j'} \left\langle a_j^\dagger a_{j'} \right\rangle_0 \quad \forall_{i,i'}.} \tag{61}$$

  This is a *self-consistency* condition.

- Eq. (61) is only a necessary condition, if there are multiple solutions for $h_{ii'}^{(0)}$ pick the one that yields the smallest bound on F, i.e. minimizes the rhs of Eq. (55).

Heuristic approach to MFT

- We can argue for the self-consistency Eq. (61) in a simpler but somewhat sloppy way, see discussion below.

- Consider full interacting H and assume state $\rho_0 \sim e^{-\beta H_0}$ with non-interacting $H_0 \rightarrow$ can apply Wick's theorem

$$\langle H \rangle_0 = \sum_i \xi_i \left\langle a_i^\dagger a_i \right\rangle_0 + \frac{1}{4} \sum_{i,i',j,j'} V_{ij,i'j'} \left(\left\langle a_i^\dagger a_{i'} \right\rangle_0 \left\langle a_j^\dagger a_{j'} \right\rangle_0 + \zeta \left\langle a_i^\dagger a_{j'} \right\rangle_0 \left\langle a_j^\dagger a_{i'} \right\rangle_0 \right) \tag{62}$$

- Pick H_0 such that $\langle H \rangle_0 \stackrel{!}{=} \langle H_0 \rangle_0$, this yields

$$\begin{aligned} H_0 &= \sum_i \xi_i a_i^\dagger a_{i0} \\ &+ \frac{1}{4} \sum_{i,i',j,j'} V_{ij,i'j'} \left(a_i^\dagger a_{i'} \left\langle a_j^\dagger a_{j'} \right\rangle_0 + \left\langle a_i^\dagger a_{i'} \right\rangle_0 a_j^\dagger a_{j'} - \left\langle a_i^\dagger a_{i'} \right\rangle_0 \left\langle a_j^\dagger a_{j'} \right\rangle_0 \right) \text{ (”Hartree} - \text{term”)} \\ &+ \frac{\zeta}{4} \sum_{i,i',j,j'} V_{ij,i'j'} \left(a_i^\dagger a_{j'} \left\langle a_j^\dagger a_{i'} \right\rangle_0 + \left\langle a_i^\dagger a_{j'} \right\rangle_0 a_j^\dagger a_{i'} - \left\langle a_i^\dagger a_{j'} \right\rangle_0 \left\langle a_j^\dagger a_{i'} \right\rangle_0 \right) \text{ (”Fock} - \text{term”)} \end{aligned}$$

  We can drop the (constant) last terms in line two and three and compare to the ansatz for H_0 in Eq. (54). If we re-label summed-over indices i, i', j, j' and use symmetries of V we reproduce the self-consistency condition (61).

- Remark: If the i, i' and j, j' refer to different types of particles (e.g. electrons with spin $\uparrow$ and $\downarrow$) the mean-field approximation is also called **Hartree-Fock approximation** with the purple terms the "Hartree-terms" involving densities of equal particles and the brown mixing "Fock-terms".

- Discussion:
  - this shortcut yields the correct self-consistency conditions, but is *not* based on variational principle
  - in the case of multiple solutions for $h_{ii'}^{(0)}$ we would not be able to decide which $h_{ii'}^{(0)}$ to pick
  - see Ex. 2.3 for a simple example case where this is crucial

Example: Electron gas (Hartree-Fock approximation)

- Consider the electron gas ($\zeta = -1$) with Coulomb interactions as in Ex. 1.5 (but keep $q = 0$ term).
- Perform mean-field decoupling. Crucial: We guess/assume spin-rotational symmetry and translation invariance $\left\langle c^\dagger_{\mathbf{k}_1+\mathbf{q},\sigma} c_{\mathbf{k}_1,\sigma'} \right\rangle_0 = \delta_{\sigma,\sigma'}\delta_{\mathbf{q},0} n_{\mathbf{k}_1}$:

$$\begin{aligned} H &= \sum_{\mathbf{k},\sigma} \varepsilon_k c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \frac{1}{2\mathcal{V}} \sum_{\mathbf{k}_{1,2},\mathbf{q}} \sum_{\sigma_{1,2}} V(q) c^\dagger_{\mathbf{k}_1+\mathbf{q},\sigma_1} c^\dagger_{\mathbf{k}_2-\mathbf{q},\sigma_2} c_{\mathbf{k}_2,\sigma_2} c_{\mathbf{k}_1,\sigma_1} \\ &\to \\ H_0 &= \sum_{\mathbf{k},\sigma} \varepsilon_k c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \frac{1}{2\mathcal{V}} \sum_{\mathbf{k}_{1,2}} \sum_{\sigma_{1,2}} \{ \\ &\quad + V(0) \left(n_{\mathbf{k}_1,\sigma_1} \left\langle \hat{n}_{\mathbf{k}_2,\sigma_2} \right\rangle_0 + \left\langle \hat{n}_{\mathbf{k}_1,\sigma_1} \right\rangle_0 n_{\mathbf{k}_2,\sigma_2} - \left\langle \hat{n}_{\mathbf{k}_1,\sigma_1} \right\rangle_0 \left\langle \hat{n}_{\mathbf{k}_2,\sigma_2} \right\rangle_0 \right) \\ &\quad - V(|\mathbf{k}_2 - \mathbf{k}_1|) \Big(\left\langle c^\dagger_{\mathbf{k}_2,\sigma_1} c_{\mathbf{k}_2,\sigma_2} \right\rangle_0 c^\dagger_{\mathbf{k}_1,\sigma_2} c_{\mathbf{k}_1,\sigma_1} + c^\dagger_{\mathbf{k}_2,\sigma_1} c_{\mathbf{k}_2,\sigma_2} \left\langle c^\dagger_{\mathbf{k}_1,\sigma_2} c_{\mathbf{k}_1,\sigma_1} \right\rangle_0 - \left\langle c^\dagger_{\mathbf{k}_2,\sigma_1} c_{\mathbf{k}_2,\sigma_2} \right\rangle_0 \left\langle c^\dagger_{\mathbf{k}_1,\sigma_2} c_{\mathbf{k}_1,\sigma_1} \right\rangle_0 \Big) \} \end{aligned}$$

- This can be written as $H_0 = \sum_{\mathbf{k},\sigma} \varepsilon^{HF}_k c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} - \text{const.}$ with

$$\begin{aligned} h^{(0)}_{ii'} \sim \varepsilon^{HF}_{\mathbf{k}} &= \varepsilon_k + \frac{1}{\mathcal{V}} \sum_{\mathbf{k}'} \sum_{\sigma'} \left(V(0) - \delta_{\sigma,\sigma'} V(|\mathbf{k} - \mathbf{k}'|) \right) n_{\mathbf{k}'} \\ &= \varepsilon_k + V(0) n - \frac{1}{\mathcal{V}} \sum_{\mathbf{k}'} V(|\mathbf{k} - \mathbf{k}'|) n_{\mathbf{k}'} \end{aligned} \tag{63}$$

  The second term is the interaction with average electron density $n = \frac{2}{\mathcal{V}} \sum_{\mathbf{k}'} n_{\mathbf{k}'}$. It is canceled against interaction with opposite ion charge. Need to solve self-consistently:

$$n_{\mathbf{k}} = 1/(e^{\beta \varepsilon^{HF}_{\mathbf{k}}} + 1). \tag{64}$$

2.2 Spontaneous symmetry breaking and MFT

- General MFT for N single-particle orbitals:
  - Self-consistency equation (61) needs to be solved for $N \times N$ matrix $h^{(0)}_{ii'}$ → difficult for large N
  - Idea: Use symmetries to restrict $h^{(0)}_{ii'}$ (c.f. Hartree-Fock for electron gas: Ansatz respects translation invariance and spin-rotation symmetry)
- Spontaneous symmetry breaking:
  The free energy bound $F_0 + \langle H - H_0 \rangle_0$ from rhs of Eq. (55) attains a global minimum for $H_0(h^{(0)})$ that breaks a symmetry.
- Note:
  - The statement that the symmetry-broken trial state $\rho_0(h^{(0)})$ approximates the true state implies ergodicity breaking and $\rho \not\propto e^{-\beta H}$, because $\rho_0(Sh^{(0)})$ with symmetry-transformed $h^{(0)} \to Sh^{(0)}$ should lead to degenerate minimum.
  - Ergodicity breaking only applies for infinite systems when the free energy barrier between state $\rho_0(h^{(0)})$ and $\rho_0(Sh^{(0)})$ is impossible to overcome.
- Example from classical physics: FM Ising model $H = -J \sum_{\langle i,j \rangle} s_i s_j$, $s_i = \pm 1$ on lattice, see Fig. 3(b).
  - H invariant under discrete spin flip symmetry $s_i \to -s_i \forall i$ and lattice translation symmetry
  - Ansatz for mean-field H_0: Maintain translation, break spin flip symmetry (for fixed m):

$$H_0 = -Jzm \sum_j s_j \tag{65}$$

    with $m = \langle s_i \rangle_0$ from self-consistency equation and z the number of nearest neighbors per site (coordination number).

  - At $T = T_c = zJ$: Free energy bound as function of m changes from single-well to double-well form.
  - Global minima move from $m = 0$ to finite $m = \pm m_0$ corresponding to finite magnetization.

- Warning: MFT can be completely wrong! It generally tends to overestimate spontaneous symmetry breaking tendencies (e.g. FM Ising model in 1d with known solution which is always disordered at $T > 0$.)

- Thermal average $\langle O \rangle$ of operator O as **order parameter**: $\langle O \rangle \neq 0$ is signature of symmetry-broken state. Examples:

broken symmetry	order parameter	sym. broken state
translation (discrete or continuous)	$\sum_{\mathbf{k}} \left\langle a^\dagger_{\mathbf{k}} a_{\mathbf{k}+\mathbf{Q}} \right\rangle = \rho(\mathbf{Q})$ for $\mathbf{Q} \neq 0$	density-wave or crystal
spin-rotation	$\langle \mathbf{S}_j \rangle$	(anti-)ferromagnet
$U(1)$ (particle number conservation)	$\langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle$	superconductor

Example: Stoner ferromagnetism from point-like interactions

- Metallic magnetism (e.g. in Fe or Ni) happens if conduction bands are formed by narrower d or f orbitals. This leads to larger and more localized interactions.

- Consider electron gas with point-like interactions $U(r) \sim \delta(r)$:

$$H = \sum_{\mathbf{k},\sigma} \xi_k c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} + \frac{U}{2\mathcal{V}} \sum_{\mathbf{k}_{1,2},\mathbf{q}} \sum_{\sigma_{1,2}} c^\dagger_{\mathbf{k}_1+\mathbf{q},\sigma_1} c^\dagger_{\mathbf{k}_2-\mathbf{q},\sigma_2} c_{\mathbf{k}_2,\sigma_2} c_{\mathbf{k}_1,\sigma_1} \tag{66}$$

- Search for **magnetic** mean-field solution which breaks spin-rotation symmetry $\left\langle c^\dagger_{\mathbf{k}+\mathbf{q},\sigma} c_{\mathbf{k},\sigma'} \right\rangle = \delta_{\sigma,\sigma'} \delta_{\mathbf{q},0} n_{\mathbf{k},\sigma}$.

- Similar steps as above yield the mean-field Hamiltonian:

$$H_0 = \sum_{\mathbf{k},\sigma} \Big(\xi_k + U \underbrace{[n_\uparrow + n_\downarrow - n_\sigma]}_{n_{\bar\sigma}} \Big) c^\dagger_{\mathbf{k},\sigma} c_{\mathbf{k},\sigma} - U \frac{\mathcal{V}}{2} \sum_{\sigma_{1,2}} n_{\sigma_1} n_{\sigma_2} + U \frac{\mathcal{V}}{2} \sum_\sigma n_\sigma^2 \tag{67}$$

  where $n_\uparrow + n_\downarrow$ comes from the Hartree and $-n_\sigma$ from the Fock terms and $n_\sigma = \mathcal{V}^{-1} \sum_{\mathbf{k}} n_{\mathbf{k},\sigma}$ is the density of electrons with spin σ and $\bar\uparrow = \downarrow$, $\bar\downarrow = \uparrow$.

- Interpretation: Repulsive interactions are only between opposite spin densities, U favors fully polarized state which costs more kinetic energy.

- Self-consistency condition:

$$n_\sigma = \mathcal{V}^{-1} \sum_{\mathbf{k}} \langle \hat{n}_{\mathbf{k},\sigma} \rangle_0 = \mathcal{V}^{-1} \sum_{\mathbf{k}} \frac{1}{\exp\left[\beta \left(\xi_k + U n_{\bar\sigma}\right)\right] + 1} \tag{68}$$

- We use $\xi_k = k^2/(2m) - \varepsilon_F$ and work at $T = 0$. The $k_{F,\sigma}$ depends on the effective $\varepsilon_{F\sigma} = \varepsilon_F - U n_{\bar\sigma}$ (c.f. Sec. 1.4) which might differ for the two spins:

$$n_\sigma = \frac{1}{(2\pi)^3} \frac{4\pi}{3} k^3_{F,\sigma} = \frac{1}{6\pi^2} \left(2m \left[\varepsilon_F - U n_{\bar\sigma}\right]\right)^{3/2} \tag{69}$$

  We introduce $n = n_\uparrow + n_\downarrow$, $\zeta = (n_\uparrow - n_\downarrow)/n$ and $\gamma = 2mUn^{1/3}/(3\pi^2)^{2/3}$. We obtain

$$(1+\zeta)^{2/3} - (1-\zeta)^{2/3} = \gamma\zeta. \tag{70}$$

- Eq. (70) has three types of solution depending on interaction and density via $\gamma \sim U n^{1/3} > 0$, see Fig. 3(c):
  - $0 < \gamma < 4/3$: $\zeta = 0 \to n_\uparrow = n_\downarrow$ (no spontaneous magnetization)
  - $4/3 < \gamma < 2^{2/3} \simeq 1.58$: $\zeta \in (0,1) \to n_\uparrow > n_\downarrow > 0$ (partial polarization, weak ferromagnet)
  - $2^{2/3} < \gamma$: $\zeta = 1 \to n_\uparrow = 1,\ n_\downarrow = 0$ (full polarization, strong ferromagnet)

Exercises

Exercise 2.1. Proof of simplified Wick theorem

Show by explicit calculation that Eq. (60), $\left\langle a_1^\dagger a_2^\dagger a_{1'} a_{2'} \right\rangle_0 = \left\langle a_1^\dagger a_{2'} \right\rangle_0 \left\langle a_2^\dagger a_{1'} \right\rangle_0 + \zeta \left\langle a_1^\dagger a_{1'} \right\rangle_0 \left\langle a_2^\dagger a_{2'} \right\rangle_0$ holds. Hint: Careful, this should hold for thermal averages of *any* non-interacting state $\rho_0 \sim e^{-\beta H_0}$ where $H_0 = \sum_{ij} a_i^\dagger h_{ij} a_j$ with h_{ij} not necessarily diagonal. Although this result holds for fermions and bosons, you may limit your efforts to the fermionic case.

Exercise 2.2. Mean-field self-consistency condition

Show the self-consistency equation (61). Start from Eq. (58) and perform the steps outlined in the lecture.

Exercise 2.3. MFT for the AFM Ising model (pitfalls of heuristic approach)

This problem illustrates the necessity to work with the variational formulation of MFT instead of the heuristic approach if one needs to go beyond the self-consistency equations. For simplicity, the model is the anti-ferromagnetic (AFM) Ising model on a square lattice with $N = L^2$ sites $\mathbf{r}_i = (x_i, y_i)$ with $x_i, y_i = 0, 1, ..., L$ and periodic boundary conditions. The Hamiltonian is

$$H = J \sum_{\langle i,j \rangle} s_i^z s_j^z \tag{71}$$

with $J > 0$ and the sum is over nearest-neighbor bonds $\langle i, j \rangle$. As the "operators" $\{s_i^z = \pm 1\}_i$ commute, the model is classical in nature (and amply studied in statistical mechanics). We drop the z-superscript in the following. As temperature is lowered below the Néel temperature T_N, we expect a phase transition between a paramagnetic phase $\langle s_i \rangle = m_i = 0$ and an AFM phase $m_i = m_a$ for i on the a sublattice ($x_i + y_i$ even) and $m_i = m_b = -m_a$ for i on the b sublattice ($x_i + y_i$ odd).

1) For the mean-field Hamiltonian, make the ansatz $H_0 = 4Jm_b \sum_{i \in a} s_i + 4Jm_a \sum_{i \in b} s_i$, insert the associated ρ_0 in the rhs of the Bogoliubov inequality (55), $F_0 + \langle H - H_0 \rangle_0 \equiv \phi(m_a, m_b)$ and find the global minimum of $\phi(m_a, m_b)$ as a function of $m_{a,b} \in [-1, 1]$. You should obtain the self-consistency conditions, confirm $T_N = 4J$ and add a 3d plot of $\phi(m_a, m_b)$ for a complete picture for $T = 5J > T_N$ and $T = 3J < T_N$.

2) In the heuristic approach start from H and replace $s_i \to \langle s_i \rangle + \delta s_i$ where $\delta s_i \equiv s_i - \langle s_i \rangle$. Neglect interacting terms of order $(\delta s)^2$. Then introduce the ansatz for $m_{a,b}$ as above. Show that this leads to

$$H_0' = -2NJm_a m_b + 4Jm_b \sum_{i \in b} s_i + 4Jm_a \sum_{j \in b} s_j. \tag{72}$$

Find the "free energy" $F_0' = -T \ln Z_0'$ with $Z_0' = \sum_{\{s_i\}_i} e^{-\beta H_0'}$ and produce a 3d plot of $F_0'(m_a, m_b)$ as a function of m_a and m_b at $T = 3J < T_N$. For which $m_{a,b}$ does $F_0'(m_a, m_b)$ assume the global minimum? On the landscape of F_0', what is the nature of the points characterizing the AFM state found in 1) above?

3 Time dependence in quantum theory

Idea:

- So far we only treated static problems: H, ρ and observables did not change over time
- Combine time-dependent Schrödinger equation with many-body framework

3.1 Schrödinger picture and evolution operator

- Schrödinger picture: State evolves in time according to **Schrödinger equation**

$$\boxed{i\frac{d}{dt}\left|\psi(t)\right\rangle = H_t\left|\psi(t)\right\rangle} \tag{73}$$

  and operators O_t and Hamiltonian H_t have only explicit time dependence denoted by subscript (e.g. time-dependent external fields in solid state experiment or laser-controlled Hamiltonian in cold-atom experiment).

- Write formal solution of Schrödinger eq. as unitary time-evolution operator $U(t, t_0)$ that mediates evolution of state from time t_0 to t:

$$\left|\psi(t)\right\rangle \quad = \quad U(t, t_0)\left|\psi(t_0)\right\rangle . \tag{74}$$

  For density matrix $\rho(t) = U(t, t_0)\rho(t_0)U(t_0, t)$ (von-Neumann eq.).

- Determine $U(t, t_0)$ from Schrödinger eq.:

$$i\frac{d}{dt}U(t, t_0) = H_t\, U(t, t_0) \tag{75}$$

  and $U(t_0, t_0) = 1$. How to solve for $U(t, t_0)$?

  - For time-independent $H_t = H$ have $U(t, t_0) = \exp\left[-i(t - t_0)H\right]$. Note: The exponential of an operator is defined by series expansion.
  - For general H_t, try:

$$U(t, t_0) \stackrel{?}{=} \exp\left[-i\int_{t_0}^{t} \mathrm{d}\tilde{t}\, H_{\tilde{t}}\right] = \sum_{n=0}^{\infty}\frac{1}{n!}\left[-i\int_{t_0}^{t}\mathrm{d}\tilde{t}_1 H_{\tilde{t}_1}\right]\left[-i\int_{t_0}^{t}\mathrm{d}\tilde{t}_2 H_{\tilde{t}_2}\right]\ldots\left[-i\int_{t_0}^{t}\mathrm{d}\tilde{t}_n H_{\tilde{t}_n}\right] \tag{76}$$

    If we act with $i\frac{d}{dt}$, use $i\frac{d}{dt}\left[-i\int_{t_0}^{t}\mathrm{d}\tilde{t}_1 H_{\tilde{t}_1}\right] = H_t$ but we need to apply product rule also to the other [...]. Problem: Since $[H_t, H_{t'}] \neq 0$ in general, the H_t does not commute with [...] and cannot be moved to the left to satisfy Eq. (75)! → Solution: Apply **time-ordering operator**.

- Definition: Time-ordering operator for general time-dependent operators $A_t, B_{t'}$ (not necessarily Hamiltonians H_t, but later also operators in Heisenberg picture). Put *later times to the left*:

$$T_t\left[A_t B_{t'}\right] = \begin{cases} A_t B_{t'} & : t > t' \\ \zeta B_{t'} A_t & : t' > t \end{cases} \tag{77}$$

  where ζ encodes the statistics, $\zeta = +1$ for bosons, $\zeta = -1$ for fermions. Remarks:

  - $H = c^\dagger c$ with c fermionic is a bosonic operator.
  - T_t generalizes to 3,4,5... operators, with a sign $\zeta^{P(p)}$ (see Eq. (59)) and p the permutation needed to achieve the time ordering

- Use time-ordering to write time evolution operator:

$$\boxed{U(t,t_0) = T_t \exp\left[-i\int_{t_0}^{t} \mathrm{d}\tilde{t}\, H_{\tilde{t}}\right] = \sum_{n=0}^{\infty} \frac{(-i)^n}{n!} \int_{t_0}^{t} \mathrm{d}\tilde{t}_1 ... \int_{t_0}^{t} \mathrm{d}\tilde{t}_n\, T_t \left(H_{\tilde{t}_1} ... H_{\tilde{t}_n}\right)} \tag{78}$$

  Due to time-ordering and since t is the largest time, H_t always appears on the left and Eq. (75) is satisfied.

- Properties of $U(t,t_0)$:
  - unitarity condition $[U(t_1,t_2)]^\dagger = U(t_2,t_1)$
  - group properties: $U(t,t) = 1$ and $U(t_3,t_2)U(t_2,t_1) = U(t_3,t_1)$

- The conjugate evolution (backward in time) is given by $U(t_0,t) = [U(t,t_0)]^\dagger = \tilde{T}_t \exp\left[i\int_{t_0}^{t} \mathrm{d}\tilde{t}\, H_{\tilde{t}}\right]$ with $\tilde{T}_t$ *anti*-time-ordering (puts later times to the right).

3.2 Heisenberg picture

- Time evolution of average of operator O_t:

$$\langle O_t \rangle (t) = \frac{1}{\mathrm{Tr}\rho(t)} \mathrm{Tr}\left[O_t \rho(t)\right] = \frac{1}{\mathrm{Tr}\rho(t)} \mathrm{Tr}\left[O_t U(t,t_0)\rho(t_0)U(t_0,t)\right] \overset{\text{cycl.}}{=} \frac{1}{\mathrm{Tr}\rho(t_0)} \mathrm{Tr}\Big[\underbrace{U(t_0,t)O_t U(t,t_0)}_{\equiv O_t(t)\text{ Heisenberg pic.}} \rho(t_0)\Big] \tag{79}$$

  The right-hand side defines the Heisenberg picture, in which operators carry the time-dependence (t) in addition to their explicit time dependence denoted in superscript.

- Equation of motion for Heisenberg picture operator $O_t(t)$:

$$\frac{d}{dt} O_t(t) = i\left[H_t(t), O_t(t)\right] + \left(\frac{dO_t}{dt}\right)(t) \tag{80}$$

  with $H_t(t) = U(t_0,t)H_t U(t,t_0)$ the time-evolved Hamiltonian and $\partial O_t/\partial t$ capturing explicit time-dependence of O_t (proof in Ex. 3.1).

- For a time-independent Hamiltonian and operator: $O(t) = e^{iH(t-t_0)} O e^{-iH(t-t_0)}$ and $H(t) = H$.

- Example: For a non-interacting and time-independent Hamiltonian $H = \sum_\nu \varepsilon_\nu a_\nu^\dagger a_\nu$, we have for $t_0 = 0$ and for Fock space operators of both fermions and bosons (proof in Ex. 3.1)

$$\boxed{a_\mu(t) = e^{-i\varepsilon_\mu t} a_\mu, \qquad a_\mu^\dagger(t) = e^{+i\varepsilon_\mu t} a_\mu^\dagger} \tag{81}$$

3.3 Interaction picture

- Split the Hamiltonian as $H = H_0 + V_t$ with H_0 time-independent (and usually "simple" in some sense, e.g. non-interacting)

- Evolve operators as in Heisenberg picture, but with respect to H_0 only,

$$O_{I,t}(t) = e^{iH_0(t-t_0)} O_t e^{-iH_0(t-t_0)} \tag{82}$$

  and the state evolves with respect to $|\psi_I(t)\rangle = U_I(t,t_0)\,|\psi(t_0)\rangle$ where

$$U_I(t,t_0) = e^{iH_0(t-t_0)} U(t,t_0) \tag{83}$$

- The $U_I(t,t_0)$ satisfies the Schrödinger eq., $i\partial_t U_I(t,t_0) = V_{I,t}(t) U_I(t,t_0)$ where $V_{I,t}(t) = e^{iH_0(t-t_0)} V_{I,t} e^{-iH_0(t-t_0)}$. This is solved similar to above as $U_I(t,t_0) = T_t \exp\left[-i\int_{t_0}^{t} \mathrm{d}\tilde{t} V_{I,\tilde{t}}(\tilde{t})\right]$.

Exercises

Exercise 3.1. Operators in Heisenberg picture

Derive the general equation of motion for operators in the Heisenberg picture in Eq. (80) and also show Eq. (81).

4 Green functions (real time)

Idea:

- Description of many-body quantum system: Wavefunction $\psi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N; t)$?
- Problem: No analytical solution known, $N \sim 10^{23}$ is very demanding for numerics, too much information (cannot measure all N particle positions)
- Alternative: GF are averages of two or more operators taken at different times, e.g. $\left\langle \Psi_{\mathbf{r}}(t)\Psi^\dagger_{\mathbf{r}'}(t')\right\rangle$ ($\rightarrow$ Heisenberg picture)
- GFs are efficient because closely related to measurement ($\rightarrow$ Sec. 6) and intuition (follow propagation in *full many-body background*), c.f. Fig. 4.
- Like the wavefunction (or density matrix), the full set of GFs characterizes many-body system

4.1 Zoo of real-time Green functions

- We define a variety of different GFs and study their mutual relations.
  This may first seem annoying, but we will see later that some of them are measurable objects while others are easier to compute.
- Operators A, B:
  - in Heisenberg picture $\rightarrow A(t), B(t')$
  - do not need to be hermitian, e.g. $A(t) = a^\dagger_\mu(t)$ or $\Psi_{\mathbf{r}}(t)$
  - $\zeta = \pm 1$ for bosonic or fermionic operators, also define $[A, B]_\zeta \equiv AB - \zeta BA$
- Zoo of GFs:
  - Greater and lesser GFs (do not care about order of times):

$$G^>_{AB}(t,t') = -i\left\langle A(t)B(t')\right\rangle$$
$$G^<_{AB}(t,t') = -i\zeta\left\langle B(t')A(t)\right\rangle$$

    For $A = \Psi_{\mathbf{r}}$, $B = \Psi^\dagger_{\mathbf{r}'}$, we have $G^>_{AB}(t,t') \sim \left\langle \Psi_{\mathbf{r}}(t)\Psi^\dagger_{\mathbf{r}'}(t')\right\rangle$ describes propagation of a particle added at $(t', \mathbf{r}')$ to $(t, \mathbf{r})$ under the full many-body dynamics (correlation)
  - Retarded and advanced GFs are averages of commutators [with $\theta(0) \equiv 1/2$]:

$$\begin{aligned} G^R_{AB}(t,t') &\equiv -i\theta(t-t')\left\langle [A(t), B(t')]_\zeta\right\rangle \\ &= +\theta(t-t')\left(G^>_{AB}(t,t') - G^<_{AB}(t,t')\right) \\ G^A_{AB}(t,t') &\equiv +i\theta(t'-t)\left\langle [A(t), B(t')]_\zeta\right\rangle \\ &= +\theta(t'-t)\left(G^<_{AB}(t,t') - G^>_{AB}(t,t')\right) \end{aligned}$$

    The retarded $G^R_{AB}(t,t')$ is only non-vanishing for $t - t' \geq 0$, the advanced $G^A_{AB}(t,t')$ for $t - t' \leq 0$. The $G^R_{AB}(t,t')$ describes the linear response of a system (measured via A) to perturbation B (Kubo formula): Thus, retarded (and advanced) Green functions are also called *response* functions.
  - Time ordered GF:

$$G^T_{A,B}(t,t') = -i\left\langle T_t A(t)B(t')\right\rangle = \theta(t-t')G^>_{AB}(t,t') + \theta(t'-t)G^<_{AB}(t,t')$$

    These GFs are useful for actual calculations and can be related to the other GFs.

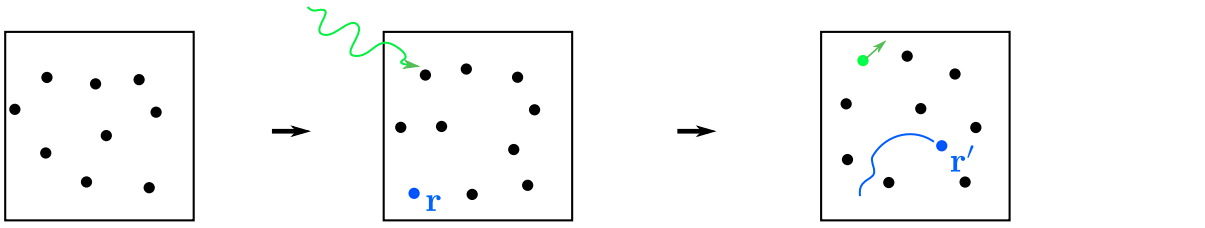

Figure 4: Sketch for two different processes in a quantum many-body systems described by appropriate Green functions.

- Relations:

$$G^{\lessgtr}_{AB}(t,t') = -G^{\lessgtr}_{B^\dagger A^\dagger}(t',t)^*, \quad G^{>}_{AB}(t,t') = \zeta G^{<}_{BA}(t',t), \tag{84}$$

$$G^{A}_{B^\dagger A^\dagger}(t',t) = G^{R}_{AB}(t,t')^*, \quad G^{A}_{BA}(t',t) = \zeta G^{R}_{AB}(t,t'). \tag{85}$$

- Temporal Fourier transform for stationary state [$G(t,t') \stackrel{!}{=} G(t-t')$, in particular for equilibrium]:

$$G(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} G(t) \tag{86}$$

$$G(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega\, e^{-i\omega t} G(\omega)$$

  Note that $\omega \in \mathbb{R}$ is continuous.

4.2 GFs in thermal equilibrium

Spectral density

- In equilibrium, we can work with single-frequency representation Eq. (86).
- Claim: All GFs can be calculated from the *spectral density:*

$$\boxed{A_{AB}(\omega) \equiv i\left(G^R_{AB}(\omega) - G^R_{B^\dagger A^\dagger}(\omega)^*\right)} \tag{87}$$

- Remark: For $A = c_\mu$, $B = c^\dagger_\mu$, the spectral density is real and non-negative and has the meaning of an energy resolution of the single-particle state $|\mu\rangle$ in the many-body system, → Ex. 4.2.
- Define "real" and "imaginary" parts of GFs (not the same as for complex numbers unless $A = B^\dagger$, thus denoted by "Gothic" letters).
  Applies for time-ordered, retarded and advanced GFs:

$$G^{T/R/A} = \mathfrak{R}G^{T/R/A} + i\mathfrak{I}G^{T/R/A} \tag{88}$$

  where

$$\begin{aligned}
\mathfrak{R}G^{T/R/A}_{A,B}(t,t') &\equiv \frac{1}{2}\left(G^{T/R/A}_{A,B}(t,t') + G^{T/R/A}_{B^\dagger,A^\dagger}(t',t)^*\right), \\
\mathfrak{I}G^{T/R/A}_{A,B}(t,t') &\equiv \frac{1}{2i}\left(G^{T/R/A}_{A,B}(t,t') - G^{T/R/A}_{B^\dagger,A^\dagger}(t',t)^*\right),
\end{aligned}$$

  or, for stationary states, after Fourier transform,

$$\begin{aligned}
\mathfrak{R}G^{T/R/A}_{A,B}(\omega) &\equiv \frac{1}{2}\left(G^{T/R/A}_{A,B}(\omega) + G^{T/R/A}_{B^\dagger,A^\dagger}(\omega)^*\right), \\
\mathfrak{I}G^{T/R/A}_{A,B}(\omega) &\equiv \frac{1}{2i}\left(G^{T/R/A}_{A,B}(\omega) - G^{T/R/A}_{B^\dagger,A^\dagger}(\omega)^*\right).
\end{aligned}$$

- Relations which follow from definitions:

$$\boxed{\Re G^R = \Re G^A = \Re G^T} \tag{89}$$

$$\Im G^R = -\Im G^A = -\frac{1}{2}A \tag{90}$$

Relation $A \leftrightarrow \Im G^T$

- Integral relation: Shift t-integration from real axis to the line $t - i\beta$ (use definition of $\langle ... \rangle$ and $A(t) = e^{iHt}Ae^{-iHt}$)

$$\int \mathrm{d}t\, e^{i\omega t} \langle A(t)B(0)\rangle = e^{\omega\beta} \int \mathrm{d}t\, e^{i\omega t} \langle B(0)A(t)\rangle \tag{91}$$

- We derive a relation between $\Im G^{R/A}_{AB}(\omega)$ and $G^{>}_{AB}(\omega)$:

$$\begin{aligned}
\Im G^R_{AB}(\omega) &= -\Im G^A_{AB}(\omega) \\
&= \frac{1}{2i}\left(G^R_{AB}(\omega) - G^R_{B^\dagger A^\dagger}(\omega)^\star\right) \\
&= \frac{1}{2i}\int_{-\infty}^{\infty} \mathrm{d}t \left(e^{i\omega t} G^R_{AB}(t,0) - e^{-i\omega t} \underbrace{G^R_{B^\dagger A^\dagger}(t,0)^\star}_{G^A_{AB}(0,t)}\right) \\
&= \frac{1}{2i}\int_{-\infty}^{\infty} \mathrm{d}t\, e^{i\omega t}\theta(t)\left(G^>_{AB}(t,0) - G^<_{AB}(t,0)\right) - e^{-i\omega t}\theta(t)\underbrace{\left(G^<_{AB}(0,t) - G^>_{AB}(0,t)\right)}_{\text{eq.: } G^<_{AB}(-t,0) - G^>_{AB}(-t,0)} \\
(\text{right} : t \to -t) &= \frac{1}{2i}\int_{-\infty}^{\infty} \mathrm{d}t\, e^{i\omega t}\theta(t)\left(G^>_{AB}(t,0) - G^<_{AB}(t,0)\right) - e^{i\omega t}\theta(-t)\left(G^<_{AB}(t,0) - G^>_{AB}(t,0)\right) \\
&= \frac{1}{2i}\int_{-\infty}^{\infty} \mathrm{d}t\, e^{i\omega t}\left(G^>_{AB}(t,0) - G^<_{AB}(t,0)\right) \\
&= -\frac{1}{2}\int_{-\infty}^{\infty} \mathrm{d}t\, e^{i\omega t}\langle A(t)B(0) - \zeta B(0)A(t)\rangle \qquad (92) \\
[(91)] &= -\frac{i}{2}\left(1 - \zeta e^{-\omega\beta}\right) G^>_{AB}(\omega) \qquad (93)
\end{aligned}$$

  Similar for time-ordered Green function:

$$\Im G^T_{AB}(\omega) = -\frac{i}{2}\left(1 + \zeta e^{-\omega\beta}\right) G^>_{AB}(\omega)$$

- Combine the last two equations, eliminate $G^>_{AB}(\omega)$, we find a relation between the imaginary parts of time-ordered Green functions and spectral density A:

$$\boxed{-\frac{1}{2}A = \Im G^R = -\Im G^A = \frac{1 - \zeta e^{-\beta\omega}}{1 + \zeta e^{-\beta\omega}} \Im G^T(\omega)} \tag{94}$$

Relation $A \leftrightarrow \Re G^{R/A/T}$ (Kramers-Kronig)

- We show that $\Im G^R_{AB} = -A_{AB}/2$ determines the full $G^R_{AB}(\omega)$.
- Use FT of step-function (η is positive infinitesimal for convergence of the FT):

$$FT[\theta(t)](\omega) = \lim_{\eta\to 0}\int_0^\infty \mathrm{d}t e^{i\omega t} e^{-\eta t} = \lim_{\eta\to 0}\frac{-1}{i\omega - \eta} = \underbrace{i\lim_{\eta\to 0}\frac{\omega}{\omega^2 + \eta^2}}_{\mathcal{P}\frac{1}{\omega}} + \underbrace{\lim_{\eta\to 0}\frac{\eta}{\omega^2 + \eta^2}}_{\pi\delta(\omega)} \tag{95}$$

  or

$$\theta(t) = \frac{1}{2\pi i}\int_{-\infty}^{+\infty} d\omega \frac{e^{i\omega t}}{\omega - i\eta} \tag{96}$$

- Find retarded Green function (use convolution theorem for FT):

$$\begin{aligned} G^R_{AB}(\omega) &= \int_{-\infty}^{\infty} \mathrm{d}t\, e^{i\omega t} \left[\theta(t)\left(G^>_{AB}(t,0) - G^<_{AB}(t,0)\right)\right] \\ &= -\frac{1}{2\pi i}\int_{-\infty}^{+\infty} \mathrm{d}\omega' \frac{1}{\omega' - \omega - i\eta} \int_{-\infty}^{\infty} \mathrm{d}t\, e^{i\omega' t} i \left\langle A(t)B(0) - \zeta B(0)A(t)\right\rangle \\ [(92)] &= \frac{1}{\pi}\int_{-\infty}^{+\infty} \mathrm{d}\omega' \frac{\Im G^R_{AB}(\omega')}{\omega' - \omega - i\eta} \\ &= -\frac{1}{2\pi}\int_{-\infty}^{+\infty} \mathrm{d}\omega' \frac{A_{AB}(\omega')}{\omega' - \omega - i\eta} \end{aligned} \tag{97}$$

Fluctuation-dissipation theorem

- Similar expressions for $G^{\gtrless}$ in terms of A:

$$\begin{aligned} G^>_{AB}(\omega) &= -\frac{iA_{AB}(\omega)}{1-\zeta e^{-\omega\beta}} \\ G^<_{AB}(\omega) &= +\frac{iA_{AB}(\omega)}{1-\zeta e^{+\omega\beta}} \end{aligned} \tag{98}$$

- Combine these expressions to find fluctuation-dissipation theorem:

$$\boxed{G^<_{AB}(\omega) + G^>_{AB}(\omega) = -iA_{AB}(\omega)\frac{e^{\beta\omega}+\zeta}{e^{\beta\omega}-\zeta}} \tag{99}$$

- Remarks:
  - Dissipation: On the rhs, imaginary part of the response functions $A \sim \Im G^R$ determines dissipation
  - Fluctuation: Correlation function $G^{\gtrless}$ on the lhs [the sum is also called Keldysh GF, $G^K_{AB}(\omega)$]
  - Recall: This only holds in equilibrium.

Lehmann representation

- Assume we have diagonalized the many-body Hamiltonian $H\,|n\rangle = E_n\,|n\rangle$. We wish to express the spectral density $A_{AB}(\omega)$ (and thus all GFs) in terms of eigenstates.
- We start from the greater GF:

$$G^>_{AB}(t) = -\frac{i}{Z}\sum_n e^{-\beta E_n}\left\langle n|A(t)B|n\right\rangle = -\frac{i}{Z}\sum_{n,n'} e^{-\beta E_n + it(E_n - E_{n'})}\left\langle n|A|n'\right\rangle\left\langle n'|B|n\right\rangle \tag{100}$$

  and after a FT [using $\int_{-\infty}^{+\infty}\mathrm{d}x\, e^{iax} = 2\pi\,\delta(a)$]

$$G^>_{AB}(\omega) = \int_{-\infty}^{\infty}\mathrm{d}t\, e^{i\omega t} G^>_{AB}(t) = -\frac{2\pi i}{Z}\sum_{n,n'} e^{-\beta E_n}\delta\left(E_n - E_{n'} + \omega\right)\left\langle n|A|n'\right\rangle\left\langle n'|B|n\right\rangle \tag{101}$$

- We find with Eq. (98):

$$\begin{aligned} A_{AB}(\omega) &= \left(1-\zeta e^{-\omega\beta}\right) iG^>_{A,B}(\omega) \\ &= \left(1-\zeta e^{-\omega\beta}\right)\frac{2\pi}{Z}\sum_{n,n'} e^{-\beta E_n}\delta\left(E_n - E_{n'} + \omega\right)\left\langle n|A|n'\right\rangle\left\langle n'|B|n\right\rangle \\ &= \frac{2\pi}{Z}\sum_{n,n'}\delta\left(E_n - E_{n'} + \omega\right)\left(e^{-\beta E_n} - \zeta e^{-\beta E_{n'}}\right)\left\langle n|A|n'\right\rangle\left\langle n'|B|n\right\rangle \end{aligned} \tag{102}$$

- The Lehmann expression is useful for explicit calculations (if we know $|n\rangle$, e.g. for small systems) or for general proofs. For example, the relations found in the previous section could have been derived in this way as well.

Exercises

Exercise 4.1. Harmonic oscillator: GFs, spectral density and equation-of-motion (EoM) technique

The Hamiltonian for a 1D quantum mechanical oscillator with mass m and frequency ω_0 reads

$$H = \frac{1}{2m}p^2 + \frac{1}{2}m\omega_0^2 x^2 \tag{103}$$

where momentum and position operators satisfy $[p, x]_- = -i$.

1. Introduce the bosonic creation operator $a = x\sqrt{m\omega_0/2} + ip/\sqrt{2m\omega_0}$ and express the Hamiltonian as $H = \omega_0(a^\dagger a + 1/2)$. Assume thermal equilibrium at temperature T and find the greater and lesser GFs $G^{\gtrless}_{aa^\dagger}$, the retarded and advanced GFs $G^{R/A}_{aa^\dagger}$ and the time ordered GF $G^{T}_{aa^\dagger}$, both in time and frequency domain. Confirm that the spectral density reads $A_{aa^\dagger} = 2\pi\delta(\omega - \omega_0)$.

2. Use your results in 1.) to find the retarded GF for the position operator,

$$G^R_{xx}(t) = -\theta(t)\frac{1}{m\omega_0}\sin(\omega_0 t)\,. \tag{104}$$

   Find the same result from the EoM technique, which does not require diagonalization of H: Apply two t-derivatives to the definition of $G^R_{xx}(t)$ and solve the resulting differential equation.

Exercise 4.2. Spectral density $A(\omega)$ and tunneling spectroscopy

Consider the equilibrium spectral density $A_{AB}(\omega)$ of Eq. (87) for the case $A = c$, $B = c^\dagger$ with c a fermionic operator. Here, we explore the meaning of $A_{cc^\dagger}(\omega)$ as the energy resolution of a particle created by $c^\dagger$ in a many-body system and discuss how it can be measured in the solid state context.

1. Show that $A_{cc^\dagger}(\omega)$...
   (a) is normalized $\frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega A_{cc^\dagger}(\omega) = 1$,
   (b) is real and non-negative (use Lehmann representation),
   (c) determines the occupation when weighted with $n_F(\omega)$, i.e. show $\langle c^\dagger c\rangle = \frac{1}{2\pi}\int_{-\infty}^{+\infty} d\omega A_{cc^\dagger}(\omega) n_F(\omega)$,
   (d) is a δ-function for a non-interacting system $H = \varepsilon_0 c^\dagger c$ and broadens if scattering with rate $1/\tau$ removes the particle from its state (start from $G^R_{cc^\dagger}(t) = -i\theta(t)e^{-i\varepsilon_0 t}e^{-t/2\tau}$ and discuss).

2. In solid state physics the spectral density can be measured by tunneling spectroscopy. Consider two pieces of metal, sample A and probe B described by - *possibly interacting* - Hamiltonians H_A and H_B. They are weakly coupled by a tunneling barrier $H_{AB} = \sum_{\nu\mu} T_{\mu\nu} c^\dagger_{A\mu} c_{B\nu}$ + h.c. with $T_{\mu\nu}$ a small complex tunneling matrix element ($T = T^\dagger$) and Greek letters denote eigenstates of $H_{A,B}$. The total Hamiltonian is $H = H_A + H_B + H_{AB}$. The tunnel current through the barrier is given by the rate of change of the charge in metal A (or B), $I = \partial_t Q_A = i[H, Q_A]$ where $Q_A = -e\sum_\mu c^\dagger_{A\mu} c_{A\mu}$. Show that

$$I = ie\sum_{\nu\mu}\left(T_{\mu\nu} c^\dagger_{A\mu} c_{B\nu} - T^\star_{\mu\nu} c^\dagger_{B\nu} c_{A\mu}\right) \tag{105}$$

   and calculate the change of I when the tunneling barrier is added via $I(t) = \int_{-\infty}^{+\infty} dt' G^R_{I,H_{AB}}(t,t')$. This is an application of the Kubo formula [→ Sec. (6)] and the retarded Green function needs to be calculated with respect to $H_A + H_B$ only (without the perturbation H_{AB}!). Assume a voltage bias $eV = \mu_A - \mu_B$ between the two metals (i.e. use $H_A \to H_A - \mu_A\sum_\mu c^\dagger_{A\mu}c_{A\mu}$ and analogous for H_B). Show that

$$I = -e\frac{1}{2\pi}\int d\omega \sum_{\nu\mu} |T_{\mu\nu}|^2 A_{c_{A\mu}c^\dagger_{A\mu}}(\omega) A_{c_{B\nu}c^\dagger_{B\nu}}(\omega + eV)\left[n_F(\omega + eV) - n_F(\omega)\right]. \tag{106}$$

   Assume that metal B (the probe) has a spectral density that does not vary strongly with ω, this means $\sum_\nu |T_{\mu\nu}|^2 A_{c_{B\nu}c^\dagger_{B\nu}}(\omega) \simeq$ const., and also assumed that $|T_{\mu\nu}|^2$ does not vary strongly with μ. Show that at low temperature, the differential conductance $dI/dV \equiv G(V)$ is proportional to $\sum_\mu A_{c_{A\mu}c^\dagger_{A\mu}}(-eV)$, i.e. the spectral density of metal A that we measure. This is the theory of tunneling spectroscopy.

Exercise 4.3. Hubbard atom: Spectral density and occupation

Consider a localized electronic orbital where an interaction $U \geq 0$ occurs in the case of double occupation with two electrons of opposite spin. The Hamiltonian is

$$H = U\hat{n}_\uparrow\hat{n}_\downarrow - \mu(\hat{n}_\uparrow + \hat{n}_\downarrow) \tag{107}$$

with $\hat{n}_\sigma = c_\sigma^\dagger c_\sigma$ the occupation operator, c_σ fermionic annihilation operators (for spin $\sigma =\uparrow,\downarrow$), and assume thermal equilibrium at temperature T. Note: This "Hubbard atom" is the local limit of the famous Hubbard model which in addition considers hopping $-tc_{j\sigma}^\dagger c_{i\sigma}$ between neighboring sites $\langle i,j\rangle$ in a lattice of such Hubbard atoms.

Diagonalize the Hamiltonian and use the Lehmann representation to find the spectral density $A_{c_\sigma c_\sigma^\dagger}(\omega)$. Does it depend on σ? Calculate the occupation $n = \langle\hat{n}_\uparrow + \hat{n}_\downarrow\rangle$ directly from the eigenstates and from the spectral density (c.f. Ex. 4.2). Plot n as a function of μ/U for $T/U = \{0.01, 0.1, 0.5\}$ and discuss your results. In the special case $\mu = U/2$, you should find $n = 1$ independent of T. Explain this observation in terms of a symmetry of H.

5 Equilibrium GF: Imaginary time and Matsubara formalism

Idea:

- Imaginary time formalism only for equilibrium, so H is always time-independent.
- In definition of GF: Compare time evolution $e^{\pm itH}$ with thermal state $\rho \sim e^{-\beta H}$
- Transform to imaginary time $it = \tau \in \mathbb{R}$ to treat both exp on equal footing. Related concept: imag. freq. $i\omega_n$
- This is just a mathematical trick without physical content!
- Pro: Resulting formalism is simple, in particular for perturbation theory ($\rightarrow$ Feynman diagrams)
- Con: Real-time/freq. quantities [e.g. $A(\omega)$] obtain from *analytical continuation* which is difficult.

5.1 Imaginary time

- We want:
  - exponentials appearing in $G_{AB}(t) \sim \langle A(t)B\rangle \sim \mathrm{Tr}\left[e^{itH}Ae^{-itH}\ B\ e^{-\beta H}\right]$ to be real
  - avoid to expand $e^{-\beta H}$ *and* $e^{\pm itH}$ when doing perturbation theory
- In the complex plane, we rotate $t \rightarrow -i\tau$ (with $\tau \in \mathbb{R}$), see Fig. 5(a).
- For the time-evolution operator we get $e^{-i(t-t_0)H} = U(t,t_0) \rightarrow U(\tau,\tau_0) = e^{-(\tau-\tau_0)H}$ ("delete the i"). The $U(\tau,\tau_0)$ is no longer unitary, but the group properties remain.
- Define the Heisenberg- and interaction picture in imaginary time, just copy from above.
- We use a Greek letter τ to indicate imaginary time evolved operators $O(\tau)$. A roman letter stands for real-time Heisenberg picture, $O(t) = e^{itH}Oe^{-itH}$.
- Heisenberg picture: $O(\tau) = e^{H\tau}Oe^{-H\tau}$ and the EoM is $\partial_\tau O(\tau) = [H, O(\tau)]$.
- Interaction picture ($H = H_0 + V$):
  - Operators: $O_I(\tau) = e^{H_0\tau}Oe^{-H_0\tau}$ and the EoM is $\partial_\tau O_I(\tau) = [H_0, O_I(\tau)]$.
  - States $|\psi_I(\tau)\rangle = U_I(\tau,\tau')\,|\psi_I(\tau')\rangle$ with $U_I(\tau,\tau') = e^{H_0(\tau-\tau')}U(\tau,\tau')$ and $\partial_\tau U_I(\tau,\tau') = -V_I(\tau)U_I(\tau,\tau')$
  - Formal solution for $U_I(\tau,\tau')$ with imaginary time ordering operator T_τ:

$$U_I(\tau,\tau') = T_\tau \exp\left[-\int_{\tau'}^{\tau} \mathrm{d}\tilde{\tau} V_I(\tilde{\tau})\right] \tag{108}$$

- Main result: Express thermal density matrix (state) in terms of evolution operator (both in Heisenberg and interaction picture)

$$\boxed{Z\rho = e^{-\beta H} = U(\beta,0) = e^{-\beta H_0}U_I(\beta,0)} \tag{109}$$

5.2 Imaginary time ordered GF

- We use the time ordering operator for imaginary times $\tau_{1,2}$ and consider operators in Heisenberg picture:

$$\boxed{\mathcal{G}_{AB}(\tau_1,\tau_2) \equiv -\langle T_\tau A(\tau_1)B(\tau_2)\rangle = -\frac{1}{Z}\mathrm{Tr}\left[e^{-\beta H}T_\tau A(\tau_1)B(\tau_2)\right]} \tag{110}$$

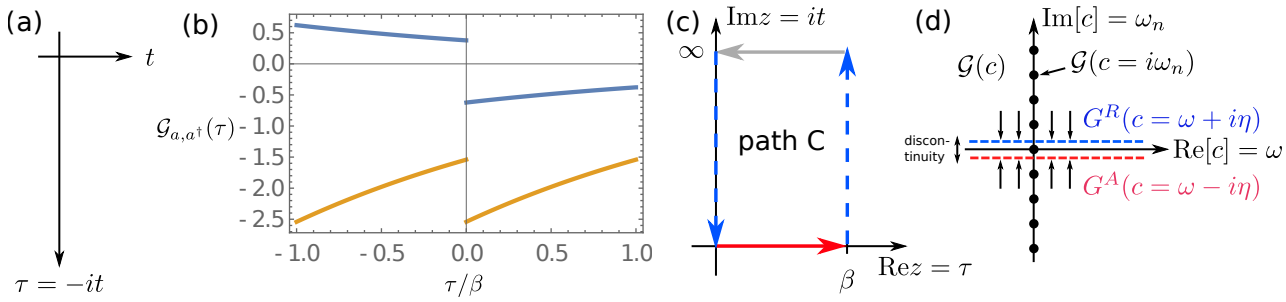

Figure 5: (a) Real and imaginary time (b) Sketch of the imaginary time ordered GF $\mathcal{G}_{aa^\dagger}(\tau)$ for $H = \xi a^\dagger a$ for bosons (red), fermions (blue) and $\xi\beta = 0.5$. (c) Integration path to connect $\mathcal{G}(\tau)$ and $G^R(\omega)$. (d) $\mathcal{G}(c)$ with complex frequency argument c.

Relation to perturbation theory

- Use Eq. (109) to write $\mathcal{G}_{AB}(\tau_1, \tau_2)$ for $H = H_0 + V$ in a compact way that is the basis of perturbation theory in V.
- Assume $\tau_1 > \tau_2$ and work with interaction picture $A(\tau_1) = U_I(0, \tau_1)A_I(\tau_1)U_I(\tau_1, 0)$:

$$\begin{aligned}\langle T_\tau A(\tau_1)B(\tau_2)\rangle &= \frac{1}{Z}\mathrm{Tr}\left[e^{-\beta H}U_I(0,\tau_1)A_I(\tau_1)U_I(\tau_1,\tau_2)B_I(\tau_2)U_I(\tau_2,0)\right] \\ &\overset{(109)}{=} \frac{1}{Z}\mathrm{Tr}\Big[e^{-\beta H_0}\underbrace{U_I(\beta,\tau_1)A_I(\tau_1)U_I(\tau_1,\tau_2)B_I(\tau_2)U_I(\tau_2,0)}_{T_\tau U_I(\beta,0)A_I(\tau_1)B_I(\tau_2)}\Big]\end{aligned}$$

  and a similar calculation holds for $\tau_1 < \tau_2$ so that we can conclude for all $\tau_{1,2}$:

$$\langle T_\tau A(\tau_1)B(\tau_2)\rangle = \frac{\mathrm{Tr}\left[e^{-\beta H_0}T_\tau\left(U_I(\beta,0)A_I(\tau_1)B_I(\tau_2)\right)\right]}{\mathrm{Tr}\left[e^{-\beta H_0}U_I(\beta,0)\right]} \tag{111}$$

  The time-ordering puts the parts of $U_I(\beta, 0) = U_I(\beta, \tau_1)U_I(\tau_1, \tau_2)U_I(\tau_2, 0)$ at their correct positions.
- We divide both numerator and denominator by $1/Z_0$ and use *"simple"* averages with respect to $e^{-\beta H_0}$ which are defined as $\langle ...\rangle_0 \equiv Z_0^{-1}\mathrm{Tr}\left[e^{-\beta H_0}...\right]$:

$$\boxed{\langle T_\tau A(\tau_1)B(\tau_2)\rangle = \frac{\langle T_\tau U_I(\beta,0)A_I(\tau_1)B_I(\tau_2)\rangle_0}{\langle U_I(\beta,0)\rangle_0}} \tag{112}$$

- Observation: The perturbation V sits only in $U_I(\beta, 0)$ and not in $A_I(\tau_1)B_I(\tau_2)$ so that no separate expansions of state and time-evolution needs to be performed.
- Before we embark in performing expansion in V ($\rightarrow$ Sec. (7)), we first consider the relation of $\mathcal{G}_{A,B}(\tau_1, \tau_2)$ to real-time GF (or rather real-frequency GF).

Matsubara frequencies

- Properties of $\mathcal{G}_{A,B}$ (proof $\rightarrow$ Ex. 5.1):
  - translation invariance in τ:

$$\mathcal{G}_{AB}(\tau_1, \tau_2) = \mathcal{G}_{AB}(\tau_1 - \tau_2, 0) \equiv \mathcal{G}_{AB}(\tau_1 - \tau_2) \tag{113}$$

  - for $\mathcal{G}_{AB}(\tau)$ to be well-defined (not divergent), the argument needs to be restricted to $\tau \in (-\beta, \beta)$. Here it is assumed that the (many-body) spectrum E_n is bounded from below, but not necessarily from above.

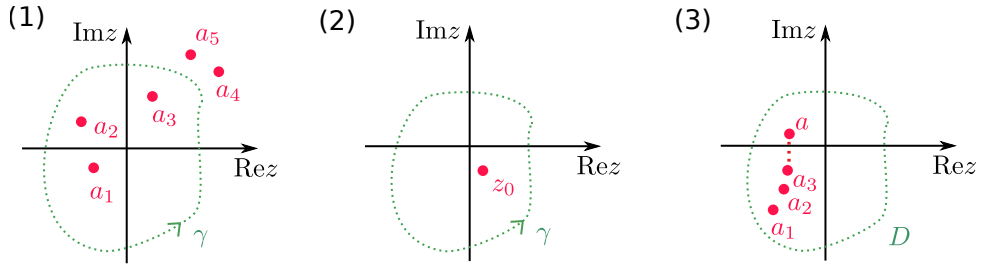

Figure 6: Sketches for reminders on complex analysis.

– (anti-)periodic boundary conditions: For $0 \leq \tau < \beta$, we have

$$\mathcal{G}_{AB}(\tau) = \zeta \cdot \mathcal{G}_{AB}(\tau - \beta). \tag{114}$$

- The boundary condition (114) means $\mathcal{G}_{AB}(\tau)$ is fully determined by its behavior for $\tau \in [0, \beta)$. However, generalizing Eq. (114), one can extend $\mathcal{G}_{AB}(\tau)$ to τ on the whole real axis, $\tau \in \mathbb{R}$ to obtain a function periodic in 2β.
- As an example, the $\mathcal{G}_{aa^\dagger}(\tau)$ for free bosons or fermions is shown in Fig. 5(b), for details see Sec. 5.5.
- It is useful to represent the periodic function $\mathcal{G}_{AB}(\tau)$ as a Fourier series with discrete coefficients that can be obtained from $\mathcal{G}(\tau)$ on $\tau \in [0, \beta)$:

$$\mathcal{G}_{AB}(\tau) \equiv T \sum_n e^{-i\omega_n \tau} \mathcal{G}_{AB}(i\omega_n) \tag{115}$$

$$\mathcal{G}_{AB}(i\omega_n) \equiv \int_0^\beta \mathrm{d}\tau\, e^{i\omega_n \tau} \mathcal{G}_{AB}(\tau) \tag{116}$$

where for $n \in \mathbb{Z}$ the **Matsubara frequencies** are:

$$\boxed{\omega_n = \begin{cases} 2\pi T n & : \text{bosons} \\ 2\pi T(n + 1/2) & : \text{fermions} \end{cases}} \tag{117}$$

This ensures β-(anti)-periodicity.

- The $\mathcal{G}_{AB}(i\omega_n)$ is known as the Matsubara GF and the complex argument is a convention. Sometimes also $\mathcal{G}_{AB}(\omega_n)$ is used in the literature.

5.3 Reminders on complex analysis

Before we can embark on showing the relation between Matsubara GF $\mathcal{G}_{AB}(i\omega_n)$ and real-frequency GFs, we need the following facts from complex analysis.

(1) Residue theorem: Consider $f : \mathbb{C} \to \mathbb{C}$, $z \to f(z)$ a complex function which is analytic on $\mathbb{C}$ (locally expandable in power series) except at the points $a_{1,2,\ldots,n}$. Then we have for the $a_{1,2,..,k}$ inside a closed path γ:

$$\oint_\gamma \mathrm{d}z\, f(z) = 2\pi i \sum_{j=1}^{k} \mathrm{Res}(f, a_j) \tag{118}$$

where $\mathrm{Res}(f, a_j)$ is the residue of f at a_j. If a_j is a pole of n-th order of $f(z)$:

$$\mathrm{Res}(f, a_j) = \frac{1}{(n-1)!} \lim_{z \to a_j} \frac{d^{n-1}}{dz^{n-1}} \left([z - a_j]^n f(z) \right) \tag{119}$$

(2) Cauchy's integral formula (follows from residue theorem): If f is analytic on $\mathbb{C}$, then for a path enclosing z_0:

$$f(z_0) = \frac{1}{2\pi i} \oint_\gamma \mathrm{d}z \, \frac{f(z)}{z - z_0} \tag{120}$$

(3) Identity theorem for complex functions: Let $f, g : D \to \mathbb{C}$ be two complex functions analytic on the domain $D \subseteq \mathbb{C}$ and consider $a_n \in D$, $n \in \mathbb{N}$ a series of complex numbers with $\lim_{n\to\infty} a_n = a \in D$. Theorem: If $f(a_n) = g(a_n)$ for all $n = 1, 2, ...$, then $f(z) = g(z)$ for all $z \in D$.
Consequence: If we know a function $f(z)$ for a series of points, we can continue it analytically to a larger region of the complex plane in a *unique* way.

5.4 Connection between Matsubara and retarded GF

- Consider the integrand in Eq. (116) but replace $\tau \to z$ (complex argument) $e^{i\omega_n z}\mathcal{G}_{AB}(z)$ and integrate along closed path $C = C_\rightarrow + C_\uparrow + C_\leftarrow + C_\downarrow$ in Fig. 5(c). Assume $\omega_n > 0$ and use residue theorem (1).
- The integrand has no singularities in C, thus

$$0 = \oint_C \mathrm{d}z \, e^{i\omega_n z}\mathcal{G}_{AB}(z) = I_\rightarrow + I_\uparrow + I_\leftarrow + I_\downarrow \tag{121}$$

We calculate the different line integrals on the rhs separately:

- $C_\rightarrow$: $z = \tau \in \mathbb{R}$, $\mathrm{d}z = \mathrm{d}\tau$: The integral is just the definition of the Matsubara GF, $I_\rightarrow = \mathcal{G}_{AB}(i\omega_n)$
- $C_\uparrow$: $z = \beta + it$, $t \in [0, \infty)$, $\mathrm{d}z = i\mathrm{d}t$: The convergence of this integral requires $\omega_n > 0$. We use the important identity $e^{i\omega_n\beta} = \zeta$.

$$\begin{aligned} I_\uparrow &= -\frac{1}{Z}\int_0^\infty i\mathrm{d}t \, e^{i\omega_n(\beta+it)} \operatorname{Tr}\left(e^{-\beta H} e^{(\beta+it)H} A e^{-(\beta+it)H} B\right) \\ &= -\frac{1}{Z}\int_0^\infty i\mathrm{d}t \, e^{-\omega_n t}\,\zeta \operatorname{Tr}\left(e^{-\beta H} B \underbrace{e^{itH} A e^{-itH}}_{A(t)}\right) \\ &= -\zeta\int_0^\infty \mathrm{d}t \, e^{-\omega_n t} i \langle BA(t)\rangle \end{aligned}$$

- $C_\leftarrow$: We have $I_\leftarrow = 0$ to due to $e^{i\omega_n z} \to 0$ if $\omega_n > 0$ and $\mathrm{Im}z \to \infty$.
- $C_\downarrow$: Similar to $C_\uparrow$, we find with $z = it$, $t \in (\infty, 0]$, $\mathrm{d}z = i\mathrm{d}t$,

$$\begin{aligned} I_\downarrow &= -\frac{1}{Z}\int_\infty^0 i\mathrm{d}t e^{i\omega_n it} \operatorname{Tr}\left(e^{-\beta H} e^{itH} A e^{-itH} B\right) \\ &= +\int_0^\infty \mathrm{d}t e^{-\omega_n t} i \langle A(t)B\rangle \end{aligned}$$

- We insert in Eq. (121) and convert $\int_0^\infty \mathrm{d}t = \int_{-\infty}^\infty \mathrm{d}t\,\theta(t)$:

$$\mathcal{G}_{AB}(i\omega_n) = \int_{-\infty}^\infty \mathrm{d}t e^{-\omega_n t} \underbrace{\theta(t)\left(-i\langle A(t)B\rangle + \zeta i\langle BA(t)\rangle\right)}_{G^R_{AB}(t)} \quad (\omega_m > 0) \tag{122}$$

Note: On the rhs, this is not the usual FT of Eq. (86) because of the missing imaginary unit in the exponent.

- What about $\omega_m < 0$? We need flip the path C to negative side of the complex plane. Similar steps lead to:

$$\mathcal{G}_{AB}(i\omega_n) = \int_{-\infty}^\infty \mathrm{d}t \, e^{\omega_n t} G^A_{AB}(t) \; (\omega_m < 0) \tag{123}$$

- To complete the argument, we need to extend defintion of FT, $G^{R/A}(\omega) = \int_{-\infty}^{\infty} dt\, e^{i\omega t} G^{R/A}(t)$ [Eq. (86)] to complex frequency variable $c = \omega + i\nu$ with $\omega, \nu \in \mathbb{R}$.

$$\boxed{G^{R/A}(c = \omega + i\nu) \equiv \int_{-\infty}^{\infty} dt\, e^{i\omega t}\, e^{-t\nu}\, G^{R/A}(t)} \tag{124}$$

- What values can ν take for convergence? Due to the $\theta(\pm t)$ in $G^{R/A}(t)$, we restrict to $\nu > 0$ for $G^R(\omega + i\nu)$ and $\nu < 0$ for $G^A(\omega + i\nu)$.

- It follows:
  - $G^R(c)$ is an analytic function on the upper half plane $\mathrm{Im} c = \nu > 0$
  - $G^A(c)$ is an analytic function on the lower half plane $\mathrm{Im} c = \nu < 0$

- Relation between Matsubara GF and response functions: With the definition Eq. (124) and Eqns. (122), (123) from contour integration of $\mathcal{G}_{AB}(\tau \to z)$, we have

$$\mathcal{G}_{AB}(i\omega_n) = \begin{cases} G^R_{AB}(i\omega_n) & : \omega_n > 0 \\ G^A_{AB}(i\omega_n) & : \omega_n < 0 \end{cases} \tag{125}$$

- Remark: The special case $\omega_n = 0$ (only for bosonic Matsubara frequencies!) will be considered in Ex. 5.2 and interpreted in Sec. 6.

Analytic continuation

- Usually $\mathcal{G}_{AB}(i\omega_n)$ is easier to calculate than other GF $\to$ assume we know $\mathcal{G}_{AB}(c = i\omega_n)$ where c is complex frequency argument. See Fig. 5(d).

- Use identity theorem (3) from complex analysis and the fact that Eq. (125) holds for infinite number of (either positive or negative) Matsubara frequencies. We conclude that there is a function $\mathcal{G}_{AB}(c)$ which is analytic for $c \notin \mathbb{R}$ which coincides with the Matsubara GF at $c = i\omega_n$ and is identical to $G^{R/A}_{AB}(\omega)$ for $c = \omega \pm i\eta$ just above or below the real axis.

- Analytic continuation:

$$\boxed{G^{R/A}_{AB}(\omega) = \lim_{\eta \to 0} \mathcal{G}_{AB}(i\omega_n \to \omega \pm i\eta)} \tag{126}$$

- Remarks:
  - For straightforward analytic continuation by simply replacing $i\omega_n \to \omega \pm i\eta$, need $\mathcal{G}_{AB}(i\omega_n)$ in the form of a rational function analytic in the upper/lower half plane.
    E.g.: One **cannot** replace $i\omega_n \to \omega \pm i\eta$ in the defining FT integral (116), the τ-integration must be performed first because we need discrete Fourier coefficients.
  - $\mathcal{G}_{AB}(c)$ has a discontinuity on the real axis, $c \in \mathbb{R}$, this is evident as $G^R_{AB}(\omega) \neq G^A_{AB}(\omega)$. See also Ex. 5.2 where $\mathcal{G}_{AB}(c)$ is expressed using the Lehmann representation.
  - For numerical data, only a finite number of Matsubara frequencies is known and there might be error bars. Then analytic continuation is not well defined.

5.5 Example: Matsubara GF for non-interacting particles

- Consider non-interacting particles described by $H_0 = \sum_\mu \xi_\mu a^\dagger_\mu a_\mu$ where for bosons $\xi_\mu > 0$ for finite occupation. We want to find the Matsubara GF $\mathcal{G}_{a_\nu a^\dagger_\nu}(\tau) \equiv \mathcal{G}_\nu(\tau)$ and $\mathcal{G}_\nu(i\omega_n)$.

- We have similar to the real-time case Eq. (81), $a_\nu(\tau) = e^{\tau H_0} a_\nu e^{-\tau H_0} = e^{-\xi_\nu \tau} a_\nu$ and $a^\dagger_\nu(\tau) = e^{+\xi_\nu \tau} a^\dagger_\nu$.

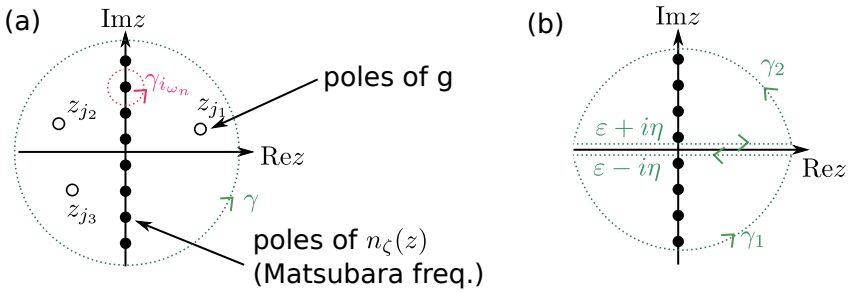

Figure 7: (a) Matsubara sum $S(\tau) = T\sum_{\omega_n} g(i\omega_n)e^{i\omega_n\tau}$ in two cases for function $g(z)$, (a) with known simple poles and (b) with a non-analyticity along the real axis.

- Insert into the definition of $\mathcal{G}_{a_\nu a_\nu^\dagger}(\tau) \equiv \mathcal{G}_\nu(\tau)$ in Eq. (110),

$$\begin{aligned}\mathcal{G}_\nu(\tau) &= -\left[\theta(\tau)\left\langle a_\nu a_\nu^\dagger\right\rangle + \zeta\theta(-\tau)\left\langle a_\nu^\dagger a_\nu\right\rangle\right] e^{-\xi_\nu\tau} \\ &= -\left[\theta(\tau)\left(1+\zeta\left\langle\hat{n}_\nu\right\rangle\right) + \zeta\theta(-\tau)\left\langle\hat{n}_\nu\right\rangle\right] e^{-\xi_\nu\tau}\end{aligned}$$

  with $\langle\hat{n}_\nu\rangle = n_\nu = 1/(e^{\beta\xi_\nu} - \zeta)$ the occupation function for bosons ($\zeta = +1$) or fermions ($\zeta = -1$). See Fig. (5)(b) for a sketch of $\mathcal{G}_\nu(\tau)$ for $\xi_\nu\beta = 0.5$.

- We perform the FT (116) to find $\mathcal{G}_\nu(i\omega_n) = \int_0^\beta \mathrm{d}\tau\, e^{i\omega_n\tau}\mathcal{G}_\nu(\tau)$. It is crucial that $\xi_\mu > 0$ for the bosonic case and $i\omega_n \neq 0$ for the fermionic case so that $\int_0^\beta \mathrm{d}\tau\, e^{(i\omega_n-\xi_\nu)\tau} = \frac{e^{(i\omega_n-\xi_\nu)\beta}-1}{i\omega_n-\xi_\nu}$. We then use $e^{i\omega_n\beta} = \zeta$ and obtain after a cancellation with $1+\zeta\langle\hat{n}_\nu\rangle$.

$$\boxed{\mathcal{G}_\nu(i\omega_n) = \frac{1}{i\omega_n - \xi_\nu}} \tag{127}$$

- Analytic continuation:

$$G_\nu^{R/A}(\omega) = \lim_{\eta\to 0}\mathcal{G}_\nu(i\omega_n \to \omega \pm i\eta) = \frac{1}{\omega \pm i\eta - \xi_\nu} \tag{128}$$

  For the bosonic case, the $G^{R/A}(\omega)$ has already been found in the Ex. (4.1) on the real-time GF of the harmonic oscillator.

5.6 Evaluation of Matsubara sums

- When working with Matsubara GFs, we will often encounter generic sums [for $\tau \in (0,\beta)$]

$$S(\tau) \equiv T\sum_{\omega_n} g(i\omega_n)e^{i\omega_n\tau} \tag{129}$$

  and ω_n are either bosonic or fermionic Matsubara frequencies and $g(i\omega_n)$ is a Matsubara GF or products thereof. Goal: Calculate $S(\tau)$.

- Trick: Use Cauchy's integral formula (120) backwards, $f(i\omega_n) = \frac{1}{2\pi i}\oint_\gamma \mathrm{d}z\, f(z)/(z - i\omega_n)$. Write the rhs of $S(\tau)$ as an integral of the complex variable z.

- Start with rewriting a single term in the sum, $g(i\omega_n)e^{i\omega_n\tau}$. See the red contour in Fig. 7(a).

- We need a function that has simple poles at $i\omega_n$, but for all n. Since $e^{i\beta\omega_n} = \zeta$ this function is the fermionic or bosonic distribution function:

$$n_\zeta(z) \equiv \frac{1}{e^{\beta z} - \zeta} \;\to\; \mathrm{Res}\left(n_\zeta(z), i\omega_n\right) = \lim_{z\to i\omega_n}\Big(\underbrace{[z - i\omega_n]}_{\delta}\frac{1}{e^{\beta z} - \zeta}\Big) = \lim_{\delta\to 0}\frac{\delta}{e^{\beta\delta}\zeta - \zeta} = \zeta\frac{1}{\beta} \tag{130}$$

- For a contour integral that encloses the point $i\omega_n$ but no singularity of $g(z)$, we have according to Cauchy's formula

$$\oint_{\gamma_{i\omega_n}} \mathrm{d}z\, g(z) n_\zeta(z) = 2\pi i \zeta \frac{1}{\beta} g(i\omega_n) \tag{131}$$

- Generalize to contour γ which encloses all $i\omega_n$ but no singularities of $g(z)$, then

$$\boxed{S(\tau) = \frac{\zeta}{2\pi i} \oint_\gamma \mathrm{d}z\, n_\zeta(z) g(z) e^{z\tau}} \tag{132}$$

- Special case (a) (perturbation theory): Function $g(z)$ with simple poles that are known, $g(z) = \Pi_j \frac{1}{z - z_j}$. Use contour $\gamma : z = Re^{i\theta}$, $\theta \in [0, 2\pi]$ and $R \to \infty$, see Fig. 7(a). The integrand contains $n_\zeta(z) e^{z\tau} = \frac{e^{z\tau}}{e^{\beta z} - \zeta}$ which vanishes in the $R \to \infty$ limit and hence

$$0 = \frac{1}{2\pi i} \oint_\gamma \mathrm{d}z\, n_\zeta(z) g(z) e^{z\tau} \tag{133}$$

  The poles of $n_\zeta(z)$ give rise to $\zeta S(\tau)$, the (few and known) poles of $g(z)$ which are also enclosed provide the rhs:

$$S(\tau) = -\zeta \sum_j \mathrm{Res}\,(g(z), z_j)\, n_\zeta(z_j) e^{z_j \tau} \tag{134}$$

- Special case (b) (full GF, fermionic $\zeta = -1$): Assume the poles of $g(z) = \mathcal{G}_{cc^\dagger}(z)$ are not known, but we know that it is analytic for z not on the real axis [follows for $\mathcal{G}_{cc^\dagger}(i\omega_n \to z)$ from Lehmann representation]. Enclose all $z = i\omega_n$ by contours $\gamma_{1,2}$ shown in Fig. 7(b). Again, the part $|z| \to \infty$ does not contribute to the integral. We have from Eq. (132)

$$\begin{aligned} S(\tau) &= -\frac{1}{2\pi i} \int_{-\infty}^{+\infty} \mathrm{d}\varepsilon\, n_F(\varepsilon) \left[\mathcal{G}_{cc^\dagger}(\varepsilon + i\eta) - \mathcal{G}_{cc^\dagger}(\varepsilon - i\eta)\right] e^{\varepsilon\tau} \\ \text{(anal. cont.)} &= -\frac{1}{2\pi i} \int_{-\infty}^{+\infty} \mathrm{d}\varepsilon\, n_F(\varepsilon) \underbrace{\left[G^R_{cc^\dagger}(\varepsilon) - G^A_{cc^\dagger}(\varepsilon)\right]}_{-iA_{cc^\dagger}(\varepsilon)} e^{\varepsilon\tau} \\ &= \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{d}\varepsilon\, n_F(\varepsilon) A_{cc^\dagger}(\varepsilon) e^{\varepsilon\tau} \end{aligned}$$

  Application: Occupation number

$$\langle c^\dagger c \rangle = -\langle T_\tau c(-\eta) c^\dagger(0) \rangle \overset{\text{def.}}{=} \mathcal{G}_{cc^\dagger}(\tau = -\eta) = T \sum_n e^{i\omega_n \eta} \mathcal{G}_{cc^\dagger}(i\omega_n) = S(\eta) \overset{\text{(b)}}{=} \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{d}\varepsilon\, n_F(\varepsilon) A_{cc^\dagger}(\varepsilon) \tag{135}$$

  This relation between occupation and spectral density was already derived by other means in Ex. 4.2.

5.7 Wick's theorem

- n-particle imaginary time ordered GF: We specialize to creation and operators $A, B = a_{\nu_j}, a^\dagger_{\nu_j}$ but generalize from the single-particle imaginary time ordered GF to n-particle (=2n-point)

$$\boxed{\mathcal{G}^{(n)}(\nu_1\tau_1, ..., \nu_n\tau_n; \nu'_1\tau'_1, ..., \nu'_n\tau'_n) \equiv (-1)^n \left\langle T_\tau a_{\nu_1}(\tau_1) ... a_{\nu_n}(\tau_n) a^\dagger_{\nu'_n}(\tau'_n) ... a^\dagger_{\nu'_1}(\tau'_1) \right\rangle} \tag{136}$$

  Note the order of the creation operators and the leading sign which might differ from author to author.

- Wick's theorem applies to $\mathcal{G}^{(n)}$ only if the average $\langle ... \rangle$ is with respect to a Hamiltonian $H_0 = \sum_{\nu',\nu} h^{(0)}_{\nu',\nu} a^\dagger_{\nu'} a_\nu$ which is quadratic in $a, a^\dagger$. We denote this case by subscript 0: $\mathcal{G}^{(n)} = \mathcal{G}^{(n)}_0$.

- We abbreviate $j = (\nu_j, \tau_j)$. The theorem states that $\mathcal{G}_0^{(n)}$ factorizes into a sum of n products of single-particle ($n = 1$) imaginary time ordered non-interacting GFs

$$\mathcal{G}_0(j, j') \equiv -\left\langle T_\tau a_{\nu_j}(\tau_j) a^\dagger_{\nu'_j}(\tau'_j) \right\rangle_0 \tag{137}$$

in the following way;

$$\boxed{\mathcal{G}_0^{(n)}\left(1, 2, ..., n; 1', 2', ..., n'\right) = \sum_{p \in S_n} \zeta^{P(p)} \mathcal{G}_0\left(1, p(1')\right) \mathcal{G}_0\left(2, p(2')\right) \cdots \mathcal{G}_0\left(n, p(n')\right)} \tag{138}$$

- Remarks:
  - $P(p) \equiv [1 - \mathrm{sgn}(p)]/2$ where $\mathrm{sgn}(p) = \pm 1$ is the sign of permutation $p \to \zeta^{P(p)} = 1$ except for an odd permutation of fermions where it is -1
  - essential: (i) fermionic or bosonic operator algebra and (ii) non-interacting H_0
  - if we consider the matrix M with elements $M_{jj'} = \mathcal{G}_0(j, j')$, the rhs of Eq. (138) is the determinant of M (for fermions, $\zeta = -1$) or the permanent of M (for bosons, $\zeta = +1$)
  - Wick's theorem and the interaction picture representation of the full $\mathcal{G}$ in Eq. (112) are the basis of perturbation theory and Feynman diagrams

Preparation for proof: EoM for $\mathcal{G}_0 = \mathcal{G}_0^{(1)}$

- Apply ∂_τ to (compare to Ex. 4.1 for real-time GF):

$$\mathcal{G}_{0,\nu\nu'}(\tau) = -\theta(\tau)\left\langle a_\nu(\tau) a^\dagger_{\nu'} \right\rangle_0 - \zeta\theta(-\tau)\left\langle a^\dagger_{\nu'} a_\nu(\tau) \right\rangle_0 \tag{139}$$

- Preparation for EoM in imaginary time Heisenberg picture: $\partial_\tau a_\nu(\tau) = [H_0, a_\nu](\tau)$:

$$[H_0, a_\nu] = \sum_{\mu',\mu} h^{(0)}_{\mu'\mu} a^\dagger_{\mu'} a_\mu a_\nu - \sum_{\mu',\mu} h^{(0)}_{\mu'\mu} \underbrace{a_\nu a^\dagger_{\mu'} a_\mu}_{\delta_{\mu'\nu} a_\mu + \zeta a^\dagger_{\mu'} a_\nu a_\mu = \delta_{\mu'\nu} a_\mu + a^\dagger_{\mu'} a_\mu a_\nu} = -\sum_\mu h^{(0)}_{\nu\mu} a_\mu \tag{140}$$

so that:

$$\partial_\tau a_\nu(\tau) = [H_0, a_\nu](\tau) = -\sum_\nu h^{(0)}_{\nu\mu} a_\mu(\tau) \tag{141}$$

- Combine this with the derivatives of the $\theta(\tau)$-functions

$$\begin{aligned} \partial_\tau \mathcal{G}_{0,\nu\nu'}(\tau) &= -\delta(\tau)\left\langle a_\nu a^\dagger_{\nu'} \right\rangle_0 + \zeta\delta(\tau)\left\langle a^\dagger_{\nu'} a_\nu \right\rangle_0 - \sum_\mu h^{(0)}_{\nu\mu} \mathcal{G}_{0,\mu\nu'}(\tau) \\ \sum_\mu \left(-\delta_{\mu\nu}\partial_\tau - h^{(0)}_{\nu\mu}\right) \mathcal{G}_{0,\mu\nu'}(\tau) &= \delta(\tau)\left\langle \left[a_\nu, a^\dagger_{\nu'}\right]_\zeta \right\rangle_0 \\ \sum_\mu \left[\mathcal{G}_0^{-1}(\tau)\right]_{\nu\mu} \mathcal{G}_{0,\mu\nu'}(\tau) &= \delta(\tau)\delta_{\nu,\nu'} \end{aligned} \tag{142}$$

- After a Fourier transform, $\left[\mathcal{G}_0^{-1}(\tau)\right]_{\nu\mu} = -\delta_{\mu\nu}\partial_\tau - h^{(0)}_{\nu\mu}$ is consistent with our finding for the non-interacting GF in Eq. (127), $1/\mathcal{G}_\nu(i\omega_n) = i\omega_n - \xi_\nu$ (here, $h^{(0)}_{\nu'\nu}$ was diagonalized before).

- Generalize to two time arguments $\tau \to \tau - \tau'$:

$$\sum_\mu \underbrace{\left(-\delta_{\mu\nu}\partial_\tau - h^{(0)}_{\nu,\mu}\right)}_{\mathcal{G}_0^{-1}(\tau\nu,\tau'\mu)} \mathcal{G}_0(\mu\tau, \nu'\tau') = \delta(\tau - \tau')\delta_{\nu,\nu'} \equiv \mathbf{1} \tag{143}$$

Proof via EoM

- Define operator

$$d_j(\sigma_j) = \begin{cases} a_{\nu_j}(\tau_j) & : j = 1, 2, ..., n \\ a^\dagger_{\nu'_{2n+1-j}}(\tau'_{2n+1-j}) & : j = n+1, n+2, ..., 2n \end{cases} \tag{144}$$

  so that $\sigma_j = \tau_j$ for $j = 1, 2, ..., n$ and $\sigma_j = \tau'_{2n+1-j}$ for $j = n+1, ..., 2n$. We then have

$$\mathcal{G}_0^{(n)}(1, 2, ..., n; 1', 2', ..., n') = (-1)^n \langle T_\tau d_1 d_2 ... d_n d_{n+1} ... d_{2n} \rangle_0 . \tag{145}$$

- Idea: Rewrite τ-ordering T_τ by summing over all possible orders of d_j ($\rightarrow$ permutations p) and pick the correct one (determined by the actual values of τ_j) by product of θ-functions:

$$\begin{aligned} \mathcal{G}_0^{(n)}(1, 2, ..., n; 1', 2', ..., n') &= (-1)^n \sum_{p \in S_{2n}} \zeta^{P(p)} \theta\left(\sigma_{p(1)} - \sigma_{p(2)}\right) \theta\left(\sigma_{p(2)} - \sigma_{p(3)}\right) ... \theta\left(\sigma_{p(2n-1)} - \sigma_{p(2n)}\right) \\ &\quad \times \left\langle d_{p(1)}(\sigma_{p(1)}) ... d_{p(2n)}(\sigma_{p(2n)}) \right\rangle_0 \end{aligned}$$

- Take ∂_{σ_i}-derivative with $i \in \{2, ..., n\}$ (if $n = 1$ there is nothing to prove): The derivative acts on σ_i which occurs at two positions: (I) Act on $d_i(\sigma_i)$ which produces the $\mathcal{G}_{0,i}^{-1}$ as in the preparation. (II) Act on the two $\theta(...)$ with σ_i in their arguments.

$$\mathcal{G}_{0,i}^{-1} \cdot \mathcal{G}_0^{(n)} = -\partial_{\sigma_i}^{(\theta)} \mathcal{G}_0^{(n)} \tag{146}$$

- For the rhs, consider the two permutations which put $\sigma_i = \tau_i$ together with τ'_j in a θ-function (neighboring in permutation, either $\tau_i > \tau'_j$ or $\tau_i < \tau'_j$). These contributions are

$$\mathcal{G}_0^{(n)} = \left[...\theta(\tau_i - \tau'_j)...\right] \left\langle ...a_{\nu_i}(\tau_i) a^\dagger_{\nu'_j}(\tau'_j) ... \right\rangle_0 + \zeta \left[...\theta(\tau'_j - \tau_i)...\right] \left\langle ...a^\dagger_{\nu'_j}(\tau'_j) a_{\nu_i}(\tau_i) ... \right\rangle_0 + ... \tag{147}$$

  And the ... are the **same** strings of θ-functions and operators in both cases. Acting with $-\partial_{\sigma_i}^{(\theta)}$ we have analogous to Eq. (142) for the single-particle case from the a-operator algebra:

$$-\partial_{\tau_i}^{(\theta)} \mathcal{G}_0^{(n)} = -\left[...\delta(\tau_i - \tau'_j)...\right] \left\langle ...\delta_{\nu_i, \nu'_j} ... \right\rangle_0 + ... \tag{148}$$

- For the other cases where τ_i is together with τ_j (corresponding to two annihilation operators placed together), we have $[a_{\nu_i}, a_{\nu_j}]_\zeta = 0$ and the contribution vanishes.

- By taking $-\partial_{\sigma_i}^{(\theta)} \mathcal{G}_0^{(n)}$ we have deleted one annihilation and one creation operator are thus left with a a sum over $\mathcal{G}_0^{(n-1)}$.

$$\mathcal{G}_{0,\sigma_i}^{-1} \cdot \mathcal{G}_0^{(n)} = \sum_{j=1}^{n} \zeta^{j+i} \delta_{\nu_i, \nu'_j} \delta(\tau_i - \tau'_j) \mathcal{G}_0^{(n-1)}\left(\nu_1\tau_1, ..., \cancel{\nu_i\tau_i}, ..., \nu_n\tau_n; \nu'_1\tau'_1, ..., \cancel{\nu'_j\tau'_j}, ..., \nu'_n\tau'_n\right) \tag{149}$$

- The sign in Eq. (148) cancels with the relative sign between $\mathcal{G}^{(n)}$ and $\mathcal{G}^{(n-1)}$ due to the deliberately chosen prefactor $(-1)^n$ in the definition of $\mathcal{G}^{(n)}$, see Eq. (136).

- The sign ζ^{j+i} comes from moving $a^\dagger_{\nu'_j}(\tau'_j)$ from position $2n + 1 - j$ to position $i + 1$ so that it sits right of $a_{\nu_i}(\tau_i)$. This causes a sign of $\zeta^{2n-i-j} = \zeta^{i+j}$.

- In Eq. (149), we now insert the EoM of the single-particle GF, $\mathcal{G}_0$ in Eq. 143 and replace:

$$\delta(\tau_i - \tau'_j)\delta_{\nu_i, \nu'_j} = \sum_\mu \mathcal{G}_0^{-1}(\tau_i\nu_i, \tau'_j\mu) \mathcal{G}_0(\mu\tau_i, \nu'_j\tau'_j) \tag{150}$$

  Multiplying with $\mathcal{G}_{0,\sigma_i}$ from the left yields:

$$\mathcal{G}_0^{(n)}(\nu_1\tau_1, ..., \nu_n\tau_n; \nu'_1\tau'_1, ..., \nu'_n\tau'_n) = \sum_{j=1}^{n} \zeta^{j+i} \mathcal{G}_0(\nu_i\tau_i, \nu'_j\tau'_j) \mathcal{G}_0^{(n-1)}\left(\nu_1\tau_1, ..., \cancel{\nu_i\tau_i}, ..., \nu_n\tau_n; \nu'_1\tau'_1, ..., \cancel{\nu'_j\tau'_j}, ..., \nu'_n\tau'_n\right) \tag{151}$$

- This is exactly the iteration formula for the determinant ($\zeta = -1$) or the permanent ($\zeta = +1$). Thus, via the remark below Eq. (138), this proves the theorem.

Exercises

Exercise 5.1. Properties of imaginary time GF $\mathcal{G}_{AB}(\tau)$

Consider the imaginary time GF of Eq. (110) and prove the properties (i) of time translation invariance in Eq. (113), (ii) the restriction $\tau \in (-\beta, \beta)$ for the argument [Hint: Use Lehmann representation] and (iii) the boundary condition in Eq. (114).

Exercise 5.2. Lehmann representation of Matsubara GF and anomalous contribution

Starting from the definition in Eq. (116), follow similar steps as in Sec. 4.2 and introduce the Lehmann representation for the Matsubara Green function (for general $\zeta = \pm 1$),

$$\mathcal{G}_{AB}\left(i\omega_n\right) \equiv -\frac{1}{Z}\sum_{m,m'} e^{-\beta E_{m'}} \left\langle m'|A|m\right\rangle \left\langle m|B|m'\right\rangle \begin{cases} \beta & : i\omega_n + E_{m'} - E_m = 0, \\ \frac{\zeta e^{(E_{m'}-E_m)\beta}-1}{i\omega_n + E_{m'} - E_m} & : \text{otherwise.} \end{cases} \tag{152}$$

The upper line is called the "anomalous" contribution (often missing in textbooks!), it can only occur for the bosonic case (why?) and we will discuss its physical meaning later in Sec. 6. For $i\omega_n \to z \notin \mathbb{R}$, Eq. (152) confirms that $\mathcal{G}_{AB}(i\omega_n \to z)$ is analytic. Derive also the Lehmann representation of the (real-frequency) retarded GF, compare to Eq. (152) and confirm that $\mathcal{G}_{AB}(i\omega_n \to \omega + i\eta) = G^R_{AB}(\omega)$ as shown in the lecture by other means.

Exercise 5.3. Polarizability of non-interacting electrons (I): Lindhard function

The polarizability describes how the charge distribution ρ is modified by a perturbing external electric field. Let the field be characterized by frequency ω and momentum $\mathbf{q} \neq 0$. In Sec. 6 we will see that under suitable experimental conditions this response is given by the retarded (real frequency) correlation function with $A = B = \rho$. We consider a spatial Fourier transform to $\rho_{\mathbf{q}}$ and work in a translation invariant electron system $H_0 = \sum_{\mathbf{k}} \sum_{\sigma=\uparrow,\downarrow} \xi_{\mathbf{k}} c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}$ (a metal, say) and wish to confirm

$$G^R_{\rho_{\mathbf{q}},\rho_{-\mathbf{q}}}(\omega) \equiv \chi^R_0(\mathbf{q},\omega) = \frac{1}{V}\sum_{\mathbf{k},\sigma} \frac{n_F(\xi_{\mathbf{k}}) - n_F(\xi_{\mathbf{k}+\mathbf{q}})}{\xi_{\mathbf{k}} - \xi_{\mathbf{k}+\mathbf{q}} + \omega + i\eta} \tag{153}$$

where V is the volume and the subscript zero reminds us on the non-interacting nature. This is known as the Lindhard function. Confirm the expression for $\chi_0(\mathbf{q},\omega)$. Hint: Define a suitable **imaginary** time ordered GF (with $n = 2$ creation an annihilation operators, respectively). Simplify this GF by using Wick's theorem, then change to Matsubara frequency. Perform the resulting Matsubara sum with the techniques developed in Sec. 5.6 and finally do the necessary analytic continuation.

Exercise 5.4. Polarizability of non-interacting electrons (II): Particle-hole excitations in a metal

In the setting of Ex. 5.3, the perturbing field can cause dissipation in the metal. In general, the dissipation is proportional to $-\mathrm{Im}\chi^R_0(\mathbf{q},\omega)$ with $\chi^R_0(\mathbf{q},\omega)$ given in Eq. 153. Assume zero temperature and a parabolic dispersion $\xi_{\mathbf{k}} = k^2/(2m) - E_F$ filled up to the Fermi energy E_F. In a the parameter plane spanned by the axes q and $\omega \geq 0$, indicate the region where the dissipation is nonzero. Interpret this result in terms of particle-hole pair creation processes which take up the energy.

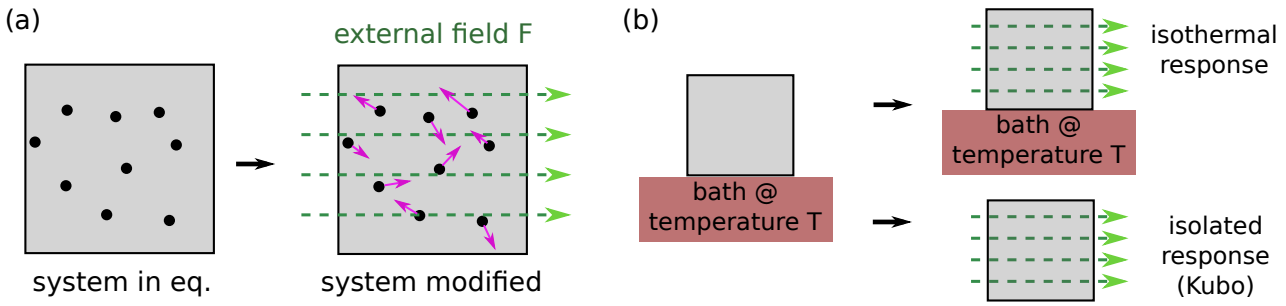

Figure 8: (a) Schematic of linear response of a system to an external perturbation ("field") F. (b) The situation depends on the presence of equilibration during the measurement.

6 Measurement: Linear response theory

Idea:

- Define measurement setup with weak probe field.
- Define susceptibility as outcome of measurement, connect to correlation function.
- Different measurement protocols relate to different correlation functions.

6.1 Measurement situations

- A system in equilibrium is exposed to a **weak** external perturbation F (electric field, magnetic field, temperature gradient, ...)
- Measure average of operator O that depends on F, $\langle O \rangle (F)$,
- The $\langle O \rangle (F)$ can be expanded in F, we are interested in the linear contribution.

$$\langle O \rangle (F) = \langle O \rangle + \frac{\partial \langle O \rangle (F)}{\partial F}|_{F=0} \cdot F + \mathcal{O}(F^2) \tag{154}$$

- The linear response term is also called the susceptibility

$$\frac{\partial \langle O \rangle (F)}{\partial F}|_{F=0} \equiv \chi \tag{155}$$

- Goal: Calculate χ theoretically. For this, it is crucial to distinguish between two experimental situations. (there are other more exotic situations)
- **Isothermal response:** The system remains coupled to the bath when F is applied (or: system that is always coupled to bath has time to equlibrate), the state is always $\rho \sim e^{-\beta H(F)}$ with β unchanged $\rightarrow$ isothermal susceptibility χ^I.
- **Isolated (Kubo) response**: The system is isolated from the bath when F is applied (or system coupled to bath has *no* time to equilibrate), the state is changed $\rho \not\sim e^{-\beta H(F)}$ $\rightarrow$ Kubo susceptibility χ^K.
- Hamiltonian in the presence of perturbation F:

$$H \rightarrow H(F) = H + \underbrace{\frac{\partial H(F)}{\partial F}|_{F=0}}_{\equiv H_1} \cdot F + \mathcal{O}(F^2) \tag{156}$$

  For linear response it is sufficient to focus on linear part.

Example: Electrons in B-field

- Consider an electron coupled to a magnetic field $\mathbf{B}$, so that we have a vector $\mathbf{F} = \mathbf{B}$. The Hamiltonian reads $H(\mathbf{B}) = H - \mathbf{m} \cdot \mathbf{B}$ with magnetic moment

$$\mathbf{m} = \mathbf{m}_S + \mathbf{m}_L = -\mathbf{H}_1 \tag{157}$$

  which splits into spin ($\mathbf{m}_S$) and "orbital" part ($\mathbf{m}_L$, due to movement of electron).

- Orbital part: $\mathbf{m}_L = -\mu_B \mathbf{L}/\hbar$ with $\mathbf{L}$ the angular momentum operator. Here, $\mu_B = e\hbar/(2m_e)$ is the Bohr magneton. The orbital part can be understood classically as a ring-current.

- Spin part: $\mathbf{m}_S = -g_e \mu_B \mathbf{S}/\hbar$ with $\mathbf{S}$ the spin operator and Landé-factor $g_e \simeq 2.0023$ (with QED correction, we approximate $g_e \equiv 2$). The spin part is of purely quantum nature. The spin part will be considered further in Ex. 6.1.

6.2 Theory of isothermal response

- We assumed that the perturbation is slow enough so that the system equilibrates $\rho \sim e^{-\beta H(F)}$, the observable is

$$\langle O \rangle (F) = \frac{1}{Z(\beta, F)} \mathrm{Tr} \left[e^{-\beta H(F)} O \right] \tag{158}$$

  with $Z(\beta, F) = \mathrm{Tr}\, e^{-\beta H(F)}$.

- Naive attempt to susceptibility:

$$\partial_F e^{-\beta H(F)} \stackrel{?}{=} \begin{cases} -\beta e^{-\beta H(F)} \partial_F H(F) \\ -\beta \left[\partial_F H(F) \right] e^{-\beta H(F)} \end{cases} \tag{159}$$

  The right hand sides are not the same unless $[H(F), \partial_F H(F)] = 0$. Correct way: Series expansion of $e^{-\beta H(F)}$, but this is complicated.

- Alternative approach: Use differential equation for auxiliary operator

$$A(\beta, F) \equiv \partial_F e^{-\beta H(F)} \tag{160}$$

- Find β-derivative of A, set $\partial_F H(F) \equiv H'(F)$: $\partial_\beta A(\beta, F) = -\partial_F \left[H(F) e^{-\beta H(F)} \right]$. Express this via $A(\beta, F)$:

$$\boxed{\partial_\beta A(\beta, F) = -H(F) A(\beta, F) - H'(F) e^{-\beta H(F)}, \quad A(\beta = 0, F) = 0} \tag{161}$$

  We thus obtained a homogeneous linear first order differential equation.

- Solution of homogeneous equation (only first term on rhs): $A_0(\beta, F) = e^{-\beta H(F)}$

- Ansatz for **in**homogeneous equation:

$$A(\beta, F) = A_0(\beta, F) \cdot G(\beta, F) = e^{-\beta H(F)} G(\beta, F) \tag{162}$$

  Insert in Eq. (161),

$$\partial_\beta G(\beta, F) = -e^{\beta H(F)} H'(F) e^{-\beta H(F)} \;\rightarrow\; G(\beta, F) = G(0, F) - \int_0^\beta \mathrm{d}\tau\, e^{\tau H(F)} H'(F) e^{-\tau H(F)} \tag{163}$$

- Insert in $A(\beta, F)$ and use initial condition:

$$A(\beta, F) = -e^{-\beta H(F)} \int_0^\beta \mathrm{d}\tau\, e^{\tau H(F)} H'(F) e^{-\tau H(F)} \tag{164}$$

- Use this result to compute the F-derivative of $\langle O\rangle(F)$ to linear order:

$$\begin{aligned}\partial_F \langle O\rangle(F) &= \partial_F\left(\frac{1}{Z(\beta,F)}\mathrm{Tr}\left[e^{-\beta H(F)}O\right]\right)\\ &= -\frac{1}{Z^2(\beta,F)}\left\{\partial_F Z(\beta,F)\right\}\mathrm{Tr}\left[e^{-\beta H(F)}O\right]+\frac{1}{Z(\beta,F)}\mathrm{Tr}\left[\partial_F e^{-\beta H(F)}O\right]\end{aligned} \tag{165}$$

  - For the curly brackets in the first term, we use:

$$\begin{aligned}\partial_F Z(\beta,F) &= \mathrm{Tr}A(\beta,F)\\ &= -\int_0^\beta \mathrm{d}\tau\,\mathrm{Tr}\left[e^{-\beta H(F)}e^{\tau H(F)}H'(F)e^{-\tau H(F)}\right]\\ \text{(cycl.)} &= -\int_0^\beta \mathrm{d}\tau\,\mathrm{Tr}\left[e^{-\beta H(F)}H'(F)\right]\\ &= -\beta\left\langle H'(F)\right\rangle Z(\beta,F)\end{aligned}$$

  - For the second term, we use:

$$\begin{aligned}\frac{1}{Z(\beta,F)}\mathrm{Tr}\Big[\underbrace{\partial_F e^{-\beta H(F)}}_{A(\beta,F)}O\Big] &= -\frac{1}{Z(\beta,F)}\int_0^\beta \mathrm{d}\tau\,\mathrm{Tr}\left[e^{-\beta H(F)}e^{\tau H(F)}H'(F)e^{-\tau H(F)}O\right]\\ &= -\frac{1}{Z(\beta,F)}\int_0^\beta \mathrm{d}\tau\,\mathrm{Tr}\left[e^{-\beta H(F)}H'(F)(\tau)O\right]\\ &= -\int_0^\beta \mathrm{d}\tau\,\left\langle H'(F)(\tau)O\right\rangle_F\end{aligned}$$

  where $\langle ...\rangle_F = \mathrm{Tr}\left[e^{-\beta H(F)}...\right]/Z(\beta,F)$.

- Insert in Eq. (165),

$$\partial_F\langle O\rangle(F) = -\int_0^\beta \mathrm{d}\tau\,\left[\left\langle H'(F,\tau)O\right\rangle_F - \left\langle H'(F)\right\rangle_F\langle O\rangle_F\right] \tag{166}$$

  and set $F=0$, use $\langle ...\rangle = \mathrm{Tr}\left[e^{-\beta H}...\right]/Z$ and recall $H'(F)|_{F=0}\equiv H_1$:

$$\begin{aligned}\chi^I_{H_1O} &\equiv \partial_F\langle O\rangle(F)|_{F=0}\\ &= -\int_0^\beta \mathrm{d}\tau\,\left[\left\langle H_1(\tau)O\right\rangle - \left\langle H_1\right\rangle\langle O\rangle\right]\end{aligned}$$

- The final result for the isothermal susceptibility is

$$\boxed{\chi^I_{H_1O} = \mathcal{G}_{H_1O}(i\omega_n=0) + \beta\left\langle H_1\right\rangle\langle O\rangle} \tag{167}$$

- Remarks and interpretation:
  - since we set $F=0$, the averages $\langle ...\rangle$ are to be computed with respect to the unperturbed system ($H_1=0$)
  - the last term on the rhs of Eq. (167) is not substantial: We can redefine $O\to O-\langle O\rangle$ to make it vanish. This means we only measure the *change* in the observable
  - imaginary time occurs naturally in this context (via differential equation):
    The isothermal response of observable O under perturbation H_1 is given by imaginary time (ordered) GF of H_1 and O averaged over *imaginary* times τ
  - this relates the Matsubara GF at zero Matsubara frequency $i\omega_n=0$ to a measurable quantity
  - since H_1 and O are bosonic, we have $\chi^I_{H_1O} = \chi^I_{OH_1}$

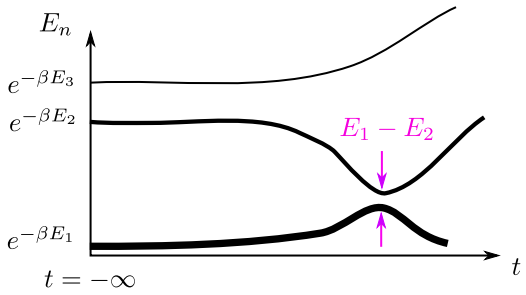

Figure 9: The instantaneous eigenenergies of $H(t) = H + F(t) \cdot H_1$, the $F(t)$ is switched on slowly starting from $t = -\infty$. The assumption for the dynamic-isolated (Kubo) response is that only the states change, not the occupations (line thickness). The occupations are taken to be the initial ones $e^{-\beta H}$ for the duration of the measurement. The pink arrows indicate the smallest gap which controls the adiabatic time scale.

6.3 Theory of isolated (Kubo) response

- As the system does not equilibrate (on the timescales considered) we treat the perturbation as dynamic $F \to F(t)$.
- Perturbation is absent at $t = -\infty$ $[F(t \to -\infty) = 0]$ and sufficiently slow (see below). Hamiltonian:

$$H(F) = H + F(t) \cdot H_1 \equiv H(t) \tag{168}$$

- To find $O(t)$, we need to know the density matrix which can be always diagonalized,

$$\rho(t) = \sum_n \lambda_n(t) \left|\psi_n(t)\right\rangle \left\langle\psi_n(t)\right|, \quad \sum_n \lambda_n(t) = 1. \tag{169}$$

- Equation of motion: Apply Schrödinger equation, $i\partial_t \left|\psi_n(t)\right\rangle = H(t) \left|\psi_n(t)\right\rangle$, find

$$\partial_t \rho(t) = -i \left[H(t), \rho(t)\right] + \sum_n \left(\partial_t \lambda_n(t)\right) \left|\psi_n(t)\right\rangle \left\langle\psi_n(t)\right| \tag{170}$$

  The first term is due to the change of the eigenstates due to the perturbation $F(t)$, the second is due to the change in occupation numbers.

- As discussed in Sec. 6.1, we start (at $t = -\infty$) in a thermal state

$$\rho = \frac{1}{Z} e^{-\beta H} = \sum_n \frac{e^{-\beta E_n}}{Z} \left|n\right\rangle \left\langle n\right| \tag{171}$$

  where $H = H(t = -\infty)$ and $H \left|n\right\rangle = E_n \left|n\right\rangle$ are eigenstates.

Assumption:

- The occupation numbers $\lambda_n(t)$ in Eq. (169) do not change with t when the perturbation is switched on:

$$\lambda_n(t) \stackrel{!}{=} \frac{e^{-\beta E_n}}{Z} \;\to\; \partial_t \lambda_n(t) = 0 \tag{172}$$

- Justification I: Absence of scattering (Fig. 9)
  - If the perturbation is slow, $F(t) \sim e^{\eta t}$ with $\eta \to 0$, then the adiabatic theorem tells us that eigenstate $\left|n\right\rangle$ of H evolve into the continuously deformed eigenstate $\left|n(t)\right\rangle$ of $H(t)$ and does not scatter into other states $\left|m(t)\right\rangle$.
  - For finite time-scale of the perturbation T_F, the adiabatic theorem still holds for $T_F \gg T_{ad} = \hbar/(E_m - E_n)$.

- Justification II: Absence of thermalization
  - If the system is strongly coupled to an external bath, then $\lambda_n(t) = e^{-\beta E_n(t)}/Z(t)$. To avoid this, we assumed that the system is isolated.
  - If the system is not perfectly isolated, then thermalization only happens after a timescale T_{th}
- In practice, require the perturbatino time scale T_F to fulfill:

$$T_{ad} \ll T_F \ll T_{th} \tag{173}$$

Then we have

$$\boxed{\partial_t \rho(t) = -i\left[H(t), \rho(t)\right], \quad \rho(t=-\infty) = \rho_0 = e^{-\beta H}/Z} \tag{174}$$

Kubo formula

- We now use the above assumption to find the "Kubo" susceptibility which tells us about the linear response of the observable at time t to the perturbation at time t':

$$\frac{\partial \langle O \rangle (t)(F)}{\partial F(t')}|_{F=0} \equiv \chi^K_{OH_1}(t,t') \tag{175}$$

- Expand density matrix $\rho(t) = \rho_0 + \rho_1(t) + \mathcal{O}(F^2)$ with ρ_1 of order F and $\rho_1(t=-\infty) = 0$. Insert in evolution equation

$$\begin{aligned} \partial_t \rho(t) &= \partial_t \rho_1(t) + \mathcal{O}(F^2) \\ &= -i\left[H + F(t)H_1, \rho_0 + \rho_1(t)\right] + \mathcal{O}(F^2) \\ &= -i\left[H, \rho_1(t)\right] - iF(t)\left[H_1, \rho_0\right] + \mathcal{O}(F^2) \end{aligned}$$

- We solve the differential equation for $\rho_1(t)$ by the ansatz $\rho_1(t) \equiv e^{-iHt} G(t) e^{+iHt}$ (like interaction picture), find with $[H, \rho_0] = 0$:

$$e^{-iHt}\left(\partial_t G(t)\right) e^{+iHt} = -iF(t)\left[H_1, \rho_0\right] \;\rightarrow\; \partial_t G(t) = -iF(t)\left[e^{itH} H_1 e^{-itH}, \rho_0\right] = -iF(t)\left[H_1(t), \rho_0\right] \tag{176}$$

where $H_1(t)$ is the Heisenberg time evolution of H_1 with respect to H.

- Integrate to find $G(t)$, use $G(t=-\infty) = 0$, $G(t) = -i\int_{-\infty}^{t} \mathrm{d}\tilde{t}\, F(\tilde{t})\left[H_1(\tilde{t}), \rho_0\right]$ and insert in $\rho_1(t)$:

$$\rho_1(t) = -i\int_{-\infty}^{t} \mathrm{d}\tilde{t}\, F(\tilde{t})\left[H_1(\tilde{t}-t), \rho_0\right] \tag{177}$$

- Compute average of observable

$$\begin{aligned} \partial_{F(t')} \langle O \rangle_t (F)|_{F=0} &= \partial_{F(t')} \mathrm{Tr}\left[O\left\{\rho_0 + \rho_1(t)\right\}\right]|_{F=0} \\ &= \partial_{F(t')} \mathrm{Tr}\left[O\rho_1(t)\right]|_{F=0} \end{aligned} \tag{178}$$

Prepare with $\partial F(\tilde{t})/\partial F(t') = \delta(\tilde{t} - t')$,

$$\partial_{F(t')} \rho_1(t) = -i\theta(t-t')\, F(t')\left[H_1(t'-t), \rho_0\right] \tag{179}$$

and find:

$$\begin{aligned} \chi^K_{OH_1}(t,t') &= \frac{\partial \langle O \rangle (t)(F)}{\partial F(t')}|_{F=0} \\ &= -i\theta(t-t')\mathrm{Tr}\left\{O\left[H_1(t'-t), \rho_0\right]\right\} = \chi^K_{OH_1}(t-t') \end{aligned}$$

- We use $H_1(t) = e^{itH} H_1 e^{-itH}$ and $[H, \rho_0] = 0$ along with the cyclic property of the trace to obtain the **Kubo formula** in its usual form:

$$\boxed{\chi^K_{OH_1}(t-t') = -i\theta(t-t') \left\langle [O(t), H_1(t')] \right\rangle = G^R_{OH_1}(t-t')} \tag{180}$$

- Remarks and interpretation:
  - averages and Heisenberg time-evolutions are to be computed with respect to the unperturbed system ($H_1 = 0$)
  - Kubo response corresponds to the retarded (real-time) GF for operators O and H_1
  - retardation is encoded in $\theta(t-t')$: No response signal before the perturbation
  - the response from the full time-trace $F(t)$ can be found via a time-integral of Eq. (180):

$$\langle O \rangle (t) = \int_{-\infty}^{+\infty} \mathrm{d}t' \; \chi^K_{OH_1}(t-t') \cdot F(t') \tag{181}$$

  - Fourier transform of $\chi^K(t)$ (perturbation with frequency ω, c.f. Eq. 86):

$$\chi^K_{OH_1}(\omega) = \lim_{\eta \to 0} \int_{-\infty}^{\infty} \mathrm{d}t \, e^{i\omega t - \eta t} \chi^K_{OH_1}(t) = G^R_{OH_1}(\omega) \tag{182}$$

Conclusion

- The Matsubara GF contains both the static-isothermal (assume $\langle O \rangle = 0$) and dynamic-isolated (Kubo) response

$$\mathcal{G}_{OH_1}(i\omega_n) \to \begin{cases} \chi^I_{OH_1} & : i\omega_n = 0 \\ \chi^K_{OH_1}(\omega) & : i\omega_n \to \omega + i\eta \end{cases} \tag{183}$$

- Question: What happens to the Kubo response $\chi^K_{OH_1}(\omega)$ in the limit $\omega \to 0$? Does it agree to the static-isothermal response $\chi^I_{OH_1}$?

$$\lim_{\omega \to 0} \chi^K_{OH_1}(\omega) \stackrel{?}{=} \chi^I_{OH_1} \tag{184}$$

- It seems that this should be the case since both sides seem to correspond to $\mathcal{G}_{OH_1}(i\omega_n = z = 0)$. However, since $\mathcal{G}_{OH_1}(z)$ is not necessarily analytic for $z \in \mathbb{R}$, the two expressions might differ:

$$\lim_{\omega \to 0} \chi^K_{OH_1}(\omega) = \lim_{\eta \to 0} \mathcal{G}_{OH_1}(i\eta) \neq \mathcal{G}_{OH_1}(0) = \chi^I_{OH_1} \tag{185}$$

  This interesting question is further analyzed in Ex. 6.3.

Exercises

Exercise 6.1. Isothermal response of single quantum spin of length S

Consider a single localized quantum spin of length S in a magnetic field B in z-direction. The Hamiltonian reads $H = hS^z$ where we abbreviate $h = 2\mu_B B$ (c.f. Sec. 6.1, no orbital contribution). Assume that the spin is in equilibrium with a thermal bath at temperature $T = 1/\beta$. From elementary QM recall the spin algebra for spin operators S^x, S^y, S^z and that S can be integer or half-integer. Obtain the partition function

$$Z = \sinh\left[\beta h(S + 1/2)\right] / \sinh\left[\beta h/2\right]. \tag{186}$$

Use the free energy $F = -T \ln Z$ and the appropriate derivative to find the magnetization $\langle S^z \rangle$,

$$\langle S^z \rangle = -\partial_h F = \frac{1}{2} \left\{ \coth\left(\frac{y}{2}\right) - (1+2S) \coth\left([S+1/2]\, y\right) \right\} \tag{187}$$

where $y \equiv \beta h$. This function is known as the *Brillouin function.*

Now set $h = 0$ (such that $H = 0$) and compute the imaginary time ordered GF $\mathcal{G}^{(h=0)}_{S^z S^z}(\tau)$ and its Fourier transform $\mathcal{G}^{(h=0)}_{S^z S^z}(i\omega_n)$. Apply *linear* response theory for the perturbation hS^z. Find the isothermal static susceptibility from $\chi^{T(h=0)}_{S^z S^z} = \mathcal{G}^{(h=0)}_{S^z S^z}(i\omega_n = 0)$ and compare to the linear-in-h term of the series expansion of the exact result 187 (which holds for any h). What is the physical reason for its divergence as $T \to 0$? Bonus: Find the Kubo susceptibility $G^{R(h=0)}_{S^z S^z}(\omega)$ and obtain its $\omega \to 0$ limit. Is it the same as $\chi^{T(h=0)}_{S^z S^z}$?

Exercise 6.2. Kubo formula for electrical conductivity

One of the most important applications of the Kubo formula is the calculation of the electrical conductivity, $\sigma^{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t')$ where $\alpha, \beta = x, y, z$ are directions in real space. In the spirit of Eq. (181), the current density in direction α at space-time point $\mathbf{r}t$ is the summed response to fields at space-time points $\mathbf{r}'t'$ and in directions β as follows:

$$j^\alpha(\mathbf{r}t) = \int \mathrm{d}t' \int \mathrm{d}\mathbf{r}' \sum_\beta \sigma^{\alpha\beta}(\mathbf{r}t, \mathbf{r}'t') E^\beta(\mathbf{r}'t') \tag{188}$$

We consider free electrons $H_0 = \frac{1}{2m}\sum_\sigma \int \mathrm{d}\mathbf{r}\, \Psi^\dagger_\sigma(\mathbf{r}) \left(-i\hbar\nabla_\mathbf{r}\right)^2 \Psi_\sigma(\mathbf{r})$ that are perturbed by the probe electric field $\mathbf{E}(\mathbf{r}t)$. We want to find an expression for the temporal Fourier transformed conductivity

$$\sigma^{\alpha\beta}(\mathbf{r}, \mathbf{r}'; \omega) \equiv \int_0^\infty \mathrm{d}t\, e^{i\omega t}\, \sigma^{\alpha\beta}(\mathbf{r}t, \mathbf{r}'0) \tag{189}$$

using the Kubo formula. The electric field is expressed via a vector potential as $\mathbf{E} = -\partial_t \mathbf{A}$ (we chose a gauge in which the electric potential vanishes, $\phi = 0$). The Hamiltonian including the perturbation is then given by (electronic charge $e < 0$, speed of light $c = 1$)

$$H = \frac{1}{2m}\sum_\sigma \int \mathrm{d}\mathbf{r}\, \Psi^\dagger_\sigma(\mathbf{r}) \left(-i\hbar\nabla_\mathbf{r} - e\mathbf{A}\right)^2 \Psi_\sigma(\mathbf{r}). \tag{190}$$

From elementary quantum mechanics recall the current density operator $\hat{\mathbf{j}} = \hat{\mathbf{j}}_p + \hat{\mathbf{j}}_d$ with paramagnetic and diamagnetic part

$$\hat{\mathbf{j}}_p = \sum_\sigma \frac{e\hbar}{2mi}\left(\Psi^\dagger_\sigma(\mathbf{r})\left[\nabla_\mathbf{r}\Psi_\sigma(\mathbf{r})\right] - \left[\nabla_\mathbf{r}\Psi^\dagger_\sigma(\mathbf{r})\right]\Psi_\sigma(\mathbf{r})\right), \qquad \hat{\mathbf{j}}_d = -\frac{e^2}{m}\mathbf{A}\sum_\sigma \Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r}). \tag{191}$$

1. Expand H to first order in $\mathbf{A}$ to define H_1 as in the lecture and use $\mathbf{A}(\mathbf{r}, \omega) = \int_{-\infty}^\infty \mathrm{d}t\, e^{i\omega t}\, \mathbf{A}(\mathbf{r}, t)$. You should find
$$F(\omega) \cdot H_1 = -\frac{1}{i\omega}\int \mathrm{d}\mathbf{r}\, \hat{\mathbf{j}}^p(\mathbf{r}) \cdot \mathbf{E}(\mathbf{r}, \omega). \tag{192}$$

2. Compute the observable current $j^\alpha(\mathbf{r}\omega) = \left\langle \hat{j}^\alpha(\mathbf{r}\omega)\right\rangle$ in first order of $E^\beta(\omega)$ and read off $\sigma^{\alpha\beta}(\mathbf{r}, \mathbf{r}', \omega)$. You should find
$$\boxed{\sigma^{\alpha\beta}(\mathbf{r}, \mathbf{r}'; \omega) = \frac{i}{\omega} G^R_{\hat{j}^\alpha_p(\mathbf{r}), \hat{j}^\beta_p(\mathbf{r}')}(\omega) - \frac{e\rho_e(\mathbf{r})}{i\omega m}\delta(\mathbf{r} - \mathbf{r}')\delta_{\alpha\beta}}. \tag{193}$$
The last term with the charge density $\rho_e(\mathbf{r}) = e\left\langle \sum_\sigma \Psi^\dagger_\sigma(\mathbf{r})\Psi_\sigma(\mathbf{r})\right\rangle$ does not come from the Kubo formula 180 as discussed in the lecture. How does it emerge? We will further evaluate $\sigma^{\alpha\beta}(\mathbf{r}, \mathbf{r}'; \omega)$ in Sec. 7.

Exercise 6.3. Long-term memory, ergodicity and the difference between χ^T and $\chi^K(\omega \to 0)$

TODO

7 Perturbation theory and Feynman diagrams

Idea:

- Evaluate Matsubara GF in perturbation theory making use of a small parameter
- Works best with fermions or bosons because we can make use of Wick's theorem
- Introduce diagrammatic language to organize the calculation
- Apply to interacting systems and to disordered systems
- Explore schemes for infinite-order resummations of subsets of diagrams

7.1 General setup for perturbation theory of the imaginary time ordered GF

- Assume thermal equilibrium at temperature T. Split Hamiltonian $H = H_0 + W$ where H_0 is "simple" and W is a perturbation.
- From Sec. 5 we recall the definition of the imaginary time ordered GF

$$\mathcal{G}_{AB}(\tau) = -\langle T_\tau A(\tau) B\rangle = \frac{1}{Z}\mathrm{Tr}\left(e^{-(\beta-\tau)H} A e^{-\tau H} B\right) \tag{194}$$

- In Eq. (112) we already found an expression for $\mathcal{G}_{AB}(\tau)$ involving $U_I(\beta,0)$, the imaginary time evolution operator in the interaction picture:

$$\boxed{\mathcal{G}_{AB}(\tau) = -\frac{\langle T_\tau U_I(\beta,0) A_I(\tau) B\rangle_0}{\langle U_I(\beta,0)\rangle_0}} \tag{195}$$

  Recall the ingredients in this expression (from Sec. 5):
  - imaginary time ordering operator T_τ
  - operator A imaginary time evolved in the interaction picture: $A_I(\tau) = e^{H_0\tau} A e^{-H_0\tau}$
  - thermal average with respect to the unperturbed Hamiltonian $\langle ...\rangle_0 \equiv Z_0^{-1}\mathrm{Tr}\left[e^{-\beta H_0}...\right]$
  - denominator, see Eq. (109):

$$\langle U_I(\beta,0)\rangle_0 = Z_0^{-1}\mathrm{Tr}\left[e^{-\beta H_0} U_I(\beta,0)\right] = Z_0^{-1}\mathrm{Tr}\left[e^{-\beta H}\right] = Z_0^{-1} Z \tag{196}$$

  - imaginary-time evolution operator in the interaction picture

$$\boxed{U_I(\beta,0) = T_\tau \exp\left[-\int_0^\beta \mathrm{d}\tau W_I(\tau)\right] = \sum_{n=0}^{\infty} \frac{(-1)^n}{n!}\int_0^\beta \mathrm{d}\tau_1 ... \int_0^\beta \mathrm{d}\tau_n\, T_\tau W_I(\tau_1)...W_I(\tau_n)} \tag{197}$$

- Perturbation theory: Insert this expansion of $U_I(\beta,0)$ in $\mathcal{G}_{AB}(\tau)$ and evaluate the sum for $n = 0, 1, ...N$ up to some tractable order N.
- It looks as if we had to expand numerator and denominator separately, but this is not the case if we use the concept of connected GF, see Ex. 7.1.
- So far, this is completely general and not specific to A, B being fermionic or bosonic Fock-space operators. Exercise 7.2 will explore perturbation theory for quantum Heisenberg spins which is somewhat cumbersome.
- The easiest case for perturbation theory is for $A, B = a, a^\dagger$ fermionic or bosonic (or composites of $a, a^\dagger$) and a H_0 that is quadratic in the Fock space operators $a, a^\dagger$. Assume that $W \sim a^\dagger a^\dagger a a$ is quartic.
  - Wick's theorem can be applied for $\left\langle T_\tau W_I(\tau_1)...W_I(\tau_n) a_{i,I}(\tau) a_j^\dagger\right\rangle_0 \sim \mathcal{G}\cdot\mathcal{G}\cdots\mathcal{G}$ (2n+1 times $\mathcal{G}$)
  - Diagrams with simple rules help organize the calculation. Rules depend on the type of the theory.
  - Start with pair interactions for fermions.

7.2 Fermionic pair interactions

- Consider fermionic field annihilation operators $\Psi(\sigma,\mathbf{r})$ where $\sigma\in\{\uparrow,\downarrow\}$ is spin. The Hamiltonian splits in quadratic and interaction terms as $H=H_0+W$, with

$$\begin{aligned} H_0 &= \sum_{\sigma}\int \mathrm{d}\mathbf{r}\ \Psi^{\dagger}(\sigma,\mathbf{r})h_0(\mathbf{r})\Psi(\sigma,\mathbf{r}),\\ W &= \frac{1}{2}\sum_{\sigma_1,\sigma_2}\int \mathrm{d}\mathbf{r}_{1,2}\ \Psi^{\dagger}(\sigma_1,\mathbf{r}_1)\Psi^{\dagger}(\sigma_2,\mathbf{r}_2)\,W\left(\sigma_2,\mathbf{r}_2;\sigma_1,\mathbf{r}_1\right)\ \Psi(\sigma_2,\mathbf{r}_2)\Psi(\sigma_1,\mathbf{r}_1) \end{aligned} \tag{198}$$

- We have assumed that the single-particle Hamiltonian is not spin dependent. Further, we chose the interaction to be of density-density type so that no spin-flips occur.

- Consider interaction-picture time evolution for operators $(e^{H_0\tau}...e^{-H_0\tau})$ and abbreviate $\Psi_I(\sigma_j,\mathbf{r}_j)(\tau_j)\equiv\Psi_j$ along with $\int_j\equiv\sum_{\sigma_j}\int\mathrm{d}\mathbf{r}_j\int_0^{\beta}\mathrm{d}\tau_j$. We dropped the subscript I since no confusion is possible.

- The Matsubara GF of Eq. (195) reads for $A=\Psi(\sigma_b,\mathbf{r}_b)$ and $B=\Psi^{\dagger}(\sigma_a,\mathbf{r}_a)$:

$$\begin{aligned} \mathcal{G}\left(b,a\right) &\equiv \mathcal{G}_{\Psi(\sigma_b,\mathbf{r}_b),\Psi^{\dagger}(\sigma_a,\mathbf{r}_a)}\left(\tau_b,\tau_a\right)=\frac{-\left\langle T_{\tau}U(\beta,0)\Psi_b\Psi_a^{\dagger}\right\rangle_0}{\langle U(\beta,0)\rangle_0}\\ &= -\frac{\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int_0^{\beta}\mathrm{d}\tau_1...\int_0^{\beta}\mathrm{d}\tau_n\left\langle T_{\tau}W(\tau_1)...W(\tau_n)\Psi_b\Psi_a^{\dagger}\right\rangle_0}{\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int_0^{\beta}\mathrm{d}\tau_1...\int_0^{\beta}\mathrm{d}\tau_n\left\langle T_{\tau}W(\tau_1)...W(\tau_n)\right\rangle_0} \end{aligned} \tag{199}$$

- The order of the operators in $W(\tau_j)$ is not arbitrary but must be kept as in Eq. (198). For this, use infinitesimal imaginary-time shifts for the creation operators $\tau_j\to\tau_j+\eta$. This shift is indicated by subscript $j_+\equiv(\sigma_j,\mathbf{r}_j,\tau_j+\eta)$:

$$\int_0^{\beta}\mathrm{d}\tau_j W(\tau_j)=\frac{1}{2}\int_j\int_{j'}\Psi_{j_+}^{\dagger}\Psi_{j'_+}^{\dagger}\underbrace{W\left(\sigma_2,\mathbf{r}_2;\sigma_1,\mathbf{r}_2\right)\delta(\tau_j-\tau_{j'})}_{W_{j,j'}}\Psi_{j'}\Psi_j \tag{200}$$

- We insert this in Eq. (199):

$$\begin{aligned} \mathcal{G}\left(b,a\right) &= \frac{-\sum_{n=0}^{\infty}\frac{(-1/2)^n}{n!}\int_{1,1'...n,n'}W_{11'}...W_{nn'}\left\langle T_{\tau}\left(\Psi_1^{\dagger}\Psi_{1'}^{\dagger}\Psi_{1'}\Psi_1\right)\cdots\left(\Psi_n^{\dagger}\Psi_{n'}^{\dagger}\Psi_{n'}\Psi_n\right)\Psi_b\Psi_a^{\dagger}\right\rangle_0}{\sum_{n=0}^{\infty}\frac{(-1/2)^n}{n!}\int_{1,1'...n,n'}W_{11'}...W_{nn'}\left\langle T_{\tau}\left(\Psi_1^{\dagger}\Psi_{1'}^{\dagger}\Psi_{1'}\Psi_1\right)\cdots\left(\Psi_n^{\dagger}\Psi_{n'}^{\dagger}\Psi_{n'}\Psi_n\right)\right\rangle_0}\\ &= \frac{\sum_{n=0}^{\infty}\frac{(-1/2)^n}{n!}\int_{1,1'...n,n'}W_{11'}...W_{nn'}\mathcal{G}_0^{(2n+1)}\left(b11'...nn';a11'...nn'\right)}{\sum_{n=0}^{\infty}\frac{(-1/2)^n}{n!}\int_{1,1'...n,n'}W_{11'}...W_{nn'}\mathcal{G}_0^{(2n)}\left(11'...nn';11'...nn'\right)} \end{aligned}$$

  and the sign is canceled by the definition of the factor $(-1)^m$ in $\mathcal{G}_0^{(m)}$.

- Apply Wick's theorem (since all time-evolution and averages are with respect to the non-interacting H_0):

$$\mathcal{G}\left(b,a\right)=\frac{\sum_{n=0}^{\infty}\frac{(-1/2)^n}{n!}\int_{1,1'...n,n'}W_{11'}...W_{nn'}\begin{vmatrix}\mathcal{G}_0\left(b;a\right)&\mathcal{G}_0\left(b;1\right)&\mathcal{G}_0\left(b;1'\right)&\cdots&\mathcal{G}_0\left(b;n'\right)\\ \mathcal{G}_0\left(1;a\right)&\mathcal{G}_0\left(1;1\right)&\mathcal{G}_0\left(1;1'\right)&\cdots&\mathcal{G}_0\left(1;n'\right)\\ \mathcal{G}_0\left(1';a\right)&\mathcal{G}_0\left(1';1\right)&\mathcal{G}_0\left(1';1'\right)&\cdots&\mathcal{G}_0\left(1';n'\right)\\ \vdots&\vdots&\vdots&\ddots&\vdots\\ \mathcal{G}_0\left(n';a\right)&\mathcal{G}_0\left(n';1\right)&\mathcal{G}_0\left(n';1'\right)&\cdots&\mathcal{G}_0\left(n';n'\right)\end{vmatrix}}{\sum_{n=0}^{\infty}\frac{(-1/2)^n}{n!}\int_{1,1'...n,n'}W_{11'}...W_{nn'}\begin{vmatrix}\mathcal{G}_0\left(1;1\right)&\mathcal{G}_0\left(1;1'\right)&\cdots&\mathcal{G}_0\left(1;n'\right)\\ \mathcal{G}_0\left(1';1\right)&\mathcal{G}_0\left(1';1'\right)&\cdots&\mathcal{G}_0\left(1';n'\right)\\ \vdots&\vdots&\ddots&\vdots\\ \mathcal{G}_0\left(n';1\right)&\mathcal{G}_0\left(n';1'\right)&\cdots&\mathcal{G}_0\left(n';n'\right)\end{vmatrix}} \tag{201}$$

- To help with the calculation of the expressions in the numerator and denominator, we represent terms of each order by a diagram.
- Diagrammatic building blocks (Fig. 10a):
  - interaction $W_{jj'}$ (wiggly lines)
  - fermion propagator $\mathcal{G}_0(j_2; j_{1+})$ (directed lines).
    The arrow on the fermion line points towards the first entry, ψ_{j_2}.
  - vertices j (dots, $\bullet_j$) where interaction lines and fermion lines connect
- First we treat the diagrammatic expansion in the denominator of Eq. (201).

Feynman rules for the denominator: n-th order "vacuum" diagram See Fig. 10(b) for the diagrams.

1) Draw a set of n wiggly interaction lines $W_{jj'}$ terminating in $2n$ vertices $\bullet_j$

2) Connect the $2n$ vertices with $2n$ (directed) fermion lines $= \mathcal{G}_0(j_2; j_{1+})$ so that one line is entering and one leaving each vertex.
There are $(2n)!$ ways of drawing the fermion lines corresponding to different diagrams for the same order n. (This corresponds to the $(2n)!$ terms in the determinant of a $2n \times 2n$ matrix.)

3) For each of the diagrams perform the sum over internal variables, at each vertex $\int_j \delta_{\sigma_j^{in},\sigma_j^{out}} = \sum_{\sigma_j} \delta_{\sigma_j^{in},\sigma_j^{out}} \int \mathrm{d}\mathbf{r}_j \int_0^\beta \mathrm{d}\tau_j$.

4) Weigh each diagram by $\frac{(-1/2)^n}{n!}(-1)^F$ and sum all diagrams.
Here, F is the number of fermion loops (= uninterrupted sequence of fermion lines starting and ending at the same vertex).

- The sign factor $(-1)^F$ comes from the signs in the determinant.
  - The product of the diagonals is the diagram with a separate fermion loop at every vertex ($F = 2n$), it has a positive sign which agrees to $(-1)^F = (-1)^{2n} = +1$.
  - All other diagrams can be constructed one by one by exchanging the endpoints of two fermion lines.
  - Each exchange gives a factor -1 and at the same time changes the number of fermion loops F, see Fig. 10.
- The diagrammatic expansion for the denominator yields the partition function (up to a factor Z_0) since $\langle U_I(\beta, 0)\rangle_0 = Z_0^{-1} Z$.
  Diagrams contributing to these expansion are also called "vacuum diagrams" (no external lines).

Feynman rules for the numerator: n-th order

- The numerator $-\left\langle T_\tau U(\beta, 0) \Psi_b \Psi_a^\dagger \right\rangle_0$ differs from the denominator by the presence of two additional **"external"** operators $\Psi_b \Psi_a^\dagger$.
- These are treated as external vertices $\bullet_a$ and $\bullet_b$. The space-time-spin points a, b are not summed over in the diagram evaluation!
- We need to adapt Feynman rules 1 and 2.

1') Draw a set of n wiggly interaction lines $W_{jj'}$ terminating in $2n$ vertices j $\bullet_j$
and add the two external vertices $\bullet_a$ and $\bullet_b$. This makes in total $2n + 2$ vertices.

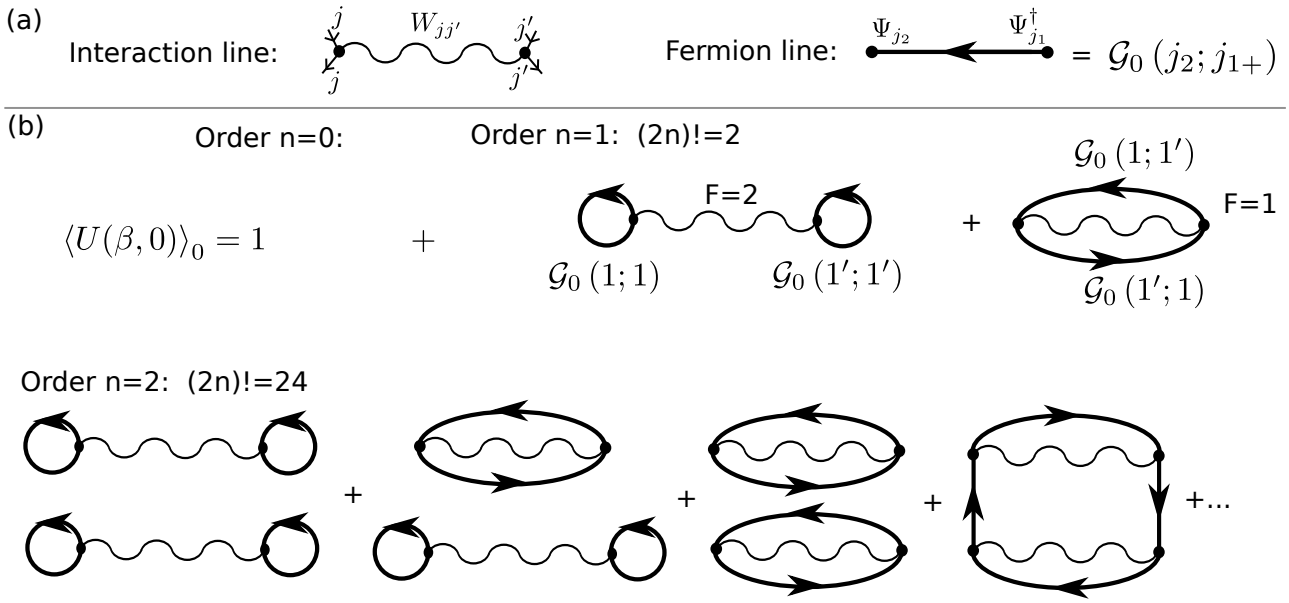

Figure 10: (a) Building blocks of Feynman diagrams and (b) vacuum diagrams for the expansion of $\langle U(\beta,0)\rangle_0$ to first order and second order (partial).

2') Connect all vertices with $2n+1$ Fermion lines:
One leaving a, one entering b, and one entering and one leaving each internal vertex j. There are $(2n+1)!$ diagrams.

- Feynman rules 3) and 4) are unchanged.
- Figure 11 shows the expansion for orders $n = 0, 1, 2$.

Cancellation of disconnected diagram parts

- Connected diagrams: Diagrams, where all internal vertices are connected to external vertices.
- Disconnected diagram: Diagrams that are not connected. They have a connected and one ore more disconnected parts.
- From the sum of all diagrams for the numerator, factor out the connected diagrams and connected parts, obtain product of two sums $(...) \times (...)$, see Fig. 11(bottom).
  - First sum: Connected diagrams.
  - Second sum: These are exactly the vacuum diagrams that appear in the expansion of $\langle U(\beta,0)\rangle_0$.
- The second sum thus cancels with the denominator.
- A formal proof is given in Ex. 7.1.

Simplified Feynman rules for $\mathcal{G}(b,a)$: Diagram topology

- It turns out that only the topology of the connected diagrams that sum up to form $\mathcal{G}(b,a)$ matters.
- Two diagrams are topological equivalent if they show the same connectivity structure when going through the diagram from the external vertices $a \to b$.
  Example: Topological equivalent pairs of $n = 1$ diagrams in second line of Fig. 11.
- At order n, out of all the connected diagrams, how many diagrams are topological equivalent at order n?
  Answer: $2^n n!$

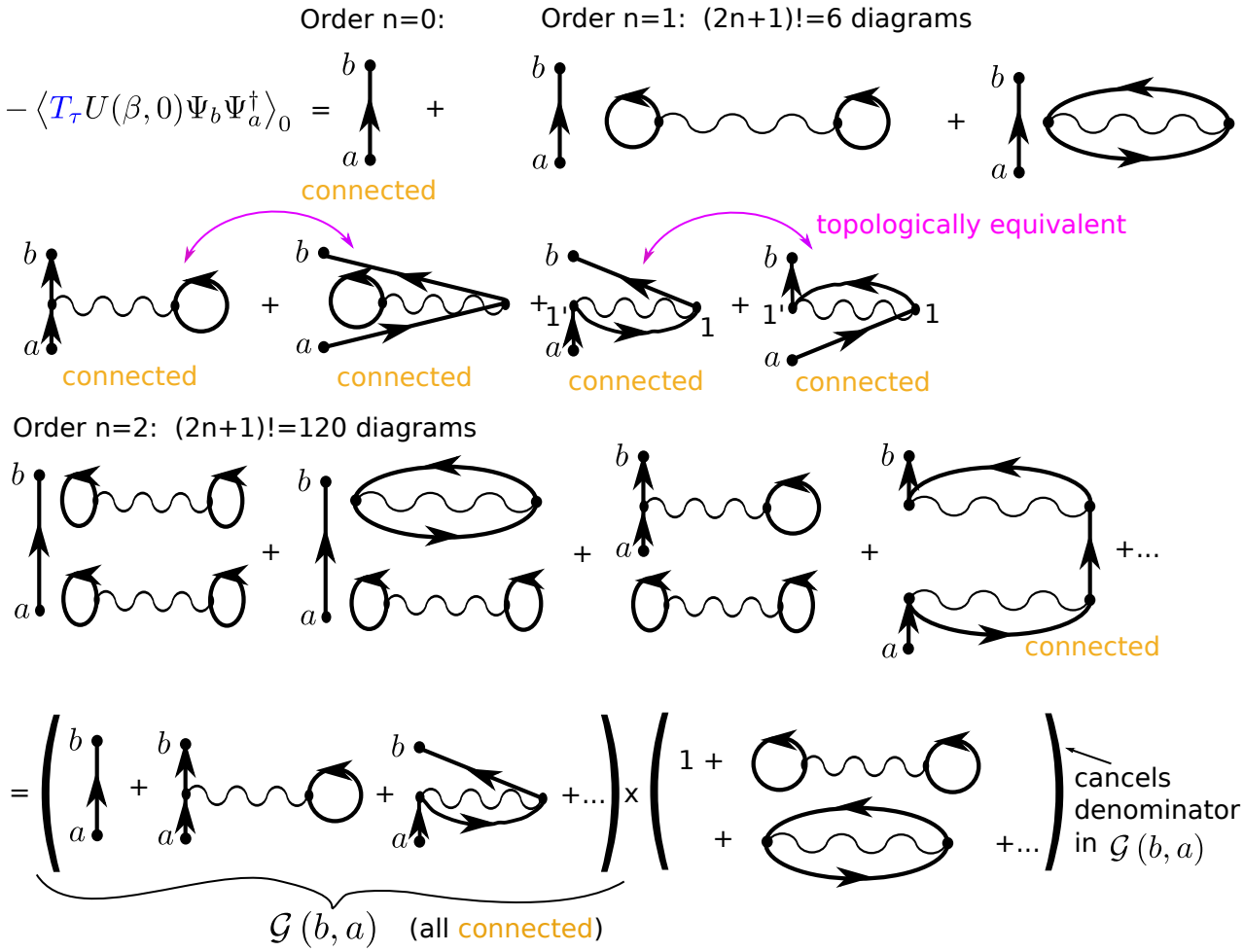

Figure 11: Building blocks of Feynman diagrams and vacuum diagrams for the expansion of the numerator in $\mathcal{G}(b,a)$ to first and second order (partially).

- For n interaction lines $W_{11'}W_{22'}...W_{nn'}$, we can associate the label-pairs $11', 22', ..., nn'$ in $n!$ ways.
- Since $W_{jj'} = W_{j'j}$, we can re-name $j \leftrightarrow j'$ (flip interaction line) $\rightarrow$ factor of 2^n for all interaction lines.

- The factor $2^n n!$ partially cancels the prefactor in Feynman rule 4). The remaining $(-1)^n$ can be absorbed into interaction line, now $-W$.

- Final Feynman rules for the expansion of $\mathcal{G}(b,a)$:

a) Draw a set of n wiggly interaction lines $-W_{jj'}$ terminating in $2n$ vertices j and add the two external vertices $\bullet_a$ and $\bullet_b$. This makes in total $2n+2$ vertices.

b) Draw all topologically different and fully connected diagrams with $2n+1$ Fermion lines: One leaving a, one entering b and one entering and one leaving each internal vertex j.

c) For each diagram topology perform the sum over internal variables, at each vertex $\int_j \delta_{\sigma_j^{in},\sigma_j^{out}} = \sum_{\sigma_j} \delta_{\sigma_j^{in},\sigma_j^{out}} \int \mathrm{d}\mathbf{r}_j \int_0^\beta \mathrm{d}\tau_j$.

d) Weigh each diagram by $(-1)^F$ and sum all diagrams.

7.3 Self-energy and Dyson's equation

- Idea: Save work by re-using lower-order diagrams as building blocks for higher order diagrams with certain properties.

Self-energy

- Definition: A diagram for $\mathcal{G}(b,a)$ is (1-line) **reducible** if the external vertices $\bullet_a$ and $\bullet_b$ can be separated by cutting a single *internal* fermion line.
  Diagrams that are not reducible are called **irreducible**. See Fig. 12(a) for some examples.

- Definition: The self energy $\Sigma(l,j)$ is the sum of all irreducible diagrams in $\mathcal{G}(b,a)$ with the external fermion lines $\mathcal{G}_0(j;a)$ and $\mathcal{G}_0(b;l)$ amputated (divided out).
  See Fig. 12(b) for the lowest order contribution to $\Sigma(l,j)$.

- The self-energy is drawn as a shaded circle. We will motivate the name below.

Dyson's equation

- We can use the self-energy to find the full GF $\mathcal{G}(b,a)$ (from now on denoted by double fermion line). All reducible diagrams are made by two or more (in the ...) self-energies connected by fermion lines $\mathcal{G}_0 \rightarrow$ Fig. 12(c)

- On the right hand side of this equation, we can identify again the full GF. This leads to **Dyson's equation** which relates $\Sigma, \mathcal{G}, \mathcal{G}_0$:

$$\mathcal{G}(b,a) = \mathcal{G}_0(b,a) + \int_{l,j} \mathcal{G}_0(b,l)\Sigma(l,j)\,\mathcal{G}(j,a) \tag{202}$$

- In practice, $\mathcal{G}_0$ is known and Σ is calculated up to some order n or approximated otherwise. Then Dyson's equation is used to find $\mathcal{G}$ which contains diagrams of infinite order!
  Unless Σ is exact, $\mathcal{G}$ from Dyson's equation is only approximate and will miss diagrams.

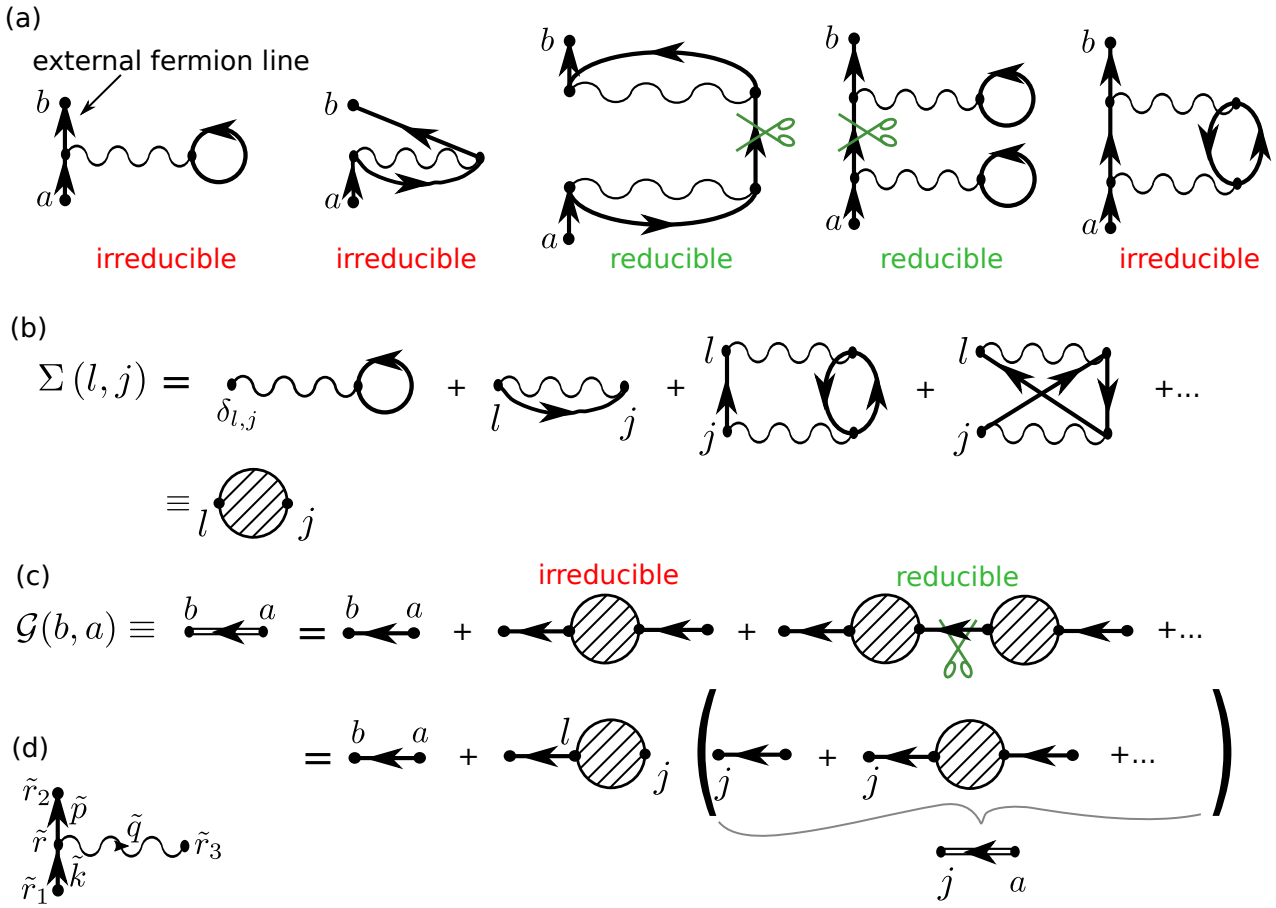

Figure 12: (a) Examples for reducible and irreducible diagrams appearing in the expansion of $\mathcal{G}(b,a)$. (b) Definition of self-energy. (c) Dyson's equation. (d) Momentum conventions for the FT at a single internal vertex.

7.4 Feynman rules in momentum and (Matsubara-) frequency representation

- Assume system is translation invariant $\rightarrow W_{jj'}$ and $\mathcal{G}_{(0)}(j,j')$ only depend on coordinate distances $\mathbf{r}_j - \mathbf{r}_{j'}$.
- These quantities will also only depend on imaginary time differences $\tau_j - \tau_{j'}$ in any case, this is due to $W_{jj'} \propto \delta(\tau_j - \tau_{j'})$, see the definition Eq. (200) and for $\mathcal{G}_{(0)}$ it was shown in Eq. (113).
- We recall the FT convention from Eq. (115) and also add the spatial FT (note the sign-convention!):

$$\mathcal{G}_{(0)}(\mathbf{r}\tau, \mathbf{r}'\tau') \equiv \frac{1}{\beta V} \sum_{\omega_n, \mathbf{k}} \mathcal{G}_{(0)}(\mathbf{k}, i\omega_n)\, e^{i\mathbf{k}\cdot(\mathbf{r}-\mathbf{r}') - i\omega_n(\tau-\tau')} \tag{203}$$

  Note: One could also start from the FT of the field operators $\Psi(\mathbf{r}, \tau)$.

- It is then convenient to also introduce the FT of the interaction line (Ω_n = bosonic Matsubara frequency, since W creates/annihilates pairs of fermions):

$$W(\mathbf{r}\tau, \mathbf{r}'\tau') \equiv \frac{1}{\beta V} \sum_{\Omega_n, \mathbf{q}} W(q) e^{i\mathbf{q}\cdot(\mathbf{r}-\mathbf{r}') - i\Omega_n(\tau-\tau')} \tag{204}$$

  We assume that $W(\mathbf{q}) = W(q)$, i.e. it only depends on magnitude q of spatial momentum $\mathbf{q}$.

- Four-momentum notation: $\tilde{k} \equiv (\mathbf{k}, i\omega_n)$, $\tilde{r} \equiv (\mathbf{r}, \tau)$ with $i\tilde{k}\cdot\tilde{r} \equiv i\mathbf{k}\cdot\mathbf{r} - i\omega_n\tau$.
- The arrows on the fermion lines and the newly added one on the interaction line indicate four-momentum.
- FT of scattering vertex, see Fig. 12(d):

$$\begin{aligned}
\int \mathrm{d}\tilde{r} \mathcal{G}_0(\tilde{r}_2, \tilde{r}) \mathcal{G}_0(\tilde{r}, \tilde{r}_1) W(\tilde{r}_3, \tilde{r}) &= \frac{\int \mathrm{d}\tilde{r}}{(\beta V)^3} \sum_{\tilde{k},\tilde{p},\tilde{q}} \mathcal{G}_0(\tilde{p}) \mathcal{G}_0(\tilde{k}) W(\tilde{q}) e^{i\left[\tilde{p}\cdot(\tilde{r}_2-\tilde{r}) + \tilde{k}\cdot(\tilde{r}-\tilde{r}_1) + \tilde{q}\cdot(\tilde{r}_3-\tilde{r})\right]} \\
&= \frac{1}{(\beta V)^2} \sum_{\tilde{k},\tilde{p},\tilde{q}} \mathcal{G}_0(\tilde{p}) \mathcal{G}_0(\tilde{k}) W(\tilde{q}) e^{i\left[\tilde{p}\cdot\tilde{r}_2 - \tilde{k}\cdot\tilde{r}_1 + \tilde{q}\cdot\tilde{r}_3\right]} \underbrace{\frac{\int \mathrm{d}\tilde{r}}{\beta V} e^{i\left[-\tilde{p}\cdot\tilde{r} + \tilde{k}\cdot\tilde{r} - \tilde{q}\cdot\tilde{r}\right]}}_{\delta_{\tilde{p}+\tilde{q},\tilde{k}}} \\
&= \frac{1}{(\beta V)^2} \sum_{\tilde{k},\tilde{p}} \mathcal{G}_0(\tilde{k}-\tilde{q}) \mathcal{G}_0(\tilde{k}) W(\tilde{q}) e^{i\left[\tilde{p}\cdot\tilde{r}_2 - \tilde{k}\cdot\tilde{r}_1 + \tilde{q}\cdot\tilde{r}_3\right]}
\end{aligned}$$

  Observations:

  - The remaining exponential is taken care of by the integrals $\int \mathrm{d}\tilde{r}_{1,2,3}$ of the neighboring vertices.
  - Four momentum is conserved at each vertex: $\tilde{k} = \tilde{p} + \tilde{q}$ (c.f. Kirchhoff rule).
  - The interaction line transfers four-momentum, but does not depend on the transferred (bosonic) Matsubara frequency.

- Modification of Feynman rules in momentum-frequency space:
  - Fermi lines are $\mathcal{G}_0(\mathbf{k}, i\omega_n)$, wiggly interaction lines are $-W(\tilde{q}) = -W(q)$
  - At vertex: Four momentum (and spin) is conserved.
  - Sum over remaining internal four-momenta and spin $\frac{1}{\beta V}\sum_{\tilde{p}}\sum_{\sigma}$
  - In "same-time" diagrams like the first two at rhs of 12(b): Recall time τ at creation operator was shifted by $+\eta$, thus $\mathcal{G}_0(\mathbf{k}, i\omega_n) \rightarrow \mathcal{G}_0(\mathbf{k}, i\omega_n)\, e^{i\omega_n\eta}$.

Dyson's equation in four-momentum

- Recall form of the non-interacting ("bare") Matsubara GF from Eq. (127): $\mathcal{G}_0(\tilde{k}) = \mathcal{G}_0(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n - \xi_\mathbf{k}}$.
- FT of Dyson's equation (202) (convolution theorem of FT):

$$\mathcal{G}(\tilde{k}) = \mathcal{G}_0(\tilde{k}) + \mathcal{G}_0(\tilde{k})\Sigma(\tilde{k})\mathcal{G}(\tilde{k}) \tag{205}$$

  This is now an algebraic equation which can be solved for the fully interacting GF $\mathcal{G}(\tilde{k})$:

$$\boxed{\mathcal{G}(\tilde{k}) = \frac{\mathcal{G}_0(\tilde{k})}{1 - \mathcal{G}_0(\tilde{k})\Sigma(\tilde{k})} = \frac{1}{i\omega_n - \xi_\mathbf{k} - \Sigma(\mathbf{k}, i\omega_n)}} \tag{206}$$

- Why the name "self-energy"?
  - The difference between non-interacting $\mathcal{G}_0(\mathbf{k}, i\omega_n)$ and full $\mathcal{G}(\mathbf{k}, i\omega_n)$ is the replacement of the "energy" $\xi_\mathbf{k} = H_{0,\mathbf{k}} \to H_{0,\mathbf{k}} + \Sigma(\mathbf{k}, i\omega_n)$.
  - Thus the (hermitian part of) the self-energy acts like an effective single-particle Hamiltonian ("energy") induced by interactions.
  - The anti-hermitian part and the $i\omega_n$-dependence go beyond this picture [→ decay time c.f. Ex. 5.6.1(d), quasiparticle weight,...]

Exercises

Exercise 7.1. Cancellation of disconnected diagrams (general case)

Consider the Hamiltonian $H = H_0 - V$ with $-V$ a perturbation and operators A and B which are not necessarily fermionic or bosonic. The expansion of the imaginary-time ordered GF in $-V$ reads [factors of $(-1)^n$ are avoided by using $-V$ as the perturbation, c.f. Eq.(199)]

$$\langle T_\tau A(\tau)B(\tau')\rangle = \frac{\sum_{n=0}^{\infty} \frac{1}{n!} \int_0^\beta \mathrm{d}\tau_1 ... \int_0^\beta \mathrm{d}\tau_n \langle T_\tau V(\tau_1)...V(\tau_n)A(\tau)B(\tau')\rangle_0}{\sum_{n=0}^{\infty} \frac{1}{n!} \int_0^\beta \mathrm{d}\tau_1 ... \int_0^\beta \mathrm{d}\tau_n \langle T_\tau V(\tau_1)...V(\tau_n)\rangle_0}. \tag{207}$$

Show that this expression can be simplified to

$$\boxed{\langle T_\tau A(\tau)B(\tau')\rangle = \sum_{n=0}^{\infty} \frac{1}{n!} \int_0^\beta \mathrm{d}\tau_1 ... \int_0^\beta \mathrm{d}\tau_n \langle T_\tau V(\tau_1)...V(\tau_n)A(\tau)B(\tau')\rangle_{0,c}} \tag{208}$$

with the subscript "c" denoting the *connected* GF. Here, connectedness of the GF (diagram) is understood with with respect to external operators $A(\tau)$, $B(\tau')$ and the formal definition is as follows:

$$\begin{aligned} \langle T_\tau V(\tau_1)...V(\tau_n)A(\tau)B(\tau')\rangle_{0,c} \;\equiv\; & \langle T_\tau V(\tau_1)...V(\tau_n)A(\tau)B(\tau')\rangle_0 \\ & - \sum_{p\in S_n} \sum_{j=0}^{n-1} \left\langle T_\tau V(\tau_{p(1)})...V(\tau_{p(j)})A(\tau)B(\tau')\right\rangle_{0,c} \left\langle T_\tau V(\tau_{p(j+1)})...V(\tau_{p(n)})\right\rangle_0 . \end{aligned} \tag{209}$$

Hint: Start from the numerator in Eq. (207) and collect all terms of order $n > m$ that contain a connected GF of order m.

Exercise 7.2. Perturbation theory for Heisenberg spins

Perturbation theory is usually employed for fermions or bosons since the Wick theorem simplifies matters enormously. Nevertheless, one can also do perturbation theory when Wick's theorem is not available, like for quantum spin operators, c.f. Ex. 6.1. This exercise considers the perturbative expansion of the spin Matsubara GF defined as the temporal Fourier transform [c.f. Eq. (116)] of

$$\mathcal{G}_{j_1 j_2}(\tau) = -\left\langle T_\tau S^z_{j_1}(\tau) S^z_{j_2}\right\rangle . \tag{210}$$

Recall that the time-ordering for spin operators works like in the bosonic case. We assume the Heisenberg spin Hamiltonian on an arbitrary lattice (with lattice sites labeled by $j = 1, 2, ..., N$),

$$H = \frac{1}{2} \sum_{j_1 \neq j_2} J_{j_1 j_2} \left(S^x_{j_1} S^x_{j_2} + S^y_{j_1} S^y_{j_2} + S^z_{j_1} S^z_{j_2} \right) \tag{211}$$

and the $N \times N$ matrix J is real and symmetric. The spin operators fulfill the spin algebra $\left[S^\alpha_{j_1}, S^\beta_{j_2} \right] = i\delta_{j_1 j_2} \sum_\gamma \epsilon^{\alpha\beta\gamma} S^\gamma_{j_1}$ where $\alpha, \beta, \gamma \in \{x, y, z\}$ and $\mathbf{S}^2_j = S(S+1)$ where S is the (integer or half-integer) spin length. We chose $H = H_0 - V$ with $H_0 = 0$ such that the interaction V is the full Heisenberg interaction. This type of perturbation theory is controlled by the smallness of the parameter βJ, i.e. it should work at large temperatures.

1. Use Eq. (208) to find the first order (in J) contribution to $\mathcal{G}_{j_1 j_2}(i\omega_n)$ in terms of the free spin GF $\mathcal{G}_0(i\omega_n) = -\int_0^\beta \mathrm{d}\tau\, e^{i\omega_n \tau} \left\langle T_\tau S^z_j(\tau) S^z_j \right\rangle_0 = -\delta_{0,\omega_n} \frac{\beta}{3} S(S+1)$, c.f. Ex. 6.1. Show that

$$\mathcal{G}^{(1)}_{j_1 j_2}(i\omega_n) = \beta^2 \delta_{0,\omega_n} J_{j_1 j_2} \left(\frac{S}{3}(S+1) \right)^2 . \tag{212}$$

   Hint: Make use of spin-rotation symmetry which forces many expectation values to vanish, e.g. $\left\langle S^\alpha_j \right\rangle_{(0)} = 0$ and $\left\langle S^\alpha_{j_1} S^\beta_{j_2} \right\rangle_{(0)} = 0$ for $\alpha \neq \beta$ (What is the precise argument?). Can you define a set of diagrammatic rules?

2. For the second order contribution $\mathcal{G}^{(2)}_{j_1 j_2}(i\omega_n)$ specialize to the non-local case $j_1 \neq j_2$ only (the local case $j_1 = j_2$ is too difficult). You should find

$$\mathcal{G}^{(1)}_{j_1 j_2}(i\omega_n)|_{j_1 \neq j_2} = \beta^3 \left(\frac{S}{3}(S+1) \right)^2 \left\{ -\delta_{n,0} \left[J \cdot J \right]_{j_1 j_2} \left(\frac{S}{3}(S+1) \right) + \left[J_{j_1 j_2} \right]^2 \left(2\frac{1-\delta_{n,0}}{(2\pi n)^2} + \delta_{n,0} \frac{1}{12} \right) \right\} . \tag{213}$$

   You will have to use the three-point free spin correlators which are non-trivial,

$$\begin{aligned} \mathcal{G}^{xyz}_0(\omega_{n1}, \omega_{n2}) &\equiv \int_0^\beta \mathrm{d}\tau_{1,2} e^{i\omega_{n1}\tau_1} e^{i\omega_{n2}\tau_2} \langle T_\tau S^x(\tau_1) S^y(\tau_2) S^z \rangle_0 \\ &= \beta \left(\frac{S}{3}(S+1) \right) \left(-\delta_{\omega_{n1},0} \Delta_{\omega_{n2}} + \delta_{\omega_{n2},0} \Delta_{\omega_{n1}} - \delta_{\omega_{n2}+\omega_{n1},0} \Delta_{\omega_{n1}} \right) , \end{aligned}$$

   where $\Delta_{\omega_n} = 1/\omega_n$ if $\omega_n \neq 0$ and zero otherwise.

Exercise 7.3. Self-energy diagrams for pair interaction

For the situation of fermionic pair interactions $W(\mathbf{q})$ as in Sec. 7.2, compute the first two self-energy diagrams $\Sigma_\sigma(\mathbf{k}, i\omega_n)$ on the rhs of Fig. 12(b), assuming external four momentum $(\mathbf{k}, i\omega_n)$. You should find $W(0)n$ (where $n = [N_\uparrow + N_\downarrow]/V$ is the total particle density) and $-\frac{1}{(2\pi)^3} \int \mathrm{d}\mathbf{p} W(|\mathbf{k} - \mathbf{p}|) n_F(\xi_\mathbf{p})$. For the Matsubara sums, use Sec. 5.6. Why is the first diagram called "Hartree-diagram", the second "Fock-diagram"? (Hint: Compare to the expression for the Hartree-Fock single particle energy in Eq. (63).)
Also compute the pair-bubble diagram which is the third term on the rhs of Fig. 12(b). Show that it can be expressed as

$$\Sigma^P_\sigma(\mathbf{k}, i\omega_n) = T \sum_{\Omega_n} \frac{1}{(2\pi)^3} \int \mathrm{d}\mathbf{q} W(|\mathbf{q}|)^2 \Pi^0(\mathbf{q}, i\Omega_n) \mathcal{G}_{0,\sigma}(\mathbf{k} - \mathbf{q}, i\omega_n - i\Omega_n) \tag{214}$$

where $\Pi^0(\mathbf{q}, i\Omega_n) = -2T \sum_{\omega_n} \frac{1}{(2\pi)^3} \int \mathrm{d}\mathbf{p} \frac{1}{i\omega_n + i\Omega_m - \xi_{\mathbf{p}+\mathbf{q}}} \cdot \frac{1}{i\omega_n - \xi_\mathbf{p}}$. No further simplifications required here.

Exercise 7.4. General structure of perturbation theory

In this exercise we explore the convergence properties of perturbative expansions. To simplify matters to the essentials, we disregard quantum mechanics and consider some caricature of a classical toy-model field theory with an action $S(x \in \mathbb{R}) = x^2/2 + gx^4$ so that the integral

$$I(g) = \int_{-\infty}^{+\infty} \frac{\mathrm{d}x}{\sqrt{2\pi}} e^{-S(x)} \tag{215}$$

represents the partition function. For $g = 0$ the integral is Gaussian and exactly solvable, $I(g = 0) = 1$. This is the non-interacting case. We consider $g > 0$ a small interaction parameter that is treated perturbatively. This means we are interested in the expansion

$$I(g) = \sum_{n=0,1,2,\ldots} g^n I_n. \tag{216}$$

1) Use Stirling's formula ($n! \sim n^n e^{-n}$) for large n to show $g^n I_n \sim \left(-\frac{16g}{e}n\right)^n$. Explain why this means that the perturbative series diverges for *any finite* g if summed to sufficiently large order n (the convergence radius is zero). What is the underlying mathematical reason for this behavior? What is the reason from the viewpoint of Feynman diagrams? Hint: Use the Gaussian integral-version of the Wick theorem where $\int_{-\infty}^{+\infty} \frac{\mathrm{d}x}{\sqrt{2\pi}} e^{-x^2/2} x^{4n}$ is the number of all possible pairings of $4n$ objects.

2) A partial summation of the series up to order N yields an error $\Delta_N = |I(g) - \sum_{n=0}^{N} g^n I_n|$. Show that for large $N \gg 1$, the error has the upper bound $\sim (16gN/e)^N$. Given $g \ll 1$ what is the optimal $N = N_{opt}$ for the smallest error? [Hint: Start from the error bound on the Taylor series in x for the integrand $\exp\left(-gx^4\right)$, that is $\left|\exp\left(-gx^4\right) - \sum_{n=0}^{N}(-gx^4)^n/n\right| \leq \left(gx^4\right)^{N+1}/(N+1)!$] .

The moral of this exercise is that general perturbative expansions should not be confused with with rigorous Taylor expansions. The former are instead *asymptotic expansions* in the sense that for weaker and weaker "interaction", a partial summation of the perturbation series to order N leads to results that improve with increasing N.

8 Interacting electron gas: Random-phase approximation and screening

Idea:

- Apply Feynman diagrams for electrons in metals with Coulomb interactions
- Learn strategy to select subclass of diagrams and perform their re-summation
- Application: Ground-state energy up to second-order in perturbation, polarization function, plasmon excitations

8.1 Setup

- Use framework of fermionic pair interactions from Sec. 7.2.
- Model electrons in a 3d metal (spinful fermions with Fermi energy ε_F), with Coulomb interactions where $e_0^2 \equiv e^2/(4\pi\varepsilon_0)$:
$$W(r) = \frac{e_0^2}{r} \;\leftrightarrow\; W(q) = \frac{4\pi e_0^2}{q^2} = \frac{e^2}{\varepsilon_0 q^2} \tag{217}$$
so that the Hamiltonian $H = H_0 + W$ reads:
$$H_0 = \sum_{\sigma,\mathbf{k}} \Psi^\dagger(\sigma,\mathbf{k})\xi_{\mathbf{k}}\Psi(\sigma,\mathbf{k}),$$
$$W = \frac{1}{2V}\sum_{\sigma_1,\sigma_2}\sum_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{q}\neq 0} W(q)\,\Psi^\dagger(\sigma_1,\mathbf{k}_1+\mathbf{q})\Psi^\dagger(\sigma_2,\mathbf{k}_2-\mathbf{q})\Psi(\sigma_2,\mathbf{k}_2)\Psi(\sigma_1,\mathbf{k}_1)$$
- Introduce:
  - Bohr radius $a_0 = \hbar^2/(me_0^2) = 0.053$nm as our unit of length
  - Rydberg $1\text{Ry} = e_0^2/(2a_0) = 13.6$eV as the unit of energy
  - Radius of a sphere r_s containing exactly one electron (in units of a_0): $\frac{4}{3}\pi(r_s a_0)^3 = 1/\rho = 3\pi^2/k_F^3$:
$$r_s = \left(\frac{9\pi}{4}\right)^{1/3}\frac{1}{a_0 k_F} \propto k_F^{-1} \tag{218}$$
- Electron density $\rho = N/V$ as a control parameter:
  - Non-interacting electrons: $E_0/N \sim \varepsilon_F \sim \rho^{2/3}$
  - Typical interaction energy: Mean electron-electron distance $a = \rho^{-1/3} \to E_{pot}/N \sim e_0^2/a \sim \rho^{1/3}$
  - it follows $E_{pot}/E_0 \sim \rho^{-1/3} \to$ interaction effects are weaker at higher density
  - use high density $r_s \to 0$ as control limit for perturbation theory
- Recall Ex. 1.5: Found ground-state energy in first order (non-diagrammatic) perturbation theory:
$$\frac{E_0^{(0)}}{N} \simeq \frac{2.21}{r_S^2}\text{Ry},\quad \frac{E_0^{(1)}}{N} \simeq -\frac{0.916}{r_s}\text{Ry} \tag{219}$$
- Fact: $E_0^{(2)}$ obtained naively would diverge! Problem: Singularity of $W(q)$ for $q \to 0$.
- Trick:
  1. Introduce screening parameter α by hand (deforms Coulomb- to Yukawa-potential)
$$W(r) = \frac{e_0^2}{r}e^{-\alpha r} \;\leftrightarrow\; W(q) = \frac{4\pi e_0^2}{q^2+\alpha^2} \tag{220}$$
  2. Diagrammatic calculation with finite α yields "self-screening" that survives for $\alpha \to 0$.

8.2 Self-energy in random-phase approximation (RPA)

- Self-energy diagrams up to order $n = 3$ (partially) are shown in Fig. 13(a).
- The first Hartree (also "tadpole") diagram has been calculated in Ex. 7.3 and it was found

$$\Sigma_\sigma^H(\mathbf{k}, i\omega_n) = W(q=0)\rho = \rho \int \mathrm{d}\mathbf{r}^3 W(r) \tag{221}$$

  This constant cancels the positive smeared-out background charge $+|e_0|\rho$ of the ions → drop the Hartree diagram and higher order diagrams where it appears as a building block.
- Above we estimated that interactions are less important for high density $r_s \propto k_F^{-1} \to 0$. Check if self-energy diagrams of lower order dominate in this case.
- Consider value of generic n-th order self-energy diagram:

$$\Sigma_\sigma^{(n)}(\mathbf{k}, i\omega_n) \propto \underbrace{\int \mathrm{d}\tilde{k}_1 ... \int \mathrm{d}\tilde{k}_n}_{n \text{ internal momenta}} \underbrace{W(...) \cdot ... \cdot W(...)}_{n \text{ interaction lines}} \times \underbrace{\mathcal{G}_0(...) \cdot ... \cdot \mathcal{G}_0(...)}_{2n-1 \text{ propagators}} \tag{222}$$

  Make integrals dimensionless:
  - measure momenta in units of k_F (i.e. replace $k = xk_F$ with x a number) and temperature T in units of $\varepsilon_F \propto k_F^2$:

$$\int \mathrm{d}\tilde{k}_1 = T \sum_{i\omega_n} \int \frac{\mathrm{d}\mathbf{k}^3}{(2\pi)^3} \propto k_F^2 k_F^3 = k_F^5 \tag{223}$$

  - for interaction lines $W(q) \propto 1/(q^2 + \alpha^2) \propto k_F^{-2}$ and for propagators $\mathcal{G}_0(i\omega_n, \mathbf{k}) = 1/(i\omega_n - \varepsilon_k) \propto k_F^{-2}$
- It follows

$$\Sigma_\sigma^{(n)}(\mathbf{k}, i\omega_n) \propto \left(k_F^5\right)^n \times \left(k_F^{-2}\right)^n \times \left(k_F^{-2}\right)^{2n-1} = k_F^{-n+2} \propto r_s^{n-2} \tag{224}$$

  which indeed means that higher-order diagrams are suppressed for high-density $r_s \to 0$.
- At a given order n, which diagrams are dominant?
  - Consider interactions line $W(|\mathbf{q}|) \overset{\alpha\to 0}{\to} 1/q^2$ where $\mathbf{q}$ is a momentum that is summed over.
  - In general the interaction lines have different momenta, e.g. $W(|\mathbf{q}|)W(|\mathbf{q}+\mathbf{p}|) \overset{\alpha\to 0}{\to} \frac{1}{q^2|\mathbf{q}+\mathbf{p}|^2}$.
  - The contribution from interaction lines is maximized for the single diagram where all n interaction lines are forced to the same loop momentum, $W(|\mathbf{q}|) \cdot ... \cdot W(|\mathbf{q}|)$.
- RPA self-energy $\Sigma_\sigma^{\mathrm{RPA}}(\mathbf{k}, i\omega_n)$: The infinite sum of all diagrams containing $W(|\mathbf{q}|)^n$ at order n, see Fig. 13(b).

Renormalized interaction in RPA

- The RPA self-energy can be formally written as a Fock diagram with a single renormalized interaction line $-W^{\mathrm{RPA}}(\mathbf{q}, i\Omega_n)$ defined in Fig. 13(c).
  Note: We now expect also a non-trivial frequency dependence!
- Ingredient for $-W^{\mathrm{RPA}}(\mathbf{q}, i\Omega_n)$: Fermion pair bubble already calculated in Ex. 7.3.

$$\chi^0(\mathbf{q}, i\Omega_n) = T \sum_{\omega_n} \frac{1}{V} \sum_{\mathbf{p},\sigma} \frac{1}{i\omega_n + i\Omega_n - \xi_{\mathbf{p}+\mathbf{q}}} \cdot \frac{1}{i\omega_n - \xi_{\mathbf{p}}} = \frac{1}{V} \sum_{\mathbf{p},\sigma} \frac{n_F(\xi_{\mathbf{q}+\mathbf{p}}) - n_F(\xi_{\mathbf{p}})}{\xi_{\mathbf{q}+\mathbf{p}} - \xi_{\mathbf{p}} - i\Omega_n} \tag{225}$$

  The Matsubara sum was performed in Ex. 5.3.

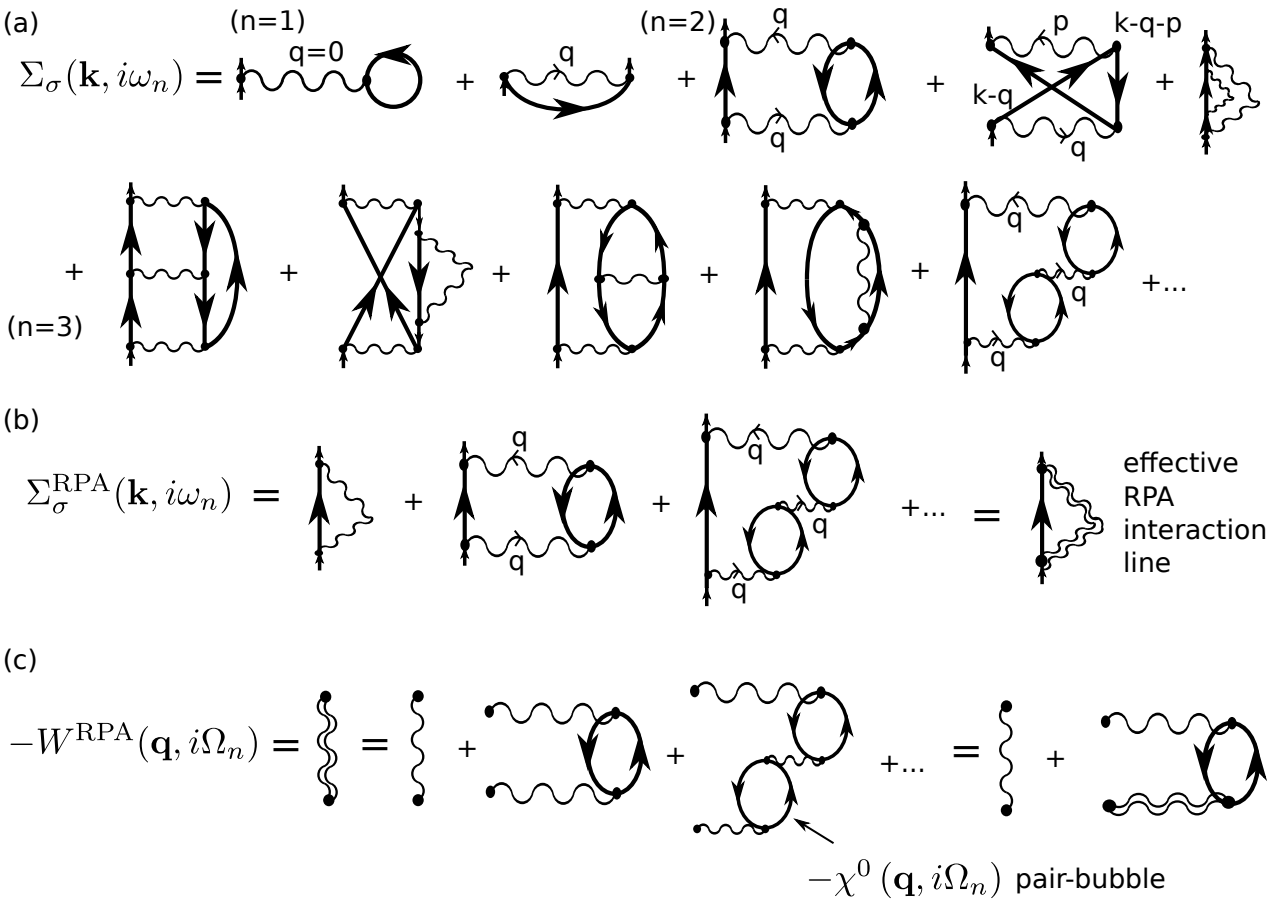

Figure 13: (a) Self-energy diagrams for Coulomb interaction up to order $n = 3$. (b) RPA diagrams with effective interaction line $-W^{RPA}$. (c) Self-consistency equation for $-W^{RPA}$.

- Find $-W^{\mathrm{RPA}}(\mathbf{q}, i\Omega_n)$ from a Dyson-like equation, see rightmost expression in Fig. 13(c):

$$-W^{\mathrm{RPA}}(\mathbf{q}, i\Omega_n) = -W(\mathbf{q}) + [-W(\mathbf{q})]\left[-\chi^0(\mathbf{q}, i\Omega_n)\right]\left[-W^{\mathrm{RPA}}(\mathbf{q}, i\Omega_n)\right] \tag{226}$$

- We solve for W^{RPA} and insert the explicit Yukawa form of $W(q) = 4\pi e_0^2/(q^2+\alpha^2)$ from Eq. (220):

$$W^{\mathrm{RPA}}(\mathbf{q}, i\Omega_n) = \frac{W(\mathbf{q})}{1 - W(\mathbf{q})\chi^0(\mathbf{q}, i\Omega_n)} = \frac{4\pi e_0^2}{q^2+\alpha^2 - 4\pi e_0^2\chi^0(\mathbf{q}, i\Omega_n)} \overset{\alpha\to 0}{\to} \frac{4\pi e_0^2}{q^2 - 4\pi e_0^2\chi^0(\mathbf{q}, i\Omega_n)} \tag{227}$$

  In the last step we have taken the limit $\alpha \to 0$, we don't need it any longer from here on.

- Observation: From the form of $W^{\mathrm{RPA}}(\mathbf{q}, i\Omega_n)$, we see that the system has created "its own" screening $+\alpha^2 \to -4\pi e_0^2\chi^0(\mathbf{q}, i\Omega_n)$.

- The screening in the static ($i\Omega_n \to 0$) and long-wavelength limit ($q \to 0$) is known as **Thomas-Fermi screening**, it is parameterized by the wavevector k_s (~ inverse screening length):

$$\begin{aligned} k_s^2 &= \lim_{q\to 0} -4\pi e_0^2\chi^0(\mathbf{q}, i\Omega_n = 0) \\ &= -4\pi e_0^2 \frac{1}{V}\sum_{\mathbf{p},\sigma} \frac{(\xi_{\mathbf{q}+\mathbf{p}} - \xi_{\mathbf{p}})\partial_{\xi_{\mathbf{p}}} n_F(\xi_{\mathbf{p}})}{\xi_{\mathbf{q}+\mathbf{p}} - \xi_{\mathbf{p}}} \\ &= 4\pi e_0^2 \int \mathrm{d}\xi\, D(\xi) \underbrace{[-\partial_\xi n_F(\xi)]}_{\to\delta(\xi)} \end{aligned}$$

  If $T \ll \varepsilon_F$, the $-\partial_\xi n_F(\xi)$ is sharply peaked and the integral is just the density of states at the Fermi surface $\xi_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu = 0$ which we denote by $D(\varepsilon_F) = mk_F/(\pi^2\hbar^2)$. We obtain with $a_0 = \hbar^2/(me_0^2)$:

$$k_s^2 = 4\pi e_0^2 D(\varepsilon_F) = \frac{4}{\pi}\frac{k_F}{a_0} \tag{228}$$

- In ordinary metals, we have $k_s^{-1} \simeq 0.1\mathrm{nm}$.

Recap: Density of states $D(E)$ (DOS)

- For a general non-interacting dispersion $\xi_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu$, the density of states $D(E)$ at energy E is defined as

$$D(E) = \frac{1}{V}\sum_{\mathbf{k},\sigma} \delta(\xi_{\mathbf{k}} - E) = \frac{1}{(2\pi)^d}\sum_\sigma \int \mathrm{d}\mathbf{k}\, \delta(\xi_{\mathbf{k}} - E) \tag{229}$$

- The DOS is helpful for momentum sums over functions $f(\xi_{\mathbf{k}})$ that depend on momentum only through the dispersion

$$\frac{1}{V}\sum_{\mathbf{k},\sigma} f(\xi_{\mathbf{k}}) = \int \mathrm{d}E\, \delta(\xi_{\mathbf{k}} - E)\frac{1}{V}\sum_{\mathbf{k},\sigma} f(E) = \int \mathrm{d}E\, D(E) f(E) \tag{230}$$

- Example: For a parabolic dispersion, $\varepsilon_{\mathbf{k}} = k^2/(2m)$ one finds in $d = 3$ dimensions

$$D(E) = \frac{2}{(2\pi)^3}\int \mathrm{d}\mathbf{k}\, \delta\left(\frac{\hbar^2 k^2}{2m} - E\right) = \frac{mk}{\pi^2\hbar^2} \tag{231}$$

8.3 Dielectric function and screening of external potentials

- We found that the effective (RPA-) interaction between two electrons is a screened Coulomb interaction, $W^{\mathrm{RPA}}(\mathbf{q}, i\Omega_n) = \frac{4\pi e_0^2}{q^2 - 4\pi e_0^2 \chi^0(\mathbf{q}, i\Omega_n)}$. In the static and long-wavelength limit $W^{\mathrm{RPA}}(\mathbf{q} \to 0, i\Omega_n = 0) = \frac{4\pi e_0^2}{q^2 + k_s^2}$ (Thomas-Fermi screening.)
- Q: Is there a similar screening of external potentials ϕ_{ext}, induced e.g. by an external point-charge as in Fig. 14(a)? Will electrons gather around this external charge to screen its bare Coulomb potential?
- To adapt to a general experimental situation, generalize from the static point charge to a generic *weak* external potential $\phi_{\mathrm{ext}}(\mathbf{r}, t)$ with arbitrary dependence on $\mathbf{r}$ and t.
- Use linear response theory in the Kubo formalism, Eq. (180), for the susceptibility. Setup:
  - Perturbation in Hamiltonian: $F \cdot H_1 = \int \mathrm{d}\mathbf{r}\, [-en(\mathbf{r})]\phi_{\mathrm{ext}}(\mathbf{r}, t)$ where n is the electron density. The "$\cdot$" now stands for an integral $\to$ coupling operator $H_1 = -en(\mathbf{r})$.
  - Observable: Induced charge $O(\mathbf{r}, t) = \rho_{\mathrm{ind}}(\mathbf{r}, t) = -e[n(\mathbf{r}, t) - n_0] = -e\delta n(\mathbf{r}, t)$ where we subtracted the charge of the background ion density $n_0 = \langle n \rangle$.
  - Kubo formula: $\chi^R_{OH_1}(\mathbf{q}, \omega) = G^R_{OH_1}(\mathbf{q}, \omega) \to \chi^R_{-e\delta n, -en}(\mathbf{q}, \omega) = G^R_{-e\delta n, -en}(\mathbf{q}, \omega)$ so that after a FT:
  $$-e\rho_{\mathrm{ind}}(\mathbf{q}, \omega) = e^2 \chi^R_{nn.c}(\mathbf{q}, \omega)\phi_{\mathrm{ext}}(\mathbf{q}, \omega) \tag{232}$$
  - The subscript c stands for connected, $\chi^R_{nn,c} = \chi^R_{\delta nn} - \langle n \rangle \langle n \rangle$.
- Experiment: Instead of the induced charge, it is easier to measure the total potential
$$\phi_{\mathrm{tot}}(\mathbf{q}, \omega) = \phi_{\mathrm{ext}}(\mathbf{q}, \omega) + \phi_{\mathrm{ind}}(\mathbf{q}, \omega) \tag{233}$$
that differs from the external potential by the induced potential $\phi_{\mathrm{ind}}(\mathbf{q}, \omega)$, see Fig. 14(a).
- The induced potential is caused by the induced charge $-e\rho_{\mathrm{ind}}(\mathbf{q}, \omega)$. Since the effect of the electrons have been already taken into account above via linear response, this happens via the **bare** (and instantenous) Coulomb interaction $W(r) = -e\rho_{\mathrm{ind}}/(4\pi\varepsilon_0 r)$
$$\phi_{\mathrm{ind}}(\mathbf{r}, t) = \int \mathrm{d}\mathbf{r}' \frac{-e\rho_{\mathrm{ind}}(\mathbf{r}', t)}{4\pi\varepsilon_0 |\mathbf{r} - \mathbf{r}'|} \to \phi_{\mathrm{ind}}(\mathbf{q}, \omega) = -\frac{1}{e} W(\mathbf{q}) \rho_{\mathrm{ind}}(\mathbf{q}, \omega) \tag{234}$$
- Combine Eqns. (232) and (234) to find relation induced and external potential:
$$\phi_{\mathrm{ind}}(\mathbf{q}, \omega) = W(\mathbf{q}) \chi^R_{nn,c}(\mathbf{q}, \omega) \phi_{\mathrm{ext}}(\mathbf{q}, \omega) \tag{235}$$
or between total and external potential
$$\phi_{\mathrm{tot}}(\mathbf{q}, \omega) = \underbrace{\left[1 + W(\mathbf{q}) \chi^R_{nn,c}(\mathbf{q}, \omega)\right]}_{\varepsilon^{-1}(\mathbf{q}, \omega)} \phi_{\mathrm{ext}}(\mathbf{q}, \omega) \tag{236}$$
- Recall from EM in materials the distinction between electric and electric displacement fields $\mathbf{E}, \mathbf{D}$. They obey the two Maxwell relations that state that $\mathbf{E}$ has total charge as source whereas $\mathbf{D}$ only changes with external (or "free") charges:
$$\begin{aligned} \partial_{\mathbf{r}} \cdot \mathbf{E} &= \varepsilon_0 \rho_{\mathrm{tot}} \\ \partial_{\mathbf{r}} \cdot \mathbf{D} &= \varepsilon_0 \rho_{\mathrm{ext}} \end{aligned}$$
- Relation $\mathbf{D}(\mathbf{q}, \omega) = \varepsilon(\mathbf{q}, \omega)\mathbf{E}(\mathbf{q}, \omega)$ defines the **dielectric function** $\varepsilon(\mathbf{q}, \omega)$. From Eq. (236), we have
$$\boxed{\frac{1}{\varepsilon(\mathbf{q}, \omega)} = 1 + W(\mathbf{q}) \chi^R_{nn}(\mathbf{q}, \omega)} \tag{237}$$

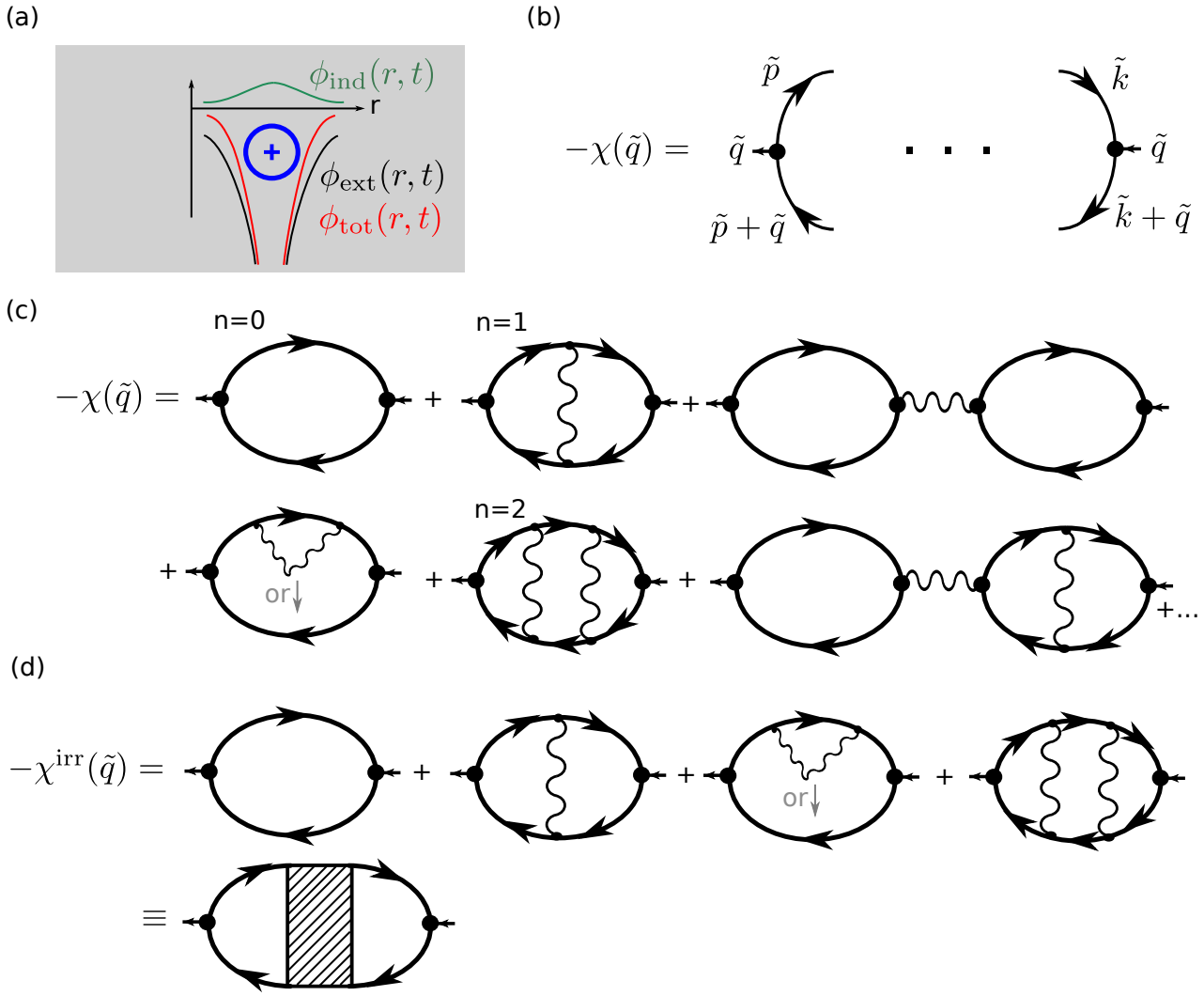

Figure 14: (a) External charge in an interacting electron gas. (b) The external vertices for the density-density correlation function. (c) Feynman diagrams for this function. (d) Irreducible part with respect to cutting interaction lines.

Calculation of $\chi^R_{nn,c}(\mathbf{q},\omega)$

- We calculate the retarded density-density correlator (with respect to the interacting but unperturbed electron gas).
- Use analytical continuation from the imaginary time correlator

$$\chi^R_{nn,c}(\mathbf{q},\tau) = -\frac{1}{V}\left\langle T_\tau n(\mathbf{q},\tau)n(-\mathbf{q},0)\right\rangle_c = -\frac{1}{V}\sum_{\mathbf{p},\mathbf{k},\sigma,\sigma'}\Big\langle T_\tau \underbrace{c^\dagger_{\mathbf{p}\sigma'}(\tau+\eta)c_{\mathbf{p}+\mathbf{q}\sigma'}(\tau)}_{A(\tau)}\underbrace{c^\dagger_{\mathbf{k}+\mathbf{q}\sigma}(\eta)c_{\mathbf{k}\sigma}}_{B}\Big\rangle_c \tag{238}$$

  where we used $n(\mathbf{q}) = \sum_{\mathbf{p},\sigma} c^\dagger_{\mathbf{p}\sigma}c_{\mathbf{p}+\mathbf{q}\sigma}$. We drop the subscripts nn, c from now on.
- We draw Feynman diagrams for $\chi(\mathbf{q}, i\Omega_m) = \chi(\tilde{q})$, the external vertices corresponding to operators A, B now have two Fermion lines to connect to, see Fig. 14(b).
- A low order expansion is shown in Fig. 14(c).
- In analogy to the Dyson's equation, we collect all diagrams that are irreducible with respect to cutting a single **interaction** line $-W$ (not Fermion line) and call this $\chi^{\text{irr}}(\tilde{q})$, see Fig. 14(d). We abbreviate this as a diagram with a hatched box.
- We express $\chi(\tilde{q})$ by $\chi^{\text{irr}}(\tilde{q})$ in analogy to Dyson's equation:

$$\begin{aligned} -\chi(\tilde{q}) &= -\chi^{\text{irr}}(\tilde{q}) + \left[-\chi^{\text{irr}}(\tilde{q})\right][-W(\mathbf{q})]\left[-\chi^{\text{irr}}(\tilde{q})\right] + \left[-\chi^{\text{irr}}(\tilde{q})\right][-W(\mathbf{q})]\left[-\chi^{\text{irr}}(\tilde{q})\right][-W(\mathbf{q})]\left[-\chi^{\text{irr}}(\tilde{q})\right] + \ldots \\ &= -\chi^{\text{irr}}(\tilde{q}) - \chi^{\text{irr}}(\tilde{q})W(\mathbf{q})\chi(\tilde{q}) \end{aligned}$$

  or

$$-\chi(\tilde{q}) = \frac{-\chi^{\text{irr}}(\tilde{q})}{1 - W(\mathbf{q})\chi^{\text{irr}}(\tilde{q})} \tag{239}$$

- We use this in the dielectric function (in Matsubara frequency!):

$$\varepsilon(\tilde{q}) = \frac{1}{1+W(\mathbf{q})\chi(\tilde{q})} = 1 - W(\mathbf{q})\chi^{\text{irr}}(\tilde{q}) = 1 - \frac{e^2}{\varepsilon_0 q^2}\chi^{\text{irr}}(\tilde{q}) \tag{240}$$

- In RPA (valid at high electron densities!), approximate $\chi^{\text{irr}}(\tilde{q})$ by the empty fermion pair-bubble, i.e. the first diagram in Fig. 14(d): $\chi^{\text{irr}}_{\text{RPA}}(\tilde{q}) = \chi_0(\tilde{q})$.
- Dielectric function in RPA (now back to real frequency)

$$\boxed{\varepsilon_{\text{RPA}}(\mathbf{q},\omega) = 1 - \frac{e^2}{\varepsilon_0 q^2}\chi^R_0(\mathbf{q},\omega)} \tag{241}$$

- Conclusion: External potentials treated in linear response are screened in the same way as the internal Coulomb interactions between the electrons:

$$\phi_{\text{tot}}(\mathbf{q},\omega) = \frac{1}{1 - \frac{e^2}{\varepsilon_0 q^2}\chi^R_0(\mathbf{q},\omega)}\phi_{\text{ext}}(\mathbf{q},\omega) \tag{242}$$

Application: Collective plasma oscillations

- Consider external potential with frequency ω, focus on high-frequency and long-wavelength perturbations $v_F q \ll \omega$ and $q \ll k_F$.
- Recall the analysis of the imaginary part of $\chi^R_0(\mathbf{q},\omega)$ in Ex. 5.4, see shaded region in Fig. 15. For the high-frequency limit in the lower left corner above the orange line, we have $\text{Im}\chi^R_0(\mathbf{q},\omega) = 0$.

- Work at low temperature, $T \ll \varepsilon_F$, and use results for $\mathrm{Re}\chi^0(\mathbf{q},\omega)$ from Ex. 8.1 [where $x \equiv q/(2k_F)$, $x_0 \equiv \omega/(4\varepsilon_F)$ and $f(x,x_0) \equiv \left[1-(x-\frac{x_0}{x})^2\right]\cdot \ln\left|\frac{x+x^2-x_0}{x-x^2+x_0}\right|$]:

$$\mathrm{Re}\chi^0(\mathbf{q},\omega) = -D(\varepsilon_F)\left(\frac{1}{2}+\frac{f(x,x_0)+f(x,-x_0)}{8x}\right) \overset{x\ll x_0}{\to} D(\varepsilon_F)\left[\frac{x^2}{3x_0^2}+\frac{x^4}{5x_0^4}\right] \tag{243}$$

- Re-insert q,ω and use $D(\varepsilon_F)=\frac{mk_F}{\pi^2}$ and $3\pi^2 n = k_F^3$ and $v_F = k_F/m$. We obtain

$$\varepsilon_{\mathrm{RPA}}(\mathbf{q},\omega) \simeq 1-\frac{\omega_p^2}{\omega^2}\left[1+\frac{3}{5}\left(\frac{qv_F}{\omega}\right)^2\right], \quad \omega_p^2 \equiv \frac{e^2 n}{\varepsilon_0 m} \tag{244}$$

  where ω_p is the characteristic "electronic plasma frequency". It is typically in the UV part of the spectrum $\omega_p \sim 10^{16}$Hz corresponding to energy ~ 10eV, so ω_p is on the same order as ε_F.

- Recall relation between external "drive" potential and the induced potential:

$$\phi_{\mathrm{tot}}(\mathbf{q},\omega) = \varepsilon^{-1}_{\mathrm{RPA}}(\mathbf{q},\omega)\phi_{\mathrm{ext}}(\mathbf{q},\omega). \tag{245}$$

  If $\varepsilon_{\mathrm{RPA}}(\mathbf{q},\omega)\to 0$ for a certain $(\mathbf{q},\omega)$, we obtain a response even if $\phi_{\mathrm{ext}}(\mathbf{q},\omega)\to 0$. In other words, the relation

$$\varepsilon_{\mathrm{RPA}}(\mathbf{q},\omega) \overset{!}{=} 0 \leftrightarrow \omega^2 = \omega_p^2\left[1+\frac{3}{5}\left(\frac{qv_F}{\omega}\right)^2\right] \tag{246}$$

  defines self-oscillations (an eigenmode) of the **interacting** electron gas. Note that there is no damping in the $q-\omega$ - regime considered ($\mathrm{Im}\chi_0^R(\mathbf{q},\omega)=0=\mathrm{Im}\varepsilon_{\mathrm{RPA}}(\mathbf{q},\omega)$).

- The dispersion $\omega(q)$ of these plasma oscillations ("plasmons") is found as (recall $v_F q \ll \omega$!)

$$\omega(q) \simeq \omega_p\sqrt{1+\frac{3}{5}\left(\frac{qv_F}{\omega_p}\right)^2} \simeq \omega_p + \frac{3}{10}\left(\frac{qv_F}{\omega_p}\right)^2 \tag{247}$$

  In Fig. 15(a) we show $\omega(q)$.

- Remarks:
  - For larger q when the $\omega(q)$ enter the shaded region with finite $\mathrm{Im}\chi_0^R(\mathbf{q},\omega)$, plasmons are damped by formation of particle-hole pairs ("Landau damping").
  - Experimentally, one or more plasmons can be excited when shooting high-energy electrons through a metal foil (spectroscopy of energy of transmitted electrons). See Fig. 15(b) for experimental data.
  - The existence of plasmons (but not the damping) can also be understood classically, see Ex. 8.3.

Exercises

Exercise 8.1. Evaluation of fermionic pair bubble: Real part

The pair-bubble in Eq. (225) describes the polarizability of a *non-interacting* electron gas $\xi_{\mathbf{k}} = \hbar^2k^2/(2m) - \varepsilon_F$ ($\to$ see Ex. 5.3 and Ex. 5.4) but also plays an important role in the RPA for the *interacting* electron gas. Consider its analytically continued (retarded) version $\chi^0(\mathbf{q},i\Omega_n\to\omega+i\eta)=\chi^0(\mathbf{q},\omega)$ and work at zero temperature:

$$\chi^0(\mathbf{q},\omega) = -\frac{2}{V}\sum_{\mathbf{k}}\frac{\Theta(\xi_{\mathbf{q}+\mathbf{k}})-\Theta(\xi_{\mathbf{k}})}{\omega-\xi_{\mathbf{q}+\mathbf{k}}+\xi_{\mathbf{k}}+i\eta} \tag{248}$$

For the real part, perform the summation over $\mathbf{p}$ and show that

$$\mathrm{Re}\chi^0(\mathbf{q},\omega) = -D(\varepsilon_F)\left(\frac{1}{2}+\frac{f(x,x_0)+f(x,-x_0)}{8x}\right) \tag{249}$$

with $x\equiv q/(2k_F)$, $x_0\equiv\omega/(4\varepsilon_F)$ and $f(x,x_0)\equiv\left[1-(x-\frac{x_0}{x})^2\right]\cdot\ln\left|\frac{x+x^2-x_0}{x-x^2+x_0}\right|$. The imaginary part is more complicated and you don't need to compute it here. However, recall that the region in the $q-\omega$ - plane where it is non-zero has been already identified in Ex. 5.4.

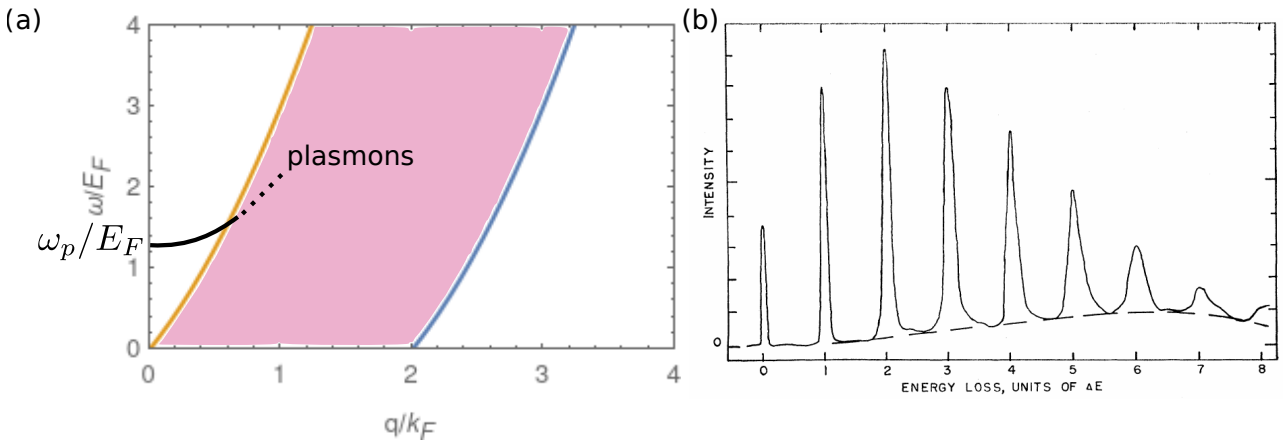

Figure 15: (a) Typical plasmon dispersion (thick line) and the region of damped charge susceptibility from Ex. 5.4. (b) Experimental observation of plasmon excitations in high-energy electron transmission through a thin aluminum foil. The peaks correspond to one or multiple plasmon excitations, $\Delta E = 14.8eV$ [from Marton *et al.*, Phys. Rev. **126**, 182 (1962)].

Exercise 8.2. Ground state energy of interacting electron gas from self-energy

Here we show that the RPA self-energy is sufficient to (approximately) calculate the ground-state energy E_0 of the interacting electron gas with Hamiltonian $H = H_0 + W$ beyond the first-order approximation of Eq. (219). This is nontrivial in sofar that naively calculating $E_0 = \lim_{T\to 0} \langle H_0 + W\rangle$ would involve the (perturbative) evaluation of the four-fermion average of the interaction W.

1) Show that by defining a deformed system $H(\lambda) \equiv H_0 + \lambda W$ ($\lambda \in [0,1]$) the following relation holds between the free energy $F = U - TS = -T\ln Z$ of the fully interacting system and the free energy of the non-interacting system $F^{(0)} = -T\ln Z^{(0)}$:

$$F - F^{(0)} = \int_0^1 \frac{\mathrm{d}\lambda}{\lambda} \langle \lambda W\rangle_\lambda \,. \tag{250}$$

Taking the limit $T \to 0$, in which $F = E_0$ is the ground-state energy it then follows $E_0 = E_0^{(0)} + \lim_{T\to 0} \int_0^1 \frac{\mathrm{d}\lambda}{\lambda} \langle \lambda W\rangle_\lambda$. Here, $\langle ...\rangle_\lambda$ is a thermal average with respect to the state $\rho_\lambda \sim \exp[-\beta H(\lambda)]$.

2) Use the equation of motion $-\partial_\tau \mathcal{G}_\sigma^\lambda(\mathbf{k},\tau) = ...$ to show that the expression for E_0 from 1) can be evaluated based *only* on the self-energy,

$$\langle \lambda W\rangle_\lambda = \frac{T}{2} \sum_{i\omega_n} \sum_{\mathbf{k},\sigma} \Sigma_\sigma^\lambda(\mathbf{k}, i\omega_n)\, \mathcal{G}_\sigma^\lambda(\mathbf{k}, i\omega_n)\, e^{i\omega_n \eta}, \tag{251}$$

and draw the (vacuum-)diagrams corresponding to this expression up to second order in W. Use renormalized interaction lines when necessary for diagram convergence. You don't need to evaluate these diagrams, but the answer for E_0 (after performing the λ-integral and adding $E_0^{(0)}$) is $E_0/N = \left(\frac{2.211}{r_s^2} - \frac{0.916}{r_s} + 0.0622\,\ln r_s - 0.094\right)$ Ry.

Exercise 8.3. Plasma oscillation - classical picture

It is possible to find the plasma frequency ω_p from classical considerations. Consider an electron gas (metal) of length L (in x-direction) and cross-section A. The electron "liquid" can move as a whole but the ions are spatially fixed. Set the electrons in motion by moving it a distance δx in the x-direction so that they feel a restoring force from the ions. Show that the frequency of the ensuing spatial oscillation is exactly ω_p.

Exercise 8.4. Coulomb interaction for electrons confined in two dimensions

Consider a translation invariant interacting electron gas confined two effectively two dimensions with parabolic dispersion $\xi_k = \hbar^2 k^2/(2m) - \varepsilon_F$. This happens for example in a semiconductor hetero-structure. The non-interacting plane-wave eigenstates for $\mathbf{k} = (k_x, k_y)$ and $\mathbf{r} = (x, y)$ are

$$\psi_{\mathbf{k},\sigma}(\mathbf{r}, z) = \frac{1}{\sqrt{L_x L_y}} e^{i\mathbf{r}\cdot\mathbf{k}} \zeta_0(z) \tag{252}$$

where $\zeta_0(z)$ is the lowest eigenstate in the z-direction (e.g. 1D potential-well eigenstates). In the following, assume the extreme 2D limit $|\zeta_0(z)|^2 \simeq \delta(z)$.

1) Show that the Coulomb interaction matrix element is $W_{2D}(q) = e^2/(2\epsilon_r\epsilon_0 q)$ where $\epsilon_r \simeq 10$ is the relative dielectric constant of the semiconductor material.

2) Find the static RPA interaction at small wavevectors and show $W_{2D}^{\mathrm{RPA}}(\mathbf{q}, i\Omega_n = 0) = \frac{e^2}{2\epsilon_r\epsilon_0[q+k_{s,2D}]}$. What is the screening wavevector $k_{s,2D}$?

9 Disordered metals and their conductivity

Idea:

- Apply perturbation theory (Feynman diagrams) for electrons in metals with impurities (potential scattering)
- Start with single impurity (foreign atom etc.) for warm-up, then consider many impurities = disorder
- Breaking of translation invariance breaks (crystal-) momentum conservation ($\neq$ Coulomb interactions)
- Disordered systems: Non-interacting but still rich and difficult
- Statistical analysis: Disorder average
- Applications: Friedel oscillations of density $n(\mathbf{r})$ close to impurity, conductivity in the presence of disorder

9.1 Single impurity and Friedel oscillations

- Problem setup [Fig. 16(a)]: Local impurity potential in 3d metal, $H = \hat{\mathbf{p}}^2/(2m) + U(\mathbf{r})$. Could also be treated with scattering theory (diagrams etc. not strictly required).
- Work with spin-less fermions for simplicity in this chapter.
- Rewrite with field operators, regard impurity potential as perturbation

$$H = -\frac{1}{2m}\int_{\mathbf{r}} \Psi^\dagger(\mathbf{r})\left(\nabla^2_{\mathbf{r}}\Psi(\mathbf{r})\right) + \int_{\mathbf{r}} \Psi^\dagger(\mathbf{r})U(\mathbf{r})\Psi(\mathbf{r}) = H_0 + H_1 \tag{253}$$

  Plane-wave basis [$\psi_{\mathbf{k}} = \frac{1}{\sqrt{V}}\int_{\mathbf{r}} e^{-i\mathbf{k}\cdot\mathbf{r}}\Psi(\mathbf{r})$] in which H_0 is diagonal. We use $U_{\mathbf{q}} = \frac{1}{V}\int_{\mathbf{r}} e^{-i\mathbf{q}\cdot\mathbf{r}}U(\mathbf{r})$.

$$H_0 = \sum_{\mathbf{k}} \underbrace{(\varepsilon_{\mathbf{k}} - \mu)}_{\xi_{\mathbf{k}}}\psi^\dagger_{\mathbf{k}}\psi_{\mathbf{k}}, \qquad H_1 = \sum_{\mathbf{p},\mathbf{q}} \psi^\dagger_{\mathbf{p}+\mathbf{q}}U_{\mathbf{q}}\psi_{\mathbf{p}} \tag{254}$$

  Note:

  - $U(\mathbf{r}) \in \mathbb{R} \to U_{\mathbf{q}} = U^\star_{-\mathbf{q}}$.
  - Clean or "bare" GF for H_0 (without the impurity)

$$\mathcal{G}^0_{\mathbf{k},\mathbf{k}'}(i\omega_n) = \delta_{\mathbf{k},\mathbf{k}'}\frac{1}{i\omega_n - \xi_{\mathbf{k}}} \equiv \delta_{\mathbf{k},\mathbf{k}'}\mathcal{G}^0_{\mathbf{k}}(i\omega_n) \tag{255}$$

  - H_1 is non-diagonal in (crystal-)momentum $\mathbf{k}$. This is due to the breaking of the (discrete-) translational invariance.

- Observables of interest: Electronic Matsubara GF, $\mathcal{G}_{\mathbf{k},\mathbf{k}'}(\tau) = -\left\langle \mathcal{T}\psi_{\mathbf{k}}(\tau)\psi^\dagger_{\mathbf{k}'}\right\rangle$ and $\mathbf{r}$-dependent density:

$$n(\mathbf{r}) = \frac{1}{V}\sum_{\mathbf{k},\mathbf{k}'} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{r}}\mathcal{G}_{\mathbf{k},\mathbf{k}'}(\tau = -\eta) \tag{256}$$

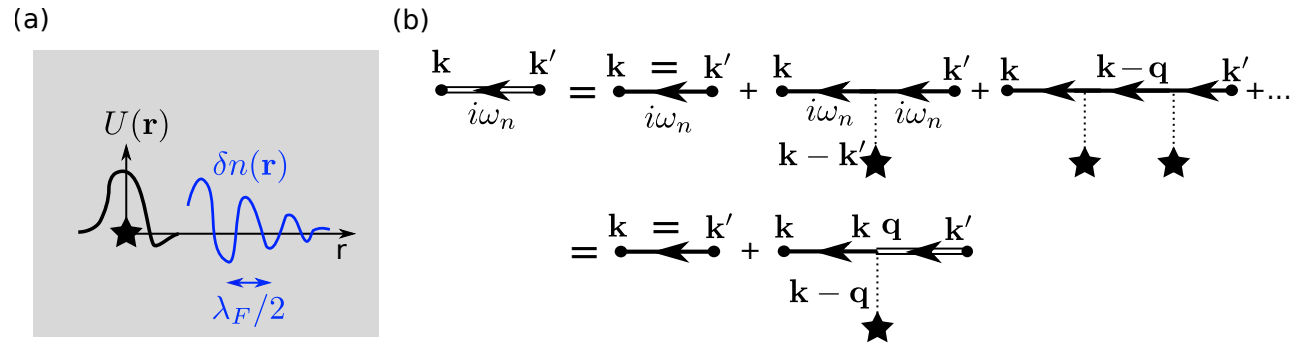

Figure 16: Single impurity in metal: (a) Impurity potential $U(\mathbf{r})$ and sketch of Friedel oscillations of density. (b) Diagrammatic perturbation theory for the electronic Matsubara GF.

Perturbation theory

- Use Eq. (208) for the perturbative evaluation of $\mathcal{G}_{\mathbf{k},\mathbf{k}'}(\tau)$:

$$\mathcal{G}_{\mathbf{k},\mathbf{k}'}(\tau) = -\left\langle T_\tau \psi_{\mathbf{k}}(\tau)\psi^\dagger_{\mathbf{k}'}\right\rangle = -\sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\int_0^\beta \mathrm{d}\tau_1 ... \int_0^\beta \mathrm{d}\tau_n \left\langle T_\tau H_1(\tau_1)...H_1(\tau_n)\psi_{\mathbf{k}}(\tau)\psi^\dagger_{\mathbf{k}'}\right\rangle_{0,c} \tag{257}$$

- Insert $H_1(\tau) = \sum_{\mathbf{p},\mathbf{q}} \psi^\dagger_{\mathbf{p}+\mathbf{q}}(\tau+\eta)U_{\mathbf{q}}\psi_{\mathbf{p}}(\tau)$

$$\mathcal{G}_{\mathbf{k},\mathbf{k}'}(\tau) = \mathcal{G}^0_{\mathbf{k},\mathbf{k}'}(\tau) + \sum_{\mathbf{p}_1,\mathbf{q}_1} U_{\mathbf{q}_1}\int_0^\beta \mathrm{d}\tau_1 \left\langle T_\tau \psi^\dagger_{\mathbf{p}_1+\mathbf{q}_1}(\tau_1+\eta)\psi_{\mathbf{p}_1}(\tau_1)\psi_{\mathbf{k}}(\tau)\psi^\dagger_{\mathbf{k}'}\right\rangle_{0,c}$$
$$-\frac{1}{2}\sum_{\mathbf{p}_{1,2},\mathbf{q}_{1,2}} U_{\mathbf{q}_1}U_{\mathbf{q}_2}\int_0^\beta \mathrm{d}\tau_{1,2}\left\langle T_\tau \psi^\dagger_{\mathbf{p}_1+\mathbf{q}_1}(\tau_1+\eta)\psi_{\mathbf{p}_1}(\tau_1)\psi^\dagger_{\mathbf{p}_2+\mathbf{q}_2}(\tau_2+\eta)\psi_{\mathbf{p}_2}(\tau_2)\psi_{\mathbf{k}}(\tau)\psi^\dagger_{\mathbf{k}'}\right\rangle_{0,c} + ...$$

- Evaluate the higher-order non-interacting correlators using Wick's theorem (138). Recall that no diagrams with vacuum parts are allowed (subscript c for connected).

$$\mathcal{G}_{\mathbf{k},\mathbf{k}'}(\tau) = \mathcal{G}^0_{\mathbf{k},\mathbf{k}'}(\tau) + \sum_{\mathbf{p}_1,\mathbf{q}_1} U_{\mathbf{q}_1}\int_0^\beta \mathrm{d}\tau_1 \mathcal{G}^0_{\mathbf{k},\mathbf{p}_1+\mathbf{q}_1}(\tau-\tau_1)\mathcal{G}^0_{\mathbf{p}_1,\mathbf{k}'}(\tau_1)$$
$$+\sum_{\mathbf{p}_{1,2},\mathbf{q}_{1,2}} U_{\mathbf{q}_1}U_{\mathbf{q}_2}\int_0^\beta \mathrm{d}\tau_{1,2}\mathcal{G}^0_{\mathbf{k},\mathbf{p}_1+\mathbf{q}_1}(\tau-\tau_1)\mathcal{G}^0_{\mathbf{p}_1,\mathbf{p}_2+\mathbf{q}_2}(\tau_1-\tau_2)\mathcal{G}^0_{\mathbf{p}_2,\mathbf{k}'}(\tau_2) + ...$$

  The prefactor $1/2$ (and more generally the $1/n!$) is canceled by the $n!$ possibilities to do the connected contraction.

- Expose the $\delta_{\mathbf{k},\mathbf{k}'}$ in the clean GF (255) and use the convolution theorem in the FT to $i\omega_n$:

$$\mathcal{G}_{\mathbf{k},\mathbf{k}'}(i\omega_n) = \delta_{\mathbf{k},\mathbf{k}'}\mathcal{G}^0_{\mathbf{k}}(i\omega_n) + \mathcal{G}^0_{\mathbf{k}}(i\omega_n)U_{\mathbf{k}-\mathbf{k}'}\mathcal{G}^0_{\mathbf{k}'}(i\omega_n) + \sum_{\mathbf{q}}\mathcal{G}^0_{\mathbf{k}}(i\omega_n)U_{\mathbf{q}}\mathcal{G}^0_{\mathbf{k}-\mathbf{q}}(i\omega_n)U_{\mathbf{k}-\mathbf{k}'-\mathbf{q}}\mathcal{G}^0_{\mathbf{k}'}(i\omega_n) + ... \tag{258}$$

- The corresponding Feynman diagrams are shown in Fig. 16(b). Interpretation:
  - Single string of clean propagator lines $\mathcal{G}^0_{\mathbf{q}}(i\omega_n)$ changing momentum $\mathbf{q}$ with impurity (star).
  - Frequency $i\omega_n$ is conserved $\leftrightarrow$ elastic scattering

- Express series as a self-consistency equation for $\mathcal{G}_{\mathbf{k},\mathbf{k}'}(i\omega_n)$ [Dyson's equation, Fig. 16(b)]:

$$\mathcal{G}_{\mathbf{k},\mathbf{k}'}(i\omega_n) = \delta_{\mathbf{k},\mathbf{k}'}\mathcal{G}^0_{\mathbf{k}}(i\omega_n) + \mathcal{G}^0_{\mathbf{k}}(i\omega_n)\sum_{\mathbf{q}}U_{\mathbf{k}-\mathbf{q}}\mathcal{G}_{\mathbf{q},\mathbf{k}'}(i\omega_n) \tag{259}$$

  For general $U(\mathbf{r})$, this would have to be solved numerically.

Point scatterer at origin and Friedel oscillations of density

- We now consider a point-scatterer, $U(\mathbf{r}) = u\delta(\mathbf{r})$ so that $U_{\mathbf{q}} = u/V$ does not depend on $\mathbf{q}$. After a sum over $\mathbf{k}$, Eq. (259) simplifies to

$$\sum_{\mathbf{k}} \mathcal{G}_{\mathbf{k},\mathbf{k}'}(i\omega_n) = \frac{\mathcal{G}^0_{\mathbf{k}'}(i\omega_n)}{1 - \frac{u}{V}\sum_{\mathbf{k}} \mathcal{G}^0_{\mathbf{k}}(i\omega_n)} \tag{260}$$

  and we re-insert his on the rhs of Eq. (259)

$$\mathcal{G}_{\mathbf{k},\mathbf{k}'}(i\omega_n) = \delta_{\mathbf{k},\mathbf{k}'}\mathcal{G}^0_{\mathbf{k}}(i\omega_n) + \frac{u}{V}\mathcal{G}^0_{\mathbf{k}}(i\omega_n)\frac{1}{1 - u\overline{\mathcal{G}^0(i\omega_n)}}\mathcal{G}^0_{\mathbf{k}'}(i\omega_n) \tag{261}$$

$$\overline{\mathcal{G}^0(i\omega_n)} \equiv \frac{1}{V}\sum_{\mathbf{k}} \mathcal{G}^0_{\mathbf{k}}(i\omega_n)$$

- We are interested in the impurity-induced modifications of the electron density $n(\mathbf{r})$, see Eq. (256). The first step is to compute the temporal FT using the recipes of Sec. 5.6 [→ Ex. 9.2]

$$\begin{aligned}\mathcal{G}_{\mathbf{k},\mathbf{k}'}(\tau = -\eta) &= T\sum_n e^{i\omega_n\eta}\mathcal{G}_{\mathbf{k},\mathbf{k}'}(i\omega_n) \\ = \delta_{\mathbf{k},\mathbf{k}'}\mathcal{G}^0_{\mathbf{k}}(\tau{=}-\eta) - \frac{u}{V}\sum_{\pm}\left(\frac{\pm 1}{2\pi i}\right)\int_{-\infty}^{+\infty} \mathrm{d}\omega \frac{e^{\omega\eta}}{1+e^{\omega\beta}}\cdot\frac{1}{\omega \pm i\eta - \xi_{\mathbf{k}}}\cdot\frac{1}{1-u\overline{G^0(\omega\pm i\eta)}}\cdot\frac{1}{\omega\pm i\eta - \xi_{\mathbf{k}'}}\end{aligned} \tag{262}$$

- In a second step, perform the spatial FT to find $n(\mathbf{r})$ from $\mathcal{G}_{\mathbf{k},\mathbf{k}'}(\tau = -\eta)$ and find in the limit of $T \to 0$ and for large distances from the impurity $r \gg k_F$,

$$\delta n(\mathbf{r}) = n(\mathbf{r}) - n^0 \simeq -\frac{\sin[\delta_0]}{4\pi^2 r^3}\cos[2k_F r + \delta_0] \tag{263}$$

  where $\delta_0 = \delta_0(\omega = 0)$ and $\delta_0(\omega) \in \mathbb{R}$ is the scattering-phase shift of electron waves at the energy ω determined by $\exp(2i\delta_0(\omega)) = \left[1 - u\overline{G^0(\omega - i\eta)}\right] / \left[1 - u\overline{G^0(\omega + i\eta)}\right]$. The calculation is done in Ex. 9.2.

- Discussion:
  - Impurity potential (at $r = 0$) perturbs the homogeneous electronic ground state of clean system
  - Impurity causes "Friedel" oscillations in the electronic density with *half* the Fermi wavelength and a $1/r^3$ decay, see Fig. 16(a)
  - Oscillations can be measured with scanning tunneling microscopy and are a characteristic feature of a Fermi surface. They also happen close to sharp edges.
  - Our calculation is non-perturbative in u!
  - One could also find the *linear* response $\propto u$ from the knowledge of the polarizability (real part of $\chi^0(\mathbf{q}, \omega)$ → Ex. 8.1)

9.2 Many impurities (disorder)

- Above the GF in the presence of a single impurity was found exactly.
- Many impurities → extended potential:

$$U(\mathbf{r}) = \sum_{j=1}^{N_{imp}} u(\mathbf{r} - \mathbf{r}_j) \tag{264}$$

  Finding the GF is not possible analytically (though numerically it is).
- However: Full disorder potential in a realistic sample is unknown (i.e. impurity positions $\mathbf{r}_j$ and impurity types unknown)

- Idea of **disorder average**: Work with statistical model for $U(\mathbf{r})$ and average over different realizations of disorder (e.g. many samples)
  - notation: $\langle ... \rangle_{\text{dis}}$
  - disorder average recovers translational invariance $\left\langle G^R_{\mathbf{r},\mathbf{r}'} \right\rangle_{\text{dis}}$ depends only on $\mathbf{r} - \mathbf{r}'$
- Disorder average in experiment:
  - measure many samples (a single large sample is enough if the observable is "self-averaging")
  - thermal cycle of one sample (measure, warm up, impurities move, cool down, repeat)

Statistical disorder model: Gaussian white noise (GWN)

- Consider $U(\mathbf{r})$ a random function with the properties
  - $\langle U(\mathbf{r}) \rangle_{\text{dis}} = 0$ (this is not really a restriction, any non-zero $\langle U(\mathbf{r}) \rangle_{\text{dis}}$ could be added to μ)
  - Disorder correlator:
$$\langle U(\mathbf{r}) U(\mathbf{r}') \rangle_{\text{dis}} = \frac{1}{2\pi D_0 \tau} \delta(\mathbf{r} - \mathbf{r}') \tag{265}$$
    where $D_0 = m k_F/(2\pi^2)$ the (spin-less) density of states at the Fermi level and τ is a parameter with units of a time, its meaning will become clear soon.
  - All higher-order disorder correlators follow from the application of (bosonic) Wick's theorem valid for a Gaussian probability distribution (hence the name "Gaussian" white noise):
$$\begin{aligned} \langle U(\mathbf{r}) U(\mathbf{r}') U(\mathbf{r}'') \rangle_{\text{dis}} &= 0 \\ \langle U(\mathbf{r}) U(\mathbf{r}') U(\mathbf{r}'') U(\mathbf{r}''') \rangle_{\text{dis}} &= \langle U(\mathbf{r}) U(\mathbf{r}') \rangle_{\text{dis}} \langle U(\mathbf{r}'') U(\mathbf{r}''') \rangle_{\text{dis}} + \langle U(\mathbf{r}) U(\mathbf{r}'') \rangle_{\text{dis}} \langle U(\mathbf{r}') U(\mathbf{r}''') \rangle_{\text{dis}} \\ &\quad + \langle U(\mathbf{r}) U(\mathbf{r}''') \rangle_{\text{dis}} \langle U(\mathbf{r}') U(\mathbf{r}'') \rangle_{\text{dis}} \end{aligned} \tag{266}$$

- For the FT of the disorder potential $U_{\mathbf{q}} = \frac{1}{V} \int_{\mathbf{r}} e^{-i\mathbf{q}\cdot\mathbf{r}} U(\mathbf{r})$, one has
$$\langle U_{\mathbf{q}} \rangle_{\text{dis}} = 0, \quad \langle U_{\mathbf{q}} U_{\mathbf{q}'} \rangle_{\text{dis}} = \frac{1}{2\pi D_0 \tau V} \delta_{\mathbf{q}+\mathbf{q}'.0} \tag{267}$$

- GWN is an oversimplified model that facilitates calculations. However, if the right parameter τ is inserted (from more elaborate microscopic calculation), it can give meaningful results.

Disorder self-energy in Born approximation

- We perform the perturbative diagrammatic treatment of $\mathcal{G}_{\mathbf{k},\mathbf{k}'}(i\omega_n)$ and copy from Sec. 9.1, see Fig. 17(a). Formally, it makes no difference if $U(\mathbf{r})$ corresponds to a single impurity or one realization of a GWN potential. Each star corresponds to $U_{\mathbf{q}}$.
- We take the disorder average using the GWN, see Fig. 17(b) to find $\langle \mathcal{G}_{\mathbf{k}}(i\omega_n) \rangle_{\text{dis}}$. All diagrams with an odd number of $U_{\mathbf{q}}$ vanish.
- In diagrams with more than two $U_{\mathbf{q}}$ the disorder potentials can be paired in multiple ways for the average, c.f. Eq. (266).
- Like in the case of interactions, we introduce the disorder self-energy $\Sigma_{\mathbf{k}}(i\omega_n)$. It is defined as the sum over all one-fermion irreducible diagrams with external fermion lines amputated. The Dyson equation connects the disorder averaged GF, self-energy and clean GF:
$$\langle \mathcal{G}_{\mathbf{k}}(i\omega_n) \rangle_{\text{dis}} = \frac{\mathcal{G}^0_{\mathbf{k}}(i\omega_n)}{1 - \mathcal{G}^0_{\mathbf{k}}(i\omega_n)\Sigma_{\mathbf{k}}(i\omega_n)} = \frac{1}{i\omega_n - \xi_{\mathbf{k}} - \Sigma_{\mathbf{k}}(i\omega_n)} \tag{268}$$

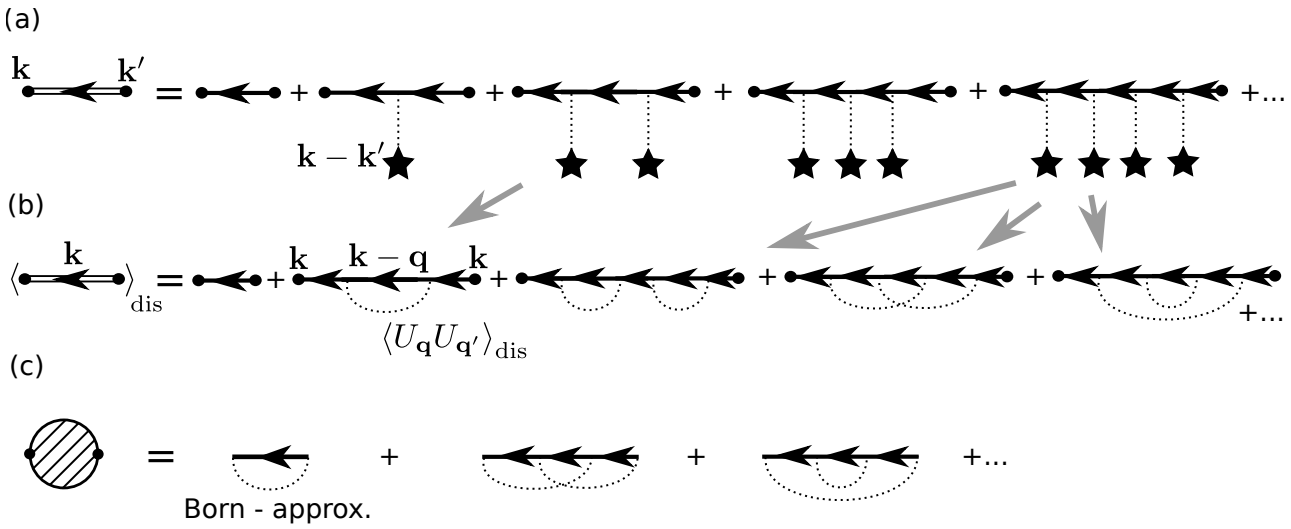

Figure 17: (a) Perturbative expansion of electronic Matsubara GF in the presence of disorder potential $U_{\mathbf{q}}$. (b) Disorder averaged GF $\langle \mathcal{G}_{\mathbf{k}}(i\omega_n)\rangle_{\rm dis}$ assuming Gaussian white noise disorder. (c) Disorder self-energy up to fourth order in $U_{\mathbf{q}}$.

- Calculation of $\Sigma_{\mathbf{k}}(i\omega_n)$ in lowest order in U ["Born approximation", first diagram on rhs of Fig. 17(c)].

$$\Sigma_{\mathbf{k}}(i\omega_n) = \frac{1}{V}\sum_{\mathbf{q}} \mathcal{G}^0_{\mathbf{k}-\mathbf{q}}(i\omega_n)\frac{1}{2\pi D_0\tau} = \frac{1}{2\pi D_0\tau}\frac{1}{(2\pi)^3}\int \mathrm{d}\mathbf{p}\,\frac{1}{i\omega_n - \xi_{\mathbf{p}}} \tag{269}$$

  We perform the analytic continuation $i\omega_n \to \omega \pm i\eta$. We disregard the real part as this can be absorbed into the Fermi energy and obtain for the imaginary part of the retarded or advanced self energy

$$\mathrm{Im}\Sigma_{\mathbf{k}}(\omega \pm i\eta) = \frac{1}{2\pi D_0\tau}\mathrm{Im}\frac{1}{(2\pi)^3}\int \mathrm{d}\mathbf{p}\,\frac{1}{\omega \pm i\eta - \xi_{\mathbf{p}}} = \mp\frac{\pi D(\omega)}{2\pi D_0\tau} \simeq \mp\frac{1}{2\tau} \tag{270}$$

  where we assumed $\omega \simeq 0$. The corresponding expression for the Matsubara self-energy is $\Sigma_{\mathbf{k}}(i\omega_n) \simeq -\frac{i}{2\tau}\mathrm{sgn}(\omega_n)$ which is not analytic at the real axis of the imaginary plane.

- We insert the above $\mathrm{Im}\Sigma_{\mathbf{k}}(\omega + i\eta)$ in the Dyson Eq. (268) and find the disorder averaged retarded propagator

$$\left\langle G^R_{\mathbf{k}}(\omega)\right\rangle_{\rm dis} = \frac{1}{\omega + i\eta - \xi_{\mathbf{k}} + i/(2\tau)} \;\to\; \left\langle G^R_{\mathbf{k}}(t)\right\rangle_{\rm dis} = \int \frac{\mathrm{d}\omega}{2\pi}\,\frac{e^{-i(\omega+i\eta)}}{\omega - \xi_{\mathbf{k}} + i/(2\tau)} \tag{271}$$

  where we can drop the infinitesimal $i\eta$ in the denominator due to the presence of the finite $i/(2\tau)$.

- The pole of $G^{R,0}_{\mathbf{k}}(\omega)$ is shifted from infinitesimally close to the imaginary axis to a finite value in the lower half-plane by the disorder. Using contour integration, we obtain

$$\left\langle G^R_{\mathbf{k}}(t)\right\rangle_{\rm dis} = -i\theta(t)\, e^{-i\xi_{\mathbf{k}}t}e^{-t/(2\tau)} = G^{R,0}_{\mathbf{k}}(t)\cdot e^{-t/(2\tau)} \tag{272}$$

  and the spectral density is a Lorentzian of width 2τ

$$\langle A_{\mathbf{k}}(\omega)\rangle_{\rm dis} = -2\mathrm{Im}\left\langle G^R_{\mathbf{k}}(\omega)\right\rangle_{\rm dis} = \frac{1/\tau}{(\omega - \xi_{\mathbf{k}})^2 + 1/(4\tau^2)} \tag{273}$$

- Interpretation → Fig. 18(a,b):
  - plane-wave states $|\mathbf{k}\rangle$ are no longer eigenstates of the system with disorder
  - microscopically, an electron injected with wavevector $|\mathbf{k}\rangle$ is scattered into a different momentum state $|\mathbf{k}'\rangle$ after a typical time τ and thus leaves the state $|\mathbf{k}\rangle$

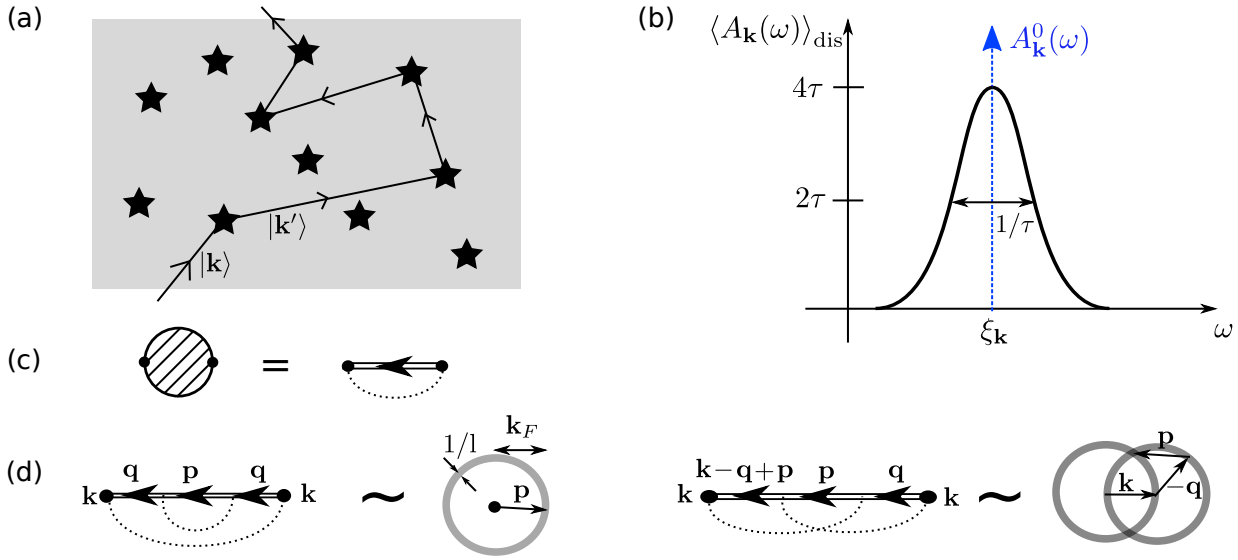

Figure 18: (a) Interpretation of the disorder averaged propagator (b) Disorder broadening of the spectral density. (c) Self-consistent Born approximation. (d) Ratio of missing and contained diagram in the self-consistent Born approximation.

- in the disorder averaged propagator $\left\langle G^R_{\mathbf{k},\mathbf{k}'}(t)\right\rangle_{\rm dis} \propto \delta_{\mathbf{k},\mathbf{k}'}$ only the latter information is encoded $\rightarrow$ exponential decay in time (with rate $1/2\tau$)
- for momenta around the Fermi surface, the distance an electron travels before scattering is the mean free path, $l = \tau v_F$.
- due to the Heisenberg uncertainty relation, the finite lifetime of an electron in state $|\mathbf{k}\rangle$ corresponds to the broadening of the energy resolution of this state in the spectral density $\langle A_{\mathbf{k}}(\omega)\rangle_{\rm dis}$

Self-consistent Born approximation and its validity in weakly disordered metals

- In the last paragraph, we approximated the full disorder self energy $\Sigma_{\mathbf{k}}(i\omega_n)$ in Fig. 17(c) by the first diagram (Born approximation).
- The self-consistent Born approximation (SCBA) in Fig. 18(c) contains the diagram of the Born approximation and all other diagrams with non-crossing impurity lines, such as the third diagram in Fig. 17(c).
- For weakly disordered metals (defined as $E_F\tau \gg 1$) the SCBA and the Born approximation yield similar results.
  Reason: We use Eq. (273) to write

$$\mathrm{Im}\Sigma^{\rm SCBA}_{\mathbf{k}}(\omega \pm i\eta) = \frac{-1/2}{2\pi D_0 \tau}\frac{1}{(2\pi)^3}\int \mathrm{d}\mathbf{p}\,\left\langle A^R_{\mathbf{p}}(\omega)\right\rangle_{\rm dis} \tag{274}$$

  and we find that the integral does not vary when $i\eta$ in the Born approximation is replaced with $i/2\tau$ in the SCBA, as long as $1/\tau$ is small compared to the scale on which the density of states $D(\omega)$ varies.
- Q: Do the crossing diagrams missing in SCBA change this picture?
- We show by a phase space argument that the crossing diagrams are suppressed relative to the non-crossing diagrams of the same order by a factor $1/(k_F l)$, see Fig. 17(d).
  We do this explicitly for the diagrams with two disorder lines exposed:
  - Non-crossing diagram (left): The 3d momentum integrals $\int_{\mathbf{q},\mathbf{p}}$ roam freely over the Fermi surface which is broadened by disorder by an amount $1/l$,

$$\int_{\mathbf{q},\mathbf{p}} \sim \left[4\pi k_F^2/l\right]^2 \sim k_F^4/l^2 \tag{275}$$

– Crossing diagram (right):
  * There is an additional restriction because the leftmost propagator comes with momentum $\mathbf{k}-\mathbf{q}+\mathbf{p}$ which must also lie on the (disorder broadened) Fermi surface.
  * If $\mathbf{k}$ is at the Fermi surface (left grey ring), and $-\mathbf{q}$ roams freely over the Fermi surface (right ring), we have only restricted configurations of $\mathbf{p}$ with length k_F that places $\mathbf{k}-\mathbf{q}+\mathbf{p}$ on the Fermi surface, i.e. back on the left ring.
  * This means the phase-space volume for the $\mathbf{p}$-integration is just the darker shaded regions which in 3d form a ring with cross-section volume $1/l$ and radius k_F, in total

$$[4\pi k_F^2/l]\times 2\pi k_F/l^2 \sim k_F^3/l^3 \tag{276}$$

– The ratio between the phase space volumes of the two diagrams is

$$\frac{v_{\text{non-cross}}}{v_{\text{cross}}}=\frac{k_F^4/l^2}{k_F^3/l^3}=k_F l=k_F v_F\tau=2E_F\tau \tag{277}$$

which in weakly disordered metals is a number much larger than one.

Electrical conductivity of disordered metal (via Kubo formula)

- We compute the electrical conductivity using the Kubo formula. Recall from Ex. 6.2 where we prepared:

$$\sigma^{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega)=\frac{i}{\omega}G^R_{j^\alpha(\mathbf{r}),j^\beta(\mathbf{r}')}(\omega)-\frac{e\rho_e(\mathbf{r})}{i\omega m}\delta(\mathbf{r}-\mathbf{r}')\delta_{\alpha\beta} \tag{278}$$

where $\mathbf{j}(\mathbf{r})=\sum_\sigma \frac{e}{2mi}\left(\Psi^\dagger_\sigma(\mathbf{r})\left[\nabla_{\mathbf{r}}\Psi_\sigma(\mathbf{r})\right]-\left[\nabla_{\mathbf{r}}\Psi^\dagger_\sigma(\mathbf{r})\right]\Psi_\sigma(\mathbf{r})\right)$ is the (paramagnetic) current density vector.

- Recall: The non-local conductivity tensor $\sigma^{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega)$ $(\alpha,\beta=x,y,z)$ gives the linear relation between perturbing electric field $E_\beta(\mathbf{r}',\omega)$ and resulting electronic current density $j_\alpha(\mathbf{r},\omega)$:

$$j_\alpha(\mathbf{r},\omega)=\int \mathrm{d}\mathbf{r}'\sum_\beta \sigma^{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega)E_\beta(\mathbf{r}',\omega) \tag{279}$$

- In a translation invariant system (after disorder average) one has $\sigma^{\alpha\beta}(\mathbf{r},\mathbf{r}';\omega)=\sigma^{\alpha\beta}(\mathbf{r}-\mathbf{r}';\omega)$ and we use momentum: $j_\alpha(\mathbf{q},\omega)=\int \mathrm{d}\mathbf{r}\, e^{-i\mathbf{q}\cdot\mathbf{r}}j_\alpha(\mathbf{r},\omega)$ and

$$\sigma^{\alpha\beta}(\mathbf{q};\omega)=\int \mathrm{d}\mathbf{r}\, e^{-i\mathbf{q}\cdot\mathbf{r}}\sigma^{\alpha\beta}(\mathbf{r};\omega)=\frac{i}{\omega}G^R_{j^\alpha(\mathbf{q}),j^\beta(-\mathbf{q})}(\omega)-\frac{e\rho_e}{i\omega m}\delta_{\alpha\beta} \tag{280}$$

with the current operator

$$\mathbf{j}(\mathbf{q})=\frac{e}{2m}\sum_{\mathbf{k},\sigma}(2\mathbf{k}+\mathbf{q})\,\psi^\dagger_{\mathbf{k},\sigma}\psi_{\mathbf{k}+\mathbf{q},\sigma} \tag{281}$$

- Order of limits for the arguments of $\sigma^{\alpha\beta}(\mathbf{q};\omega)$:
  – We are interested in the DC conductivity, i.e. $\omega\to 0$.
  – The conductivity should be defined with respect to the internal electric field in the conductor (c.f. 4-point measurement)
  – The internal field might differ from the external field $E_\beta(\mathbf{r}',\omega)$ that the calculation is done for by induced fields generated by (i) screening charges and (ii) fields generated by time-dependent currents (for $\omega\neq 0$, these currents generate magnetic fields which generate their own electric fields).
  – Claim: Induced fields are negligible for the precise order of limits $\lim_{\omega\to 0}\lim_{q\to 0}$.
  – Why? (i) No screening charges build up because the there is no time to redistribute charge in $\sim 1/\omega$ over diverging distance $\sim 1/q$. (ii) No magnetic fields are generated because frequency is too low.

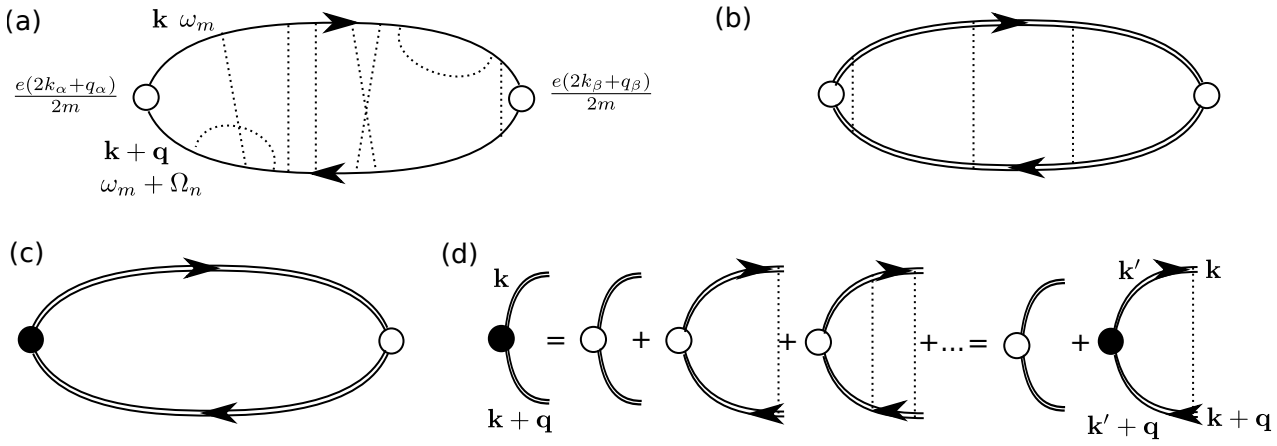

Figure 19: Electrical (Kubo-)conductivity for a disordered metal (GWN disorder). (a) Example for a term in the diagrammatic expansion on the rhs of Eq. 19

- We now do a calculation using a disorder average withing the GWN model and analytic continuation. We start from

$$G^R_{j^\alpha(\mathbf{q}),j^\beta(-\mathbf{q})}(\omega) = \mathcal{G}_{j^\alpha(\mathbf{q}),j^\beta(-\mathbf{q})}(i\Omega_n \to \omega + i\eta) \tag{282}$$

- Fig. 19(a) shows a typical diagram for perturbation theory in $U(\mathbf{r})$ after the disorder average has been taken.
  - The fermionic backbone would also contain two disconnected diagrams, but they would only give rise to a contribution $\delta_{i\Omega_n}$ which is not relevant for analytical continuation.
  - The empty circles are the (bare) current vertices $\Gamma^0_\alpha(\mathbf{k}, i\omega_m; \mathbf{k}+\mathbf{q}, i\omega_m + i\Omega_n) = \frac{e(2k_\alpha+q_\alpha)}{2m}$.
  - The disorder average is already taken, all types of connections (within one of the two legs and intra-leg) are allowed.
- We neglect any crossed impurity lines due to a phase space argument similar to the one above.
- Thus obtain the approximate "ladder" diagram in Fig. 19(b) with full fermionic propagator lines.
- Fig. 19(c): All the ladder rungs can be associated to the left current vertex which then becomes a full dot Γ_α ("vertex correction").
- The definition of the full vertex is shown in Fig. 19(d). We also find a self-consistency equation for Γ_α :

$$\begin{aligned}\Gamma_\alpha(\mathbf{k}, i\omega_m; \mathbf{k}+\mathbf{q}, i\omega_m + i\Omega_n) &= \Gamma^0_\alpha(\mathbf{k}, i\omega_m; \mathbf{k}+\mathbf{q}, i\omega_m + i\Omega_n) \\ &+ \frac{1}{2\pi D_0 \tau V} \sum_{\mathbf{k}'} \langle \mathcal{G}_{\mathbf{k}'}(i\omega_m)\rangle_{\rm dis} \langle \mathcal{G}_{\mathbf{k}'+\mathbf{q}}(i\omega_m + i\Omega_n)\rangle_{\rm dis} \Gamma_\alpha(\mathbf{k}', i\omega_m; \mathbf{k}'+\mathbf{q}, i\omega_m + i\Omega_n)\end{aligned}$$

- We multiply with $\langle \mathcal{G}_{\mathbf{k}}(i\omega_m)\rangle_{\rm dis} \langle \mathcal{G}_{\mathbf{k}+\mathbf{q}}(i\omega_m + i\Omega_n)\rangle_{\rm dis}$ and sum over $\mathbf{k}$. Then we re-insert the last equation. This yields a self-consistency condition:

$$\Gamma_\alpha(\mathbf{k}, i\omega_m; \mathbf{k}+\mathbf{q}, i\omega_m + i\Omega_n) = \frac{e}{2m}\left[2k_\alpha + q_\alpha + \frac{\sum_{\mathbf{k}'} (2k'_\alpha + q_\alpha) \langle \mathcal{G}_{\mathbf{k}'}(i\omega_m)\rangle_{\rm dis} \langle \mathcal{G}_{\mathbf{k}'+\mathbf{q}}(i\omega_m + i\Omega_n)\rangle_{\rm dis}}{2\pi D_0 \tau V - \sum_{\mathbf{k}'} \langle \mathcal{G}_{\mathbf{k}'}(i\omega_m)\rangle_{\rm dis} \langle \mathcal{G}_{\mathbf{k}'+\mathbf{q}}(i\omega_m + i\Omega_n)\rangle_{\rm dis}}\right]$$

- Anticipate the limit $\mathbf{q} \to 0$, then the numerator of the large fraction goes to zero by symmetry since the terms $\propto \pm k'_\alpha$ cancel. This means $\lim_{\mathbf{q}\to 0} \Gamma_\alpha = \Gamma^0_\alpha$, there is no vertex correction.
- Remarks:
  - The absence of vertex correction is only true for the simple dispersion that we considered and for GWN disorder. It is not expected on general grounds.

– A finite vertex correction leads to a difference between impurity scattering lifetime τ (time to scattering even) and the transport mean-free time τ_{tr} (time to change direction appreciably).

- We return to the evaluation of the Matsubara current-current correlator from diagram Fig. 19(c). We already take the limit $\mathbf{q} \to 0$ and get a factor of two from the spin-sum:

$$\begin{aligned} \mathcal{G}_{\alpha\beta}(i\Omega_n) &\equiv \lim_{\mathbf{q}\to 0} \mathcal{G}_{j^\alpha(\mathbf{q}),j^\beta(-\mathbf{q})}(i\Omega_n) \\ &= \frac{2T}{V} \sum_{\mathbf{k},\omega_m} \langle \mathcal{G}_{\mathbf{k}}(i\omega_m)\rangle_{\text{dis}} \langle \mathcal{G}_{\mathbf{k}}(i\omega_m + i\Omega_n)\rangle_{\text{dis}} \end{aligned}$$

- The Matsubara sum is done in the standard way, but now there is a branch-cut in the complex plane both at $z \in \mathbb{R}$ and at $z + i\Omega_n \in \mathbb{R}$. This yields in total four real-frequency integrals. After analytical continuation $i\Omega_n \to \omega + i\eta$ (and dropping the infinitesimal $i\eta$ against the $i/2\tau$ in the disorder-averaged propagators) we find

$$\begin{aligned} G^R_{\alpha\beta}(\omega) &= \mathcal{G}_{\alpha\beta}(i\Omega_n \to \omega + i\eta) \\ &= \frac{e^2/m^2}{2\pi i V} \sum_{\mathbf{k}} k_\alpha k_\beta \int \mathrm{d}\xi \, \tanh\frac{\xi-\mu}{2T} \times \\ &\times \Big[\frac{1}{\xi - \varepsilon_{\mathbf{k}} + i/2\tau} \cdot \frac{1}{\xi + \omega - \varepsilon_{\mathbf{k}} + i/2\tau} - \frac{1}{\xi - \varepsilon_{\mathbf{k}} - i/2\tau} \cdot \frac{1}{\xi + \omega - \varepsilon_{\mathbf{k}} + i/2\tau} \\ &+ \frac{1}{\xi - \omega - \varepsilon_{\mathbf{k}} - i/2\tau} \cdot \frac{1}{\xi - \varepsilon_{\mathbf{k}} + i/2\tau} - \frac{1}{\xi - \omega - \varepsilon_{\mathbf{k}} - i/2\tau} \cdot \frac{1}{\xi - \varepsilon_{\mathbf{k}} - i/2\tau}\Big] \end{aligned}$$

- We perform a partial integration to obtain a sharp spike as $T \to 0$,

$$G^R_{\alpha\beta}(\omega) = \frac{e^2/m^2}{4\pi i T} \int \mathrm{d}\xi \, \cosh^{-2}\left(\frac{\xi-\mu}{2T}\right) \left(\frac{1}{\omega} - \frac{1}{\omega + i/\tau}\right) \frac{1}{V} \sum_{\mathbf{k}} k_\alpha k_\beta \ln \frac{(\xi - \varepsilon_{\mathbf{k}})^2 - (\omega + i/2\tau)^2}{(\xi - \varepsilon_{\mathbf{k}})^2 + 1/4\tau^2}$$

- The $\mathbf{k}$-integral brings a factor $\delta_{\alpha\beta}$ by symmetry and we can use isotropy $k_\alpha^2 \to \frac{1}{3}k^2 = \frac{1}{3} \times 2m\varepsilon_{\mathbf{k}}$. Then we can change to a an energy integral and obtain

$$G^R_{\alpha\beta}(\omega) = -\frac{\rho_e e \delta_{\alpha\beta}}{(1 - i\omega\tau)m} \tag{283}$$

- We substitute this into the final expression for the conductivity (280) and obtain

$$\sigma^{\alpha\beta}(q \to 0, \omega) = -\frac{i}{\omega}\frac{\rho_e e \delta_{\alpha\beta}}{(1 - i\omega\tau)m} - \frac{e\rho_e}{i\omega m}\delta_{\alpha\beta} = \frac{\rho_e e\tau}{m\,(1 - i\omega\tau)}\delta_{\alpha\beta} \tag{284}$$

  In the limit $\omega \to 0$ this yields the well-known Drude formula $\sigma^D = \frac{\rho_e e\tau}{m}$ from elementary solid-state physics. Recall that the Drude formula is a purely classical result which does not even take into account the concept of Fermi surface.

- This course has to end here, but the virtue of the formalism developed is that quantum corrections to the Drude conductivity can be treated. A famous example is the weak localization correction which is rooted in quantum interference and reduces the conductivity. It can be seen as the precursor for Anderson localization ($\sigma_{T=0} = 0$) which in 3d only happens for very strong disorder.

Exercises

Exercise 9.1. Clean retarded and advanced propagators in real space

Consider a metal with clean dispersion $\xi_q = q^2/(2m) - \mu$. In the presence of impurities where translational invariance is broken it is often required to use the real-space representation of the clean retarded propagator. Show via explicit momentum space integration that

$$G^{0,R}(\omega, \mathbf{r} \neq 0) = \frac{1}{V} \sum_{\mathbf{q}} e^{i\mathbf{q}\cdot\mathbf{r}} \frac{1}{\omega + i\eta - q^2/(2m) + \mu} = -\frac{m}{2\pi} \frac{e^{+ikr}}{r} \tag{285}$$

where k is the solution of $\omega + i\eta - k^2/(2m) + \mu = 0$ with $\mathrm{Im}\, k > 0$. In the advanced case ($\eta \to -\eta$), one has $G^{0,A}(\omega) = [G^{0,R}(\omega)]^\star$. Hint: Replace the momentum sum by an integration and use spherical coordinates and the residue theorem for the final radial integral.

Exercise 9.2. Friedel oscillations

1) Derive Eq. (262) from Eq. (261) using the techniques for Matsubara summation of Sec. 5.6.

2) Derive Eq. (263) from a spatial FT of Eq. (262), $n(\mathbf{r}) = \mathcal{G}_{\mathbf{r},\mathbf{r}}(\tau = -\eta)$. Use a linearized spectrum around k_F, $\xi_k = v_F(k - k_F)$ with $v_F = k_F/m$. Perform the following steps:

- Recall that $\mathrm{Im}\overline{G^0(\omega + i\eta)} = -\pi D(\omega)$ with $D(\omega)$ the (spin-less) density of states at energy ω and also show
$$\frac{u}{1 - u\overline{G^0(\omega \pm i\eta)}} = -\frac{\sin\delta_0(\omega)}{\pi D(\omega)} e^{\pm i\delta_0(\omega)} \tag{286}$$
- Insert this and the propagators of Ex. 9.1 into Eq. (262) and perform the sum.
- Use partial integration to expose $-\partial_\omega n_F(\omega)$ and assume $\delta_0(\omega)$ and $D(\omega)$ vary slowly with ω compared to $\omega r/v_F$.
- Take the limit $T \to 0$.