Lecture notes FY8305

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Digitialized lecture notes for the course "FY8305 - Functional Integral Methods in Condensed Matter Physics".

These notes follow the pdf containing the hand written lecture notes for the course "FAG 74986 Funksjonal-integral metoder HØST 1996". Website: https://www.ntnu.edu/studies/courses/FY8305

Contributors

- Karl Kristian Ladegård Lockert
- Snorre Bergan

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1 Uncertainties/mistakes

- Something weird in the derivation of (2.28).
- The indices in equation (4.2) seems off.
- In the proof in section 4.1 i think there should be a creation operator on one of the last lines in the proof, not annihilation operator as it stands in the notes. $ae^{\varphi a^\dagger}|0\rangle$ instead of $ae^{\varphi a}|0\rangle$
- It is a somewhat unclear purpose of Equations (4.31) to (4.35).
- The ordering of headlines and equations in section 4 is a bit weird, and some things seem a bit unmotivated.
- The notes uses partial derivative where one really should use functional derivative. The functional derivative w.r.t the linear sources reduces to regular total derivative, so there is a factor 1/2 difference.
- Fixed on the "most important paths" part in feynman path integral.
- Double check the labeling on states/ sub indices in (5.19) and the previous few eqs.
- Justify why one can take the infinitesimal limit on one of the functions in a product in the integral (9.26).
- The limits in (9.44) seems a bit odd, but is probably correct. There is also some slight confusion in the signs inside the ln-functions, which also comes with a statement "not entirely correct" in the notes.

2 Short recap of second quantization for fermions and bosons

Pages 2-10 in lecture notes.

Notation: $\mu =$ set of quantum numbers that define a one-particle state.

2.1 Many particle basis

Ex 1.

$$\mu = (\vec{k}, \sigma) : \text{Wave number, spin}$$
$$\mu = (i, \sigma) : \text{Lattice point, spin}$$
$$\mu = (n, i) : \text{Orbital, lattice point}$$

A many-particle basis can be written $|\phi\rangle = |n_\mu, n_\nu, \ldots, n_{\mu_N}\rangle$. Many particle states are built by combining many one-particle states, but where the one-particle states are not necessarily independent. If one of the set of quantum numbers, μ_i, are changed, this scattering will generally have consequences for the distribution of quantum numbers for the remaining sets $\{\mu_j\}_{j\neq i}$. We generally imagine that many-particle states can be built as a linear combination of $|\phi\rangle$'s;

$$|\Psi\rangle = \sum_{n_{\mu_1},\ldots,n_{\mu_N}} \phi_{\mu_1,\ldots,n_{\mu_N}} |\mu_1, \ldots, n_{\mu_N}\rangle . \tag{2.1}$$

A definite one-state vector $|n_\mu, \ldots, n_{\mu_N}\rangle$ can be demanded from a vacuum state (where there is no filled one-particle states) $|0\rangle$ via creation operators.

bosons :	$a_\mu^\dagger$
fermions :	$c_\mu^\dagger$

A quanta in a one-particle state can be destroyed by the annihilation operators.

bosons :	a_μ
fermions :	c_μ

These operators satisfy some commutation relations:

$$[a_\mu, a_\nu] = [a_\mu^\dagger, a_\nu^\dagger] = 0 \tag{2.2}$$
$$[a_\mu, a_\nu^\dagger] = \delta_{\mu\,\nu} \tag{2.3}$$
$$[A, B] = AB - BA \tag{2.4}$$
$$\{c_\mu^\dagger, c_\nu^\dagger\} = \{c_\mu, c_\nu\} = 0 \tag{2.5}$$
$$\{c_\mu, c_\nu^\dagger\} = \delta_{\mu\,\nu} \tag{2.6}$$
$$\{A, B\} = AB + BA \tag{2.7}$$

These will automatically satisfy the Pauli principle as well, which gives symmetri/ antisymmetric solutions by exchange, dependent if the particles are bosons/fermions.

2.2 From classical formulation to second quantization of one-particle operators

For one-particle operators we usually have a kinetic energy function on a form like

$$T = \sum_i T\left(\vec{r}_i, \vec{p}_i\right) = \sum_i T\left(\vec{r}_i, \frac{\partial}{\partial r}\right) \tag{2.8}$$

Ex 2. External electrostatic potential:

$$T = \sum_i V_{\text{ext}}\left(\vec{r}_i\right) \tag{2.9}$$

Ex 3. Kinetic energy:

$$T = \sum_i \frac{p^2}{2m} = -\sum_i \frac{\hbar^2}{2m}\nabla_i^2 \tag{2.10}$$

Ex 4. Crystal-potential:

$$T = \sum_i \sum_j v_{\text{cryst}}\left(\vec{r}_i, \vec{R}_j\right) \tag{2.11}$$

Second quantization by an operator on this form can be written

$$T = \sum_{\mu,\nu} T_{\mu\nu} c_\mu^\dagger c_\nu, \tag{2.12}$$

where

$$T_{\mu\,\nu} = \langle \mu | T\left(\vec{r}, \vec{p}\right) | \nu \rangle \,. \tag{2.13}$$

Note: The matrix element of one-particle operators are determined by matrix elements in the Hilbert space of one-particle states.

2.3 From classical formulation to second quantization of two-particle operators

Typically, we consider pair-potentials

$$V = \sum_{i,j} V\left(\vec{r}_i, \vec{r}_j\right). \tag{2.14}$$

Ex 5. Exchange interaction of two charges

$$V = \frac{e^2}{2} \sum_{i \neq j} \frac{1}{|\vec{r}_i - \vec{r}_j|} \tag{2.15}$$

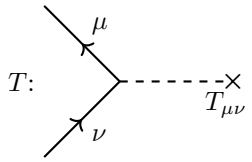


Figure 1: Scattering from an external potential $v_{\mu\nu}c_\mu^\dagger c_\nu$

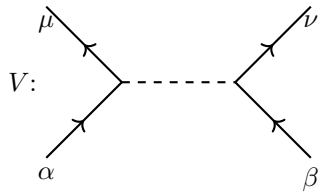


Figure 2: Exchange interaction between two particles.

The second quantization versions of these are

$$V = \sum_{\mu,\ldots,\beta} V_{\mu\nu\alpha\beta} c_\mu^\dagger c_\nu^\dagger c_\alpha c_\beta, \tag{2.16}$$

where again

$$V_{\mu\nu\alpha\beta} = \langle \mu\nu | V(\vec{r}_i, \vec{r}_j) | \beta\alpha \rangle \tag{2.17}$$

Note: The matrix element of two-particle operators are determined by matrix elements in the Hilbert room of two-particle states.

The Hamiltonian:

$$H = T + V \tag{2.18}$$

$$T = -\sum_i \frac{\hbar^2}{2m} \nabla_i^2 \tag{2.19}$$

So far, we have just presented second quantization for fermion operators, but an equivalent statement will of course hold for the second quantization version of the Hamiltonian for an interacting, material, bosonic system, which has the same identical form as (2.18). Notice that each term in H has just as many $c_\mu^\dagger$ as c_ν.

2.4 Statistical mechanics

Assume that we know the spectrum E_N^n for an interacting many-particle system, defined by a state $|\psi_N\rangle_n$, where N is the number of particles in the system and n is an index that indicates what excited state $|\psi_N\rangle_n$ the system is in. $|\psi_N\rangle$ is also assumed to be known, such that the matrix product of observables can be calculated:

$$H |\psi\rangle_n = E_N |\psi\rangle_n . \tag{2.20}$$

To do statistical mechanics, we need to introduce temperature. We do this by using the canonical partition function

$$Z_N = \sum_n \mathrm{e}^{-\beta E_N^n}. \tag{2.21}$$

Note, in (2.21) we sum over states, not the energy levels E_N^n.

$$\begin{aligned} Z &= \sum_n {}_n\langle\psi_N|\mathrm{e}^{-\beta H}|\psi_N\rangle_n \\ &= \mathrm{Tr}\left(\mathrm{e}^{-\beta H}\right) = \mathrm{Tr}\left(S^{-1}S\mathrm{e}^{-\beta H}\right) \\ &= \mathrm{Tr}\left(S\mathrm{e}^{-\beta H}S^{-1}\right) \\ &= \sum_{n'} {}_{n'}\langle\phi_N|\mathrm{e}^{-\beta H}|\phi_N\rangle_{n'}\,. \end{aligned} \tag{2.22}$$

We see in (2.22) that we can use an arbitrary basis to calculate the partition function. The most convenient basis is often a basis where the Hamiltonian is diagonal, but not always.

We write the statistical mean value of an operator as

$$\begin{aligned} \left\langle\hat{O}\right\rangle &\equiv \frac{1}{Z}\,\mathrm{Tr}\left(\hat{O}\mathrm{e}^{-\beta H}\right) \\ &= \frac{1}{Z}\sum_n {}_n\langle\psi_N|\hat{O}\mathrm{e}^{-\beta H}|\psi_N\rangle_n \\ &= \frac{1}{Z}\sum_{n,n'} {}_n\langle\psi_N|\hat{O}|\psi_N\rangle_{n'}\underbrace{{}_{n'}\langle\psi_N|\mathrm{e}^{-\beta H}|\psi_N\rangle_n}_{\delta_{nn'}\mathrm{e}^{-\beta E_{n'}}}. \end{aligned} \tag{2.23}$$

Thus, we have

$$\left\langle\hat{O}\right\rangle = \frac{1}{Z}\sum_n \underbrace{{}_n\langle\psi_N|\hat{O}|\psi_N\rangle_n}_{\text{QM matrix element}}\ \mathrm{e}^{-\beta E_N^n}. \tag{2.24}$$

Notice how the temperature, T only appears in the last factor in (2.24). Let us now consider the ground state ($n = 0$) in the low temperature limit with energy E_0 corresponding to the state $|\psi_N\rangle_0$.

$$\begin{aligned} \left\langle\hat{O}\right\rangle &\simeq \frac{1}{Z_{\beta=\infty}}\mathrm{e}^{-\beta E_0}{}_0\langle\psi_N|\hat{O}|\psi_N\rangle_0 \\ &= \frac{\mathrm{e}^{-\beta E_0}}{\mathrm{e}^{-\beta E_0}}{}_0\langle\psi_N|\hat{O}|\psi_N\rangle_0\,, \end{aligned}$$

such that

$$\left\langle\hat{O}\right\rangle \overset{\beta\to\infty}{=} {}_0\langle\psi_N|\hat{O}|\psi_N\rangle_0\,. \tag{2.25}$$

We now have a way to calculate the statistical mean value in the ground state at zero temperature. Let us now now assume that the energy spectrum

is such that the ground state is separated from excited states by a gap (band insulators, semiconductors, superconductors). This way, we can express the excited state energies as

$$E_N^1 = E_N^0 + \Delta_N \tag{2.26}$$

such that

$$E_N^2, E_N^3, \cdots \geq E_N^1. \tag{2.27}$$

This way, we get from (2.24)

$$\begin{aligned}
\left\langle \hat{O} \right\rangle &= \frac{1}{Z} \sum_n {}_n \left\langle \psi_N | \hat{O} | \psi_N \right\rangle_n \mathrm{e}^{-\beta E_N^n} \\
&= \frac{\sum_n {}_n \left\langle \psi_N | \hat{O} | \psi_N \right\rangle_n \mathrm{e}^{-\beta E_N^n}}{\sum_n \mathrm{e}^{-\beta E_N^n}} \\
&= \cdots \\
&= \frac{{}_0 \left\langle \psi_N | \hat{O} | \psi_N \right\rangle_0 \mathrm{e}^{-\beta E_N^0 \left(1 + \mathrm{e}^{-\beta\Delta} \ldots\right)}}{\mathrm{e}^{-\beta E_N^0} \left(1 + \mathrm{e}^{-\beta\Delta} \ldots\right)}
\end{aligned} \tag{2.28}$$

and we find that as $\beta\Delta >> 1$, $\hat{O} \simeq {}_0 \left\langle \psi_N | \hat{O} | \psi_N \right\rangle_0$. In semiconductors we find $\Delta \sim 10\text{mev} \sim 1000\text{K}$.

3 Coherent states and introduction to Grassmann variables

Pages 10-17 in lecture notes.

3.1 Coherent states

A coherent state (both for fermions and bosons) is defined as an eigenstate to an annihilation operator

$$a_\mu |\phi\rangle = \varphi_\mu |\phi\rangle \qquad \textbf{Bosons} \tag{3.1}$$
$$c_\mu |\psi\rangle = \xi_\mu |\psi\rangle \qquad \textbf{Fermions} \tag{3.2}$$

Both $|\psi\rangle$ and $|\phi\rangle$ must contain a component with the least (≥ 0) quantum number (quant), but it is clear that neither $|\psi\rangle$ nor $|\phi\rangle$ can be states with a sharply defined number of particles. They are therefore also "hard to destroy". This also explains why we chose to define them as eigenstates of the annihilation operators, not the creation operators. We will get back to the creation of these coherent states.

We will first look at the bosonic case:

Bosonic case

$$a_\mu |\phi\rangle = \varphi_\mu |\phi\rangle \tag{3.3}$$

$$\begin{aligned} &[a_\mu, a_\nu] = 0 \\ &\quad \Rightarrow (a_\mu a_\nu - a_\nu a_\mu) |\phi\rangle = 0 \\ &\quad = (\varphi_\mu \varphi_\nu - \varphi_\nu \varphi_\mu) |\phi\rangle \\ &\qquad\qquad \Rightarrow [\varphi_\mu, \varphi_\nu] = 0. \end{aligned} \tag{3.4}$$

Equation (3.4) will always be satisfied if $\varphi_\mu \in \mathbb{C}$. **The eigenvalues to coherent boson states can be chosen as complex numbers. This is something we can state without knowing anything about how these states are constructed.**

Fermionic case

$$c_\mu |\psi\rangle = \xi_\mu |\psi\rangle \tag{3.5}$$

$$\begin{aligned} &\{c_\mu, c_\nu\} = 0 \\ &\quad \Rightarrow (c_\mu c_\nu + c_\nu c_\mu) |\psi\rangle = 0 \\ &\quad = (\xi_\mu \xi_\nu + \xi_\nu \xi_\mu) |\psi\rangle \\ &\qquad\qquad \Rightarrow \{\xi_\mu, \xi_\nu\} = 0. \end{aligned} \tag{3.6}$$

If $\xi_\mu \in \mathbb{C}$, (3.6) will only be satisfied if $\{\xi_\mu\} = 0$, trivial eigenvalues. **The eigenvalues for coherent fermion states must be chosen as anti-commuting numbers, Grassmann-variables.**

3.2 Grassmann variables

Fundamentals

Equation (3.6) states the fundamental property of Grassmann variables, and it immediately follows that

$$\xi_\mu^2 = 0, \tag{3.7}$$

the squares of the Grassmann variables vanish! Similarly we have that $\xi^n = \xi^2\xi^{n-2} = 0, n \geq 2$. An arbitrary series expansion in Grassmann variables

$$\begin{aligned} f(\xi) &= \sum_n c_n \xi^n \\ &= c_0 + c_1\xi + \dots \\ &= c_0 + c_1\xi \end{aligned} \tag{3.8}$$

is linear. We can also consider $f(\xi^*) = c_0 + c_1\xi^*$, where $(\xi^*)^* = \xi$. An arbitrary function of ξ, ξ^* can be written on the forms

$$A(\xi, \xi^*) = c_0 + c_1\xi + c_2\xi^* + c_3\xi\xi^* \tag{3.9}$$

$$= c_0 + c_1\xi + c_2\xi^* + d_3\xi^*\xi \tag{3.10}$$

We will now look into some of the properties of functions of Grassmann variables.

Differentiation

Differentiation with respect to Grassman variables follows

$$\frac{\partial\xi}{\partial\xi} = 1 \qquad \frac{\partial\xi}{\partial\xi^*} = 0 \tag{3.11}$$

$$\frac{\partial\xi^*}{\partial\xi} = 0 \qquad \frac{\partial\xi^*}{\partial\xi^*} = 1 \tag{3.12}$$

$$\frac{\partial(\xi\xi^*)}{\partial\xi} = \xi^* \tag{3.13}$$

$$\frac{\partial(\xi\xi^*)}{\partial\xi^*} = -\frac{\partial(\xi^*\xi)}{\partial\xi^*} = -\xi \tag{3.14}$$

$$\frac{\partial f(\xi)}{\partial\xi^*} = 0 \tag{3.15}$$

$$\frac{\partial f(\xi)}{\partial\xi} = c_1 = \frac{\partial f(\xi^*)}{\partial\xi^*}, \tag{3.16}$$

and for functions defined as in (3.9), we have

$$\frac{\partial}{\partial \xi} A\left(\xi, \xi^*\right) = c_1 + c_3 \xi^* = c_1 - d_3 \xi^* \tag{3.17}$$

$$\frac{\partial}{\partial \xi^*} A\left(\xi, \xi^*\right) = c_2 - c_3 \xi = c_2 + d_3 \xi. \tag{3.18}$$

Integration

Integrating with respect to Grassmann variables are motivated from the properties of "normal" Riemann integrals, that if $f\left(x = \pm\infty\right) = 0$, then

$$\int_{-\infty}^{\infty} \mathrm{d}x \, \frac{\mathrm{d}f}{\mathrm{d}x} = 0. \tag{3.19}$$

Equivalently we define

$$\int \mathrm{d}\xi \cdot 1 = \int \mathrm{d}\xi \, \frac{\mathrm{d}\xi}{\mathrm{d}\xi} = 0 \tag{3.20}$$

$$\int \mathrm{d}\xi^* = 0, \tag{3.21}$$

in other words, the integral of a total differential is zero.

$$\int \mathrm{d}\xi \, \xi = \int \mathrm{d}\xi^* \, \xi^* = 1 \tag{3.22}$$

is a "normalization" criteria. These relations define what we mean by Grassmann-integration.

Now, we have

$$\int \mathrm{d}\xi \, f\left(\xi\right) = c_1 \tag{3.23}$$

$$\frac{\partial f}{\partial \xi} = c_1 \tag{3.24}$$

$$\begin{aligned} \int \mathrm{d}\xi \, A\left(\xi, \xi^*\right) &= \int \mathrm{d}\xi \left(x_0 + c_1 \xi + c_2 \xi^* + c_3 \xi \xi^*\right) \\ &= c_1 + c_3 \xi^*. \end{aligned} \tag{3.25}$$

As we can see by comparing (3.25) with (3.17), "integration" = "derivation". The somewhat hand wavy definition of integration is motivated by the fact that it gives results that reminds us about results from the theory for complex functions.

The number operator

Generally, we have that

$$a_\mu^\dagger |\phi\rangle \neq |\phi\rangle \qquad\qquad c_\mu^\dagger |\xi\rangle \neq |\xi\rangle \,, \tag{3.26}$$

and so

$$a_\mu^\dagger a_\mu |\phi\rangle \neq N_\mu^\phi |\phi\rangle \tag{3.27}$$

$$c_\mu^\dagger c_\mu |\xi\rangle \neq N_\mu^\xi |\xi\rangle \,. \tag{3.28}$$

The coherent states are <u>not</u> eigenstates of the counting operator. $|\phi\rangle, |\xi\rangle$ are not states with a fixed number of "quants".

Algebra

Consider a vector space with the following additional properties:

1)	$(xy)z = x(yz)$
2)	$x(y+z) = xy + xz$
3)	$(x+y)z = xz + yz$
4)	$\alpha xy = x\alpha y.$

In Abelian algebra, $xy = yx$, while in Grassmann algebra $xy = -yx$. <u>Complex numbers</u> are generators for the Abelian algebra over the field $\mathbb{G}$ of commuting numbers. <u>Grassmann numbers</u> are generators for the algebra over the field $\mathbb{G}$ of anticommuting numbers.

4 Construction of coherent states for bosons, and its properties

Pages 18-26 in lecture notes.

4.1 Construction

The definition of a coherent boson state $|\phi\rangle$ is stated in (3.1). We make an ansatz – a qualified guess – that $|\phi\rangle$ can be created as

$$|\phi\rangle = \mathrm{e}^{\sum_\mu \varphi_\mu a_\mu^\dagger} |0\rangle \,. \tag{4.1}$$

We claim that

$$a_\mu \mathrm{e}^{\sum_\nu \varphi_\nu a_\nu^\dagger} |0\rangle = \varphi_\mu \mathrm{e}^{\sum_\nu \varphi_\nu a_\nu^\dagger} |0\rangle \tag{4.2}$$

Proof.

$$a \sum_{n=0} \frac{\left(\varphi a^\dagger\right)^n}{n!} |0\rangle = a \sum_{n=1} \frac{\varphi^n}{n!} \left(a^\dagger\right)^n |0\rangle \,.$$

Note that $\left(a^\dagger\right)^n a \,|0\rangle = 0$, and so we wish to "commute a through".

$$\begin{aligned}
\left[a, f\left(a^\dagger\right)\right] &= \sum_{n=1} c_n \left[a, \left(a^\dagger\right)^n\right] \\
&= \sum_{n=1} n c_n \left(a^\dagger\right)^{n-1} \\
f\left(a^\dagger\right) &= \sum_{n=0}^{\infty} c_n \left(a^\dagger\right)^n \\
&\implies \left[a, f\left(a^\dagger\right)\right] = \frac{\partial}{\partial a^\dagger} f\left(a^\dagger\right) .
\end{aligned}$$

More generally:

$$\begin{aligned}
\left[g(a), f(a^\dagger)\right] &= g\left(\frac{\partial}{\partial a^\dagger}\right) f\left(a^\dagger\right) \\
\left[a, \left(a^\dagger\right)^n\right] &= n \left(a^\dagger\right)^{n-1} \\
\left[(a)^m, \left(a^\dagger\right)^n\right] &= \frac{n!}{(n-m)!} \left(a^\dagger\right)^{n-m} \\
\left\{c, f\left(c^\dagger\right)\right\} &= \frac{\partial}{\partial c^\dagger} f\left(c^\dagger\right) \\
\left\{g(c), f(c^\dagger)\right\} &= g\left(\frac{\partial}{\partial c^\dagger}\right) f\left(c^\dagger\right)
\end{aligned}$$

To find out what the commutator $\left[a, \left(a^\dagger\right)^n\right]$ is, we use that

$$[A, BC] = [A, B]C + B[A, C], \tag{4.3}$$

with $A = a, B = a^\dagger, C = \left(a^\dagger\right)^{n-1}$ to get

$$\begin{aligned}
\left[a, \left(a^\dagger\right)^n\right] &= \left(a^\dagger\right)^{n-1} + a^\dagger \left[a, \left(a^\dagger\right)^{n-1}\right] \\
&= a \left(a^\dagger\right)^{n-1} \\
\implies a \left(a^\dagger\right)^n |0\rangle &= n \left(a^\dagger\right)^{n-1} |0\rangle \\
\implies a \mathrm{e}^{\varphi a^\dagger} |0\rangle &= \sum_{n=1}^{\infty} \frac{\varphi^n n \left(a^\dagger\right)^{n-1}}{n!} |0\rangle \\
&= \varphi \sum_{n=1}^{\infty} \frac{\left(\varphi a^\dagger\right)^{n-1}}{(n-1)!} |0\rangle \\
&= \varphi \mathrm{e}^{\varphi a^\dagger} |0\rangle .
\end{aligned}$$

□

Then, for more modes (quantum numbers), we get

$$|\phi\rangle = \mathrm{e}^{\sum_\mu \varphi_\mu a_\mu^\dagger} |0\rangle \tag{4.4}$$

with the φ_μ's satisfying

$$a_\mu |\phi\rangle = \varphi_\mu |\phi\rangle . \tag{4.5}$$

Coherent states: "difficult to destroy".

We also could have done this in a more direct way: Assume

$$|\phi\rangle = \prod_\mu f_\mu \left(\varphi, a_\mu^\dagger\right) |0\rangle \tag{4.6}$$

with

$$a_\mu = \varphi_\mu |\phi\rangle . \tag{4.7}$$

Then, we need that

$$a_\mu f_\mu \left(\varphi, a_\mu^\dagger\right) |0\rangle = \varphi_\mu f_\mu \left(\varphi, a_\mu^\dagger\right) |0\rangle , \tag{4.8}$$

but

$$\begin{aligned}
a_\mu f_\mu |0\rangle &= [a_\mu, f_\mu] |0\rangle && (4.9)\\
&\implies \frac{\partial}{\partial a_\mu^\dagger} f_\mu = \varphi_\mu f_\mu && (4.10)\\
\implies \frac{\mathrm{d} f_\mu}{f_\mu} &= \varphi_\mu \, \mathrm{d} a_\mu^\dagger && (4.11)\\
\ln f_\mu &= \varphi_\mu a_\mu^\dagger && (4.12)\\
f_\mu &= \mathrm{e}^{\varphi_\mu a_\mu^\dagger}. && (4.13)
\end{aligned}$$

4.2 Properties

We will now look at some of the properties of coherent bosonic states.

$$a_\mu^\dagger |\phi\rangle = a_\mu^\dagger \mathrm{e}^{\sum_\mu \varphi_\nu a_\nu^\dagger} |0\rangle \tag{4.14}$$

$$= \frac{\partial}{\partial \varphi_\mu} |\phi\rangle \tag{4.15}$$

$$\langle\phi| = \langle 0| \mathrm{e}^{\sum_\mu \varphi_\mu^* a_\mu} \implies \tag{4.16}$$

$$\langle\phi| a_\mu = \frac{\partial}{\partial \varphi_\mu^*} \langle\phi| \tag{4.17}$$

The overlap of two coherent bosonic states are

$$\langle\phi|\sigma\rangle = \langle 0|\mathrm{e}^{\sum_\mu \varphi_\mu^* a_\mu} \mathrm{e}^{\sum_\nu \sigma_\nu a_\nu^\dagger}|0\rangle\,. \tag{4.18}$$

Now define

$$A = \sum_\mu \varphi_\mu^* a_\mu$$

$$B = \sum_\nu \sigma_\nu a_\nu$$

such that

$$\langle\phi|\sigma\rangle = \langle 0|\mathrm{e}^A \mathrm{e}^B|0\rangle\,. \tag{4.19}$$

We see that

$$\langle 0|\mathrm{e}^B \mathrm{e}^A|0\rangle = 1. \tag{4.20}$$

Baker-Hausdorff:

$$e^{A+B} = \mathrm{e}^A \mathrm{e}^B \mathrm{e}^{-\frac{1}{2}[A,B]} \tag{4.21}$$

$$= \mathrm{e}^B \mathrm{e}^A \mathrm{e}^{-\frac{1}{2}[B,A]}, \tag{4.22}$$

where $[A, B]$ commutes with A, B.

$$\implies \mathrm{e}^A \mathrm{e}^B = \mathrm{e}^B \mathrm{e}^A \mathrm{e}^{[A,B]} \tag{4.23}$$

$$[A, B] = \sum_{\mu,\nu} \varphi_\mu^* \sigma_\nu \underbrace{\left[a_\mu, a_\nu^\dagger\right]}_{\delta_{\mu\nu}} \tag{4.24}$$

$$= \sum_\mu \varphi_\mu^* \sigma_\mu \tag{4.25}$$

$$\implies \tag{4.26}$$

$$\langle\phi|\sigma\rangle = \mathrm{e}^{\sum_\mu \varphi_\mu^* \sigma_\mu} \underbrace{\langle 0|\mathrm{e}^B \mathrm{e}^A|0\rangle}_{=1} \tag{4.27}$$

$$= \mathrm{e}^{\sum_\mu \varphi_\mu^* \sigma_\mu}, \tag{4.28}$$

the states are not orthogonal!

For the normalization of $|\phi\rangle$ we have

$$\langle\phi|\phi\rangle = \mathrm{e}^{\sum_\mu \varphi_\mu^* \varphi_\mu} \tag{4.29}$$

$$= \mathrm{e}^{\langle N\rangle}. \tag{4.30}$$

$\langle N\rangle$ is the average number of particles in the state $|\phi\rangle$

$$\frac{\langle\phi|\sum_\mu a_\mu^\dagger a_\mu|\phi\rangle}{\langle\phi|\phi\rangle} = \langle N\rangle \tag{4.31}$$

$$= \sum_\mu \varphi_\mu^* \varphi_\mu \tag{4.32}$$

$$\left\langle (\Delta N)^2 \right\rangle = \frac{1}{\langle\phi|\phi\rangle}\left[\langle\phi|\hat{N}^2|\phi\rangle - \Big(\langle\phi|\hat{N}|\phi\rangle\Big)^2\right] \tag{4.33}$$

$$= \frac{1}{\langle\phi|\phi\rangle}\left[\langle\phi|\sum_{\mu,\nu} a_\mu^\dagger a_\mu a_\nu^\dagger a_\nu|\phi\rangle - \left(\sum_\mu \varphi_\mu^*\varphi_\mu\right)^2\right] \tag{4.34}$$

$$= \sum_\mu \varphi_\mu^*\varphi_\mu = N. \tag{4.35}$$

Coherent states for a one-bosonic oscillator

Following the construction from (4.1), we have

$$|z\rangle = \mathrm{e}^{z a^\dagger}\,|0\rangle \tag{4.36}$$

$$= \sum_{n=0}^{\infty} \frac{z^n \left(a^\dagger\right)^n}{n!}|0\rangle = \sum_n \frac{z^n}{\sqrt{n!}}\frac{\left(a^\dagger\right)}{\sqrt{n!}}|0\rangle \tag{4.37}$$

$$= \sum_n \frac{z^n}{\sqrt{n!}}|n\rangle \tag{4.38}$$

$$\frac{1}{2\pi i}\int \mathrm{d}z\,\mathrm{d}z^*\,\mathrm{e}^{-z^*z}\,|z\rangle\langle z| \tag{4.39}$$

$$= \frac{1}{2\pi i}\int \mathrm{d}z\,\mathrm{d}z^*\,\mathrm{e}^{-zz^*}\sum_{n,m}\frac{z^n}{\sqrt{n!}}\frac{(z^*)^m}{\sqrt{m!}}|m\rangle\langle m| \tag{4.40}$$

$$= \frac{1}{2\pi i}\sum_{n,m}\frac{1}{\sqrt{n!m!}}|n\rangle\langle m|\int \mathrm{d}z\,\mathrm{d}z^*\,\mathrm{e}^{-zz^*}z^n\,(z^*)^m \tag{4.41}$$

$$= \frac{1}{\pi}\sum_{n,m}\frac{1}{\sqrt{n!m!}}|n\rangle\langle m|\int \mathrm{d}x\,\mathrm{d}y\,\mathrm{e}^{-\left(x^2+y^2\right)}\,(x+iy)^n)\,(x-iy)^m\,. \tag{4.42}$$

Now, the integral in (4.42) is

$$\begin{aligned}
&\frac{1}{\pi}\int \mathrm{d}x\,\mathrm{d}y\,\mathrm{e}^{-\left(x^2+y^2\right)}\left(x+iy\right)^n)\left(x-iy\right)^m \\
&= \frac{1}{\pi}\int \mathrm{d}\rho\,\rho\,\mathrm{d}\theta\,\mathrm{e}^{-\rho^2}\left(\rho\mathrm{e}^{i\theta}\right)^n\left(\rho\mathrm{e}^{-i\theta}\right)^m \\
&= \frac{1}{\pi}\underbrace{\int \mathrm{d}\theta\,\mathrm{e}^{i\theta(n-m)}}_{2\pi\delta_{nm}}\int \mathrm{d}\rho\,\rho^{n+m+1}\mathrm{e}^{-\rho^2} \\
&= 2\delta_{nm}\int \mathrm{d}\rho\,\rho^{2n+1}\mathrm{e}^{-\rho^2} \\
&= \delta_{nm}\int_0^\infty \mathrm{d}r\,r^{-\frac{1}{2}}r^{\frac{2n+1}{2}}e^{-r} = \int_0^\infty \mathrm{d}r\,r^n\mathrm{e}^{-r} \\
&= \delta_{nm}n!, \qquad (4.43)
\end{aligned}$$

such that (4.39) becomes

$$\begin{aligned}
\frac{1}{2\pi i}\int \mathrm{d}z\,\mathrm{d}z^*\,\mathrm{e}^{-z^*z}\left|z\right\rangle\!\left\langle z\right| &= \sum_{n,m}\frac{1}{\sqrt{n!m!}}\left|n\right\rangle\!\left\langle m\right|\cdot\delta_{nm}n! \\
&= \sum_n \left|n\right\rangle\!\left\langle n\right| = 1.
\end{aligned}$$

Coherent states stays coherent under the propagation of time, but with a different label:

$$\begin{aligned}
\mathrm{e}^{\frac{-iHt}{\hbar}}\left|z\right\rangle &= \mathrm{e}^{\frac{-i\hbar\omega a^\dagger at}{\hbar}}\left|z\right\rangle = \mathrm{e}^{-i\omega ta^\dagger a}\left|z\right\rangle \\
&= \mathrm{e}^{-i\omega ta^\dagger a}\sum_n\frac{z^n}{\sqrt{n!}}\left|n\right\rangle = \sum_n\frac{z^n}{\sqrt{n!}}\mathrm{e}^{-i\omega ta^\dagger a}\left|n\right\rangle \\
&= \sum_n\frac{z^n}{\sqrt{n!}}\mathrm{e}^{-i\omega tn}\left|n\right\rangle = \sum_n\frac{\left(z\mathrm{e}^{-i\omega t}\right)^n}{\sqrt{n!}}\left|n\right\rangle \\
&= \left|z\mathrm{e}^{-i\omega t}\right\rangle
\end{aligned}$$

The propagator in this basis is thus very simple:

$$\begin{aligned}
\left\langle z_n\right|\mathrm{e}^{\frac{-iHt}{\hbar}}\left|z_0\right\rangle &= \left\langle z_n\middle|z_0\mathrm{e}^{-i\omega t}\right\rangle \qquad (4.44)\\
&= \mathrm{e}^{z_n^*z_0\mathrm{e}^{-i\omega t}} \qquad (4.45)
\end{aligned}$$

The completeness relation for coherent boson states

$$
\begin{aligned}
&\int \left(\prod_{\mu} \frac{\mathrm{d}\varphi_\mu^* \, \mathrm{d}\varphi_\mu}{2\pi i} \right) \mathrm{e}^{-\sum_\mu \varphi_\mu^* \varphi_\mu} \, |\phi\rangle\langle\phi| \\
&= \int \left(\prod_{\mu} \frac{\mathrm{d}\varphi_\mu^* \, \mathrm{d}\varphi_\mu}{2\pi i} \right) \mathrm{e}^{-\sum_\mu \varphi_\mu^* \varphi_\mu} \mathrm{e}^{\sum_\mu \varphi_\mu a_\mu^\dagger} \, |0\rangle\langle 0| \, \mathrm{e}^{-\sum_\mu a_\mu \varphi_\mu^*} \\
&= \int \left(\prod_{\mu} \frac{\mathrm{d}\varphi_\mu^* \, \mathrm{d}\varphi_\mu}{2\pi i} \right) \mathrm{e}^{-\sum_\mu \varphi_\mu^* \varphi_\mu} \\
&\cdot \sum_{n_\mu=0}^{\infty} \frac{\varphi_\mu^{n_\mu}}{\sqrt{n_\mu!}} \sum_{n_\nu=0}^{\infty} \frac{\varphi_\nu^{n_\nu}}{\sqrt{n_\nu!}} \cdots |n_\mu, n_\nu, \ldots\rangle \\
&\cdot \sum_{m_\mu=0}^{\infty} \frac{\left(\varphi_\mu^*\right)^{m_\mu}}{\sqrt{m_\mu!}} \sum_{m_\nu=0}^{\infty} \frac{\left(\varphi_\nu^*\right)^{m_\nu}}{\sqrt{m_\nu!}} \cdots \langle m_\mu, m_\nu, \ldots| \\
&= \underbrace{\sum_{n_\mu=0}^{\infty} \sum_{n_\nu=0}^{\infty} \cdots}_{\sum_{\{n_\mu\}}} |n_\mu, n_\nu, \ldots\rangle\langle n_\mu, n_\nu, \ldots| \\
&= I
\end{aligned}
$$

5 Coherent states for fermions

5.1 Construction

We will also in the fermionic case make an ansatz on the construction of coherent fermionic states, somewhat similar to (4.1):

$$|\psi\rangle = \mathrm{e}^{-\sum_\mu \xi_\mu c_\mu^\dagger} |0\rangle \tag{5.1}$$

$$= \prod_\mu \left(1 - \xi_\mu c_\mu^\dagger\right) |0\rangle \tag{5.2}$$

It is simpler to show that the ansatz satisfies the definition (3.2) ($c_\mu |\psi\rangle = \xi_\mu |\psi\rangle$) for fermions than it was for bosons. Use the fact that $\xi_\mu^2 = 0$ to express the expansion of the exponential function.

$$c_\mu \prod_\nu \left(1 - \xi_\nu c_\nu^\dagger\right) |0\rangle = c_\mu |\psi\rangle \tag{5.3}$$

affects one of the products:

$$c_\mu \left(1 - \xi_\mu c_\mu^\dagger\right) |0\rangle = +\xi_\mu \underbrace{c_\mu c_\mu^\dagger}_{1 - c_\mu^\dagger c_\mu} |0\rangle \tag{5.4}$$

$$= +\xi_\mu |0\rangle \tag{5.5}$$

$$= \xi_\mu \left(1 - \xi_\mu c_\mu^\dagger\right) |0\rangle \tag{5.6}$$

$$\Longrightarrow$$

$$c_\mu |\psi\rangle = \xi_\mu |\psi\rangle , \tag{5.7}$$

where we used the anticommutation relations $\{\xi_\mu, c_\mu\} = \{\xi_\mu, c_\mu^\dagger\} = 0$.

5.2 Properties

Creation operator

Acting with the creation operator on a coherent fermion state:

$$\begin{aligned} c_\mu^\dagger |\psi\rangle &= c_\mu^\dagger \left(1 - \xi_\mu c_\mu^\dagger\right) \prod_{\nu \neq \mu} \left(1 - \xi_\nu c_\nu^\dagger\right) |0\rangle \\ &= -\frac{\partial}{\partial \xi_\mu} \left(1 - \xi_\mu c_\mu^\dagger\right) \prod_{\nu \neq \mu} \left(1 - \xi_\nu c_\nu^\dagger\right) |0\rangle \\ &= -\frac{\partial}{\partial \xi_\mu} |\psi\rangle . \end{aligned}$$

Similarly, on the "bra" vectors:

$$\begin{aligned}\langle\psi|\, c_\mu &= \prod_\mu \langle 0|\left(1+\xi_\mu^* c_\mu\right) c_\mu \\ &= \frac{\partial}{\partial \xi_\mu^*} \prod_\mu \langle 0|\left(1+\xi_\mu^* c_\mu\right) \\ &= \frac{\partial}{\partial \xi_\mu^*} \langle\psi|\end{aligned}$$

NB: Note the plus sign in the product.

Overlap

The overlap between two coherent fermion states:

$$\begin{aligned}\langle\psi|\psi'\rangle = \langle 0|\prod_{\mu,\nu}\left(1+\xi_\nu^* c_\nu\right)\left(1-\xi_\mu c_\mu^\dagger\right)|0\rangle \\ = \prod_{\mu,\nu}\langle 0|\left(1+\xi_\nu^* c_\nu \xi_\mu c_\mu^\dagger\right)|0\rangle \\ = \prod_{\nu\neq\mu}\cdot 1 \prod_\mu\left(1+\xi_\mu^*\xi_\mu\right) \\ = \prod_\mu\left(1+\xi_\mu^*\xi_\mu\right)\end{aligned}$$

$$\text{Re-exponentiation} \implies \langle\psi|\psi'\rangle = \mathrm{e}^{\sum_\mu \xi_\mu^*\xi_\mu}.$$

We have used $\{c_\mu, \xi_\mu\} = 0$.

Completeness relation

The completeness relation for fermion coherent states is

$$\int \prod_\mu \mathrm{d}\xi_\mu^*\, \mathrm{d}\xi_\mu \mathrm{e}^{-\sum_\mu \xi_\mu^*\xi_\mu}\, |\xi\rangle\langle\xi| = 1. \tag{5.8}$$

Proof. **For one mode:**

$$
\begin{aligned}
&\int \mathrm{d}\xi\, \mathrm{d}\xi^*\, \mathrm{e}^{-\xi^*\xi} \mathrm{e}^{-\xi c^\dagger} \left|0\right\rangle\!\left\langle 0\right| \mathrm{e}^{-c\xi^*} \\
&= \int \mathrm{d}\xi\, \mathrm{d}\xi^*\, (1-\xi^*\xi)\left(1-\xi c^\dagger\right) \left|0\right\rangle\!\left\langle 0\right| (1-c\xi^*) \\
&= \int \mathrm{d}\xi\, \mathrm{d}\xi^*\, \left[1-\xi^*\xi-\xi^\dagger\right] \left|0\right\rangle\!\left\langle 0\right| (1+\xi^* c) \\
&= \int \mathrm{d}\xi\, \mathrm{d}\xi^*\, \left[(1-\xi^*\xi)\left|0\right\rangle - \xi c^\dagger \left|0\right\rangle\right] \left[\left\langle 0\right| + \xi^* \left\langle 0\right| c\right] \\
&= \int \mathrm{d}\xi\, \mathrm{d}\xi^*\, \Big[(1-\xi^*\xi)\left|0\right\rangle\!\left\langle 0\right| - \xi c^\dagger \left|0\right\rangle\!\left\langle 0\right| \\
&\qquad\qquad + (1-\xi^*\xi)\left|0\right\rangle \xi^* \left\langle 0\right| c - \xi c^\dagger \left|0\right\rangle \xi^* \left\langle 0\right| c\Big] \\
&= \int \mathrm{d}\xi\, \mathrm{d}\xi^*\, [(1-\xi^*\xi)\left|0\right\rangle\!\left\langle 0\right| - \xi \left|1\right\rangle\!\left\langle 0\right| \\
&\qquad\qquad + (1-\xi^*\xi)\,\xi^* \left|0\right\rangle\!\left\langle 1\right| + \xi\xi^* \left|1\right\rangle\!\left\langle 1\right|] \\
&= \left|0\right\rangle\!\left\langle 0\right| + \left|1\right\rangle\!\left\langle 1\right| = 1
\end{aligned}
$$

For multiple modes:

$$
\begin{aligned}
&\int \prod_\mu \mathrm{d}\xi_\mu\, \mathrm{d}\xi^*{}_\mu\, \mathrm{e}^{-\sum_\mu \xi_\mu^*\xi_\mu} \left|\xi\right\rangle\!\left\langle \xi\right| \\
&= \int \prod_\mu \mathrm{d}\xi_\mu\, \mathrm{d}\xi^*\, \mu \mathrm{e}^{-\sum_\mu \xi_\mu^*\xi_\mu} \mathrm{e}^{-\sum_\mu \xi_\mu c_\mu^\dagger} \left|0\right\rangle\!\left\langle 0\right| \mathrm{e}^{-\sum_\mu c_\mu \xi_\mu^*} \\
&= \int \left(\prod_\mu \mathrm{d}\xi_\mu^*\, \mathrm{d}\xi_\mu\right) \left(\prod_\mu (1-\xi_\mu^*\xi_\mu)\right) \left(\prod_\mu (1-\xi_\mu c_\mu^\dagger)\right) \\
&\qquad\qquad \times \left|0\right\rangle\!\left\langle 0\right| \left(\prod_\mu (1+\xi_\mu^* c_\mu)\right)
\end{aligned}
$$

We can treat $\xi_\mu^*\xi_\mu, \xi_\mu c_\mu^\dagger$ etc. as ordinary numbers when we change places, since they commute.

□

The trace of an operator:

$$\begin{aligned}
\operatorname{Tr} A &= \sum_n \langle n|A|n\rangle \\
&= \int \prod_\mu \mathrm{d}\xi_\mu^* \, \mathrm{d}\xi_\mu \mathrm{e}^{-\sum_\mu \xi_\mu^* \xi_\mu} \sum_n \langle n|\xi\rangle \, \langle \xi|A|n\rangle \\
&= \int \prod_\mu \mathrm{d}\xi_\mu^* \, \mathrm{d}\xi_\mu \mathrm{e}^{-\sum_\mu \xi_\mu^* \xi_\mu} \underbrace{\sum_n \langle -\xi|A|n\rangle \, \langle n|\xi\rangle}_{\langle -\xi|A|\xi\rangle} \\
&= \int \prod_\mu \mathrm{d}\xi_\mu^* \, \mathrm{d}\xi_\mu \mathrm{e}^{-\sum_\mu \xi_\mu^* \xi_\mu} \, \langle -\xi|A|\xi\rangle
\end{aligned} \tag{5.9}$$

$\hat{N} = \sum_\mu c_\mu^\dagger c_\mu$is the number operator, as usual. What is the mean value of this operator in a fermion coherent state?

$$\frac{\langle \xi|\hat{N}|\xi\rangle}{\langle \xi|\xi\rangle} = \sum_\mu \frac{\langle \xi|c_\mu^\dagger c_\mu|\xi\rangle}{\langle \xi|\xi\rangle} \tag{5.10}$$

$$= \sum_\mu \xi_\mu^* \xi_\mu \tag{5.11}$$

This is neither a real nor complex number! It is therefore meaningless to talk about the mean value of number of fermions in a coherent state.

In (5.9) we used a property that is not true in general, but is under the integral.

$$\begin{aligned}
\langle \psi|\xi\rangle &= c_0 + c_1 \xi \\
\langle \xi|\psi\rangle &= d_0 + d_1 \xi^*
\end{aligned}$$

Terms linear in ξ, ξ^* is zero under Grassmann integration

$$\begin{aligned}
|\xi\rangle &\equiv \mathrm{e}^{\xi c^\dagger} |0\rangle \\
|-\xi\rangle &= \mathrm{e}^{-\xi c^\dagger} |0\rangle \\
&\neq -|\xi\rangle
\end{aligned}$$

Such that

$$\langle \psi|\xi\rangle \, \langle \xi|\psi\rangle \neq \langle -\xi|\psi\rangle \, \langle \psi|\xi\rangle \,, \tag{5.12}$$

but it comes out correct in the integral. We used this as

$$\int \mathrm{d}\xi \, \mathrm{d}\xi^* \, \langle \psi|\xi\rangle \, \langle \xi|\psi\rangle = \int \mathrm{d}\xi \, \mathrm{d}\xi^* \, \langle -\xi|\psi\rangle \, \langle \psi|\xi\rangle \tag{5.13}$$

The reason for this fundamental difference between Bosonic and fermionic coherent states lies in the Pauli exclusion principle and the definition of coherent states.

With a given set of one-particle states, together with the Pauli princliple, a physical state must have a fixed, determinable number of particles, and cannot be an eigenstate of a annihilation operator. The fermionic coherent states therefore lay outside the Hilbert space of physical states, and need not represent observable states. For bosons, the symmetric property means that even with a given set of quantum numbers, physical states can be an eigenstate of the annihilation operator. This is because each one particle state can assume an arbitrary number of quants. Boson coherent states are thus physical. They are in fact physical states naturally occurring when taking the classical limit of a quantum field theory. Also in lasers.

When we considered the trace (eq (5.9)) of an operator A for both for both fermionic and bosonic coherent states, we had to consider the matrix elements

$$\begin{aligned} \langle \phi | A | \phi \rangle & \qquad \textbf{(Bosons)} \\ \langle -\psi | A | \psi \rangle & \qquad \textbf{(Fermions)} \end{aligned}$$

For bosons: Assume that $A(a_\mu^\dagger, a_\mu)$ are normal ordinals ; all a_μ are placed to the right of $a_\mu^\dagger$-

$$a_\mu \left| \phi \right\rangle = \varphi_\mu \left| \phi \right\rangle \tag{5.14}$$

$$\left(a_\mu\right)^n \left| \phi \right\rangle = \left(\varphi_\mu\right)^n \left| \phi \right\rangle \tag{5.15}$$

$$A\left(a_\mu\right) \left| \phi \right\rangle = A\left(\varphi_\mu\right) \left| \phi \right\rangle, \tag{5.16}$$

thus

$$\langle \phi | A\left(a_\mu^\dagger, a_\mu\right) | \phi' \rangle = A\left(\varphi_\mu^*, \varphi_{\mu'}\right) \langle \phi | \phi' \rangle \tag{5.17}$$

$$= A\left(\varphi_\mu^*, \varphi_{\mu'}\right) \mathrm{e}^{\sum_\mu \varphi_\mu^* \varphi_{\mu'}}. \tag{5.18}$$

Similarly,

$$\langle \psi | A\left(c_\mu^\dagger, c_\mu\right) | \psi' \rangle = A\left(\xi_\mu^*, \xi_\mu'\right) \mathrm{e}^{\sum_\mu \xi_\mu^* \xi_\mu'} \tag{5.19}$$

Thus, the calculation of expectation values reduces to quadratures; multiple integrals over $(\varphi_\mu^*, \varphi_\mu)$ or (ξ_μ^*, ξ_μ).

6 Gaussian integrals

In a functional integral formalism of quantum field theory, a free non-interacting theory will have the form of a multiple gaussian integral. These integrals are therefore very important. We have also seen that the trace of a operator can be expressed as a integral over c-numbers or Grassmann-numbers with gaussian weight. This motivates the study of such integrals. We look at the following scenarios:

- real variables
- complex variables
- Grassmann-variables

The basic formula that we need is

$$\int_{-\infty}^{\infty} \mathrm{d}x\, \mathrm{e}^{-ax^2} = \sqrt{\frac{\pi}{a}} \implies \int_{-\infty}^{\infty} \frac{\mathrm{d}x}{\sqrt{2\pi}} \mathrm{e}^{-\frac{a}{2}x^2} = \frac{1}{a}. \tag{6.1}$$

Mutiple gaussian integrals over real variables

$$I = \int \frac{\mathrm{d}x_1}{\sqrt{2\pi}} ... \frac{\mathrm{d}x_n}{\sqrt{2\pi}} \mathrm{e}^{-\frac{1}{2}x_i A_{ij} x_j + x_i J_i} \tag{6.2}$$

where we use Einstein convention in the exponent, J_i is a real number and A_{ij} is a positive-definite, symmetric matrix.

Look at the exponent:

$$\begin{aligned} -\frac{1}{2}x_i A_{ij} x_j + x_i J_i &= -\frac{1}{2}x_i A_{ij} x_j + \frac{1}{2}(x_i J_i + x_j J_j) \\ &= -\frac{1}{2}(x_i - A^{-1}_{ij} J_j) A_{ij} (x_j - A^{-1}_{ij} J_i) + \frac{1}{2} J_i A^{-1}_{ij} J_j \end{aligned}$$

and by $y_i = x_i - A^{-1}_{ij} J_j \quad (i \leftrightarrow j)$ change of variables, we end up with

$$Z(J) = \mathrm{e}^{\frac{1}{2}J_i A^{-1}_{ij} J_j} \int \frac{\mathrm{d}y_1}{\sqrt{2\pi}} ... \frac{\mathrm{d}y_n}{\sqrt{2\pi}} \mathrm{e}^{-\frac{1}{2}y_i A_{ij} y_j} \tag{6.3}$$

And by doing an orthogonal transformation and thereby diagonalizing A_{ij}

$$y_i A_{ij} y_j = \mathbf{y}^T \mathbf{A} \mathbf{y} = \mathbf{z}^T \mathbf{D} \mathbf{z} = \lambda_n z_n^2.$$

Inserting this into the formula for $Z(J)$, we end up with

$$Z(J) = \mathrm{e}^{\frac{1}{2}J_i A^{-1}_{ij} J_j} \int \frac{\mathrm{d}z_1}{\sqrt{2\pi}} ... \frac{\mathrm{d}z_n}{\sqrt{2\pi}} \mathrm{e}^{-\frac{1}{2}\lambda_n z_n^2} = \mathrm{e}^{\frac{1}{2}J_i A^{-1}_{ij} J_j} \prod_n \frac{1}{\sqrt{2\pi}} \sqrt{\frac{2\pi}{\lambda_n}} =$$
$$\mathrm{e}^{\frac{1}{2}J_i A^{-1}_{ij} J_j} \frac{1}{\sqrt{\det(\mathbf{A})}} = Z(\{J\}).$$

Note that if we define the expectation value of a quantity that depends on x_i, we end up with the nice result

$$\langle A(x_i)\rangle = \frac{1}{Z(0)}\int \frac{\mathrm{d}x_1}{\sqrt{2\pi}}...\frac{\mathrm{d}x_n}{\sqrt{2\pi}}A(x_i)\mathrm{e}^{-\frac{1}{2}x_iA_{ij}x_j+x_iJ_i} = \frac{1}{Z(0)}\int \frac{\mathrm{d}x_1}{\sqrt{2\pi}}...\frac{\mathrm{d}x_n}{\sqrt{2\pi}}A\Big(\frac{\delta}{\delta J_i}\Big)\mathrm{e}^{-\frac{1}{2}x_iA_{ij}x_j+x_iJ_i}$$
$$= \frac{1}{Z(0)}A\Big(\frac{\delta}{\delta J_i}\Big)\int \frac{\mathrm{d}x_1}{\sqrt{2\pi}}...\frac{\mathrm{d}x_n}{\sqrt{2\pi}}\mathrm{e}^{-\frac{1}{2}x_iA_{ij}x_j+x_iJ_i} = \frac{1}{Z(0)}A\Big(\frac{\delta}{\delta J_i}\Big)\ Z(\{J\})\Big|_{J=0}.$$

In particular,

$$\langle x_i\rangle = 0$$

since the derivative gives terms linear in J, which we set to 0.

$$\langle x_ix_j\rangle = \frac{\delta}{\delta J_i}\frac{\delta}{\delta J_j}\mathrm{e}^{\frac{1}{2}J_{i'}A^{-1}_{i'j'}J_{j'}}\Big|_{J=0} = \frac{\delta}{\delta J_i}\left(\frac{1}{2}J_{i'}A^{-1}_{i'j'}\delta_{j',j}+\frac{1}{2}\delta_{i',j}A^{-1}_{i'j'}J_{j'}\right)\mathrm{e}^{\frac{1}{2}J_{i'}A^{-1}_{i'j'}J_{j'}}\Big|_{J=0} =$$
$$(\frac{1}{2}\delta_{i',i}A^{-1}_{i'j'}\delta_{j',j}+\frac{1}{2}\delta_{i',j}A^{-1}_{i'j'}\delta_{j',i}\delta_{i',j}+...)\mathrm{e}^{\frac{1}{2}J_{i'}A^{-1}_{i'j'}J_{j'}}\Big|_{J=0} = A^{-1}_{ij}$$

Where we have excluded terms which evidently become 0 when we set $J=0$. We have also added a mark on the indicies in the exponent to explicitly show that they are different from the indicies in the expenctation value. We call $Z(\{J\})$ a generating functional. We will see that it's suitable for calculation of physical observables.

Next we look at multible gaussian integrals over complex variables (which corresponds to the boson-case for traces over coherent states).

$$\prod_i\int\frac{\mathrm{d}x_i^*\mathrm{d}x_i}{2\pi i}\mathrm{e}^{-x_i^*A_{ij}x_j+x_iJ_i^*+h.c.} = \prod_i\int\frac{\mathrm{d}z_i^*\mathrm{d}z_i}{2\pi i}\mathrm{e}^{-z_i^*A_{ij}z_j+J_i^*A^{-1}_{ij}J_j}$$
$$= \mathrm{e}^{J_i^*A^{-1}_{ij}J_j}\prod_i\int\frac{\mathrm{d}\tilde{z}_i^*\mathrm{d}z_i}{2\pi i}\mathrm{e}^{-\lambda_n\tilde{z}_n^*z_n}$$

where we treat $\tilde{z}$ and z as separate fields.

$$\tilde{z} = r\mathrm{e}^{i\theta} = \sqrt{u^2+v^2}\mathrm{e}^{i\theta}$$
$$\mathrm{d}z\mathrm{d}\tilde{z}^* = 2i\mathrm{d}u\mathrm{d}v \quad \tilde{z}^*z = u^2+v^2$$

which implies

$$\mathrm{e}^{J_i^*A^{-1}_{ij}J_j}\prod_i\int\frac{\mathrm{d}\tilde{z}_i^*\mathrm{d}z_i}{2\pi i}\mathrm{e}^{-\lambda_n\tilde{z}_n^*z_n} = \mathrm{e}^{J_i^*A^{-1}_{ij}J_j}\int\prod_n\frac{\mathrm{d}u\mathrm{d}v}{\pi}\mathrm{e}^{-\lambda_n(u^2+v^2)}$$
$$= \frac{1}{\det(\mathbf{A})}\mathrm{e}^{J_i^*A^{-1}_{ij}J_j} \qquad (6.4)$$

Note that the determinant is located in the numerator.

The last case we look at is integration over Grassmann-variables, which is relevant when we are calculating the trace of fermionic coherent states

$$\prod_i \int \mathrm{d}\xi_i^* \mathrm{d}\xi_i \mathrm{e}^{-\xi_i^* A i j \xi_j + \xi_i J_i^* + \xi_i^* J_i}.$$

Note that the J's are also Grassmann variables.

$$\begin{aligned} \prod_i \int \mathrm{d}\tilde{\xi}_i^* \mathrm{d}\tilde{\xi}_i \mathrm{e}^{-\tilde{\xi}_i^* A i j \tilde{\xi}_j + J_i^* A_{ij}^{-1} J_j} = \mathrm{e}^{J_i^* A_{ij}^{-1} J_j} \prod_i \int \mathrm{d}\tilde{\xi}_i^* \mathrm{d}\tilde{\xi}_i \mathrm{e}^{-\tilde{\xi}_i^* A i j \tilde{\xi}_j} \\ = \mathrm{e}^{J_i^* A_{ij}^{-1} J_j} \prod_i \int \mathrm{d}\tilde{\eta}_i^* \mathrm{d}\eta_i \mathrm{e}^{-\lambda_n \eta_n^* \eta_n} = \mathrm{e}^{J_i^* A_{ij}^{-1} J_j} \prod_i \int \mathrm{d}\tilde{\eta}_i^* \mathrm{d}\eta_i (1 - \lambda_n \eta_n^* \eta_n) = \\ \mathrm{e}^{J_i^* A_{ij}^{-1} J_j} \prod_n \lambda_n = \det(\mathbf{A}) \mathrm{e}^{J_i^* A_{ij}^{-1} J_j}. \end{aligned} \tag{6.5}$$

Here we have used the usual expansion-, anticommutation- and integration rules for Grassmann-variables. Note that for the fermionic integral, the determinant is in the numerator, as oppose to the bosonic case where it is in the denominator. This formally results from the linear expantion of Grassmanian functions. This ultimately reflects the Pauli principle.

$$\det(\mathbf{A})^{-\xi} = \mathrm{e}^{-\xi \ln(\det(\mathbf{A}))} = \mathrm{e}^{-\xi \operatorname{tr}(\ln(\mathbf{A}))}$$

Thus we can combine the result for bosons and fermions:
Bosons ($\xi = 1$):

$$I = \mathrm{e}^{J_i^* A_{ij}^{-1} J_j} \mathrm{e}^{-\operatorname{tr}(\ln(\mathbf{A}))} \tag{6.6}$$

Where the J's are complex variables.
Fermions ($\xi = -1$):

$$\mathrm{e}^{J_i^* A_{ij}^{-1} J_j} \mathrm{e}^{\operatorname{tr}(\ln(\mathbf{A}))} \tag{6.7}$$

Where the J's are Grassmann-variables.

Functional integral formulation of many-particle physics

A functional f is a mathematical map from a vector-space onto a field of scalars, usually the real- or complex numbers. Let this mapping be defined with some domain $\mathrm{D}(f)$:

$$f : \mathrm{D}(f) \to K, \quad K \in \{\mathbb{R}, \mathbb{C}\}$$

We will eventually write the partition function Z of a many-particle system as a function like the one defined above. In that case, the domain is the Hilbert space or the phase space and the co-domain is the real numbers. $mathrmD$ is then an integral or a sum over configurations of states a system can be in, namely a functional integral.

This functional integral formulation will reduce computations of physical observables to a type of product which we can treat systematically using different approximation schemes.

In order to build up such a functional integral formulation of many-particle physics, we first look at a quantum mechanical system of a single particle which does not depend explicitly on time.

The Hamiltonian is given by

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x})$$

such that the particle moves in a external potential $V(x)$ (e.g. band-structure problem). The evolution operator for the corresponding one-particle state in the Schrodinger picture is given by

$$|\psi(t_f)\rangle = U(t_f, t_i)\,|\psi(t_i)\rangle = \mathrm{e}^{-iH(t_f - t_i)}\,|\psi(t_i)\rangle$$

where i and f stands for initial and final, respectively. Now define the matrix element of $U(t_f, t_i)$ between initial and final eigenstates of the position operator, $|x_i\rangle$ and $|x_f\rangle$

$$U(x_f, t_f; x_i, t_i) = \langle x_f|\,\mathrm{e}^{-iH(t_f - t_i)}\,|x_i\rangle\,.$$

This matrix element can in general not be calculated exactly. We wish to approximate it in a controlled fashion: there should exist a "smallness" parameter which control the approximation.

Split up the interval $t_f - t_i$ into discrete pieces:

$$\varepsilon = \frac{t_f - t_i}{M} \implies U(x_f, t_f; x_i, t_i) = \langle x_f|\left(\mathrm{e}^{-iH\varepsilon}\right)^M|x_i\rangle\,,$$

since H doesn't explicitly depend on time and commute with itself. Now, write out the M exponential factors out and insert completeness relations,

$$\int \mathrm{d}x_n \, |x_n\rangle \, \langle x_n|$$

$$U = \int \prod_{k=1}^{M-1} \mathrm{d}x_k \, \langle x_f| \, \mathrm{e}^{-iH\varepsilon} \, |x_{M-1}\rangle \, \langle x_{M-1}| \, \mathrm{e}^{-iH\varepsilon} \, |x_{M-2}\rangle \cdots \langle x_1| \, \mathrm{e}^{-iH\varepsilon} \, |x_i\rangle \, .$$

So far this is an exact result. The next step is to find a "good" approximation for the matrix element of $\mathrm{e}^{-iH\varepsilon}$. First we rewrite $x_f = x_M$ and $x_i = x_0$, so that we have the starting- and ending points (x_0, t_0) and (x_M, t_M). Each integral is then over all the possible positions x_n you can have at time t_n, one integral for each time-step. This product of integrals is therefore a summation of all the possible paths a particle can travel between the starting and ending points. That is to say: A path integral.

We first start with the calculation of

$$\langle x_n| \, \mathrm{e}^{-iH\varepsilon} \, |x_{n-1}\rangle = \int \mathrm{d}p_n \, \langle x_n|p_n\rangle \, \langle p_n| \, \mathrm{e}^{-i\varepsilon H(x,p)} \, |x_{n-1}\rangle$$

where

$$\langle x_n|p_n\rangle = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{ip_n x_n} \quad \langle p_n|x_{n-1}\rangle = \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-ip_n x_{n-1}}.$$

To proceed any further with this new matrix element

$$\langle p_n| \, \mathrm{e}^{-i\varepsilon H(x,p)} \, |x_{n-1}\rangle \, ,$$

we first observe that if we can write

$$\mathrm{e}^{-i\varepsilon H} = \sum_{m,m'} C_{mm'} A_m(p) B_{m'}(x)$$

we can have $A_m(p)$ act to the left and $B_{m'}(x)$ act to the right such that

$$\sum_{m,m'} C_{mm'} A_m(p_n) B_{m'}(x_{n-1}) \mathrm{e}^{-ip_n x_{n-1}} = \mathrm{e}^{-i\varepsilon H(p_n, x_{n-1})} \mathrm{e}^{-ip_n x_{n-1}}.$$

However, its not that easy. The p_n's and x_n's doesn't commute and $\mathrm{e}^{-i\varepsilon H(p,x)}$ doesn't have an expansion with that kind of ordering in each term. To obtain such an expansion, we defined the normal ordering:

$$N\left(\mathrm{e}^{-i\varepsilon H(p,x)}\right) = :\mathrm{e}^{-i\varepsilon H(p,x)}: = \sum_{m=0}^{\infty} \frac{(-i\varepsilon)^m}{m!} :\left(\frac{p^2}{2m} + V(x)\right)^m : \qquad (6.8)$$

such that the operators respect the binomial formula:

$$(a+b)^m = \sum_{k=0}^{n} \frac{n!}{k!(n-k)!} a^{n-k} b^k$$

$$:\left(\frac{p^2}{2m} + V(x)\right)^m := \sum_{k=0}^{m} \frac{m!}{k!(m-k)!} \left(\frac{p^2}{2m}\right)^{m-k} (V(x))^k .$$

In that way, we get all the p_n's to the left of all the x_n's.

$$:\mathrm{e}^{-i\varepsilon H(p,x)}:= \sum_{m=0}^{\infty} \frac{(-i\varepsilon)^m}{m!} \sum_{k=0}^{m} \frac{m!}{k!(m-k)!} \left(\frac{p^2}{2m}\right)^{m-k} (V(x))^k .$$

Note that the first two terms in the expansion are already normal ordered! We therefor get the relation

$$\mathrm{e}^{-i\varepsilon H(p,x)} =:\mathrm{e}^{-i\varepsilon H(p,x)}: +\mathcal{O}\big(\varepsilon^2\big).$$

$M \to \infty \implies \varepsilon \to 0$. We can therefore treat the exponent as normal ordered in the limit of continuous time-steps. As we already have seen, this simplifies the problem drastically.

$$\begin{aligned}
\langle x_n| \mathrm{e}^{-i\varepsilon H(p,x)} |x_{n-1}\rangle &= \langle x_n| :\mathrm{e}^{-i\varepsilon H(p,x)}: |x_{n-1}\rangle + \mathcal{O}\big(\varepsilon^2\big) \\
&= \int \mathrm{d}p_n \frac{1}{\sqrt{2\pi}} \mathrm{e}^{ip_n x_n} \mathrm{e}^{-i\varepsilon H(p_n, x_{n-1})} \frac{1}{\sqrt{2\pi}} \mathrm{e}^{-ip_n x_{n-1}} + \mathcal{O}\big(\varepsilon^2\big) \\
&= \int \frac{\mathrm{d}p_n}{2\pi} \mathrm{e}^{ip_n(x_n - x_{n-1}) - i\varepsilon \frac{p_n^2}{2m} - i\varepsilon V(x_{n-1})} + \mathcal{O}\big(\varepsilon^2\big) \\
&= \sqrt{\frac{m}{2\pi i\varepsilon}} \mathrm{e}^{i\varepsilon\left[\frac{m}{2\varepsilon^2}(x_n - x_{n-1})^2 - V(x_{n-1})\right]} + \mathcal{O}\big(\varepsilon^2\big).
\end{aligned}$$

And from this, we get a controlled approximation of our path integral:

$$U = \lim_{M\to\infty} \int \left(\prod_{k=1}^{M-1} \mathrm{d}x_k \sqrt{\frac{m}{2\pi i\varepsilon}} \right) \mathrm{e}^{i\varepsilon\left[\sum_{k=1}^{M-1} \frac{m}{2\varepsilon^2}(x_n - x_{n-1})^2 - V(x_{n-1})\right]}.$$

In the limit of $\varepsilon \to 0$, we write

$$\frac{x_k - x_{k-1}}{\varepsilon} \to \frac{\mathrm{d}x}{\mathrm{d}t} \qquad \varepsilon \sum_{k=1}^{M-1} \to \int_{t_i}^{t_f} \mathrm{d}t$$

$$\lim_{M\to\infty} \int \left(\prod_{k=1}^{M-1} \mathrm{d}x_k \sqrt{\frac{m}{2\pi i\varepsilon}} \right) \to \int_{x_i,t_i}^{x_f,t_f} \mathcal{D}[x(t)].$$

And we get our final result

$$U = \int_{x_i,t_i}^{x_f,t_f} \mathcal{D}[x(t)] \mathrm{e}^{i\int_{t_i}^{t_f} \mathrm{d}t \left[\frac{m}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 - V(x)\right]} = \int_{x_i,t_i}^{x_f,t_f} \mathcal{D}[x(t)] \mathrm{e}^{iS[x(t)]}. \tag{6.9}$$

S is a functional and U is a functional integral, the sum over all possible paths the action describes.

$$L\left[x(t)\right] = \left[\frac{m}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 - V(x)\right]$$
$$S\left[x(t)\right] = \int_{t_i}^{t_f} \mathrm{d}t L\left[x(t)\right]$$

Which paths contributes the most to $U(x_f, t_f; x_i, t_i)$? To make an example out of this, we reinsert $\hbar$. From the Schodinger equation, we get

$$i\hbar\partial_t \left|\psi(t)\right\rangle = H\left|\psi(t)\right\rangle$$

which has the formal solution

$$\left|\psi(t)\right\rangle = \mathrm{e}^{-i\frac{Ht}{\hbar}}\left|\psi(0)\right\rangle.$$

Thus, we have to insert $\frac{\varepsilon}{\hbar}$ for every time ε appeared in the previous calculation. We end up with

$$U = \int_{x_i,t_i}^{x_f,t_f} \mathcal{D}[x(t)] \mathrm{e}^{i\frac{S[x(t)]}{\hbar}}.$$

We look at a free particle in order to get a proper intuition of which paths that are most "important". When $\frac{L}{\hbar}$ get big, the integrand in the exponent oscillates fast and yields zero or little contribution to the path integral.

$$\frac{m}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}t}\right)^2 < 1 \implies |x_k - x_{k-1}| < \sqrt{\frac{2\varepsilon\hbar}{m}}.$$

That is: in the case of a free particle, the most important contributions are the smoothest paths. Another way of looking at it is that the dominant paths are the once that make S stationary, $\delta S = 0$, which are the classically allowed paths. In the case of a free particle, this corresponds to the particle travelling in a straight line, which indeed is quite smooth.

7 Statistical mechanics for a single quantum mechanical particle

From what we have done so far, we can almost immediately do statistical mechanics. Remeber the partition function

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

Look at the partition function of one particle. After the derivation of the path integral, it's a natural choice to start with a coordinate basis to evaluate the trace

$$Z = \int \mathrm{d}x \, \langle x| \, \mathrm{e}^{-\beta H} \, |x\rangle \, .$$

Now the integrand has the same form as the one used for calculating $U(x_f, t_f; x_i, t_i)$, with

$$\begin{aligned} x_i = x(0) = x_f = x(\beta) = x \\ \beta = i(t_f - t_i) = \tau \qquad \mathrm{d}t = -i\mathrm{d}\tau \\ \frac{\mathrm{d}}{\mathrm{d}t} = i\frac{\mathrm{d}}{\mathrm{d}\tau} \qquad x(t) \to x(\tau) \end{aligned}$$

Hence we use directly the result for $U(x_f, t_f; x_i, t_i)$ and end up with

$$\begin{aligned} \langle x| \, \mathrm{e}^{-\beta H} \, |x\rangle &= \int_{x(0)=x(\beta)=x} \mathcal{D}\left[x(\tau)\right] \mathrm{e}^{-i\frac{i}{\hbar}\int_0^\beta \mathrm{d}\tau\left[-\frac{m}{2}\left(\frac{\mathrm{d}x}{\mathrm{d}\tau}\right)^2 - V(x(\tau))\right]} \\ Z = \int \mathrm{d}x \, \langle x| \, \mathrm{e}^{-\beta H} \, |x\rangle &= \int_{x(0)=x(\beta)} \mathcal{D}\left[x(\tau)\right] \mathrm{e}^{-\frac{1}{\hbar}\int_0^\beta \mathrm{d}\tau H[x(\tau)]} \end{aligned} \tag{7.1}$$

where we have identified the Hamiltonian of the system. Note that the change from Lagrangian to Hamiltonian results from the introduction of τ, being the imaginary time. Again we see that (consider free particle) that the most important paths are

$$\varepsilon \frac{m}{2} \frac{(x_k - x_{k-1})^2}{\varepsilon^2 \hbar} < 1 \implies |x_k - x_{k-1}| < \sqrt{\frac{2\varepsilon\hbar}{m}}$$

and $x_k = x_{k-1}$ (independent of τ) in the classical limit $\hbar \to 0$. Then we get

$$Z = \sqrt{\frac{m}{2\pi\beta}} \int \mathrm{d}x \mathrm{e}^{-\beta V(x)}$$

which is the well known configuration integral, where the measure in the path integral differential $\mathcal{D}\left[x(\tau)\right]$ corresponds to the momentum integral in phase space.

The partition function

$$Z = \int \mathrm{d}x \int_{x(0)=x(\beta)=x} \mathcal{D}\left[x(\tau)\right] \mathrm{e}^{-\frac{1}{\hbar}\int_0^\beta \mathrm{d}\tau H[x(\tau)]} = \int_{x(0)=x(\beta)} \mathcal{D}\left[x(\tau)\right] \mathrm{e}^{-\frac{1}{\hbar}\int_0^\beta \mathrm{d}\tau H[x(\tau)]}$$

is in fact, in this formulation, an imaginary-time path integral, or rather functional integral, with the aforementioned periodicity $x(0) = x(\beta)$.

This is the most central formulation when it comes to calculating quantum-statistics. Classically one can use e.g. Monte-Carlo simulations,

$$Z = \sum_{\{n_i\}} e^{-\beta H[\{n_i\}]}$$

where $\{n_i\}$ represents some sum over phase space configurations for which the classical system can be in. The expression above generalizes to the quantum case. We see that effectively, the classical Boltzmann factor has been replaced by an integral

$$\mathrm{e}^{-\frac{1}{\hbar}\int_0^\beta \mathrm{d}\tau H[x(\tau)]}$$

which effectively gives the system another dimension. We therefore get the correspondence. A quantum mechanical d-dimensional system is therefore equivalent to a classical d+1-dimensional system, in this sense. The statistical mechanics we have done for a one-particle system generalizes directly to a many-particle system. Since we in the latter case deal with more than one particle, statistics become more important, in particular the symmetries involved by interchanging particle-states.

$$Z = \mathrm{Tr}\left(\mathrm{e}^{-\beta H}\right) = \frac{1}{N!}\sum_P \xi^P \int \prod_i \mathrm{d}x_i \left\langle x_{P_N}, \cdots x_{P_1}\right| \mathrm{e}^{-\beta H} \left|x_1, \cdots x_N\right\rangle$$

where $\xi = -1$ for fermions and $\xi = 1$ for bosons.

The sum in this equation is over all permutations of the set $(1, \cdots, N)$, where the permutations are obtained by transpositions, i.e. pair-interchanging.

Example:

$$\begin{aligned} (1,2,3) \\ (2,1,3) &= -(1,2,3) \\ (2,3,1) = -(2,1,3) &= (1,2,3) \end{aligned}$$

We need

$$\langle x_{P_N}, \cdots x_{P_1}| \, \mathrm{e}^{-\beta H} \, |x_1, \cdots x_N\rangle$$

and remember

$$\langle x| \, \mathrm{e}^{-\beta H} \, |x\rangle = \int_{x(0)=x(\beta)=x} \mathcal{D}\left[x(\tau)\right] \mathrm{e}^{-\frac{1}{\hbar}\int_0^\beta \mathrm{d}\tau H[x(\tau)]}.$$

And thus the generalization is obvious

$$\langle x_{P_N}, \cdots x_{P_1}| \, \mathrm{e}^{-\beta H} \, |x_1, \cdots x_N\rangle = \prod_{i=1}^{N} \int \mathcal{D}\left[x_i(\tau)\right] \mathrm{e}^{-\frac{1}{\hbar}\int_0^\beta \mathrm{d}\tau H[\{x_i(\tau)\}]} \tag{7.2}$$

where we have

$$\begin{aligned} x_i(0) &= x_{P_i}(\beta) \\ i &= 1, 2, \cdots, N. \end{aligned}$$

Again periodicity, because

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

is such that only diagonal matrix elements contribute.

Many-free particles in external potential:

$$H\left[\{x_i(\tau)\}\right] = \sum_{i=1}^{N} \left[\frac{m}{2}\left(\frac{\mathrm{d}x_i}{\mathrm{d}\tau}\right)^2 + V\left[x_i(\tau)\right]\right]$$

Interacting electrons in external potential:

$$H\left[\{x_i(\tau)\}\right] = \sum_{i=1}^{N} \left[\frac{m}{2}\left(\frac{\mathrm{d}x_i}{\mathrm{d}\tau}\right)^2 + V_{ext}\left[x_i(\tau)\right] + \frac{1}{2}\sum_{i\neq j} V\left[x_i(\tau) - x_j(\tau)\right]\right].$$

So far, we have calculated $Z = \mathrm{Tr}\left(\mathrm{e}^{-\beta H}\right)$ in the basis of eigenstates of the position operator. We know that we can use any basis. Now we are going to use the results above to write down and calculate the partition function with coherent states as basis. An important result which makes it easy for us to use the formalism with coherent states, is that in the path integral approach we have, to $\mathcal{O}\left(\varepsilon^2\right)$, been able to use operators which we didn't have to normal order.

8 Functional integrals over coherent states

Now we define a many-particle evolution operator $U(\varphi_{\alpha f}, t_f; \varphi_{\alpha i}, t_i)$ using

$$\langle\varphi_f|\,\mathrm{e}^{-iH(t_f-t_i)}\,|\varphi_i\rangle$$

$|\varphi_f\rangle$: coherent final-state at time t_f, with components labeled by λ, $|\varphi_{\lambda f}\rangle$.

And similar for coherent initial-state at time t_i (notation φ for bosons). Again we split the time interval into M intervals.

$$\begin{aligned} t_i = t_0 \quad & |\varphi_{\lambda i}\rangle = |\varphi_{\lambda 0}\rangle \\ t_M = t_f \quad & |\varphi_{\lambda M}\rangle = |\varphi_{\lambda f}\rangle \end{aligned}$$

where $t_k = t_0 + k\varepsilon$, as usual. Between each time-step, we define coherent states $|\varphi_k\rangle$, with components $|\varphi_{\lambda k}\rangle$ and insert the completeness relation

$$\int \prod_\lambda \frac{\mathrm{d}\varphi^*_{\lambda k}\mathrm{d}\varphi_{\lambda k}}{2\pi i}\mathrm{e}^{-\sum_\lambda \varphi^*_{\lambda k}\varphi_{\lambda k}}\,|\varphi_{\lambda k}\rangle\,\langle\varphi_{\lambda k}| = 1.$$

$$\mathrm{e}^{-i\varepsilon H(a^\dagger,a)} =: \mathrm{e}^{-i\varepsilon H(a^\dagger,a)}: + \mathcal{O}\big(\varepsilon^2\big)$$

where normal ordering in this case means placing all creation operators to the left of all annihilation operators.

We get:

$$\langle\varphi_f|\,\mathrm{e}^{-iH(t_f-t_i)}\,|\varphi_i\rangle = \langle\varphi_f|\,\mathrm{e}^{-\frac{i}{\hbar}H\varepsilon}\cdots\mathrm{e}^{-\frac{i}{\hbar}H\varepsilon}\,|\varphi_i\rangle$$

Now insert the completeness relation for coherent states $M-1$ times between each exponential factor, and take the limit $M\to\infty$.

$$\begin{aligned} &\lim_{M\to\infty}\int\prod_{k=1,\lambda}^{M-1}\frac{\mathrm{d}\varphi^*_{\lambda k}\mathrm{d}\varphi_{\lambda k}}{2\pi i}\mathrm{e}^{-\sum_\lambda\sum_{k=1}^{M-1}\varphi^*_{\lambda k}\varphi_{\lambda k}} \\ &\langle\varphi_{\lambda M}|\,\mathrm{e}^{-\frac{i}{\hbar}H\varepsilon}\,|\varphi_{\lambda M-1}\rangle\cdots\langle\varphi_{\lambda 1}|\,\mathrm{e}^{-\frac{i}{\hbar}H\varepsilon}\,|\varphi_{\lambda 0}\rangle \\ =\ &\lim_{M\to\infty}\int\prod_{k=1,\lambda}^{M-1}\frac{\mathrm{d}\varphi^*_{\lambda k}\mathrm{d}\varphi_{\lambda k}}{2\pi i}\mathrm{e}^{-\sum_\lambda\sum_{k=1}^{M-1}\varphi^*_{\lambda k}\varphi_{\lambda k}} \\ \langle\varphi_{\lambda M}|\,&:\mathrm{e}^{-\frac{i}{\hbar}H\varepsilon}:\,|\varphi_{\lambda M-1}\rangle\cdots\langle\varphi_{\lambda 1}|\,:\mathrm{e}^{-\frac{i}{\hbar}H\varepsilon}:\,|\varphi_{\lambda 0}\rangle + \mathcal{O}\big(M\varepsilon^2\big) \end{aligned}$$

We know already how to treat these matrix elements

$$\begin{aligned} &\langle\varphi_{\lambda n}|\,:\mathrm{e}^{-\frac{i}{\hbar}H\varepsilon}:\,|\varphi_{\lambda n-1}\rangle \\ =\ &\mathrm{e}^{-\frac{i}{\hbar}H(\{\varphi^*_{\lambda n},\varphi_{\lambda n-1}\})\varepsilon}\mathrm{e}^{\varphi^*_{\lambda k}\varphi_{\lambda k-1}} \\ \Longrightarrow\ &\langle\varphi_n|\,:\mathrm{e}^{-\frac{i}{\hbar}H\varepsilon}:\,|\varphi_{n-1}\rangle \\ =\ &\mathrm{e}^{-\frac{i}{\hbar}H(\{\varphi^*_{\lambda n},\varphi_{\lambda n-1}\})\varepsilon}\mathrm{e}^{\sum_\lambda\varphi^*_{\lambda k}\varphi_{\lambda k-1}}. \end{aligned}$$

Note that we get new exponentials due to differences in the completeness relation for coherent and eigenstate basis. Now we insert this result into the expression above, and get

$$\lim_{M\to\infty}\int\prod_{k=1,\lambda}^{M-1}\frac{\mathrm{d}\varphi^*_{\lambda k}\mathrm{d}\varphi_{\lambda k}}{2\pi i}\mathrm{e}^{-\sum_\lambda\sum_{k=1}^{M-1}(\varphi^*_{\lambda k}\varphi_{\lambda k}-\varphi^*_{\lambda k}\varphi_{\lambda k-1})}\mathrm{e}^{-\frac{i}{\hbar}\sum_\lambda\sum_{k=1}^{M-1}H(\{\varphi^*_{\lambda n},\varphi_{\lambda n-1}\})\varepsilon}$$

Where the factors in the first exponential comes from the completeness relation and the inner-product in the matrix element, respectively. Instead of the k-index, define a time variable t, similar to what we did before.

$$\begin{aligned}
\varepsilon\sum_{k=1}^{M-1}&\to\int_{t_i}^{t_f}\mathrm{d}t\\
H(\{\varphi^*_{\lambda n},\varphi_{\lambda n-1}\})&\to H(\{\varphi^*_\lambda(t),\varphi_\lambda(t)\})\\
\frac{(\varphi^*_{\lambda k}\varphi_{\lambda k}-\varphi^*_{\lambda k}\varphi_{\lambda k-1})}{\varepsilon}&\to\varphi^*_\lambda(t)\frac{\partial\varphi_\lambda(t)}{\partial t}\\
\lim_{M\to\infty}\int\prod_{k=1,\lambda}^{M-1}\frac{\mathrm{d}\varphi^*_{\lambda k}\mathrm{d}\varphi_{\lambda k}}{2\pi i}&\to\int_{\varphi_\lambda(t_i)=\varphi_{\lambda 0}}^{\varphi_\lambda(t_f)=\varphi_{\lambda M}}\mathcal{D}\left[\varphi^*_\lambda(t),\varphi_\lambda(t)\right]
\end{aligned}$$

where the limits in the last integral are fixed. Using these relations, he exponents translates to

$$\begin{aligned}
-\sum_\lambda\sum_{k=1}^{M-1}(\varphi^*_{\lambda k}\varphi_{\lambda k}-\varphi^*_{\lambda k}\varphi_{\lambda k-1})-\frac{i}{\hbar}\sum_\lambda\sum_{k=1}^{M-1}H(\{\varphi^*_{\lambda n},\varphi_{\lambda n-1}\})\varepsilon&\\
=i\varepsilon\sum_{k\lambda}i\left(\frac{\varphi^*_{\lambda k}\left(\varphi_{\lambda k}-\varphi_{\lambda k-1}\right)}{\varepsilon}\right)-\frac{1}{\hbar}H(\{\varphi^*_{\lambda n},\varphi_{\lambda n-1}\})&\\
\to i\sum_\lambda\int_{t_i}^{t_f}\mathrm{d}t\left[i\varphi^*_\lambda(t)\frac{\partial\varphi_\lambda(t)}{\partial t}-\frac{1}{\hbar}H(\{\varphi^*_\lambda(t),\varphi_\lambda(t)\})\right]=i\int_{t_i}^{t_f}\mathrm{d}tL(t).&
\end{aligned}$$

It is now clear how we do a functional integral formulation:

$$H(a^\dagger,a)\to H(\varphi^*_\lambda,\varphi_\lambda)$$

For each type of field operator in Fock space $\mathcal{F}$, in the second quantization formalism, we get a term

$$\varphi^*_\lambda(t)\frac{\partial\varphi_\lambda(t)}{\partial t}\qquad(a^\dagger,a)\to(\varphi^*_\lambda,\varphi_\lambda)$$

The new fields entering in the functional integral must respect the algebra of the operators. In particular, for bosons $(\varphi^*_\lambda,\varphi_\lambda)$ are c-numbers, while they are Grassmann numbers in the fermionic case.

Therefore:

$$U(\varphi_M, t_M; \varphi_0, t_0) = \int_{\varphi_\lambda(t_i)=\varphi_{\lambda 0}}^{\varphi_\lambda(t_f)=\varphi_{\lambda M}} \mathcal{D}\left[\varphi_\lambda^*(t)\right] \mathcal{D}\left[\varphi_\lambda(t)\right] \mathrm{e}^{iS(t_f,t_i)}$$

$$S(t_f, t_i) = \int_{t_i}^{t_f} \mathrm{d}t L(t).$$

Completely analogous to the path integral formulation in position-space. Note that $\frac{1}{\hbar}$ is not a common factor in the whole exponent. It only enters in the Hamiltonian H part of L. The classical limit is therefore very altered, compared to the case in position space $U(x_f, t_f; x_i, t_i)$, where the dominant paths were the smoothest once. It is less obvious what kind of paths that dominates in the coherent states case.

In the fermionic case, we write $\xi_\lambda(t)$ instead of $\varphi_\lambda(t)$ to explicitly clarify the algebra of the fields.

$$U(\xi_M, t_M; \xi_0, t_0) = \int_{\xi_\lambda(t_i)=\xi_{\lambda 0}}^{\xi_\lambda(t_f)=\xi_{\lambda M}} \mathcal{D}\left[\xi_\lambda^*(t)\right] \mathcal{D}\left[\xi_\lambda(t)\right] \mathrm{e}^{iS(t_f,t_i)}$$

$$S(t_f, t_i) = \int_{t_i}^{t_f} \mathrm{d}t L(t) = \int_{t_i}^{t_f} \mathrm{d}t \sum_\lambda \left[i\xi_\lambda^*(t) \frac{\partial \xi_\lambda(t)}{\partial t} - \frac{1}{\hbar} H(\{\xi_\lambda^*(t), \xi_\lambda(t)\}) \right].$$

Exactly the same form as in the bosonic case, only now the fields are Grassmann numbers instead of ordinary c-numbers. The partition function $Z = \mathrm{Tr}\left(\mathrm{e}^{-\beta H}\right)$: Bosons:

$$\mathrm{Tr}\,(A) = \int \prod_\lambda \frac{\mathrm{d}\varphi_\lambda^* \mathrm{d}\varphi_\lambda}{2\pi i} \mathrm{e}^{-\sum_\lambda \varphi_\lambda^* \varphi_\lambda} \left\langle \varphi \right| A \left| \varphi \right\rangle$$

Fermions:

$$\mathrm{Tr}\,(A) = \int \prod_\lambda \frac{\mathrm{d}\xi_\lambda^* \mathrm{d}\xi_\lambda}{2\pi i} \mathrm{e}^{-\sum_\lambda \xi_\lambda^* \xi_\lambda} \left\langle -\xi \right| A \left| \xi \right\rangle$$

Common notation:

$$\mathrm{Tr}\,(A) = \int \prod_\lambda \frac{\mathrm{d}\varphi_\lambda^* \mathrm{d}\varphi_\lambda}{N} \mathrm{e}^{-\sum_\lambda \varphi_\lambda^* \varphi_\lambda} \left\langle \xi\varphi \right| A \left| \varphi \right\rangle$$

where $N = 1$ and $\xi = -1$ in the fermionic case and $N = 2\pi i$ and $\xi = 1$ in the bosonic case. The element $|\varphi\rangle$ has components $|\varphi_{\lambda i}\rangle = |\varphi_{\lambda 0}\rangle$ and $|\xi\varphi\rangle$ has components $|\xi\varphi_{\lambda f}\rangle = |\xi\varphi_{\lambda M}\rangle$.

$$Z = \int_{\varphi_{\lambda 0} = \xi\varphi_{\lambda M}} \prod_\lambda \frac{\mathrm{d}\varphi_{\lambda M}^* \cdots \mathrm{d}\varphi_{\lambda 0}}{N} \mathrm{e}^{-\sum_\lambda \varphi_{\lambda M}^* \varphi_{\lambda M}} \left\langle \xi\varphi \right| \mathrm{e}^{-\beta H} \left| \varphi \right\rangle.$$

In order to find $\langle \xi\varphi | \, \mathrm{e}^{-\beta H} \, |\varphi\rangle$, we introduce imaginary time, as in the case of a single-particle:

$$\beta = \tau \qquad \mathrm{d}t = -i\mathrm{d}\tau \qquad \frac{\mathrm{d}}{\mathrm{d}t} = i\frac{\mathrm{d}}{\mathrm{d}\tau}$$

Inserting this into the expression for the action S:

$$\begin{aligned} S &= i\sum_\lambda \int_{t_i}^{t_f} \mathrm{d}t \left[i\varphi_\lambda^*(t)\frac{\partial\varphi_\lambda(t)}{\partial t} - \frac{1}{\hbar}H(\{\varphi_\lambda^*(t),\varphi_\lambda(t)\})\right] \\ &= -i^2\sum_\lambda \int_0^\beta \mathrm{d}\tau \left[\frac{i}{-i}\varphi_\lambda^*(\tau)\frac{\partial\varphi_\lambda(\tau)}{\partial\tau} - \frac{1}{\hbar}H(\{\varphi_\lambda^*(\tau),\varphi_\lambda(\tau)\})\right] \\ &= -\sum_\lambda \int_0^\beta \mathrm{d}\tau \left[\varphi_\lambda^*(\tau)\frac{\partial\varphi_\lambda(\tau)}{\partial\tau} + \frac{1}{\hbar}H(\{\varphi_\lambda^*(\tau),\varphi_\lambda(\tau)\})\right]. \end{aligned}$$

Then the partition function becomes

$$Z = \int_{\varphi_\lambda(0)=\xi\varphi_\lambda(\beta)} \mathcal{D}\left[\varphi_\lambda^*(\tau)\right]\mathcal{D}\left[\varphi_\lambda(\tau)\right]\mathrm{e}^S \tag{8.1}$$

$$S = -\sum_\lambda \int_0^\beta \mathrm{d}\tau \left[\varphi_\lambda^*(\tau)\frac{\partial\varphi_\lambda(\tau)}{\partial\tau} + H(\{\varphi_\lambda^*(\tau),\varphi_\lambda(\tau)\})\right]$$

Where the ξ's refer to the same values as above, and we have reinstated $\hbar = 1$. We see that the formalism differentiate between fermions and bosons in that the fields $\varphi_\lambda(\tau)$ have different periodicity on the interval $\tau \in [0, \beta]$.

During the calculation, we dropped the terms $\mathrm{e}^{-\sum_\lambda \varphi_{\lambda m}^*\varphi_{\lambda m}}$. We can treat these as "surface-terms", negligible compared to $\int_0^\beta \mathrm{d}\tau\varphi_\lambda^*(\tau)\frac{\partial\varphi_\lambda(\tau)}{\partial\tau}$. We did something like this in earlier calculations for $U(x_f, t_f; x_i, t_i)$. We could have kept them in both cases, and they would have cancelled in Z! [1]

[1] Proof of some relations regarding the trace before moving on to free electron gas: $M = ABC \implies \mathrm{Tr}(M) = M_{ii} = A_{il}B_{ln}C_{ni} = C_{ni}A_{il}B_{ln} = K_{nn} = \mathrm{Tr}(K)\,\mathrm{Tr}(B) = \mathrm{Tr}\big(BSS^{-1}\big) = \mathrm{Tr}\big(S^{-1}BS\big) = \mathrm{Tr}(D) = \sum_n \lambda_n$

9 Two important examples of the formalism

9.1 Free electron gas

We start with the Hamiltonian

$$\begin{aligned}\mathcal{H} &= \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} \\ &= \sum_{\sigma} \int \mathrm{d}x\, \psi^\dagger_\sigma(x) \varepsilon(\nabla) \psi_\sigma(x). \end{aligned} \tag{9.1}$$

The partition function is

$$\mathcal{Z} = \int \mathcal{D}\left[\varphi^*(\tau)\right] \mathcal{D}\left[\varphi(\tau)\right] \mathrm{e}^{\mathcal{S}} \tag{9.2}$$

where $\varphi_\lambda(0) = -\varphi_\lambda(\beta)$ (antiperiodic for fermions) and

$$\mathcal{S} = -\sum_\lambda \int_0^\beta \mathrm{d}\tau \left[\varphi^*_\lambda \frac{\partial \varphi_\lambda}{\partial \tau} + \mathcal{H}\left(\{\varphi^*_\lambda, \varphi_\lambda\}\right) \right] \tag{9.3}$$

Now choose quantum numbers $\lambda = (k, \sigma)$ because $\mathcal{H}$ is diagonal in the plane wave basis. Then,

$$\mathcal{S} = -\sum_{k,\sigma} \int_0^\beta \mathrm{d}\tau\, \varphi^*_{k\sigma}(\tau) \left(\frac{\partial}{\partial \tau} + \varepsilon_k \right) \varphi_{k\sigma}(\tau) \tag{9.4}$$

where $\{\varphi_{k\sigma}(\tau)\}$ are Grassman variables. $\mathcal{Z}$ now becomes a Gaussian integral over Grassmann variables, which we have seen earlier. By direct insertion of this result, we find

$$\begin{aligned}\mathcal{Z} &= \mathrm{e}^{\mathrm{Tr}\ln(\partial_\tau + \varepsilon_k)} \\ &\stackrel{?}{=} \prod_{k,\sigma} \left(1 + \mathrm{e}^{-\beta\varepsilon_k}\right) \end{aligned} \tag{9.5}$$

with

$$\mathrm{Tr} = \sum_{k,\sigma} \int_0^\beta \mathrm{d}\tau \cdot \mathrm{tr} \tag{9.6}$$

where "tr" here is the trace of the operator $\ln\left(\partial_\tau + \varepsilon_k\right)$

$$\mathrm{tr}\ln\left(\partial_\tau + \varepsilon_k\right) = \sum_n \left\langle n | \ln\left(\partial_\tau + \varepsilon_k\right) | n \right\rangle. \tag{9.7}$$

To be able to get a <u>local</u> expression for $\ln\left(\partial_\tau + \varepsilon_k\right)$, the choice of a plane wave basis for $|n\rangle$ is convenient.

$$|n\rangle = u_{nk} = \frac{1}{\sqrt{\beta}} \mathrm{e}^{i(\mathbf{k}\cdot\mathbf{r}-\omega_n\tau)} \tag{9.8}$$

where

$$\omega_n = \frac{(2n+1)\,\pi}{\beta}. \tag{9.9}$$

The reason for this choice of ω_n is that we see that this ensures $u_{nk}(\tau)$ to have the same antiperiodic properties as $\varphi_\lambda(\beta)$ When we take the trace only over such states, the requirement $\varphi_\lambda(0) = -\varphi_\lambda(\beta)$ is automatically satisfied.

$$\begin{aligned}
&\sum_n \langle n|\ln\left(\partial_\tau + \varepsilon_k\right)|n\rangle \\
&= \frac{1}{\beta} \sum_{\omega_n} \mathrm{e}^{-i(\mathbf{k}\cdot\mathbf{r}-\omega_n\tau)} \ln\left(\partial_\tau + \varepsilon_k\right) \mathrm{e}^{i(\mathbf{k}\cdot\mathbf{r}-\omega_n\tau)}.
\end{aligned} \tag{9.10}$$

Before we continue, we investigate the trace of an arbitrary operator

$$\operatorname{tr} \ln A = \sum_n \langle n|A|n\rangle\,. \tag{9.11}$$

$\ln A$ is defined by its series expansion

$$\begin{aligned}
\ln A &= \ln(1 + A - 1) \\
&= \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k} \left(A-1\right)^k,
\end{aligned} \tag{9.12}$$

such that

$$\operatorname{tr} \ln A = \sum_{k=1}^{\infty} \frac{(-1)^{k+1}}{k} \operatorname{tr}\left[\left(A-1\right)^k\right]. \tag{9.13}$$

Define $B = A - 1$. Now choose S such that $S^{-1}BS = S^{-1}AS - 1 = D - 1$, i.e. such that A is diagonalized.

$$\begin{aligned}
\operatorname{tr}\left(B^k\right) &= \operatorname{tr}\left[\left(D-1\right)^k\right] \\
&= \sum_m \left(\lambda_m - 1\right)^k \implies \\
\operatorname{tr} \ln A &= \sum_m \sum_k \frac{(-1)^{k+1}}{k} (\lambda_m - 1)^k \\
&= \sum_m \ln(1 + \lambda_m - 1) \\
&= \sum_m \ln \lambda_m = \ln\left(\prod_m \lambda_m\right) \\
\implies \operatorname{tr} \ln A &= \ln \det A.
\end{aligned} \tag{9.14}$$

When we use (9.14) in (9.10), we get

$$\sum_n \langle n|\ln\left(\partial_\tau + \varepsilon_k\right)|n\rangle = \frac{1}{\beta}\sum_{\omega_n} \ln\left(-i\omega_n + \varepsilon_k\right) \tag{9.15}$$

$$\begin{aligned} \mathcal{Z} &= \mathrm{e}^{\sum_{k,\sigma} \frac{1}{\beta}\int_0^\beta \mathrm{d}\tau \sum_{\omega_n} \ln(-i\omega_n+\varepsilon_k)} \\ &= \mathrm{e}^{\sum_{k,\sigma} \sum_{\omega_n} \ln(-i\omega_n+\varepsilon_k)} \\ &= \prod_{k,\sigma} \mathrm{e}^{\sum_{\omega_n} \ln(-i\omega_n+\varepsilon_k)}. \end{aligned} \tag{9.16}$$

To get any further, we need to execute the summation over the Matsubara frequencies ω_n. To do this, observe that $i\omega_n$ are the poles of the Fermi distribution

$$f(z) = \frac{1}{1+\mathrm{e}^{\beta z}} \tag{9.17}$$

If a complex valued function $g(z)$ defined on $\mathbb{C}$ has a simple pole at $z = z_0$, Cauchy's residue theorem tells us that

$$\oint \mathrm{d}z\, g(z) = 2\pi i \,\mathrm{Res}\left[g(z_0)\right] \tag{9.18}$$

$$\mathrm{Res}\left[g(z_0)\right] = \lim_{z\to z_0}\left[(z-z_0)g(z)\right] \tag{9.19}$$

So for the Fermi distribution in (9.17), we get

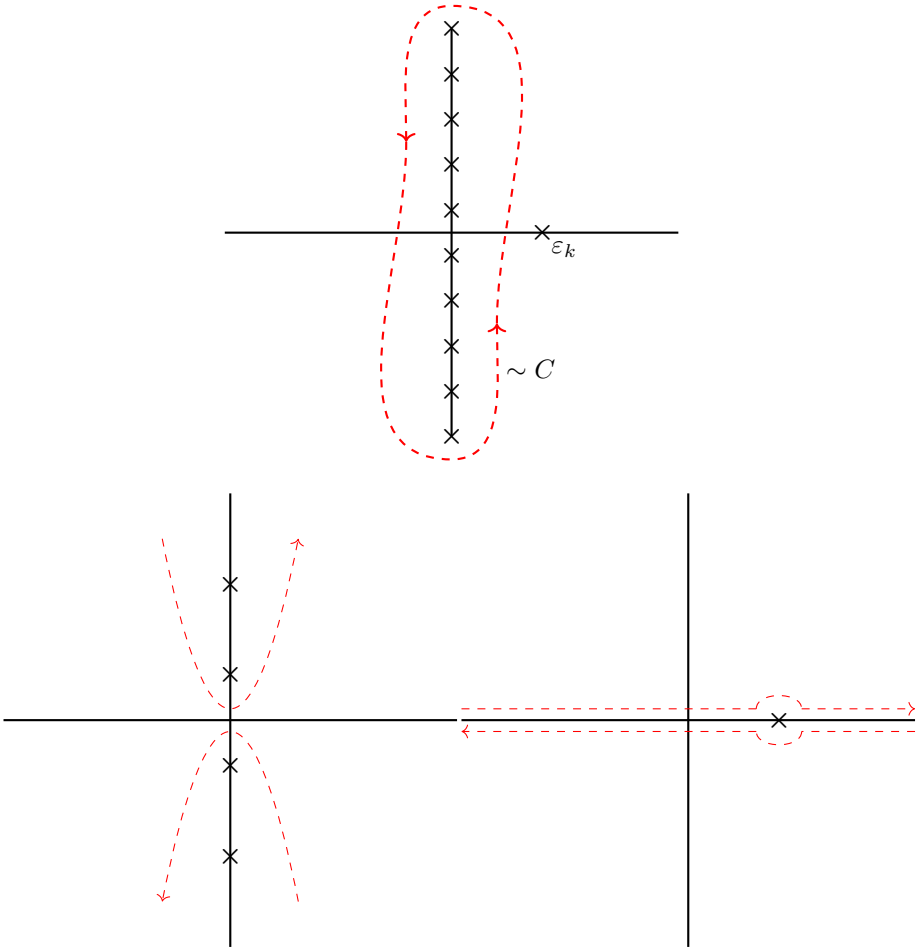
$$\begin{aligned} \mathrm{Res}\left[f(i\omega_n)\right] &= \lim_{z\to i\omega_n}\left[(z-i\omega_n)f(z)\right] \\ &= \lim_{z\to i\omega_n} \frac{1}{1+\mathrm{e}^{\beta(z-i\omega_n+i\omega_n)}} \\ &= \lim_{z\to i\omega_n} \frac{1}{1-\mathrm{e}^{\beta(z-i\omega_n)}} \\ &= \lim_{z\to i\omega_n} \frac{1}{1-1-\beta(z-i\omega_n)+\ldots} \\ &= \lim_{z\to i\omega_n} -\frac{1}{\beta}\frac{1}{z-i\omega_n} \implies \\ \mathrm{Res}\left[f(i\omega_n)\right] &= -\frac{1}{\beta} \end{aligned} \tag{9.20}$$

We then have

$$\oint \mathrm{d}z\, f(z) = 2\pi i \,\mathrm{Res}\, f(z_0) \tag{9.21}$$

$$= -\frac{2\pi i}{\beta} \implies \tag{9.22}$$

$$\sum_{\substack{i\omega_n \\ \omega_n \mathrm{odd}}} g(i\omega_n) = -\frac{\beta}{2\pi i}\oint \mathrm{d}z\, g(z)f(z) \equiv I \tag{9.23}$$



where the path encloses all simple poles of the Fermi distribution (9.17) and

$$g(i\omega_n) = \ln(-i\omega_n + \varepsilon_k) \tag{9.24}$$

Deform the path C in a way that does not enclose new poles. We have to avoid the pole in $g(i\omega_n) = \ln(-i\omega_n + \varepsilon_k)$.

Consider

$$\tilde{I} = \frac{\beta}{2\pi i} \int_{-\infty}^{\infty} \mathrm{d}\varepsilon \left[f(\varepsilon + i\delta) \ln\left(-\varepsilon - i\delta + \varepsilon_k\right) - f(\varepsilon - i\delta) \ln\left(-\varepsilon + i\delta + \varepsilon_k\right) \right]. \tag{9.25}$$

2

[2] I found no better placement as it stands on a separate page in the notes. The contribution

This is equal to

$$\tilde{I} = \frac{\beta}{2\pi i} \int_{-\infty}^{\infty} \mathrm{d}\varepsilon \, f(\varepsilon) \left[\ln(-\varepsilon - i\delta + \varepsilon_k) - \ln(-\varepsilon + i\delta + \varepsilon_k) \right]. \tag{9.26}$$

We have to be careful, since the ln-function has multiple values $\ln(z) = \ln(z) + i\varphi$, where $\varphi = 2\pi n$ for $n \in \mathbb{Z}$. We impose a branch cut off to separate the branches from one another on the Riemann surface. To eliminate the problem with a multivalued function, we define the function on specified Riemann-surfaces. The branch cut off separates one Riemann surface from another. Having multivalued functions means problems and meaninglessness when considering the computation of physical quantities. Moral of the story: Always (properly) examine the analytic structure of a function $g(z)$ that is included in $\sum_{\omega_n} g(i\omega_n)$.

For $\varepsilon < \varepsilon_k$, we have $\mathrm{Im}(\ln z) = \pi^-$ over the real axis, and $\mathrm{Im}(\ln z) = \pi^+$ under the real axis.

$$\begin{aligned} &\ln(-\varepsilon - i\delta + \varepsilon_k) - \ln(-\varepsilon + i\delta + \varepsilon_k) \\ &= \ln|-\varepsilon + \varepsilon_k| + i\pi^- - \ln|-\varepsilon + \varepsilon_k| - i\pi^+ \\ &= i(\pi^- - \pi^+) = 0^3 \end{aligned} \tag{9.27}$$

We thus have no contribution from $\varepsilon < \varepsilon_k$!
For $\varepsilon > \varepsilon_k$, $\mathrm{Im}(\ln z) = 0$ over the real axis and 2π below.

$$\begin{aligned} &\ln(-\varepsilon - i\delta + \varepsilon_k) - \ln(-\varepsilon + i\delta + \varepsilon_k) \\ &= \ln|-\varepsilon + \varepsilon_k| - \ln|-\varepsilon + \varepsilon_k| + i \cdot 0 - 2\pi i = -2\pi i \end{aligned} \tag{9.28}$$

Now we can return to the integral

$$\tilde{I} = -\frac{2\pi i}{2\pi i}\beta \int_{\varepsilon_k}^{\infty} \mathrm{d}\varepsilon \, f(\varepsilon) \tag{9.29}$$

$$= -\beta \int_{\varepsilon_k}^{\infty} \mathrm{d}\varepsilon \, \frac{1}{\mathrm{e}^{\beta\varepsilon} + 1} \tag{9.30}$$

$$= -\beta \int_{\varepsilon_k}^{\infty} \mathrm{d}\varepsilon \, \frac{\mathrm{e}^{-\beta\varepsilon}}{1 + \mathrm{e}^{-\beta\varepsilon}} \tag{9.31}$$

$$= \int_{\varepsilon_k}^{\infty} \mathrm{d}\varepsilon \, \frac{\mathrm{d}}{\mathrm{d}\varepsilon} \ln\left(1 + \mathrm{e}^{-\beta\varepsilon}\right) \tag{9.32}$$

$$= -\ln\left(1 + \mathrm{e}^{-\beta\varepsilon_k}\right). \tag{9.33}$$

from the pole is

$$= -\frac{1}{2\pi i} \int_0^{2\pi} \mathrm{d}\theta \, R \ln\left(R\mathrm{e}^{i\theta}\right) = -\frac{1}{2\pi i} R \left[2\pi \ln R + i\frac{4\pi^2}{2} \right] \overset{R \to 0}{\to} 0,$$

so no contribution.

[3] According to the notes, this is not entirely correct but here the signs on π is also swapped.

Thus

$$I = \sum_{\omega_n} \ln(-i\omega_n + \varepsilon_k) = \ln\left(1 + \mathrm{e}^{-\beta\varepsilon_k}\right). \tag{9.34}$$

This lets us calculate the partition function in (9.5) with the definition in (9.6) as

$$\begin{aligned}\mathcal{Z} &= \mathrm{e}^{\sum_{k\sigma}\sum_{\omega_n}\ln(-i\omega_n+\varepsilon_k)} = \mathrm{e}^{\sum_{k\sigma}\ln\left(1+\mathrm{e}^{-\beta\varepsilon_k}\right)} \\ &= \prod_{k,\sigma}\left(1+\mathrm{e}^{-\beta\varepsilon_k}\right).\end{aligned} \tag{9.35}$$

Equation (9.35) is a well known result for fermions. This is the partition function for a free fermion gas with Hamiltonian

$$\mathcal{H} = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma}. \tag{9.36}$$

9.2 Free Boson gas

We are now considering free, spin less bosons without any inner structure. For example phonons, magnons, solitons in one-dimensional conductors, etc..)

The Hamiltonian is

$$\mathcal{H} = \sum_q \omega_q a^\dagger_q a_q \tag{9.37}$$

As for free electron gas, we are to compute the partition function in (9.2), repeated here as

$$\mathcal{Z} = \int \mathcal{D}\left[\varphi^*(\tau)\right]\mathcal{D}\left[\varphi(\tau)\right]\mathrm{e}^{\mathcal{S}}. \tag{9.38}$$

This time, however, $\varphi_\lambda(0) = \varphi_\lambda(\beta)$, periodic for bosons.

$$\mathcal{S} = -\sum_q \int_0^\beta \mathrm{d}\tau\, \varphi^*_q(\tau)\left(\partial_\tau + \omega_q\right)\varphi_q(\tau) \tag{9.39}$$

$\mathcal{Z}$ now become a multiple Gaussian integral over complex variables, since the φ's now are eigenvalues for coherent boson states. We calculated this before;

$$\mathcal{Z} = \mathrm{e}^{-\operatorname{Tr}\ln(\partial_\tau+\omega)}$$

$$\operatorname{Tr} = \sum_q \int_0^\beta \mathrm{d}\tau\, \mathrm{tr}$$

We thus have to find a local expression for

$$\ln(\partial_\tau + \omega_q). \tag{9.40}$$

Since we are taking the trace over periodic states, $\varphi_\lambda(\tau = 0) = \varphi_\lambda(\tau = \beta)$, we introduce the plane wave basis

$$u_{\nu q} = \frac{1}{\sqrt{\beta}} \mathrm{e}^{i(\mathbf{q}\cdot\mathbf{r} - \omega_\nu \tau)}$$
$$\omega_\nu = \frac{2\nu\pi}{\beta}$$

The ω_ν's are the Matsubara boson frequencies. These basis functions are periodic on the interval $\tau \in [0, \beta)$. We have

$$\begin{aligned} \operatorname{tr} \ln(\partial_\tau + \omega) &= \sum_\nu \langle \nu | \ln(\partial_\tau + \omega_q) | \nu \rangle \\ &= \frac{1}{\beta} \sum_{\omega_\nu} \ln(-i\omega_\nu + \omega_q), \end{aligned}$$

which in turn implies that

$$\mathcal{Z} = \mathrm{e}^{-\sum_q \sum_{\omega_\nu} \ln(-i\omega_\nu + \omega_q)} \tag{9.41}$$

To compute (9.41), we need a result for

$$\sum_{\omega_\nu} \ln(-i\omega_\nu + \omega_q). \tag{9.42}$$

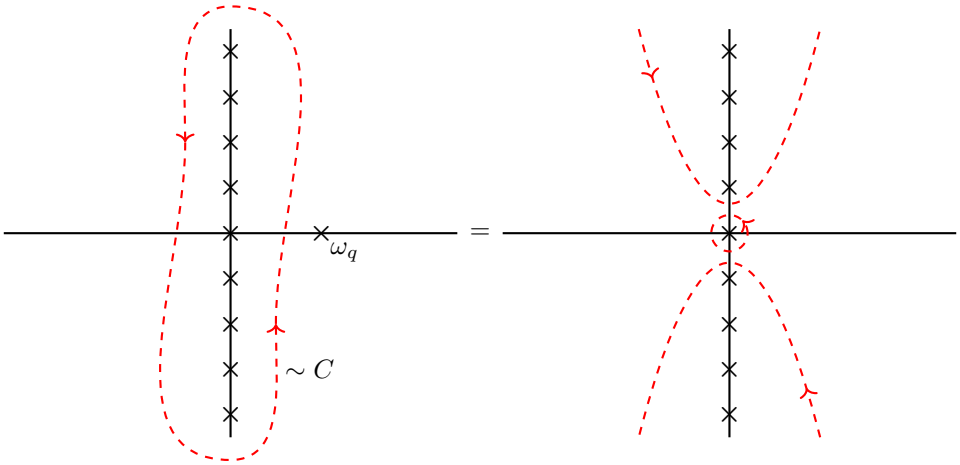
Using the same technique as we did in section 9.1, we observe that $i\omega_\nu$ are poles in the Bose-Einstein distribution

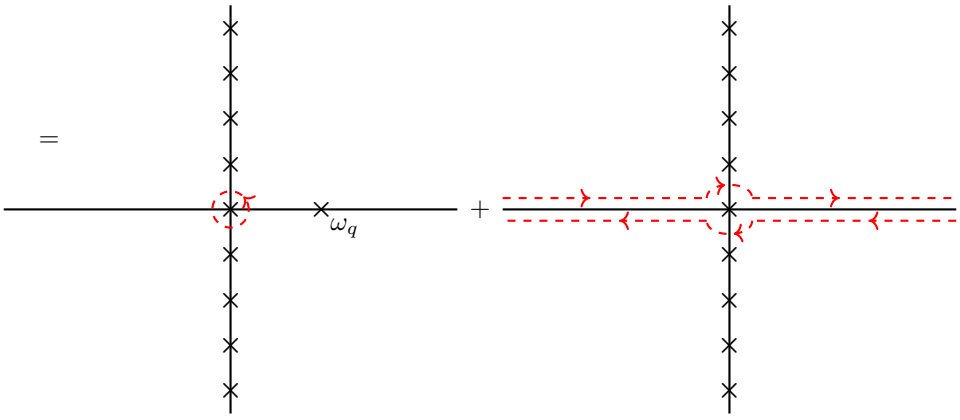
$$b(z) = \frac{1}{\mathrm{e}^{\beta z} - 1}, \tag{9.43}$$

with $\operatorname{Res} b(i\omega_\nu) = 1/\beta$. As seen in the figures, the contributions from the pole in the origin cancel. Using this and Cauchy's residue theorem gives, with $g(i\omega_\nu) = \ln(-i\omega_\nu + \omega_q)$

$$\begin{aligned} \sum_{\omega_\nu} g(i\omega_\nu) &= +\frac{\beta}{2\pi i} \oint_{\mathcal{C}} \mathrm{d}z \, g(z) b(z) \\ &= \frac{\beta}{2\pi i} \int_{-\infty}^{0^-} \mathrm{d}\varepsilon \, b(\varepsilon) \left[\ln(-\varepsilon - i\delta + \omega_q) - \ln(-\varepsilon + i\delta + \omega_q) \right] \\ &+ \frac{\beta}{2\pi i} \int_{0^+}^{\omega_q} \mathrm{d}\varepsilon \, b(\varepsilon) \left[\ln(-\varepsilon - i\delta + \omega_q) - \ln(-\varepsilon + i\delta + \omega_q) \right] \\ &= \beta \int_{\omega_q}^{\infty} \mathrm{d}\varepsilon \, b(\varepsilon) \left[\ln(-\varepsilon - i\delta + \omega_q) - \ln(-\varepsilon + i\delta + \omega_q) \right] \end{aligned} \tag{9.44}$$

The contribution from $\varepsilon < \omega_q$ disappear from the exact same reason as in the case of fermions. The contribution from $\varepsilon > \omega_q$ is easier, since the difference in


ω_q
$\sim C$
=


=
ω_q
+

the logarithms is $-2\pi i$, so that

$$\begin{aligned} -\beta \int_{\omega_q}^{\infty} \mathrm{d}\varepsilon \, b(\varepsilon) &= -\beta \int_{\omega_q}^{\infty} \mathrm{d}\varepsilon \, \frac{\mathrm{e}^{-\beta\varepsilon}}{1-\mathrm{e}^{-\beta\varepsilon}} \\ &= -\frac{\beta}{\beta} \left[\ln\left(1-\mathrm{e}^{-\beta\varepsilon}\right) \right]_{\omega_q}^{\infty} \\ &= \ln\left(1-\mathrm{e}^{-\beta\omega_q}\right). \end{aligned}$$

We then have

$$\begin{aligned} \mathcal{Z} &= \mathrm{e}^{-\sum_q \sum_{\omega_\nu} \ln(-i\omega_\nu+\omega_q)} \\ &= \mathrm{e}^{-\sum_q \ln\left(1-\mathrm{e}^{-\beta\omega_q}\right)} \\ &= \prod_q \frac{1}{1-\mathrm{e}^{-\beta\omega_q}} \\ &= \mathrm{e}^{-\beta F}. \end{aligned} \tag{9.45}$$

We recognize (9.45) as the partition function for a free boson gas, with free energy

$$F = \frac{1}{\beta} \sum_q \ln\left(1-\mathrm{e}^{-\beta\omega_q}\right). \tag{9.46}$$

The answers we have gotten for both the free fermion gas and free boson gas could easily have been found by simple counting arguments. These calculations have however illustrated what hides behind exact expressions as for example $\operatorname{Tr} A(\partial_\tau)$. In addition, the methods are familiar for interacting problems, which we will consider later.

10 Green's functions, $T > 0$

First we are going to look at the derivation of one-particle Green's functions for bosons and fermions. Recall the definition of a one-particle Green's function at $T = 0$:

$$G_\lambda(x,t) = -i \langle\psi|T_t \left(c_\lambda(x,t)c_\lambda^\dagger(0,0)\right)|\psi\rangle$$

where $|\psi\rangle$ is the exact many-particle state of the Hamiltonian H, T_t is the time ordering symbol defined as

$$\begin{aligned} T_t(A(t_1),B(t_2)) &= A(t_1)B(t_2), \quad t_1 > t_2 \\ &\pm B(t_2)A(t_1), \quad t_2 > t_1 \end{aligned}$$

where the $+$ is for bosons and the $-$ is for fermions. T_t thus (re-)arranges the elements in a time ordered way from right to left, respecting the commutation properties of the fields. We have the following interpretation of the Green's function: $G_\lambda(x,t)$ is the probability amplitude for a particle, initially in state λ at the origin at time $t = 0$, to still be in state λ at (x,t). We generalize this to the case of $T > 0$.

$$G_\lambda(x,\tau) = -\langle\psi|T_\tau \left(c_\lambda(x,\tau)c_\lambda^\dagger(0,0)\right)|\psi\rangle$$

where T_τ is the time ordering symbol, now for imaginary time τ. $G_\lambda(x,\tau)$ has a similar interpretation as for the case of $T = 0$. Further, we write

Fermions:

$$G(k,\sigma,\tau) = -\langle\psi|T_\tau \left(c_{k\sigma}(x,\tau)c_{k\sigma}^\dagger(0,0)\right)|\psi\rangle$$

where the quantum numbers (k σ) have to be the same in both operators, since the corresponding states are orthonormal.

Bosons:

$$D(q,\tau) = -\langle\psi|T_\tau \left(a_q(x,\tau)a_q^\dagger(0,0)\right)|\psi\rangle$$

where q is a set of quantum numbers, which can include spin. Similarly, we can define the Fourier transformed Green's functions.

Fermions:

$$G(k,i\omega_n) = \int_0^\beta \mathrm{d}\tau G(k,\tau)\mathrm{e}^{i\omega_n\tau}$$

Bosons:

$$D(q,i\omega_\nu) = \int_0^\beta \mathrm{d}\tau D(q,\tau)\mathrm{e}^{i\omega_\nu\tau}$$

where $\omega_n = \frac{(2n+1)\pi}{\beta}$ and $\omega_\nu = \frac{2\pi\nu}{\beta}$ for $n, \nu \in \mathbb{Z}$ are the Matsubara frequencies. The inverted expressions becomes sums, since the frequencies are discrete:

$$G(k,\tau) = \frac{1}{\beta}\sum_{\omega_n} G(k, i\omega_n)\mathrm{e}^{-i\omega_n\tau}$$
$$D(q,\tau) = \frac{1}{\beta}\sum_{\omega_\nu} G(k, i\omega_\nu)\mathrm{e}^{-i\omega_\nu\tau}.$$

In the functional integral formalism, we define the expectation value of an operator as

$$\begin{aligned}
\langle A\rangle &= \frac{1}{Z}\operatorname{Tr}\left(e^{-\beta H}A\right)\\
&= \frac{1}{Z}\int_{\varphi_\lambda(0)=\xi\varphi_\lambda(\beta)} \mathcal{D}[\varphi^*]\mathcal{D}[\varphi]A(\{\varphi^*_\lambda,\varphi_\lambda\})\mathrm{e}^{S}.\\
S &= -\sum_\lambda \int_0^\beta \mathrm{d}\tau\left[\varphi^*_\lambda\frac{\partial\varphi_\lambda}{\partial\tau} + H(\{\varphi^*_\lambda,\varphi_\lambda\})\right] = S_0 + S_I.\\
S_0 &= -\sum_\lambda\int_0^\beta \mathrm{d}\tau\left[\varphi^*_\lambda(\partial_\tau+\varepsilon)\varphi_\lambda\right]\\
S_I &= -\sum_\lambda\int_0^\beta \mathrm{d}\tau H_I(\{\varphi^*_\lambda,\varphi_\lambda\}).
\end{aligned}$$

where we have explicitly written the expressions for the interacting and non-interacting part of the exponent S. Further, we write

$$\begin{aligned}
Z_0 &= \int_{\varphi_\lambda(0)=\xi\varphi_\lambda(\beta)} \mathcal{D}[\varphi^*]\mathcal{D}[\varphi]\mathrm{e}^{S_0}\\
\langle A\rangle_0 &= \int_{\varphi_\lambda(0)=\xi\varphi_\lambda(\beta)} \mathcal{D}[\varphi^*]\mathcal{D}[\varphi]A(\{\varphi^*_\lambda,\varphi_\lambda\})\mathrm{e}^{S_0}\\
Z &= \int_{\varphi_\lambda(0)=\xi\varphi_\lambda(\beta)} \mathcal{D}[\varphi^*]\mathcal{D}[\varphi]\mathrm{e}^{S_I}\mathrm{e}^{S_0} = Z_0\left\langle \mathrm{e}^{S_I}\right\rangle_0\\
\langle A\rangle &= \frac{1}{Z_0\left\langle e^{S_I}\right\rangle_0}\int_{\varphi_\lambda(0)=\xi\varphi_\lambda(\beta)} \mathcal{D}[\varphi^*]\mathcal{D}[\varphi]\left(A\mathrm{e}^{S_I}\right)\mathrm{e}^{S_0} = \frac{\left\langle A\mathrm{e}^{S_I}\right\rangle_0}{\left\langle \mathrm{e}^{S_I}\right\rangle_0}
\end{aligned}$$

In the last expression, the denominator cancels all non-connected diagrams in perturbation theory, to all orders in S_I. $\left\langle \mathrm{e}^{S_I}\right\rangle_0$ represents all vacuum-fluctuations, or rather the fluctuations the system exhibits without the precence of A. In $\langle A\rangle$, we are interested in finding the systems response to the operator A. The vacuum fluctuations are not of interested in this case, and the factor $\left\langle \mathrm{e}^{S_I}\right\rangle_0$ in the denominator makes sure that they don't contribute to $\langle A\rangle$.

Now we define a generating functional for Green's functions:

$$W\left(\{\varphi_\lambda^*, \varphi_\lambda\}\right) = \frac{1}{Z}\int_{\varphi_\lambda(0)=\xi\varphi_\lambda(\beta)} \mathcal{D}[\varphi^*]\mathcal{D}[\varphi]\mathrm{e}^{S+F}$$
$$F = \sum_\lambda \int_0^\beta \mathrm{d}\tau \left(J_\lambda^*(\tau)\varphi_\lambda(\tau) + J_\lambda(\tau)\varphi_\lambda^*(\tau)\right)$$

where the sources $J_\lambda(\tau)$ are c-numbers in the case of bosonic fields, and Grassmann-numbers in the case of fermionic fields. In the latter case, the order of the fields and sources is important.

$$\langle W\rangle = \frac{\left\langle \mathrm{e}^F \mathrm{e}^{S_I}\right\rangle_0}{\left\langle \mathrm{e}^{S_I}\right\rangle_0}$$
$$\langle A\rangle = \frac{\left\langle A\mathrm{e}^{S_I}\right\rangle_0}{\left\langle \mathrm{e}^{S_I}\right\rangle_0} = \frac{1}{\left\langle \mathrm{e}^{S_I}\right\rangle_0} A\left(\frac{\delta}{\delta J_\lambda}, \frac{\delta}{\delta J_\lambda^*}\right)\left\langle \mathrm{e}^{S_I}\mathrm{e}^F\right\rangle\Big|_{J=0}$$

where after putting the sources to zero, the expression becomes identical to the one defined above.

10.1 Non-interacting case

Now the functional integral becomes Gaussian, and we have looked at these kind of integrals before in detail.

$$\left\langle \mathrm{e}^F\right\rangle_0 = \frac{1}{Z_0}\int_{\varphi_\lambda(0)=\xi\varphi_\lambda(\beta)} \mathcal{D}[\varphi^*]\mathcal{D}[\varphi]\mathrm{e}^S$$
$$S = \sum_\lambda \int_0^\beta \mathrm{d}\tau \left[\varphi_\lambda^*(\partial_\tau + \varepsilon)\varphi_\lambda + J_\lambda^*(\tau)\varphi_\lambda(\tau) + J_\lambda(\tau)\varphi_\lambda^*(\tau)\right].$$

This has the same form as

$$\int\left(\prod_k \frac{\mathrm{d}\varphi_k^*\mathrm{d}\varphi_k}{N}\right)\mathrm{e}^{-(\varphi_i^* A_{ij}\varphi_j + J_i^*\varphi_i + J_i\varphi_i^*)}$$
$$= \mathrm{e}^{J_i^* A_{ij}^{-1} J_i}\mathrm{e}^{-\xi\,\mathrm{Tr}\ln A} = Z_0\mathrm{e}^{J_i^* A_{ij}^{-1} J_i}$$

where again $\xi = +1$ corresponds to bosons, and $\xi = -1$ corresponds to fermions. Thus we get

$$\left\langle \mathrm{e}^F\right\rangle_0 = \mathrm{e}^{\sum_\lambda \int_0^\beta \mathrm{d}\tau J_\lambda^*(\tau)(\partial_\tau+\varepsilon)^{-1}J_\lambda(\tau)}.$$

We can use this result to calculate free-particle Green's functions at $T > 0$.

$$G(k,\sigma,\tau) = -\langle\psi|T_\tau\left(c_{k\sigma}(\tau)c^\dagger_{k\sigma}(0)\right)|\psi\rangle \to -\langle T_\tau\left(\varphi_{k\sigma}(\tau)\varphi^*_{k\sigma}(0)\right)\rangle_0$$
$$= -\left[\theta(\tau)\langle\varphi_{k\sigma}(\tau)\varphi^*_{k\sigma}(0)\rangle_0 - \theta(-\tau)\langle\varphi^*_{k\sigma}(0)\varphi_{k\sigma}(\tau)\rangle_0\right]$$

where we have explicitly gone from second quantized form to functional integral form, by introducing the coherent eigenstates. Now consider the case $\tau_1 > \tau_2$ and define $\lambda_1 = k_1, \sigma_1$ and $\lambda_2 = k_2, \sigma_2$.

$$-\left\langle\varphi_{\lambda_1}(\tau_1)\varphi^*_{\lambda_2}(\tau_2)\right\rangle = -\frac{\delta}{\delta J^*_{\lambda_1}(\tau_1)}\frac{\delta}{\delta J_{\lambda_2}(\tau_2)}\left\langle \mathrm{e}^F\right\rangle\Big|_{J=0}$$
$$= (\partial_\tau + \varepsilon)^{-1}_{\tau_1,\tau_2}\delta_{\lambda_1,\lambda_2} = G_0(\lambda_1,\lambda_2,\tau_1,\tau_2)$$

where the resulting Green's function should be interpreted as a matrix with indicies τ_1, τ_2. This is the continuous/infinitesimal edition of an operator tanking the system from imaginary time τ_1 to τ_2 (Trotter slice). This matrix is therefore non-diagonal, and inverting it is therefore non-trivial. Now for the case of $\tau_2 > \tau_1$:

$$\left\langle\varphi^*_{\lambda_2}(\tau_2)\varphi_{\lambda_1}(\tau_1)\right\rangle = \frac{\delta}{\delta J_{\lambda_2}(\tau_2)}\frac{\delta}{\delta J^*_{\lambda_1}(\tau_1)}\left\langle \mathrm{e}^F\right\rangle\Big|_{J=0}$$
$$= (\partial_\tau + \varepsilon)^{-1}_{\tau_2,\tau_1}\delta_{\lambda_1,\lambda_2}$$

we therefore see that we don't have to use time ordering explicitly, due to the definition of our statistical average. Now set $\lambda_1 = \lambda_2 = \lambda$ and $\tau = \tau_1 - \tau_2$. Then we get the equation for the Green's function:

$$(\partial_\tau + \varepsilon)G_0(\lambda,\tau) = \delta(\tau)$$
$$\int_0^\beta \mathrm{d}\tau \mathrm{e}^{i\omega_n\tau}(\partial_\tau + \varepsilon)G_0(\lambda,\tau) = 1$$
$$\frac{1}{\beta}\int_0^\beta \mathrm{d}\tau \mathrm{e}^{i\omega_n\tau}(\partial_\tau + \varepsilon)\sum_{\omega_m}\mathrm{e}^{-i\omega_m\tau}G_0(\lambda,i\omega_m) = 1$$
$$\sum_{\omega_m}\frac{1}{\beta}\int_0^\beta \mathrm{d}\tau \mathrm{e}^{i(\omega_n-\omega_m)\tau}(-i\omega_m + \varepsilon)\mathrm{e}^{-i\omega_m\tau}G_0(\lambda,i\omega_m) = 1$$
$$G_0(\lambda,i\omega_n) = \frac{-1}{i\omega_n - \varepsilon} \qquad D_0(q,i\omega_\nu) = \frac{-1}{i\omega_\nu - \omega_q}$$

for fermions and bosons, respectively.

10.2 Examples on how to use these propagators

Say that you want to look at the leading order correction to a free boson-propagator. From $T = 0$ perturbation theory, we know that such corrections

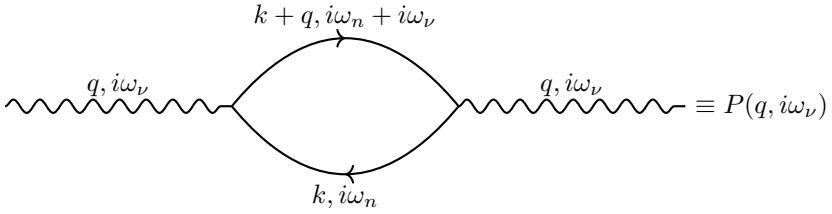


Figure 4: Feynman diagram

corresponds to Feynman diagrams like in Figure 4

$$P(q, i\omega_\nu) \sim \frac{1}{\beta} \sum_{k,\omega_n} G_0(k, i\omega_n) G_0(k+q, i\omega_n + i\omega_\nu)$$
$$= \sum_k \frac{1}{\beta} \sum_{\omega_n} \frac{1}{i\omega_n - \varepsilon_k} \frac{1}{i\omega_n + i\omega_\nu - \varepsilon_{k+q}}$$

The frequency summation is easy:

$$\frac{1}{\beta} \sum_{\omega_n} \frac{1}{i\omega_n - \varepsilon_k} \frac{1}{i\omega_n + i\omega_\nu - \varepsilon_{k+q}}$$
$$= \frac{1}{i\omega_\nu + \varepsilon_k - \varepsilon_{k+q}} \frac{1}{\beta} \sum_{\omega_n} \left(\frac{1}{i\omega_n - \varepsilon_k} - \frac{1}{i\omega_n + i\omega_\nu - \varepsilon_{k+q}} \right)$$

Now look at the general expression

$$\frac{1}{\beta} \sum_{\omega_n} \frac{1}{i\omega_n - x} = -\frac{1}{2\pi i} \oint \mathrm{d}z \frac{f(z)}{z - x} = \frac{-2\pi i}{-2\pi i} f(x) = f(x),$$

making the path deformation like in Figure 5. This expression implies

$$P(q, i\omega_\nu) \sim \frac{[f(\varepsilon_k) - f(\varepsilon_{k+q})]}{i\omega_\nu + \varepsilon_k - \varepsilon_{k+q}}.$$

The f-factors contain all T-effects. Now we can analytically continue:

$$i\omega_\nu \to \omega \pm i\delta \qquad \delta = 0^+$$

where + and − correspond to retarded and advanced greens functions respectively. From this, we get a dynamical responsefunction for $\omega > 0$ at $T > 0$.

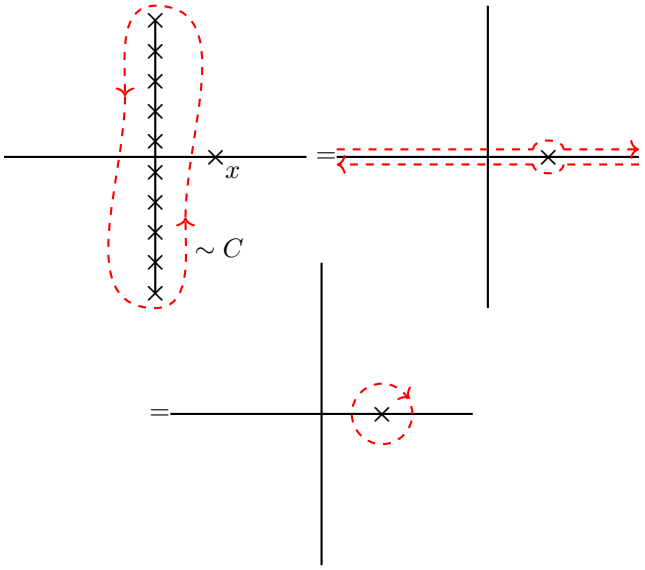


Figure 5: Path deformation

11 Interacting fermion-systems and the Hubbard-Stratonovich de-coupling

$$Z = \int \mathcal{D}\left[\varphi^*\right] \mathcal{D}\left[\varphi\right] \mathrm{e}^{S_0+S_I}$$

where S_I contain the interaction terms. These terms are typically of the form $\sim \varphi^*\varphi\varphi\varphi^*$, which makes it impossible to calculate the partition function exactly. If S_I is sufficiently small, one uses perturbation theory, which is assumed to be good if S_I doesn't cause qualitative changes in Z relative to Z_0 (phase-changes).

If S_I on the other hand is sufficiently big, which means that it's strong enough to cause phase transitions, we wouldn't be able to detect such changes using perturbation theory at any order. Our strategy will therefore be to approximate Z non-perturbatively around some known free theory. The trick that makes such a calculation possible is the Hubbard-Stratonovich de-coupling of the interacting part of S, making $S \to S_{eff}$ into some effective action of the theory.

$$\mathrm{e}^{S_I} = \mathrm{e}^{-\sum_\lambda \int_0^\beta \mathrm{d}\tau H_I(\{\varphi_\lambda^*,\varphi_\lambda\})}$$

In order to decouple something like this expression, we use the identity

$$\mathrm{e}^{-\operatorname{Tr}\ln A}\mathrm{e}^{J^*A^{-1}J} = \int \mathcal{D}a^\dagger \mathcal{D}a \mathrm{e}^{-a^\dagger A a + J^* a + J a^\dagger}$$

where $a, a^\dagger$ are bosonic fields and the sources J, J^* are c-numbers. Now we make the following substitutions

$$J = \varphi\varphi \qquad A^{-1} = V$$

and we get

$$e^{S_I} = \mathrm{e}^{-\operatorname{Tr}\ln A} \int \mathcal{D}a^\dagger \mathcal{D}a \mathrm{e}^{-a^\dagger V^{-1} a + \varphi^* \varphi^* a + \varphi\varphi a^\dagger}$$

where the first exponent is just a number we can set = 1, since this only define the zero-point in the free energy.

Inserting this substitution for e^{S_I} into the partition function, we end up with

$$Z = \int \mathcal{D}\left[\varphi^*\right] \mathcal{D}\left[\varphi\right] \mathcal{D}a^\dagger \mathcal{D}a \mathrm{e}^{-\varphi^*(\partial_\tau + \varepsilon)\varphi + \varphi^* a \varphi^* + \varphi a^\dagger \varphi - a^\dagger V^{-1} a}.$$

The point here is that now the fermion part (φ's) of the theory is Gaussian, which means that we can integrate out the fermion part of the theory exactly! The interacting fermion theory is formally equivalent to a free fermion theory, coupled to some background bosonic fields.

$$Z = \int \mathcal{D}a^\dagger \mathcal{D}a \mathrm{e}^{-a^\dagger V^{-1} a} \mathrm{e}^{\frac{1}{2}\operatorname{Tr}\ln G^{-1}} \tag{11.1}$$

where we have inserted the results from

$$-\varphi^*(\partial_\tau + \varepsilon)\varphi + \varphi^* a \varphi^* + \varphi a^\dagger \varphi =$$
$$-\frac{1}{2}\begin{pmatrix}\varphi^* & \varphi\end{pmatrix}\begin{pmatrix}\partial_\tau + \varepsilon & -2a \\ -2a^\dagger & \partial_\tau - \varepsilon\end{pmatrix}\begin{pmatrix}\varphi \\ \varphi^*\end{pmatrix} = -\frac{1}{2}\varphi^* G^{-1}\varphi$$

where we have introduced fermion spinor notation $\varphi = \begin{pmatrix}\varphi \\ \varphi^*\end{pmatrix}$ and performed a partial integration in S_I, resulting in a sign change in the lower right cell of the matrix.

$$Z = \int \mathcal{D}a^\dagger \mathcal{D}a \mathrm{e}^{S_{eff}}$$
$$S_{eff}(a^\dagger, a) = -\sum_\lambda \int_0^\beta \mathrm{d}\tau a_\lambda^\dagger(\tau) V^{-1} a_\lambda(\tau) + \frac{1}{2}\operatorname{Tr}\ln G^{-1}$$

Now we have converted our interacting fermion theory into an effective, interacting boson-theory, with effective action $S_eff(a^\dagger, a)$. A priori, this seems like a much more complicated theory compared to the fermion theory we started out with. So what have we accomplished?

The main point here is that the saddle-point approximation over c-numbers makes sense. A corresponding approximation with Grassmann-numbers doesn't exist. The reason for this is very simple. Say that you want to approximate the integral

$$I = \int \mathrm{d}x \mathrm{e}^{f(x)}.$$

Now if $f(x)$ has some stable minimum at $x = x_0$, the integral is dominated by the parts close to that minimal value

$$f(x) = f(x_0) + \frac{1}{2}(x - x_0)f^{''}(x_0) + \cdots$$
$$I = \approx \mathrm{e}^{-f(x_0)} \int \mathrm{d}x \mathrm{e}^{-\frac{1}{2}(x-x_0)^2 f^{''}(x_0)} = \sqrt{\frac{2\pi}{f^{''}(x_0)}} \mathrm{e}^{-f(x_0)}$$

Now, if x is a Grassmann-variable, then the taylor expansion is linear $f(x) = c_1 + c_2 x$, and this integral approximation wouldn't have made any sense. We have avoided the problem of calculating the Grassmannian fermion integral approximately, because our Hubbard-Stratonovich de-coupling (HS) mapping made it possible to calculate it exactly! The boson part $a^\dagger, a$ can we, however, try to calculate using our saddle-point approximation. Another way of interpreting this: boson-theories have classical counterparts, whereas fermions doesn't.

Some remarks:

i) The partition function

$$Z = \int \mathcal{D}\left[\varphi^*\right] \mathcal{D}\left[\varphi\right] \mathcal{D}a^\dagger \mathcal{D}a \mathrm{e}^{J^* a + J a^\dagger - a^\dagger V^{-1} a + S_0(\{\varphi^*, \varphi\})}$$

can be interpreted as the partition function for a non-interacting fermion system which is coupled to a dynamical boson-field, where $S_{eff}(a^\dagger, a)$ is the free energy to this system for a particular configuration of the external fields $a^\dagger, a$. The total free energy is the sum of the free energies of each of the configurations.

ii) It's important to notice that there is an ambiguity in choosing how to HS decouple the non-interacting part in the fermion sector. We could have just as well chosen to substitute

$$J = \varphi^* \varphi \qquad J^* = \varphi^* \varphi$$

instead of our previous choice

$$J = \varphi\varphi \qquad J = \varphi^*\varphi^*.$$

The important thing to note here is that as long as we compute the boson functional integral exactly, it doesn't matter what choice we make. On the other hand, if we compute the boson functional integral approximately, then the choice does matter. Then the choice of decouple scheme is determined by what kind of physics we expect in the end.

Now we HS decouple S_I in the following manner:

$$J = \varphi_\downarrow(x,\tau)\varphi_\uparrow(x,\tau)$$
$$J^* = \varphi^*_\uparrow(x,\tau)\varphi^*_\downarrow(x,\tau)$$

where now J, J^* is pair-fields and $a, a^\dagger$ is their corresponding conjugated fields. Now recall that the trace-exponential, which corresponed to the zero-point energy, was put to zero. Then we get

$$\mathrm{e}^{S_I} = \mathrm{e}^{VJ^*J} = \int \mathcal{D}a^\dagger \mathcal{D}a \mathrm{e}^{-a^\dagger \frac{1}{V} a + J^* a + J a^\dagger} \tag{11.2}$$

$$\implies \mathrm{e}^{S_I} = \int \mathcal{D}a^\dagger \mathcal{D}a \mathrm{e}^{-\sum_x \left[\frac{1}{V}|a(x)|^2 - \varphi^*_\uparrow(x,\tau)\varphi^*_\downarrow(x,\tau)a(x) - \varphi_\downarrow(x,\tau)\varphi_\uparrow(x,\tau)a^\dagger\right]} \tag{11.3}$$

And we get the partition function

$$Z = \int \mathcal{D}\left[\varphi^*\right]\mathcal{D}\left[\varphi\right]\mathcal{D}a^\dagger\mathcal{D}a\mathrm{e}^{-\sum_x \frac{1}{V}a^\dagger a + A_z}$$
$$A_z = S_0 + \sum_x \left[a^\dagger\varphi_\downarrow(x,\tau)\varphi_\uparrow(x,\tau) + a\varphi^*_\uparrow(x,\tau)\varphi^*_\downarrow(x,\tau)\right]$$

Now we define the Nambu-formalism, which means writing the conjugate fields $\varphi_\uparrow, \varphi_\downarrow$ as a 2-component spinor in the following way

$$\Psi(x) = \begin{pmatrix}\varphi_\uparrow(x)\\ \varphi^*_\downarrow(x)\end{pmatrix} \qquad \Psi^\dagger = \begin{pmatrix}\varphi^*_\uparrow(x) & \varphi_\downarrow(x)\end{pmatrix}$$

Now we see that

$$\sum_x \left[a^\dagger \varphi_\downarrow(x,\tau)\varphi_\uparrow(x,\tau) + a\varphi_\uparrow^*(x,\tau)\varphi_\downarrow^*(x,\tau)\right]$$
$$= \sum_x \Psi^\dagger(x) \begin{pmatrix} 0 & a(x) \\ a^\dagger(x) & 0 \end{pmatrix} \Psi(x)$$
$$S_0 = -\sum_{x,y} \left[\varphi_\uparrow^*(x)(\partial_\tau + \varepsilon - \mu)\varphi_\uparrow(y) + \varphi_\downarrow^*(x)(\partial_\tau + \varepsilon - \mu)\varphi_\downarrow(x)\right]$$
$$= -\sum_{x,y} \begin{pmatrix} \varphi_\uparrow^* & \varphi_\downarrow \end{pmatrix} \begin{pmatrix} (\partial_\tau + \varepsilon - \mu) & 0 \\ 0 & (\partial_\tau - (\varepsilon - \mu)) \end{pmatrix} \begin{pmatrix} \varphi_\uparrow \\ \varphi_\downarrow^* \end{pmatrix}$$
$$= -\sum_{x,y} \Psi^\dagger(x) \left[-G_0^{-1}(x,y)\right] \Psi(y)$$

Combining all expressions, we get

$$A_z = -\sum_{x,y} \Psi^\dagger(x) \left[-G^{-1}(x,y)\right] \Psi(x)$$
$$-G^{-1}(x,y) = -G_0^{-1}(x,y) - B(x)\delta_{x,y}$$
$$B(x) = \begin{pmatrix} 0 & a(x) \\ a^\dagger(x) & 0 \end{pmatrix}$$

Note that here the fermion propagator $G \sim -\left\langle \Psi\Psi^\dagger \right\rangle$ is a 2x2-matrix acting in Nambu spinor-space. The partition function now becomes

$$Z = \int \mathcal{D}\left[\Psi^\dagger\right] \mathcal{D}\left[\Psi\right] \mathcal{D}a^\dagger \mathcal{D}a \mathrm{e}^{-\sum_x \frac{1}{V} a^\dagger a - \sum_{x,y} \Psi^\dagger(x)\left[-G^{-1}(x,y)\right]\Psi(x)}$$
$$= \int \mathcal{D}a^\dagger \mathcal{D}a \mathrm{e}^{-\sum_x \frac{1}{V} a^\dagger a + \mathrm{Tr}\ln\left(-G^{-1}\right)}$$
$$= \int \mathcal{D}a^\dagger \mathcal{D}a \mathrm{e}^{S_{eff}(a^\dagger, a)}$$
$$S_{eff} = -\sum_x \frac{1}{V} a^\dagger a + \mathrm{Tr}\ln\left(-G_0^{-1}(x,y) - B(x)\delta_{x,y}\right)$$

This partition function has now been transformed into a pure bosonic problem. Saddle-point approximation to this integral gives mean field theory. Here the trace $\mathrm{Tr} = \sum_x \mathrm{tr}$, where tr is a 2x2-matrix trace.

Mean field theory (MFT): $a(x) \to a$ constant.

$$\mathrm{Tr}\ln\left(-G^{-1}(x,y)\right) = \sum_x \mathrm{tr}\ln\left(-G^{-1}(x,y)\right) = \sum_k \mathrm{tr}\ln\left(-G^{-1}(k)\right)$$

11.1 BCS-theory

$$
\begin{aligned}
Z &= \int \mathcal{D}\varphi^* \mathcal{D}\varphi \mathrm{e}^S \\
S = S_0 + S_I &= -\sum_\lambda \varphi_\lambda^* \frac{\partial \varphi_\lambda}{\partial \tau} + H\left(\varphi_\lambda^*, \varphi_\lambda\right) \\
S_0 &= \sum_{x,y,\sigma} \varphi_\sigma^*(x)\left(\partial_\tau + \varepsilon - \mu\right)\varphi_\sigma(y) \\
H_I &= -V \sum_x n_\uparrow(x) n_\downarrow(x) \qquad V > 0 \\
S_I &= V \sum_x n_\uparrow(x) n_\downarrow(x) \qquad V > 0
\end{aligned}
$$

Attractive interaction for electrons with opposite spin (Retarded).

$$
\begin{aligned}
S_I &= V \sum_x \varphi_\uparrow^*(x)\varphi_\downarrow^*(x)\varphi_\downarrow(x)\varphi_\uparrow(x) \\
\mathrm{e}^{S_I} &= \int \mathcal{D}a^\dagger \mathcal{D}a \mathrm{e}^{-\sum_x \left(\frac{a^\dagger a}{V} - a\varphi_\uparrow^*\varphi_\downarrow^* - a^\dagger \varphi_\downarrow \varphi_\uparrow\right)} \\
\varphi &= \begin{pmatrix} \varphi_\uparrow \\ \varphi_\downarrow^* \end{pmatrix} \qquad \varphi^\dagger = \begin{pmatrix} \varphi_\uparrow^* & \varphi_\downarrow \end{pmatrix} \\
\mathrm{e}^{S_I} &= \int \mathcal{D}a^\dagger \mathcal{D}a \mathrm{e}^{-\sum_x \left(\frac{a^\dagger a}{V} + \sum_x \varphi^\dagger(x) B(x) \varphi(x)\right)}
\end{aligned}
$$

Where $B(x)$ is the same matrix as in the last section.

$$
S_0 = -\sum_{k,\sigma} \int_0^\beta \mathrm{d}\tau \left[\varphi_{k\sigma}^*(\tau)\left(\partial_\tau + \varepsilon_k - \mu\right)\varphi_{k\sigma}(\tau)\right]
$$

where we have done the following partial Fourier transformation

$$
\varphi_\sigma^*(x,\tau) \to \varphi_{k\sigma}^*(\tau).
$$

Now we do the spin summation:

$$
-\sum_k \int_0^\beta \mathrm{d}\tau \left[\varphi_{\uparrow k}^*(\tau)\left(\partial_\tau + \varepsilon_k - \mu\right)\varphi_{\uparrow k}(\tau) + \varphi_{\downarrow k}^*(\tau)\left(\partial_\tau + \varepsilon_k - \mu\right)\varphi_{\downarrow k}(\tau)\right].
$$

Look at the last term:

$$\begin{aligned}
&\sum_k \int_0^\beta \mathrm{d}\tau \left[\varphi_{\downarrow k}^*(\tau)\left(\partial_\tau + \varepsilon_k - \mu\right)\varphi_{\downarrow k}(\tau)\right] \\
&= \sum_k \int_0^\beta \mathrm{d}\tau \left[\varphi_\downarrow{}^*(k)\frac{\partial\varphi_{\downarrow k}}{\partial\tau} + \varphi_{\downarrow k}^*(\tau)\left(\varepsilon_k - \mu\right)\varphi_{\downarrow k}(\tau)\right] \\
&= \sum_k \varphi_{\downarrow k}^*\varphi_{\downarrow k}\Big|_0^\beta + \int_0^\beta \mathrm{d}\tau \left[\varphi_\downarrow(k)\frac{\partial\varphi_{\downarrow k}^*}{\partial\tau} - \varphi_{\downarrow k}(\tau)\left(\varepsilon_k - \mu\right)\varphi_{\downarrow k}^*(\tau)\right] \\
&= \sum_k \int_0^\beta \mathrm{d}\tau \left[\varphi_\downarrow(k)\frac{\partial\varphi_{\downarrow k}^*}{\partial\tau} - \varphi_{\downarrow k}(\tau)\left(\varepsilon_k - \mu\right)\varphi_{\downarrow k}^*(\tau)\right]
\end{aligned}$$

where we have performed a partial integration, which effectively reduced to changing the derivative and sign since the fields are periodic on $[0, \beta]$. This change of sign is cancelled by the anti-commutation of the fermionic fields. The sign of the last term also changed due to interchange of the fields. Fourier transforming back into real space and combining this with the other part of S_0, we get

$$\begin{aligned}
S_0 &= -\sum_{x,y}\left[\varphi_\uparrow^*(x)(\partial_\tau + \varepsilon)\varphi_\uparrow(y) + \varphi_\downarrow(x)(\partial_\tau - \varepsilon)\varphi_\downarrow^*(y)\right] \\
&= -\sum_{x,y}\varphi^\dagger(x)\begin{pmatrix}(\partial_\tau + \varepsilon) & 0\\ 0 & (\partial_\tau - \varepsilon)\end{pmatrix}\varphi(y)
\end{aligned}$$

$$\begin{aligned}
Z &= \int \mathcal{D}\varphi^\dagger\mathcal{D}\varphi\mathcal{D}a^\dagger\mathcal{D}a\mathrm{e}^{-\sum_x \frac{a^\dagger(x)a}{V}}\mathrm{e}^{-\sum_{x,y}\varphi(x)^\dagger G^{-1}(x,y)\varphi(y)} \\
G^{-1}(x,y) &= G_0^{-1}(x,y) - B(x)\delta_{x,y} \\
G_0^{-1}(x,y) &= \begin{pmatrix}(\partial_\tau + \varepsilon) & 0\\ 0 & (\partial_\tau - \varepsilon)\end{pmatrix}
\end{aligned}$$

Now perform the φ integrations:

$$\begin{aligned}
&\int \mathcal{D}a^\dagger\mathcal{D}a\mathrm{e}^{S_{eff}[a,a^\dagger]} \\
S_{eff}[a,a^\dagger] &= -\sum_x \frac{a^\dagger(x)a(x)}{V} + \mathrm{Tr}\ln[G^{-1}],
\end{aligned}$$

which is an exact result! Now we move on to mean field approximation: $a(x) \to a$.

$$\mathrm{Tr}\ln[G^{-1}] = \frac{1}{\beta}\sum_k\sum_{\omega_n}\mathrm{tr}\ln G^{-1}(k,i\omega_n),$$
$$G^{-1}(k,i\omega_n) = \begin{pmatrix} -i\omega_n+\varepsilon_k & -a \\ -a^\dagger & -i\omega_n-\varepsilon_k \end{pmatrix}$$

$$\mathrm{tr}\ln G^{-1} = \ln\det\{G^{-1}\} = \ln\Big((i\omega_n)^2 - \mathrm{e}_k^2 - |a|^2\Big) = \ln(i\omega_n - E_k) + \ln(i\omega_n + E_k)$$
$$\implies S_{eff}^{MF} = -\frac{N\beta|a|^2}{V} + \sum_k \ln\left[(1+\mathrm{e}^{-\beta E_k})(1+\mathrm{e}^{\beta E_k})\right] = -\beta F^{MF}$$
$$\implies f^{MF} = \frac{F^{MF}}{N} = \frac{|a|^2}{V} + \frac{1}{\beta}\frac{1}{N}\sum_k \ln\left[(1+\mathrm{e}^{-\beta E_k})(1+\mathrm{e}^{\beta E_k})\right].$$

Since S_{eff} is exact, we automatically have a recipe for how we can correct mean-field theory, and also a recipe for how to check it's stability.

$$G^{-1}(k) = \begin{pmatrix} -i\omega_n+\varepsilon_k & -a \\ -a^\dagger & -i\omega_n-\varepsilon_k \end{pmatrix}$$
$$\implies G(k) = \frac{-1}{(i\omega_n)^2 - E_k^2}\begin{pmatrix} i\omega_n+\varepsilon_k & a \\ a^\dagger & i\omega_n-\varepsilon_k \end{pmatrix} = \left\langle \Phi\Phi^\dagger \right\rangle$$

where $E_k = \sqrt{\varepsilon_k^2 + |a|^2}$ and we compare with

$$G(k) \to -G_F(k) \implies G_F = -\left\langle \Phi\Phi^\dagger \right\rangle$$

$$\mathrm{tr}\ln\left[-G_f^{-1}(k)\right] = \ln\det(-G_F - 1(k)) = \ln(i\omega_n - E_k) + \ln(i\omega_n + E_k)$$
$$\sum_k \mathrm{tr}\ln\left[-G_f^{-1}(k)\right] = \sum_k \frac{1}{\beta}\sum_{\omega_n}\left[\ln(i\omega_n - E_k) + \ln(i\omega_n + E_k)\right]$$

Earlier we showed that

$$\frac{1}{\beta}\sum_{\omega_n}\ln(i\omega_n - x) = \ln\big(1+\mathrm{e}^{-\beta x}\big)$$
$$\implies \sum_x \mathrm{tr}\ln\big(-G_F^{-1}(k)\big) = \sum_k\left[\ln\big(1+\mathrm{e}^{-\beta E_k}\big) + \ln\big(1+\mathrm{e}^{\beta E_k}\big)\right]$$

$$\sum_x \frac{|a(x)|^2}{V} = \beta N \frac{|a|^2}{V}$$

$$Z_{MF} = \mathrm{e}^{-\beta F_{MF}} = \mathrm{e}^{-\beta N \frac{|a|^2}{V}} \mathrm{e}^{\sum_k \left[\ln\left(1+\mathrm{e}^{-\beta E_k}\right)+\ln\left(1+\mathrm{e}^{\beta E_k}\right)\right]}$$

$$\frac{F_{MF}}{N} = \frac{|a|^2}{V} - \frac{1}{\beta}\frac{1}{N}\sum_k \left[\ln\left(1+\mathrm{e}^{-\beta E_k}\right)+\ln\left(1+\mathrm{e}^{\beta E_k}\right)\right]$$

where a is determined by minimizing the free energy.

$$\frac{\partial}{\partial a} f_{MF} = 0 \implies \frac{2a}{V} - \frac{1}{N}\sum_k \frac{2a}{2E_k}\left(\frac{e^{\beta E_k}}{1+\mathrm{e}^{\beta e_k}} - \frac{e^{-\beta E_k}}{1+\mathrm{e}^{-\beta e_k}}\right) = 0$$

$$2a\left[\frac{1}{V} - \frac{1}{N}\sum_k \frac{1}{2E_k}\left(\frac{e^{\beta E_k}}{1+\mathrm{e}^{\beta e_k}} - \frac{e^{-\beta E_k}}{1+\mathrm{e}^{-\beta e_k}}\right)\right] = 0$$

$$\frac{1}{V} = \frac{1}{N}\sum_k \frac{\tanh\left(\frac{\beta E_k}{2}\right)}{2E_k}$$

This is the gap-equation for BCS-theory! The advantage of solving it this way, is that now we know how to include fluctuations.

To check that this is in fact a minimum, we check the curvature of the free energy at this value a_0

$$\frac{\partial^2 f_{MF}}{\partial a^2} = \frac{\partial}{\partial a} 2a\left[\frac{1}{V} - \frac{1}{N}\sum_k \frac{1}{2E_k}\left(\frac{e^{\beta E_k}}{1+\mathrm{e}^{\beta e_k}} - \frac{e^{-\beta E_k}}{1+\mathrm{e}^{-\beta e_k}}\right)\right]$$

$$= 2\left[\frac{1}{V} - \frac{1}{N}\sum_k \frac{1}{2E_k}\left(\frac{e^{\beta E_k}}{1+\mathrm{e}^{\beta e_k}} - \frac{e^{-\beta E_k}}{1+\mathrm{e}^{-\beta e_k}}\right)\right]$$

$$-2a\frac{1}{N}\sum_k \frac{\partial}{\partial E_k}\left(\frac{1}{2E_k}\tanh\left(\frac{\beta E_k}{2}\right)\right)\frac{\partial E}{\partial a}.$$

By the gap-equation, we see that the first term is 0 at a_0. Taking the derivative of the last term, we end up with

$$\frac{a^2}{N}\sum_k \frac{1}{E_k^3}\frac{1}{\cosh^2(\frac{\beta E_k}{2})}\left(\sinh(\beta E_k) - \beta E_k\right) > 0 \quad \forall \beta E_k.$$

Thus the free energy has a global minimum at $a = a_0$, which means that the solution is unique in the case of contact-interactions.

11.2 Stationary point condition

$$\frac{\partial f^{MF}}{\partial b^2} = 0 \implies -\lambda + \frac{1}{N}\sum_k \frac{\mathrm{e}^{-\beta\varepsilon_k}}{1+\mathrm{e}^{-\beta\varepsilon_k}}\frac{\partial \varepsilon_k}{\partial b^2} = 0$$
$$\frac{\partial f^{MF}}{\partial \lambda} = 0 \implies -1 + b^2 + \frac{1}{N}\sum_k \frac{\mathrm{e}^{-\beta\varepsilon_k}}{1+\mathrm{e}^{-\beta\varepsilon_k}}\frac{\partial \varepsilon_k}{\partial \lambda} = 0.$$

We also have the constraint

$$n = -\frac{\partial f^{MF}}{\partial \mu} = \frac{1}{N}\sum_k f(\varepsilon_k),$$

which is the number of fermion constraint

$$\implies n = 1 - b^2 \implies n + b^2 = 1.$$

Look at the spectrum compared to the free theory

$$\varepsilon_k^{MF} = -2tb^2\gamma_k - (\lambda + \mu)$$
$$\varepsilon_k^{free} = -2t\gamma_k\mu$$

We see that λ renormalizes the chemical potential μ in order for $\langle Q_i \rangle = 1$ to be fulfilled. We also see that b^2 renormalizes the gap-width, correlation effect, $Q_i = n + b^2 = 1$.

Now look at the case $n = 1$, i.e. half-filled band. Thus $b^2 = 0$, and therefore

$$\varepsilon_k = -(\lambda + \mu) = \varepsilon_k$$

The energy spectrum is independent of k! This means that we have localized fermions. No movement, no momentum exitations k. Thus, in mean-field theory, we have an insulator at $U = \infty$ half-filled band. Mean field theory also predict that $b^2 > 0; n < 1$, i.e. that when the system is doped away from half-filled band. In this case, still using mean field theory, we get a metal. Thus by doping the system away from half-filled bands, we go from an insulator to a metal. Near half-filled band, the gap is very small, i.e. that the quasiparticels are effectively very massive

$$m^* \sim \frac{1}{b^2} \qquad b \to 0 \implies m^* \to \infty$$

Preciely at half-filled band, the model is a very simple insulator. It reduces to the Heisenberg model

$$H = -J\sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j \qquad J \sim \frac{t^2}{U} \to 0 \quad ; \quad U \to \infty$$

$$S_{eff} = -\sum_i \int_0 \beta \mathrm{d}\tau b_i^\dagger(\partial_\tau + i\lambda_i)b_i + i\sum_i \int_0 \beta\lambda_i(\tau) + \mathrm{Tr}\ln\big(G^{-1}\big)$$

$$S_{eff}^{MF} = -N\beta(b^2-1)\lambda\sum_k \ln\big(1+\mathrm{e}^{-\beta\varepsilon_k}\big)$$

$$\varepsilon_k = -2tb^2\gamma_k - (\lambda+\mu)$$

Again, the exact expression makes it possible to do corrections to mean field theory. We may come back to this later.

In this saddle point approximation, we have $\langle b\rangle \neq 0$. Look at the Hamiltonian

$$H = -\sum_{i,j,\sigma} t_{ij} d_{i\sigma}^\dagger b_i b_j^\dagger d_{j\sigma}.$$

We see that the following symmetry isn't broken

$$b_i \to b_i \mathrm{e}^{i\theta}$$
$$d_i \to d_i \mathrm{e}^{i\theta}$$

since the creation operators $b^\dagger, d^\dagger$ cancel the phase-factor, which again keeps the Hamiltonian invariant. Thus the Hamiltonian is still invariant under global $U(1)$ transformations, even tho $\langle b\rangle \neq 0$. On the other hand, by introducing the bosons $b^\dagger, b$, the symmetry has improved to a local $U(1)$ symmetry

$$b_i \to b_i \mathrm{e}^{i\varphi_i}$$
$$d_i \to d_i \mathrm{e}^{i\varphi_i}.$$

It is this symmetry which is broken at the saddle-point, because then the boson-fields have acquired a finite expectation value $\langle b\rangle \neq 0$. If the local $U(1)$ symmetry had not been broken, the expectation value would have vanished due to the fluctuations associated with the symmetry. Again $\langle b\rangle$ can be interpreted as a order parameters, but for what? To answer this, we look at the spectrum, similar to what we did in the superconductor case

$$\varepsilon_k = -2tb^2\gamma_k - (\lambda+\mu).$$

When $b \neq 0$, we have dispersion, but when $b = 0$, ε_k is independent of k. Localized quasiparticles in the system implies that the system is an insulator. b is therefore an order parameter for metal.

Equivalently: The local $U(1)$ invariance means that we have conservation of particle number at each site i. This means that the particles in the system are confined/localized. If we again look at the original Hamiltonian

$$H = -t \sum_{\langle i,j \rangle} c^\dagger_{i\sigma} c_{j\sigma} - \mu \sum_{i,\sigma} c^\dagger_{i\sigma} c_{i\sigma},$$

we see that as long as we have hopping t, there are no local $U(1)$ invariance. As long as the fermions are moving, this symmetry is broken. If however the hopping isn't operative, which implies localized fermions, the system has local $U(1)$. Again we reach the conclusion that if the local $U(1)$ symmetry is broken, the number of localized fermions is not conserved, which means that they are mobile, i.e. metallic system. $\langle b \rangle \neq 0 \implies$ broken local $U(1)$ invariance $\implies \langle b \rangle$ order parameter for metal.

Generally, the conductivity of a translationally invariant system is of the form

$$\sigma(\omega) = D\delta(\omega) + \sigma_{reg}(\omega).$$

Thus a translationally invariant system has infinite d.c. conductivity. D is often called the rigid conductivity, or the Drude-weight. In our model, $D \sim b^2$. Many years ago, Walter Kohn suggested using D as the order parameter for a metallic system (non-zero drude weight). Our example above show that this wasn't a bad suggestion.

The problem of describing an insulator-metal phase transitions is a notoriously hard problem. The fact that we find this using this very simple approximation really show the potential of the functional integral formalism, especially in strongly correlated systems. Free theory with half-filled band is a good metal, not an insulator. It would have been hopeless to find this transitions using perturbation theory, similarly for the metal-superconductor phase transition. Note that this mean field theory predict that, even for $U \to \infty$, the Hubbard model is always a Fermi fluid away from half-filled band. In one dimention, we know this is wrong, since every interacting one-dimensional system is a Luttinger fluid. This is a quantum fluid without low-energy one-particle exitations. In one dimention, interactions are always effective, because of the restriction of the kinematics. Particles cannot pass each other without colliding in one-dimention, in contrast to higher dimensional systems, where Fermi fluids are possible.

In three dimension, our mean field theory should be qualitatively correct. In two-dimension, there are indications that strongly correlated systems can have non-fermi fluid behaviour, so mean field theory is not the end of the story. We might later on look at what happens when we turn on fluctuations in this model. Then the quasiparticles starts interacting with the fermions we found using mean field theory. The result is: superconductivity!

12 Broken continuous symmetries and Goldstone-modes

Both of the previous examples, the BCS- and Hubbard-model, have shown that a system where the Hamiltonian is invariant under a continuous symmetry group ($U(1)$ in both cases), the ground state, which the system chooses, doesn't need to respect the symmetry. This are examples of broken symmetries, and because the system "brakes it on its own", we say that the systems have spontaneously broken (continuous) symmetries. In the following, we will examine an important consequence of these broken symmetries. Note that this does not apply to discrete symmetries, like e.g. Ising-model.

BCS-model:

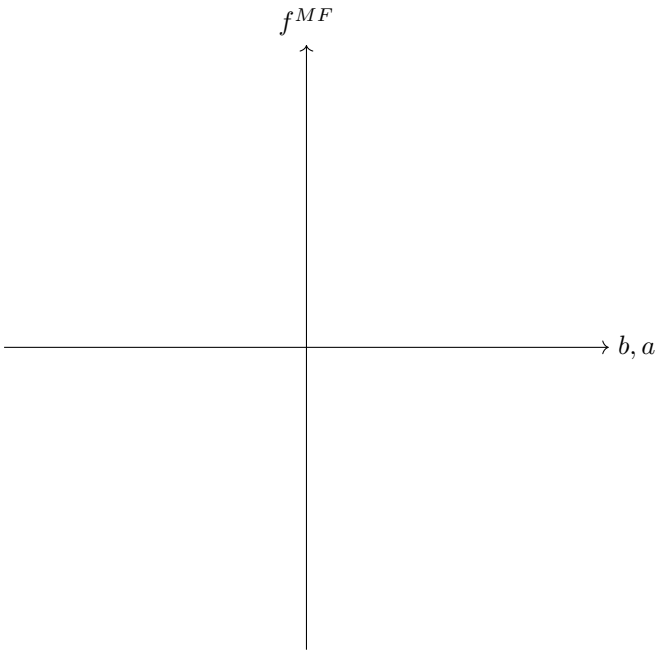
$$f^{MF}(a^\dagger, a) = f(|a|^2) \quad \left\langle a^\dagger \right\rangle \neq 0 \neq \langle a \rangle .$$

$U = \infty$ Hubbard model:

$$f^{MF}(b^\dagger, d) = f(|b|^2)$$

$$|\Delta| = |a|, |b|.$$

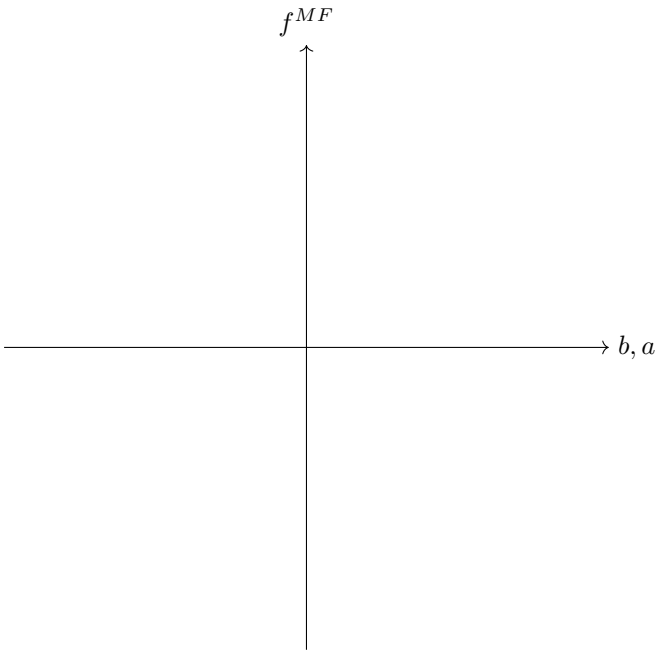
$$|\Delta| \neq 0 :$$



Here we see that there is two global minima of f^{MF} for non-zero Δ's. These are both stable.

$$\frac{\partial f^{MF}(\Delta^2)}{\partial \Delta} = 2\Delta f^{'}(\Delta^2)$$

$$|\Delta| = 0 :$$



Here we see that f^{MF} has one global minima at $\Delta = 0$. This minima is also stable.

We have seen that generally $\langle a \rangle$ and $\langle b \rangle$ are complex order parameters. We can therefore treat f^{MF} as a function of a complex variable, while it is independent of the phase of the complex number. In the case of $|\Delta| = 0$, the phase is ill-defined at f^{MF}_{min}. In the case of $|\Delta| \neq 0$, the situation is a little bit different. Then we can rotate the corresponding graph around the y-axis (f^{MF}), and we obtain the following kind of graph

We see that the minima of the free energy is infinetly degenerate, because it is independent of the phase φ:

$$f^{MF}(\Delta, \Delta^*) = f^{MF}(|\Delta|, \varphi) = f^{MF}(|\Delta|)$$
$$\Delta = |\Delta| \mathrm{e}^{i\varphi}.$$

This means that phase fluctuations cost no energy, but fluctuations in the radial $|\Delta|$ direction does.

$|\Delta|$-amplitude fluctuations: Longitudinal fluctuations.

φ-fluctuations: Transverse fluctuations.

We say that the longitudinal fluctuations are "massive" and the traversal fluctuations are "massless". The massless fluctuations correspond to Goldstone-modes, which has a finite interaction range. We have seen that a broken symmetry ($\Delta \neq 0$) means that there exist Goldstone-modes.

In our case, the order parameter where comples, which means that it has two real components. Here we got one infinite degeneracy in the phase, which corresponded to one Goldstone mode. Generally in our study, if Δ has n components, we get $n-1$ Golstone-modes.

The existence of the Goldstone-modes makes it apparently problematic to define a fluctuation-calculation around the stationary point, since the Goldstone-modes corresponds to (at least one) zero eigenvalue of the fluctuation propagators.

$$S = S^{MF} + \operatorname{Tr} \ln D^{-1}$$
$$Z = \mathrm{e}^{S^{MF}} \frac{1}{\det D^{-1}}$$
$$D^{-1} = \prod_i \lambda_i \qquad \exists j : \lambda_j = 0$$

In order to investigate small fluctuations around a mean-field theory, it is of course intolerable to have this problem. It turns out that this is an apparent problem which we can avoid, as we will see.

We will look at Gaussian fluctuations around a spontaneously broken continuous symmetry. The following effective action isn't approximated, but we will for the sake of the argument and simplicity look at a real field with real rotational invariance (e.g. XY-model, where the spins can point in any direction in the plane). I emphasise however that the discussion is general.

$$Z = \int \mathcal{D}\varphi \mathrm{e}^{S[\varphi]}$$
$$\frac{\delta S}{\delta \varphi} = 0 \qquad \varphi = \varphi_0$$

where φ is a function of $x = (\vec{x_0}, \tau)$. φ_0 contains a parameter θ which describe the symmetry-transformation of the symmetry that is spontaneously broken. It can e.g. be the parameter describing the ground state degeneracy ("circular minimum") in the rotated graph of f^{Mf} above. We expand to gaussian order in S:

$$Z = \mathrm{e}^{S^{MF}} \int \mathcal{D}\varphi \mathrm{e}^{-\frac{1}{2}\sum_{x,y}(\varphi(x)-\varphi_0(x))A(\varphi(y)-\varphi_0(y))}$$
$$A = \frac{\delta^2 S}{\delta\varphi_0(x)\delta\varphi_0(y)}$$

Naively, this will be something like

$$Z = \mathrm{e}^{S^{MF}} \frac{1}{\sqrt{\det A}}$$

but because of the Goldstone-modes, there is an apparent divergence in the fluctuations due to the zero eigenvalue. It seems like any attempt at doing mean-field theory when the symmetry is broken is doomed to fail. Nevertheless, we know that e.g. the mean-field theory of BCS-theory is a very good approximation without any divergences. There must be a reason for why this is the case.

In order to avoid such divergences, the idea is to split the fluctuations into longitudinal- and transverse components. Recall that the longitudinal components are the "massless" components, which are associated to the degeneracy of the ground state, and the transverse are the "massive" components associated to the fluctuations in the radial, or amplidude, direction. The functional derivative

$$A = \frac{\delta^2 S}{\delta\varphi_0(x)\delta\varphi_0(y)}$$

must be diagonalized in order to find the fluctuation corrections. The problem is, however, that the presence of zero eigenvalues makes this impossible. The corresponding eigenvectors of these eigenvalues, namely the Goldstone-modes, are the components of the fluctuation vector $\varphi(x) - \varphi_0(x,\theta)$ with zero eigenvalue.

$$\begin{aligned} A \cdot x &= \lambda x \\ A \cdot x_G &= 0 \\ A \cdot x_\perp &\neq 0 \\ x_\perp \cdot x_G &= 0 \end{aligned}$$

Define the "inner-probduct"

$$\int \mathrm{d}x(\varphi(x) - \varphi_0(x))_\perp(\varphi(x) - \varphi_0(x))_G$$

At the stationary point, we have (independent of the value of θ)

$$\begin{aligned} \frac{\delta S}{\delta\varphi_0(x,\theta)} = 0 \implies \frac{\partial}{\partial\theta}\left(\frac{\delta S}{\delta\varphi_0(x,\theta)}\right) = 0 \implies \int \mathrm{d}y \frac{\delta^2 S}{\delta\varphi_0(x)\delta\varphi_0(y)} \frac{\partial\varphi_0(y,\theta)}{\partial\theta} \\ = \int \mathrm{d}y A(x,y) \frac{\partial\varphi_0(y,\theta)}{\partial\theta} = A \cdot \frac{\partial\varphi_0(y,\theta)}{\partial\theta} = 0 \implies \frac{\partial\varphi_0(y,\theta)}{\partial\theta} = x_G \end{aligned}$$

where we have identified the explicit form of the Goldstone-mode. The next step is to split up the fluctuations into the Goldstone-mode and components "vertical" to this. We do this by using the inner-product as a projection, defining

$$f(\theta) = \int \mathrm{d}x \frac{\partial \varphi_0(y,\theta)}{\partial \theta}[-\varphi(x) + \varphi_0(x)].$$

the components of $[-\varphi(x)+\varphi_0(x)]$ orthogonal to the Goldstone-mode $\frac{\partial \varphi_0(y,\theta)}{\partial \theta}$, the verical components, are therefore the once corresponding to $f(\theta) = 0$. We can therefore write:

$$\varphi(x) - \varphi_0(x,\theta) = \begin{pmatrix} \frac{\partial \varphi_0(y,\theta)}{\partial \theta} \\ (\varphi(x) - \varphi_0(x,\theta))_\perp \end{pmatrix}$$

using this notation, we can write

$$(\varphi(x) - \varphi_0(x))A(x,y)(\varphi(y) - \varphi_0(y))$$
$$= \begin{pmatrix} \frac{\partial \varphi_0(y,\theta)}{\partial \theta} & (\varphi(x) - \varphi_0(x,\theta))_\perp \end{pmatrix} \begin{pmatrix} A_G & 0 \\ 0 & A_\perp \end{pmatrix} \begin{pmatrix} \frac{\partial \varphi_0(y,\theta)}{\partial \theta} \\ (\varphi(x) - \varphi_0(x,\theta))_\perp \end{pmatrix}$$

The problem now amounts to $A_G = 0$.

$$\det A = \det A_G \det A_\perp = 0$$

$A_G = 0$ because the energies associated with the quadratic Goldstone-mode fluctuations is zero. The trick now is to define $A_G = \varepsilon$ (one Goldstone-mode), such that the determinant $\det A = \varepsilon \det A_\perp \neq 0$. After the gaussian integrations have been done, ε is set to zero. Do we get something finite?

We wish to split the functional integral into two contributions, one over Goldstone-modes, $f = 1$, and one over longitudinal modes, $f = 0$.

$$\int \mathrm{d}f \delta(f) = 1$$
$$\int \mathrm{d}\theta \frac{\mathrm{d}f}{\mathrm{d}\theta} \delta(f) = 1$$

The point here is: the delta function $\delta(f)$ only contributes when $f = 0$.

$$Z = \mathrm{e}^{S_{MF}} \int \mathcal{D}\psi \mathrm{e}^{-\frac{1}{2}\sum_{x,y}\psi(x)A\psi(y)}$$

General fluctuations vector

$$\psi = \phi(x) - \phi_0(x,\theta) = 1Z = Z = \mathrm{e}^{S_{MF}} \int \mathcal{D}\psi \int \mathrm{d}\theta \frac{\mathrm{d}f}{\mathrm{d}\theta} \delta(f) \mathrm{e}^{-\frac{1}{2}\sum_{x,y}\psi(x)A\psi(y)}$$

Look at the two extra factors in the integral:

$$\begin{aligned} f'(\theta) &= \frac{\mathrm{d}}{\mathrm{d}\theta} \int \mathrm{d}x \frac{\partial \phi_0}{\partial \theta} \left[-\phi(x) + \phi_0(x,\theta)\right] \\ &= \int \mathrm{d}x \left[-\frac{\partial^2 \phi_0}{\partial \theta^2}\psi + \left(\frac{\partial \phi_0}{\partial \theta}\right)^2 \right] \\ \delta(f) &= \int \frac{\mathrm{d}\alpha}{2\pi} \mathrm{e}^{i\alpha f} \end{aligned}$$

where the α-integration projects out the Goldstone-mode contribution to the fluctuations. This procedure is very similar to Abrikosov's trick.

$$\begin{aligned} Z &= Z_{MF} \int \mathcal{D}\psi \mathrm{d}\theta \frac{\mathrm{d}\alpha}{2\pi} \int \mathrm{d}x \left[-\frac{\partial^2 \phi_0}{\partial \theta^2}\psi + \left(\frac{\partial \phi_0}{\partial \theta}\right)^2 \right] \mathrm{e}^S \\ S &= -\frac{1}{2}\sum_{x,y}\psi(x)A(x,y)\psi(y) + i\alpha \sum_x \frac{\partial \phi_0(x,\theta)}{\partial \theta}\psi(x). \end{aligned}$$

The first term in the x-integral is zero, since it is linear in the ψ-fields. The ψ-integral can be solved exactly

$$\begin{aligned} &\int \mathcal{D}\psi \mathrm{e}^{-\frac{1}{2}\sum_{x,y}\psi(x)A(x,y)\psi(y) + i\alpha \sum_x \frac{\partial \phi_0(x,\theta)}{\partial \theta}\psi(x)} \\ &\qquad = \frac{1}{\sqrt{\det A}} \mathrm{e}^{-\frac{\alpha^2}{2}\sum_{x,y}\frac{\partial \phi_0(x)}{\partial \theta}A^{-1}\frac{\partial \phi_0(y)}{\partial \theta}}. \end{aligned}$$

The partition then becomes

$$Z = Z_{MF} \frac{1}{\sqrt{\det A}} \int \mathrm{d}\theta \frac{\mathrm{d}\alpha}{2\pi} \int \mathrm{d}x \left[\left(\frac{\partial \phi_0}{\partial \theta}\right)^2 \right] \mathrm{e}^{-\frac{\alpha^2}{2}\sum_{x,y}\frac{\partial \phi_0(x)}{\partial \theta}A^{-1}\frac{\partial \phi_0(y)}{\partial \theta}}.$$

Now the α integration is Gaussian! We proceed looking at the exponent:

$$\begin{aligned} &\sum_{x,y} \frac{\partial \phi_0(x)}{\partial \theta} A^{-1}(x,y) \frac{\partial \phi_0(y)}{\partial \theta} \\ &\qquad A = \begin{pmatrix} \varepsilon & 0 \\ 0 & A_\perp \end{pmatrix} \end{aligned}$$

where we have introduced $\varepsilon \neq 0$ as an eigenvalue for the Goldstone-mode.

$$\begin{aligned}
\sum_y A(x,y)\frac{\partial \varphi_o(y)}{\partial \theta} &= \varepsilon \frac{\partial \varphi_o(x)}{\partial \theta} \\
\Longrightarrow \sum_{x,y} \frac{\partial \phi_0(x)}{\partial \theta} A^{-1}(x,y) \frac{\partial \phi_0(y)}{\partial \theta} & \\
= \sum_{x,y,y'} \frac{\partial \phi_0(x)}{\partial \theta} A^{-1}(x,y) \frac{A(y,y')}{\varepsilon} \frac{\partial \varphi_0(y')}{\partial \theta} & \\
\sum_y A^-1(x,y)A(y,y') &= \frac{1}{\varepsilon}\delta_{x,y'} \\
\Longrightarrow \sum_{x,y,y'} \frac{\partial \phi_0(x)}{\partial \theta} A^{-1}(x,y) \frac{A(y,y')}{\varepsilon} \frac{\partial \varphi_0(y')}{\partial \theta} & \\
= \sum_{x,y'} \frac{1}{\varepsilon} \frac{\partial \phi_0(x)}{\partial \theta} \frac{\partial \phi_0(y')}{\partial \theta} \delta_{x,y'} & \\
= \frac{1}{\varepsilon} \sum_x \left(\frac{\partial \phi_0(x)}{\partial \theta} \right)^2 = \frac{1}{\varepsilon} g(\theta)^2 &
\end{aligned}$$

were we have identified $g(\theta)$, which is equal to the factor in the x-integral. The α-integral becomes

$$\int \frac{\mathrm{d}\alpha}{2\pi} \mathrm{e}^{-\frac{\alpha^2}{2}\frac{g(\theta)}{\varepsilon}} = \frac{1}{2\pi}\sqrt{\frac{2\pi\varepsilon}{g(\theta)}} = \frac{1}{\sqrt{2\pi}}\sqrt{\frac{\varepsilon}{g(\theta)}}.$$

Recall that the α-integration projects out the goldstone mode ($f = 1$). We have integrated out the effect of the Goldstone mode and obtained an effective theory given by Z.

$$\begin{aligned}
Z &= Z_{MF} \int \frac{\mathrm{d}\theta}{\sqrt{2\pi}} g(\theta) \sqrt{\frac{\varepsilon}{g(\theta)}} \frac{1}{\sqrt{\det A}} \\
&= Z_{MF} \int \frac{\mathrm{d}\theta}{\sqrt{2\pi}} \sqrt{g(\theta)} \sqrt{\frac{\varepsilon}{\varepsilon \det A_\perp}} \\
= Z_{MF} \frac{1}{\sqrt{\det A_\perp}} \left\{ \int \frac{\mathrm{d}\theta}{\sqrt{2\pi}} \sqrt{g(\theta)} \right\} &= Z_{MF} \frac{1}{\sqrt{\det A_\perp}} Z_{GM}
\end{aligned}$$

which becomes finite in the limit $\varepsilon \to 0$. The factor Z_{GM} contains all effects of the Goldstone-mode and $\det A_\perp \neq 0$, which corresponds to the trace of massive fluctuations of the theory. We expect that the dominant fluctuations are the transverse fluctuations, since they don't alter the expectation value of the fields a, b.

If we had done a similar analysis in the case of complex fields

$$Z = Z_{MF} \int \mathcal{D}\varphi^* \mathcal{D}\varphi \mathrm{e}^{-\sum_{x,y} \varphi^*(x) A(x,y) \varphi(y)}$$

we would have ended up with

$$Z = Z_{MF} \frac{1}{\det A_\perp} \int \frac{\mathrm{d}\theta}{\sqrt{2\pi}} \sqrt{g(\theta)}$$
$$g(\theta) = \int \mathrm{d}x \left| \frac{\partial \varphi_0(x)}{\partial \theta} \right|^2$$

12.1 Goldstone mode contributions to fluctuations in the BCS-model

Fluctuation vectors and A (which is hard to calculate)

$$\varphi^\dagger = \begin{pmatrix} a^\dagger & a \end{pmatrix} \qquad \varphi = \begin{pmatrix} a \\ a^\dagger \end{pmatrix}$$
$$A = D^{-1}$$
$$\varphi_0(x,\theta) = \varphi_0(\theta) = |a| \mathrm{e}^{i\theta} \implies \frac{\partial \varphi_0}{\partial \theta} = i\varphi_0$$
$$\left| \frac{\partial \varphi_0}{\partial \theta} \right|^2 = |a|^2$$
$$g(\theta) = \int \mathrm{d}x |a|^2 = \sum_x \int_0^\beta \mathrm{d}\tau |a|^2 = N\beta |a|^2$$

where N is the volume of the system.

$$\int_0^{2\pi} \mathrm{d}\theta \sqrt{\frac{g(\theta)}{2\pi}} = \sqrt{2\pi}\sqrt{\beta N}|a| = \sqrt{2\pi\beta N}|a|$$
$$S = S_{MF} - \mathrm{Tr} \ln\left(D_\perp^{-1}\right) + \ln\left(\sqrt{2\pi\beta N}|a|\right).$$

If we neglect the contribution from D, we can easily calculate the corrected amplitude $|a|$. Note that this is a phase-fluctuation giving contributions to the amplitude fluctuations (explain!). Note also that the Goldstone mode contribution to the fluctuations doesn't contain any information about A, only information about the eigenvectors with eigenvalue zero. This is because the information disappears in the expression

$$\sum_{x,y} \frac{\partial \varphi_0(x)}{\partial \theta} A(x,y) \frac{\partial \varphi_0(y)}{\partial \theta} = 0.$$

13 An introduction to Fermi liquid theory

A free electron gas has the following Hamiltonian

$$H = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma}$$

with $T = 0$ single-particle propagator

$$\begin{aligned} G_0(k,\omega) &= F[G_0(x,t)] \\ G_0(x,t) &= -i\left\langle T(\psi_\sigma(x,t)\psi^\dagger_\sigma(0,0))\right\rangle \\ G_0(k,\omega) = \frac{\Theta(\varepsilon_k - \varepsilon_F)}{\omega - \varepsilon_k + i\delta} + \frac{\Theta(\varepsilon_F - \varepsilon_k)}{\omega - \varepsilon_k - i\delta} &= \frac{1}{\omega - \varepsilon_k + i\delta_k} \\ \delta_k = \delta\text{sign}(\varepsilon_k - \varepsilon_F) \quad \delta = 0^+. & \end{aligned}$$

$G(k,\omega)$ has a singular pole which gives the excitation spectrum of the system. The fact that the pole is singular means that the single-particle excitations, described by the operators $c^\dagger_{k\sigma}, c_{k\sigma}$, are well-defined with lifetime $\tau_k = \frac{1}{2\delta_k} \to \infty$, i.e. long-lived exitations. If we include interactions between the Fermions, we can write the following exact expression for the full single-particle propagator (Dyson equation):

$$G^{-1}(k,\omega) = G_0^{-1}(k,\omega) - \Sigma(k,\omega).$$

All effects from the interactions are included in Σ, which is often called the self-energy. The question is: when can we write $G(k,\omega)$ on the same form as $G_0(k,\omega)$? This question is equivalent to: when does an interacting fermionic system look like a free electron system?

Assum that we can write Σ like

$$\Sigma = \Sigma_R + i\Sigma_I \qquad \Sigma_I \ll \Sigma_R.$$

This assumption means that the damping of the single-particle exitations isn't to big. The pole in the full-propagator $G(k,\omega)$ are now given by

$$\omega - \varepsilon_k - \Sigma_R - i\Sigma_I = 0.$$

To 0'th order, we get

$$\begin{aligned} \omega &= \varepsilon_k + \Sigma_R(k,\omega) \\ \varepsilon^*_k &= \varepsilon_k + \Sigma_R(k,\varepsilon^*_k). \end{aligned}$$

This corresponds to a shift of the real pole given by ε_k^*, which is the solution of the self-consisting equation below. Now we include Σ_I to first order.

$$\omega - (\varepsilon_k + \Sigma_R(k,\omega)) - i\Sigma_I(k,\varepsilon_k^*) = 0$$

$$\Sigma_R(k,\omega) = \Sigma_R(k,\varepsilon_k^*) + (\omega - \varepsilon_k^*)\left.\frac{\partial \Sigma_R}{\partial \omega}\right|_{\omega=\varepsilon_k^*}$$

$$\omega \to \varepsilon_k^* + ix$$

$$\varepsilon_k^* + ix - (\varepsilon_k + \Sigma_R(k,\varepsilon_k^*)) - (\varepsilon_k^* + ix - \varepsilon_k^*)\left.\frac{\partial \Sigma_R}{\partial \omega}\right|_{\omega=\varepsilon_k^*} - i\Sigma_I = 0$$

$$ix\left(1 - \left.\frac{\partial \Sigma_R}{\partial \omega}\right|_{\omega=\varepsilon_k^*}\right) = i\Sigma_I \qquad x = \frac{\Sigma_I}{1 - \left.\frac{\partial \Sigma_R}{\partial \omega}\right|_{\omega=\varepsilon_k^*}} \equiv \frac{\Sigma_I}{1 - \frac{\partial \Sigma_R}{\partial \omega}}$$

$$\omega = \varepsilon_k^* + i\frac{\Sigma_I}{1 - \frac{\partial \Sigma_R}{\partial \omega}} = \varepsilon_k^* + i\frac{1}{2\tau_k}$$

$$G = \frac{1}{\omega - \varepsilon_k^* - (\omega - \varepsilon_k^*)\frac{\partial \Sigma_R}{\partial \omega} - i\Sigma_I}$$

$$= \frac{1}{\omega(1 - \frac{\partial \Sigma_R}{\partial \omega}) - \varepsilon_k^*(1 - \frac{\partial \Sigma_R}{\partial \omega}) - i\Sigma_I}$$

$$= \frac{Z_k}{\omega - \varepsilon_k^* + i\frac{1}{2\tau_k}}$$

where $Z_k = \frac{1}{1 - \frac{\partial \Sigma_R}{\partial \omega}}$ is the quasi-particle residue and $\frac{1}{2\tau_k} = \frac{-\Sigma_I}{1 - \frac{\partial \Sigma_R}{\partial \omega}}$. Remember that

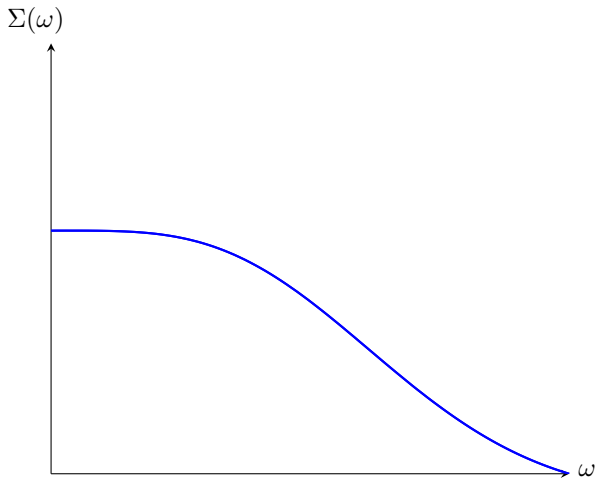
$$G_0(k,\omega) = \frac{1}{\omega - \varepsilon_k + i\delta_k}.$$

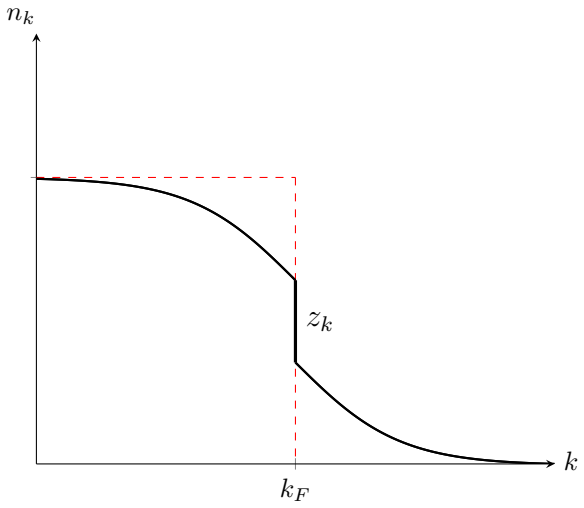
From this, one can deduce the effects of interactions. First of all, we have the relative shift of the spectrum given by the self-consistent equation $\varepsilon_k \to \varepsilon_k^* = \varepsilon_k + \Sigma_R(k,\varepsilon_k^*)$. We also have the lifetime τ_k of the excitation given by $\delta_k = \frac{1}{2\tau_k}$. In the non-interacting case the lifetime is infinite, but when one turns on interactions, it becomes finite. Lastly, we have that the pole-residue Z_k deviates from the value $Z_k = 1$. Typically, we have

where $\frac{\partial \Sigma}{\partial \omega} < 0 \implies \frac{1}{1 - \frac{\partial \Sigma}{\partial \omega}} < 1$.

In general, we say that if $Z_k \neq 0$, the system is a Fermi liquid.

If we start out with non-interacting electron gas, H_0, and turn on interactions, there will be a one-to-one correspondence between low-energy excitation's in H_0 and the low-energy excitation's in interacting case. By low-energy excitation's we mean around the Fermi-level, where the excitation energy is far less


$\Sigma(\omega)$
ω


n_k
z_k
k
k_F

than the Fermi-energy, ε_F. In a typical Fermi-liquid, we have

$$\Sigma_I \sim (\omega - \varepsilon_F)^2$$

which means that at $\omega \to \varepsilon_F$, the damping of the one-particle excitation's goes down quicker than $\omega - \varepsilon_F$. These excitation's therefore become well defined at Fermi-level, as appose to far away from the Fermi-level, where the damping is significant. Fermi-liquid: $Z_{k=k_F} \neq 0$.

14 General discussion on broken symmetries

A symmetry of a system described by a Lagrange density, $\mathcal{L}(\{\varphi_\lambda^*, \varphi_\lambda\})$, is defined as follows: Let T_λ be a transformation that acts on the fields, either in field-space or its spacetime coordinates

$$T_\lambda \varphi_\lambda = \varphi_\lambda^{'}$$
$$T_\lambda \varphi_\lambda^* = \varphi_\lambda^{'*}.$$

Then T_λ is a symmetry if it leaves the Lagrangian invariant, i.e.

$$\mathcal{L}(\{T_\lambda \varphi_\lambda^*, T_\lambda \varphi_\lambda\}) = \mathcal{L}(\{\varphi_\lambda^{*'}, \varphi_\lambda'\}) = \mathcal{L}(\{\varphi_\lambda^*, \varphi_\lambda\}).$$

This means that the equations of motion, given by the solutions of the Euler-Lagranges equation of the classical fields $\varphi_\lambda^*, \varphi_\lambda$, are not altered by the transformation T_λ. The transformation maps the solutions onto new solutions of the field equation.

Now that we have defined a symmetry, we can formulate Noether's theorem: for every continuous symmetry of the system, there is a corresponding conserved quantity. We divide these symmetries into two categories. First of all, we have spacetime symmetries. If a system is invariant under time-translation, the energy of the system is conserved. If a system is invariant under space-translations, the momentum is conserved. If a system is invariant under rotations, angular momentum is conserved. Then we have internal symmetries. These are symmetries of field-space, like e.g. $\varphi \to \mathrm{e}^{i\theta}\varphi$ which corresponds to conservation of electric charge.

These conserved quantities are directly related to a corresponding conserved current, like e.g. charge and electric current, energy and energy-flow, etc. If the symmetry is broken, the current is no longer conserved.

Say that we have a set of transformations

$$T_\eta \varphi_\lambda(x) \to \varphi^{'}(x;\eta)$$
$$\varphi^{'}_\lambda(x;0) = \varphi_\lambda(x).$$

Define

$$Q_\lambda(x) = \frac{\mathrm{d}}{\mathrm{d}\eta}\, \varphi_\lambda(x;\eta)\Big|_{\eta=0},$$

which can be compensated by a change of coordinates

$$x_\mu \to x_\mu(x;\eta)$$
$$\frac{\mathrm{d}}{\mathrm{d}\eta}\, x^{'}_\mu(x;\eta)\Big|_{\eta=0} \equiv R_\mu.$$

Then the system has the following conserved current

$$\partial_\mu J^\mu = 0; J^\mu = \prod_\lambda Q_\lambda(x^\mu) - R^\mu \mathcal{L}$$

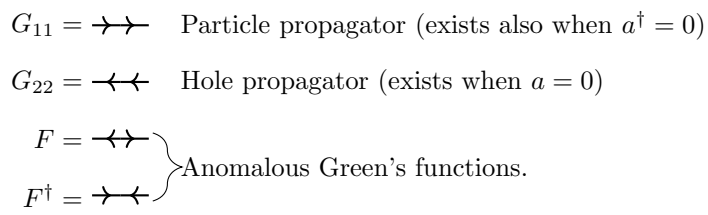


Figure 6: Propagators of the system

15 Mean field Green's function

Physical interpretation if the saddle point.

$$\psi = \begin{pmatrix} \varphi_\uparrow \\ \varphi_\downarrow^\dagger \end{pmatrix} \qquad \psi^\dagger = \begin{pmatrix} \varphi_\uparrow^\dagger & \varphi_\downarrow \end{pmatrix} \tag{15.1}$$

Green's function

$$\begin{aligned} \mathcal{G}_F &= -\left\langle \psi\psi^\dagger \right\rangle \\ &= -\left\langle \begin{pmatrix} \varphi_\uparrow \\ \varphi_\downarrow^\dagger \end{pmatrix} \begin{pmatrix} \varphi_\uparrow^\dagger & \varphi_\downarrow \end{pmatrix} \right\rangle \\ &= \begin{pmatrix} -\left\langle \varphi_\uparrow \varphi_\uparrow^\dagger \right\rangle & -\left\langle \varphi_\uparrow \varphi_\downarrow \right\rangle \\ -\left\langle \varphi_\downarrow^\dagger \varphi_\uparrow^\dagger \right\rangle & -\left\langle \varphi_\downarrow^\dagger \varphi_\downarrow \right\rangle \end{pmatrix} \\ \mathcal{G}_F(k) &= \begin{pmatrix} G_{11}(k) & F(k) \\ F^\dagger(k) & G_{22}(k) \end{pmatrix} \\ &= \frac{1}{(i\omega_n)^2 - \varepsilon_k^2} \cdot \begin{pmatrix} i\omega_n + \varepsilon_k & a \\ a^\dagger & i\omega_n - \varepsilon_k \end{pmatrix} \end{aligned}$$

The Green's function of the fermionic system in the presence of a static boson field that creates and annihilates electron pairs. In absence ($a = a^\dagger = 0$):

$$\mathcal{G}_F(\mathbf{k}, i\omega_n) = \begin{pmatrix} \frac{1}{i\omega_n - \varepsilon_k} & 0 \\ 0 & \frac{1}{i\omega_n + \varepsilon_k} \end{pmatrix} \tag{15.2}$$

$$= \begin{pmatrix} G_{11} & 0 \\ 0 & G_{22} \end{pmatrix} \tag{15.3}$$

With the particle propagator G_{11} and hole propagator G_{22} which is as for a free electron gas. See Figure 6. $F \sim a, F^\dagger \sim a^\dagger$. These two functions do not exist in the normal state, since $a = a^\dagger = 0$ in this state. Now, we are able to interpret what it means to have $a \neq 0, a^\dagger \neq 0$. Notice that

$$\begin{aligned} \langle \varphi_\downarrow \varphi_\uparrow \rangle &\sim a \\ \left\langle \varphi_\uparrow^\dagger \varphi_\downarrow^\dagger \right\rangle &\sim a^\dagger \end{aligned} \tag{15.4}$$

NB! Remember: when we Hubbard-Stratonovich decoupled S_I, we used the terms $a^\dagger\varphi_\downarrow\varphi_\uparrow$ and $a\varphi_\uparrow^\dagger\varphi_\downarrow^\dagger$. a, $a^\dagger$ are pair field that are conjugated to the order parameters $\langle\varphi_\downarrow\varphi_\uparrow\rangle$ and $\left\langle\varphi_\uparrow^\dagger\varphi_\downarrow^\dagger\right\rangle$, analog to the case of a spin system in an external magnetic field. This field is a magnetic field that are conjugated to the order parameter of the spin system, which is the magnetization, $\mathbf{M}\sim\mathbf{H}$. The order parameters of a superconductor is as in (15.4). When these are nonzero, there is a spontaneously broken symmetry of the problem. Returning to $\mathcal{H}$;

$$\mathcal{H}=\sum_x\varphi^*\varepsilon(\boldsymbol{\nabla})\varphi+V\sum_x\varphi^*\varphi\varphi^*\varphi \tag{15.5}$$

This model has a continous symmetry

$$\begin{aligned}\varphi(x)&\to\varphi(x)\mathrm{e}^{i\theta(x)}\\ \mathcal{H}&\to\mathcal{H},\end{aligned}$$

which is a $U(1)$-symmetry. However, in $\langle\varphi_\downarrow\varphi_\uparrow\rangle$, the phases do not cancel, but instead goes to $\left\langle\varphi_\downarrow\varphi_\uparrow\mathrm{e}^{2i\theta}\right\rangle$. If this phase is completely undetermined, this average will be zero. Thus, having $\langle\varphi_\downarrow\varphi_\uparrow\rangle\neq0$ must mean that θ is a known quantity, i.e. the symmetry is spontaneously broken. More generally:

When we assume a saddle point in a functional integral, and also assume $\mathcal{S}_{\mathit{eff}}$ is a minimum for finite values of $\langle a\rangle, \left\langle a^\dagger\right\rangle$, this is quivalent to the assumption of some spontaneous breaking of symmetry (most often).

Thus: To choose a suitable decoupling scheme, we have to chose the "right type" of bosons in the H-S transformations. This choice is decided by the physcis we expect.

15.1 The spectra E_k

The consequence of the broken symmetry discussed above is a gap in the spectrum.

$a=0$:

$$\mathcal{H}=\sum_{k,\sigma}\left(\varepsilon_k-\mu\right)c_{k\sigma}^\dagger c_{k\sigma}. \tag{15.6}$$

$a\neq0$:

$$\mathcal{H}=E_0+\sum E_k\left(\gamma_k^\dagger\gamma_k-\eta_k^\dagger\eta_k\right) \tag{15.7}$$

$a\neq0\implies$ zero resistivity and Meissner effect. Superconduction. NB: We started with a Hamiltonian defined for fermions. We then proceeded by introducing the partition function and an effective action, $\mathcal{S}_{\text{eff}}$ (the Lagrange function)

$$\begin{aligned}\mathcal{H}\left(\varphi^*,\varphi\right)&\to\varphi^*\frac{\partial\varphi}{\partial\tau}+\mathcal{H}\left(\varphi^*,\varphi\right)\\ &=\mathcal{S}_0+\mathcal{S}_I.\end{aligned} \tag{15.8}$$

Notice that the dynamic term, $\varphi^* \frac{\partial \varphi}{\partial \tau}$, in (15.8) only acts in the fermion sector. We then H-S-decoupled $\mathcal{S}_I$

$$\mathrm{e}^{\mathcal{S}_I} = \int \mathcal{D}a^\dagger \mathcal{D}a \, \mathrm{e}^{-\frac{1}{v} a^\dagger a + a\varphi_\uparrow^\dagger \varphi_\downarrow^\dagger + a^\dagger \varphi_\downarrow \varphi_\uparrow} \tag{15.9}$$

But: We don't get any dynamic $a^\dagger \frac{\partial a}{\partial \tau}$-terms. The $(a^\dagger, a)$-bosons do not exist in the Hamilton formalismm. This means that they don't have their own dynamics. It is generated by the fermions, by $\mathrm{Tr} \ln \mathcal{G}^{-1}$.

15.2 Fluctuations

Later we will come back to how we correct the mean field approximations to $\mathcal{S}_{\text{eff}}[a^\dagger, a]$. We can do this by developing to Gaussian order (2.order) in the fluctuations in the boson fields $a^\dagger, a$, near the saddle point. A coarse structure of this will be the following. Define

$$A = \begin{pmatrix} \delta a^\dagger \\ \delta a \end{pmatrix}, A^\dagger = \begin{pmatrix} \delta a & \delta a^\dagger \end{pmatrix} \tag{15.10}$$

$$\begin{aligned} \mathcal{S}_{\text{eff}} &\simeq \mathcal{S}_{\text{MF}} - \sum_q A^\dagger D^{-1}(q) A \\ \mathcal{Z} &\simeq \mathrm{e}^{\mathcal{S}_{\text{MF}}} \int \mathcal{D}A^\dagger \mathcal{D}A \mathrm{e}^{-\sum_q A^\dagger D^{-1} A} \\ \mathcal{Z} &= \mathrm{e}^{\mathcal{S}_{\text{MF}}} \mathrm{e}^{-\mathrm{Tr} \ln D^{-1}} \end{aligned} \tag{15.11}$$

where D^{-1} is a 2×2 matrix. A constraint (claim) to stability of the saddle point is that D^{-1} have to be positive definite, i.e. it must have only positive eigenvalues. With $\mathcal{Z} = \mathrm{e}^{-\beta F}$ we have

$$F = F_{\text{MF}} + \frac{1}{\beta} \mathrm{Tr} \ln D^{-1}. \tag{15.12}$$

We can now correct the mean field values for $a, a^\dagger$ by minimizing (15.12) with respect to $a, a^\dagger$.

$$\frac{\partial F}{\partial a} = 0 = \frac{\partial F_{\text{MF}}}{\partial a} + \underbrace{\frac{\partial}{\partial a} \left(\frac{1}{\beta} \mathrm{Tr} \ln D^{-1} \right)}_{\text{Correction term}}. \tag{15.13}$$

This means that we can find the fluctuation corrections to T_c etc. We expect these corrections to be significant when T_c becomes large. As of October 1996', no such calculations on the fluctuations has been made.[4]

[4] As of 2019, it has probably been done thoroughly.

16 The Hubbard model ($U = \infty$)

Consider the Hamiltonian

$$\mathcal{H} = -\sum_{i,j} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma}. \tag{16.1}$$

At $U = 0$, the Hamiltonian (16.1) transforms to

$$\mathcal{H} = \sum_{k,\sigma} (\varepsilon_k - \mu)\, c^\dagger_{k\sigma} c_{k\sigma} \tag{16.2}$$

with nearest neighbour hopping

$$\varepsilon_k = -2t \sum_{i=1}^{d} \cos k_i \equiv -2t\gamma_k$$

For intermediate $0 < U < \infty$ we have a very complicated problem with little or nothing known.

For $U = \infty$ the problem simplifies, but cannot be solved exact. The simplified Hamiltonian then reads

$$\mathcal{H} = -\sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} \tag{16.3}$$

with an extra constraint on each lattice site; that there is a maximum of one fermion per lattice site at all times t.

$$\sum_\sigma \hat{n}_{i\sigma} |\psi\rangle \sum_\sigma n_{i\sigma} |\psi\rangle$$

with

$$\sum_\sigma n_{i\sigma} \leq 1$$

Constraints like these, i.e. constraints represented by inequalities are difficult to deal with.

16.1 Hubbard operators

Before we continue, we introduce Hubbard operators. Consider states $|\alpha, i\rangle$ where $\alpha \in 0, \sigma, 2$ and $\sigma = \uparrow, \downarrow$. These are empty, simple, or doubly occupied states. Next, define

$$X^{\alpha\beta}_i = |\alpha, i\rangle\langle\beta, i|\,. \tag{16.4}$$

$$\begin{aligned} \hat{O} &= \sum_{\alpha,\beta} |\alpha, i\rangle\ \langle\alpha, i|\hat{O}|\beta, i\rangle\, \langle\beta, i| \\ &= \sum_{\alpha,\beta} X^{\alpha\beta}_i \langle\alpha, i|\hat{O}|\beta, i\rangle \end{aligned}$$

Ex 6.

$$\begin{aligned} c_{i\sigma} &= \sum_{\alpha,\beta} X_i^{\alpha\beta} \langle \alpha, i | c_{i\sigma} | \beta, i \rangle \\ &= X_i^{0\sigma} + X_i^{-\sigma 2} \\ c_{i\sigma}^\dagger &= X_i^{\sigma 0} + X_i^{2-\sigma} \end{aligned}$$

If we let $U = \infty$, we see from (16.1) that we can drop the operators involving doubly occupied states $X_i^{-\sigma 2}, X_i^{2-\sigma}$ such that we can write[5]

$$c_{i\sigma} = X_i^{0\sigma} \tag{16.5}$$

$$c_{j\sigma}^\dagger = X_j^{\sigma 0} \tag{16.6}$$

This means that the Hamiltonian in the Hubbard model can be written

$$\mathcal{H} = -t \sum_{i,j,\sigma} X_i^{\sigma 0} X_j^{0\sigma} \tag{16.7}$$

Here we thus have hopping with no double-occupancy-constraint. We have restrictions on the creation and annihilation operators, but no restriction on the Hubbard operators $X_i^{\sigma 0}$. Unfortunately, the problem is more complicated then what it seems. The reason is that the Hubbard operators satisfy much more complicated commutation relations. By the definition (16.4), these are

$$\begin{aligned} \left[X_i^{\alpha\beta}, X_j^{\gamma\eta} \right]_\pm &= |\alpha i\rangle \langle \beta i | \gamma j \rangle \langle \eta j | \pm | \gamma j \rangle \langle \eta j | \alpha i \rangle \langle \beta i | \\ &= \delta_{ij} \delta_{\beta\gamma} X_i^{\alpha\eta} \pm \delta_{ij} \delta_{\eta\alpha} X_j^{\gamma\beta} \\ &= \delta_{ij} \left[\delta_{\beta\gamma} X_i^{\alpha\eta} \pm \delta_{\eta\alpha} X_i^{\gamma\beta} \right] \end{aligned} \tag{16.8}$$

Now, we introduce canonical boson- and fermion operators to represent X by these.

$$\begin{aligned} X_i^{00} &= |0i\rangle\langle 0i| \\ &\Leftrightarrow b_i^\dagger b_i \\ X_i^{\sigma 0} &= |\sigma i\rangle\langle 0i| \\ &\Leftrightarrow f_{i\sigma}^\dagger b_i \\ X_i^{0\sigma} &= |0i\rangle\langle \sigma i| \\ &\Leftrightarrow b_i^\dagger f_{i\sigma} \\ X_i^{\sigma\sigma'} &= |\sigma i\rangle\langle \sigma' i| \\ &\Leftrightarrow f_{i\sigma}^\dagger f_{i\sigma'} \end{aligned}$$

[5] Comment in the notes: " This is valid when the doubly occupied states gets projected out of the Hilbert space"

Using these representations, we get the correct commutation relations for the Hubbard operators.

$$\begin{aligned}\left[X_i^{0\sigma}, X_i^{\sigma'0}\right]_+ &= X_i^{0\sigma}X_i^{\sigma'0} + X_i^{\sigma'0}X_i^{0\sigma} \\ &= \delta_{\sigma\sigma'}X_i^{00} + X_i^{\sigma'\sigma} \\ &= \delta_{\sigma\sigma'}b_i^\dagger b_i + f_{i\sigma}^\dagger f_{i\sigma'}\end{aligned} \tag{16.9}$$

Or,using the representations directly:

$$\begin{aligned}\left[b_i^\dagger f_{i\sigma}, f_{i\sigma'}^\dagger b_i\right]_+ &= f_{i\sigma'}^\dagger f_{i\sigma}\left(1 + b_i^\dagger b_i\right) + b_i^\dagger b_i\left(\delta_{\sigma\sigma'} - f_{i\sigma'}^\dagger f_{i\sigma}\right) \\ &= \delta_{\sigma\sigma'}b_i^\dagger b_i + f_{i\sigma'}^\dagger f_{i\sigma} \\ &= \delta_{\sigma\sigma'}X_i^{00} + X_i^{\sigma'\sigma}.\end{aligned} \tag{16.10}$$

We see that (16.9) and (16.10) are equal and thus this representation gives the correct commutation relations. We still have the completeness relation

$$\begin{aligned}1 &= \sum_\alpha |\alpha i\rangle\langle\alpha i| \\ &= X_i^{00} + \sum_\sigma X_i^{\sigma\sigma} \\ &= b_i^\dagger b_i + \sum_\sigma f_{i\sigma}^\dagger f_{i\sigma}\end{aligned} \tag{16.11}$$

16.2 Reformulating constraint

We now return to the general problem of constraint govern by an inequality. We wish to convert this constraint to an equality, and we develop methods for solving such problems. The trick is to introduce a boson, b_i, which keeps track of when a lattice site i is unoccupied.

Using our previously defined Hubbard operators, we associate, using (16.5), $c_{i\sigma}^\dagger = X_i^{\sigma 0} \Leftrightarrow f_{i\sigma}^\dagger b_i$ and $c_{i\sigma} = X_i^{0\sigma} \Leftrightarrow b_i^\dagger f_{i\sigma}$.

$f_{i\sigma}^\dagger$: Creation operator for a fermion on the lattice site i . b_i: Creation operator for an unoccupied lattice site. $f_{i\sigma}^\dagger f_{i\sigma}$: The number of fermions on the lattice site i.

Either the site is occupied with one fermion, or the site is empty. This is expressed with the condition

$$b_i^\dagger b_i + \sum_\sigma f_{i\sigma}^\dagger f_{i\sigma} = 1, \tag{16.12}$$

which is now a leading constraint expressed with an equality.

The Hamiltonian (16.7)of the problem is written on the form

$$\mathcal{H} = -\sum_{i,j,\sigma} t_{ij} f_{i\sigma}^\dagger b_i b_j^\dagger f_{j\sigma}. \tag{16.13}$$

Equations (16.12) and (16.13) define our problem, which we are to solve. Define

$$Q_i \equiv \sum_\sigma f_{i\sigma}^\dagger f_{i\sigma} + b_i^\dagger b_i \tag{16.14}$$

such that $Q_i = 1$ is our condition. Abrikosovs' trick: [6]

$$\prod_{i,\tau} \int_{-\pi}^{\pi} \frac{\mathrm{d}\lambda_i}{2\pi} \mathrm{e}^{-i\int_0^\beta \lambda_i(\tau)(Q_i-1)\mathrm{d}\tau} = \prod_{i,\tau} \delta_{Q_i,1} \tag{16.15}$$

The partition function is given by

$$\mathcal{Z} = \int \mathcal{D}\varphi^* \mathcal{D}\varphi \mathcal{D}b^* \mathcal{D}b \left(\prod_i \prod_\tau \delta_{Q_i,1} \right) \mathrm{e}^{\mathcal{S}} \tag{16.16}$$

where the factor in parentheses ensures that the functional integral is limited to include states where the lattice sites are not doubly occupied.

$$\begin{aligned} \mathcal{S} = &- \sum_{i,\sigma} \int_0^\beta \mathrm{d}\tau \left[\underbrace{b_i^* \frac{\partial b_i}{\partial \tau}}_{\text{NB!}} + \varphi_{i\sigma}^* \frac{\partial \varphi_{i\sigma}}{\partial \tau} \right] \\ &+ \sum_{i,j,\sigma} \int_0^\beta \mathrm{d}\tau\, \varphi_{i\sigma}^*(\tau) b_i(\tau) t_{ij} b_j^*(\tau) \varphi_{j\sigma}(\tau) \end{aligned} \tag{16.17}$$

NB: Note that we now have to keep all the terms involving $b_i^* \frac{\partial b_i}{\partial \tau}$. This is because the b-bosons also exist in the Hamilton formulation of the theory. This is an essential difference from what we had earlier because the b-bosons has their own intrinsic dynamics. We rewrite (16.17) as

$$\begin{aligned} \mathcal{S} = &- \sum_i \int_0^\beta \mathrm{d}\tau\, b_i^* \frac{\partial b_i}{\partial \tau} \\ &- \sum_{i,j,\sigma} \int_0^\beta \mathrm{d}\tau\, \varphi_{i\sigma}^* \left(\partial_\tau \delta_{ij} - t_{ij} b_i b_j^* \right) \varphi_{j\sigma}. \end{aligned} \tag{16.18}$$

Now introduce Abrikosov's trick

$$\mathcal{Z} = \int \mathcal{D}\varphi^* \mathcal{D}\varphi \mathcal{D}b^* \mathcal{D}b \mathcal{D}\lambda\, \mathrm{e}^{\tilde{\mathcal{S}}} \tag{16.19}$$

$$\begin{aligned} \tilde{\mathcal{S}} = &- \sum_i \int_0^\beta \mathrm{d}\tau\, b_i^* (\partial_\tau + i\lambda_i) b_i + i \sum_i \int_0^\beta \lambda_i \,\mathrm{d}\tau \\ &\underbrace{- \sum_{i,j,\sigma} \int_0^\beta \mathrm{d}\tau\, \varphi_{i\sigma}^* \left[\delta_{ij} (\partial_\tau + i\lambda_i) - t_{ij} b_i b_j^* \right] \varphi_{j\sigma}}_{\text{Gaussian fermion sector}} \end{aligned}$$

[6] Alexei Alexeyevich Abrikosov (1928-2017), awarded with the Nobel price in physics 2003

Now we can integrate out the fermion sector in an exact manner!

$$\mathcal{Z} = \int \mathcal{D}b^\dagger \mathcal{D}b \mathcal{D}\lambda \mathrm{e}^{\mathcal{S}_{\mathrm{eff}}[b^\dagger, b, \lambda]}, \tag{16.20}$$

with

$$\begin{aligned} \mathcal{S}_{\mathrm{eff}} = &- \sum_i \int_0^\beta \mathrm{d}\tau \, b_i^\dagger \left(\partial_\tau + i\lambda\right) b_i + i \sum_i \int_0^\beta \mathrm{d}\tau \, \lambda_i \\ &+ \mathrm{Tr} \ln \mathcal{G}^{-1} \end{aligned} \tag{16.21}$$

$$\mathcal{G}^{-1} = \left(\partial_\tau + i\lambda_i\right) \delta_{ij} - t_{ij} b_i b_i^\dagger \tag{16.22}$$

We have thus converted a strongly correlated fermionic system to an interacting bosonic system. The resulting boson-theory is again too complicated for direct calculation of $\mathcal{Z}$. We therefore resort to the stationary point approximation. Let $b_i = b, i\lambda_i = \lambda$ (physical explanation will follow).

$$\mathcal{G}^{-1} = (\partial_\tau + \lambda)\delta_{ij} - |b|^2 t_{ij}. \tag{16.23}$$

To compute (16.23), we may resort to the Fourier transform of $\mathcal{G}^{-1}$.

$$\begin{aligned} \mathcal{F}(\delta_{ij}) &\Rightarrow 1 \\ \mathcal{F}(t_{ij}) &\Rightarrow \tilde{\gamma}_k = 2t \underbrace{\sum_i \cos(k_i)}_{\gamma_k} \\ \partial_\tau &\Rightarrow -i\omega_n. \end{aligned}$$

Using these relations, we find

$$\mathrm{Tr} \ln \mathcal{G}^{-1} = \frac{1}{\beta} \sum_{k, \omega_n} \ln(-i\omega_n + \varepsilon_k) \tag{16.24}$$

$$= \frac{1}{\beta} \sum_{k, \omega_n} \ln(i\omega_n - \varepsilon_k), \tag{16.25}$$

$$\varepsilon_k = -2tb^2 \sum_i \cos(k_i) + \lambda, \tag{16.26}$$

or, if we had included the chemical potential all the way from the start,

$$\begin{aligned} \varepsilon_k &= -2tb^2\gamma_k - (\mu + \lambda) \\ \mathcal{S}_{\mathrm{eff}}^{\mathrm{MF}} &= -N\beta b^2 \lambda + N\beta\lambda + \sum_k \ln\left(1 + \mathrm{e}^{-\beta\varepsilon_k}\right) \\ f^{\mathrm{MF}} &= (b^2 + 1)\lambda - \frac{1}{N\beta} \sum_k \ln\left(1 + \mathrm{e}^{-\beta\varepsilon_k}\right) \end{aligned}$$

16.3 Mean-field

$$\mathcal{G}^{-1} = -i\omega_n + \varepsilon_k \tag{16.27}$$

$$\mathcal{G}_F(k, i\omega) = \frac{1}{i\omega - \varepsilon_k} = -\left\langle \varphi\varphi^\dagger \right\rangle \tag{16.28}$$

where

$$\varepsilon_k = -2tb^2\gamma_k - (\mu + \lambda). \tag{16.29}$$

$\mathcal{G}_F(k, i\omega)$: Green's function for a free quasi particle with renormalized band structure (lower bandwidth, correlation effect) and renormalized chemical potential. Both of these types of renormalization originate in the "no double occupancy constraint".

17 The Anderson and Kondo models

Imagine that we have a system defined by free, itinerant electrons, described by a conduction band with dispersion relation ε_k and, for the sake of simplicity, assume that the one-particle density of state has a simple form as shown in Figure 7. The bandwidth of this system is $2D$, and the system has a Hamiltonian

$$\mathcal{H}_c = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma}. \tag{17.1}$$

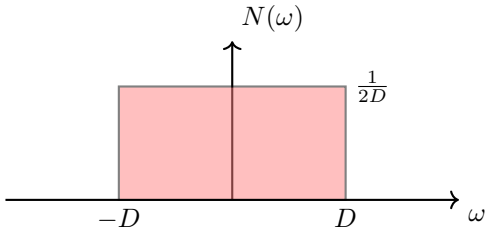


Figure 7: Density of states

We will study the effect of including a magnetic impurity in the problem, where the magnetic impurity couples to the charged electrons, but is localized in space. First we consider the system with exactly one impurity. The Hamiltonian for this impurity is given by

$$\mathcal{H}_f = E_0 \sum_m f^\dagger_m f_m + U f^\dagger_{\frac{1}{2}} f^\dagger_{-\frac{1}{2}} f_{-\frac{1}{2}} f_{\frac{1}{2}}, \tag{17.2}$$

where m are quantum numbers determining the z-component of the spin of the impurity. $(f_m, f^\dagger_m)$ are annihilation and creation operators for the impurity, in state m. $s = \frac{1}{2} : m = \pm 1$. U is the Coulomb energy associated with double occupancy of the magnetic impurity. We will later assume that this is the largest energy in the system. The coupling between the charges and the localized impurity is given by

$$\mathcal{H}_{cf} = \sum_{\mathbf{k},\sigma,m} \left(V_{m\sigma}(\mathbf{k}) f^\dagger_m c_{\mathbf{k}\sigma} + \text{h.c.} \right). \tag{17.3}$$

In (17.3), $V_{m\sigma}(\mathbf{k})$ is the matrix element transfering an electron from the impurity to the conduction band, or opposite. The total Hamiltonian is

$$\mathcal{H} = \mathcal{H}_c + \mathcal{H}_f + \mathcal{H}_{cf}. \tag{17.4}$$

$\mathcal{H}$ is often called the Anderson model. This model is the fundament for our understanding of heavy fermion systems. We will now use the techniques to study the effects of including a magnetic impurity in the conduction band. One important effect of magnetic impurities is that a metal will exhibit a minima in

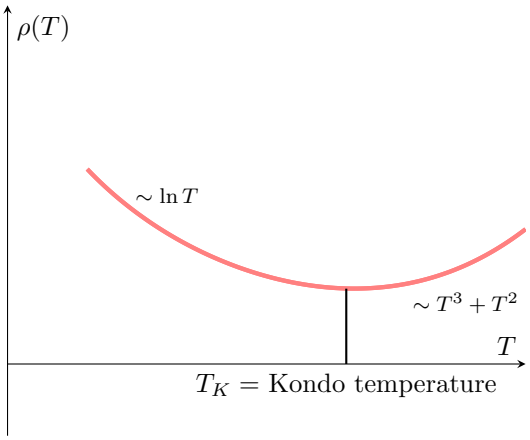


Figure 8: Resistivity

resistivity (see Figure 8). T_K is only a couple of Kelvin, but the Fermi-energy is of order 10^4K. How can an energy scale this small arise when the basis is that the relevant energy scale is $\varepsilon_F \sim 10^4$K? If magnetic impurities are excluded, the resistivity is uniformly decreasing. Jun Kondo found that $\rho(T) \sim -\ln T$ diverges in perturbation theory at low temperatures[7]. A new problem then arises; how can we give a consistent description of low temperaturre physics, $T << T_K$, in systems with a minima in resistivity? This problem is often referred to as the "Kondo problem".

What we will do, is to see how the energy scale T_K, The Kondo temperature, arises, as well as to give a consistent description of the lowæ-temperature physics in metals doped with magnetic impurities, in a saddle point approxiimation. Typical materials described by these theories are metals like aluminium and gold, doped with other rare materials. These materials are then the magnetic impurities in the problem. Rare materials: Lanthanides and actinides. Most studied: Cerium (Lanthanide) and Uranium (actinide). In the lanthanides the valence electrons are in the 4f-shell, and in actinides they are in the 5f-shell (hence $f_m^\dagger, f_m$)). Regularly studied materials are $CeAl_2$ (lanthanide) and UPt_3 (Actinide). UPt_3 is a very odd superconductor with $T_C \sim 1$mK and a very complicated order parameter.

Let us simplify the Anderson model;

i): $U = \infty$.

Doubly occupancy of the magnetic impurities are not allowed. If there already exist a spin on the lattice site of the impurity, a conducting electron can not enter this localized orbital.

ii): We assume that the coupling between f- and c-electrons are such that $m = \sigma$, i.e.

$$V_{m\sigma}(k) = \delta_{m\sigma} V(k), \tag{17.5}$$

[7]Progress of Theoretical Physics, Vol. 32, No. 1, pp. 37-49

and that $V(k)$ is k-independent (completely localized coupling)

$$V_{m\sigma}(k) = V\delta_{m\sigma} \tag{17.6}$$

which implies

$$\mathcal{H}_{cf} = V\sum_{\sigma k}\left(f_\sigma^\dagger c_{k\sigma} + h.c.\right). \tag{17.7}$$

Thus, we have the model

$$\begin{aligned}\mathcal{H} &= E_0\sum_\sigma f_\sigma^\dagger f_\sigma + \sum_{k,\sigma}\varepsilon_k c_{k\sigma}^\dagger c_{ck}^\dagger \\ &= V\sum_{k,\sigma}\left[f_\sigma^\dagger c_{k\sigma} + h.c.\right],\end{aligned} \tag{17.8}$$

with $\sum_m f_m^\dagger f_m \leq 1$. It is the restiriction on the occupation number on the impurities that makes this a hard problem.

For later reference, we first solve the problem with $U = 0$.

17.1 $U = 0$

$$\mathcal{Z} = \int \mathcal{D}c^\dagger \mathcal{D}c\mathcal{D}f^\dagger \mathcal{D}f \mathrm{e}^{\mathcal{S}} \tag{17.9}$$

$$\mathcal{S} = -\int\left(\sum_{k,\sigma} c_{k\sigma}^\dagger \frac{\partial c_{k\sigma}}{\partial\tau} + \sum_m f_m^\dagger \frac{\partial f_m}{\partial\tau} + \mathcal{H}\right)\mathrm{d}\tau \tag{17.10}$$

$$\begin{aligned}\mathcal{S} = &-\int_0^\beta \sum_{k,\sigma} c_{k\sigma}^\dagger\left(\partial_\tau + \varepsilon_k\right)c_{k\sigma}\,\mathrm{d}\tau \\ &-\int_0^\beta \sum_\sigma f_\sigma^\dagger\left(\partial_\tau + E_0\right)f_\sigma\,\mathrm{d}\tau \\ &-\int_0^\beta V\sum_{k,\sigma}\left(f_\sigma^\dagger c_{k\sigma} + h.c.\right)\mathrm{d}\tau\end{aligned} \tag{17.11}$$

$\mathcal{Z}$ can be computed exactly by a linear shift og the fermion operators $(c_{k\sigma}, c_{k\sigma}^\dagger)$. Introduce $\mathcal{G}_0^{-1} = \partial_\tau + \varepsilon_k$. Consider now the quantity

$$\begin{aligned}&\sum_{k,\sigma}\left[c_{k\sigma}^\dagger \mathcal{G}_0^{-1} c_{k\sigma} + V f_\sigma^\dagger c_{k\sigma} + V c_{k\sigma}^\dagger f_\sigma\right] \\ &= \sum_{k\sigma}\left(c_{k\sigma}^\dagger + V f_\sigma^\dagger \mathcal{G}_0\right)\mathcal{G}_0^{-1}\left(c_{k\sigma} + V\mathcal{G}_0 f_\sigma\right) - \sum_{k,\sigma} V^2 f_\sigma^\dagger \mathcal{G}_0 f_\sigma \\ &= \sum_{k\sigma}\tilde{c}_{k\sigma}^\dagger \mathcal{G}_0^{-1}\tilde{c}_{k\sigma} - \sum_\sigma f_\sigma^\dagger\left(\sum_k V^2\mathcal{G}_0\right)f_\sigma.\end{aligned} \tag{17.12}$$

Inserting (17.12) into the action, we get

$$S = -\sum_{k,\sigma} \tilde{c}^{\dagger}_{k\sigma} \mathcal{G}_0^{-1} \tilde{c}_{k\sigma} - \sum_{\sigma} f^{\dagger}_{\sigma} \left(\partial_\tau + E_0 - V^2 \sum_k \frac{1}{\partial_\tau + \varepsilon_k} \right) f_\sigma. \tag{17.13}$$

As we can see in (17.13), the action is quadratic in the c- and f- sectors.

$$\mathcal{Z} = \int \mathcal{D}\tilde{c}^{\dagger} \mathcal{D}\tilde{c} \mathcal{D} f^{\dagger} \mathcal{D} f \, \mathrm{e}^{\mathcal{S}} = \mathcal{Z}_c \cdot \mathcal{Z}_f, \tag{17.14}$$

where

$$\mathcal{Z}_c = \mathrm{e}^{\mathrm{Tr}\ln\left(\mathcal{G}_0^{-1}\right)} \qquad \mathcal{Z}_f = \mathrm{e}^{\mathrm{Tr}\ln\left(\mathcal{G}_f^{-1}\right)} \tag{17.15}$$

$$\mathcal{G}_0^{-1} = \partial_\tau + \varepsilon_k \qquad \mathcal{G}_f^{-1} = \partial_\tau + E_0 - V^2 \sum_k \frac{1}{\partial_\tau + \varepsilon_k}. \tag{17.16}$$

$\mathcal{Z}_c$ is the partition function for free electron gas, and $\mathcal{Z}_f$ is the partition function for the impurities, coupled to a free electron gas.

we have already considered

$$\mathrm{Tr}\ln \mathcal{G}_0^{-1} = \sum_{k,\sigma} \ln\left(1 + \mathrm{e}^{-\beta\varepsilon_k}\right). \tag{17.17}$$

(17.17) is the free energy for non-interacting electron gas, as we have seen earlier (see the derivation of (**??**)).

$$\mathrm{Tr}\ln\left(\mathcal{G}_f^{-1}\right) = \sum_{\sigma} \sum_{\omega_n} \ln\left(-i\omega_n + E_0 + V^2 \sum_k \frac{1}{i\omega_n - \varepsilon_k} \right) \tag{17.18}$$

Consider now the last k-summation in (17.18).

$$\begin{aligned} \sum_k \frac{1}{i\omega_n - \varepsilon_k} &= \frac{1}{2D} \int_{-D}^{D} \mathrm{d}\varepsilon \, \frac{1}{i\omega_n - \varepsilon} \\ &= \frac{1}{2D} \ln\left(\frac{D + i\omega_n}{-D + i\omega_n} \right) \\ &= -\frac{1}{2D} \ln\left(\frac{\omega_n + iD}{\omega_n - iD} \right) \end{aligned} \tag{17.19}$$

This is evaluated as

$$\ln\left(\frac{z}{z^*}\right) = \ln\left(\frac{|z| e^{i\varphi}}{|z| \mathrm{e}^{-i\varphi}} \right) = 2i\varphi. \tag{17.20}$$

Here, $\varphi = \tan^{-1}\left(\frac{D}{\omega_n}\right) \simeq \frac{\pi}{2}\mathrm{sgn}(\omega_n)$ as $T \to 0$. This implies that we can write the k-sum in (17.19) as

$$\sum_k \frac{1}{i\omega_n - \varepsilon_k} \simeq -i \frac{\pi \cdot 2}{2 \cdot 2D} \mathrm{sgn}(\omega_n) \tag{17.21}$$

$$= -i\pi\rho_0 \mathrm{sgn}(\omega_n) \tag{17.22}$$

where we introduced $\rho_0 = 1/2D$. Define $\Delta_0 \equiv \pi\rho_0 V^2$. Going back to (17.18), we now have

$$\sum_k \frac{1}{i\omega_n - \varepsilon_k} = \sum_\sigma \sum_{\omega_n} \ln\left(-i\omega + E_0 - i\Delta_0 \mathrm{sgn}(\omega_n)\right). \tag{17.23}$$

Following the same methods as we have seen earlier, we have

$$\begin{aligned}\sum_{\omega_n} \ldots &= \frac{-\beta}{2\pi i} \oint \mathrm{d}z\, f(z) \ln(-z + E_0 - i\Delta_0 \mathrm{sgn}(\mathrm{Im}\{z\})) \\ &= -\frac{\beta}{2\pi i} \int_{-D}^{D} \mathrm{d}\varepsilon\, f(\varepsilon) \left[\ln(-\varepsilon + E_0 - i\Delta_0) - \ln(-\varepsilon + E_0 + i\Delta_0)\right] \\ &= \frac{\beta}{\pi} \int_{-D}^{D} \mathrm{d}\varepsilon\, f(\varepsilon) \tan^{-1}\left(\frac{\Delta_0}{E_0 - \varepsilon}\right). \end{aligned} \tag{17.24}$$

Thus, after the spin-summation, our total action is

$$\mathcal{S} = -2\sum_k \ln\left(1 + \mathrm{e}^{-\beta\varepsilon_k}\right) + \frac{2\beta}{\pi} \int_{-D}^{D} \mathrm{d}\varepsilon\, f(\varepsilon) \tan^{-1}\left(\frac{\Delta_0}{E_0 - \varepsilon}\right). \tag{17.25}$$

$\mathcal{S}$ describes a free electron gas, plus a scattering resonance at the energy E_0 caused by the coupling between f- and c-electrons. Notice that if $|E_0| >> D$,the second term in (17.25) can be neglected. The impurities are far from the conduction band, and does not matter. When $U = \infty$, this will drastically change this result, as we shall now see.

NB! The Green's functions:

$$\begin{aligned} -\left\langle f f^\dagger \right\rangle &= -\left(\partial_\tau + E_0 - V^2 \sum_k \frac{1}{\partial_\tau + \varepsilon_k}\right)^{-1} \\ &\to \left(i\omega_n - E_0 + V^2 \sum_k \frac{1}{i\omega_n - \varepsilon_k}\right)^{-1} \\ -\left\langle \tilde{c}\tilde{c}^\dagger \right\rangle &= -\frac{1}{\partial_\tau + \varepsilon_k} \\ &\to \frac{1}{i\omega_n - \varepsilon_k}, \end{aligned}$$

but the $\tilde{c}$-"electrons" are <u>not</u> physical electrons. We defined them as $\tilde{c} = c + V\mathcal{G}_0 f_\sigma \Rightarrow c = \tilde{c} - V\mathcal{G}_0 f_\sigma$. Then, the conducting-electron-propagator is modified;

$$\begin{aligned} -\left\langle c c^\dagger \right\rangle &= -\left[\left\langle (\tilde{c} - V\mathcal{G}_0 f_\sigma)(\tilde{c}^\dagger - V\mathcal{G}_0 f_\sigma^\dagger) \right\rangle\right] \\ &= -\mathcal{G}_0 + V\mathcal{G}_0 \left\langle \tilde{c} f^\dagger \right\rangle + V\mathcal{G}_0 \left\langle f \tilde{c}^\dagger \right\rangle - V^2 \mathcal{G}_0 \left\langle f f^\dagger \right\rangle \mathcal{G}_0 \end{aligned}$$

The propagator for the conducting electrons is then

$$\mathcal{G}(\partial_\tau, \varepsilon_k) = -\left[\mathcal{G}_0(\partial_\tau, \varepsilon_k) + V^2 \mathcal{G}_0(\partial_\tau, \varepsilon_k) \mathcal{G}_f(\partial_\tau) \mathcal{G}_0(\partial_\tau, \varepsilon_k)\right] \tag{17.26}$$

17.2 $U = \infty$

Remember that U is the energy of the Coloumb interaction from double occupancy of the impurities defined in (17.2).

$$\mathcal{H} = E_0 \sum_\sigma F_\sigma^\dagger F_\sigma + \sum_{k,\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + V \sum_{k,\sigma} \left(F_\sigma^\dagger c_{k\sigma} + c_{k\sigma}^\dagger F_\sigma \right) \tag{17.27}$$

Our constraint reads

$$\sum_m F_m^\dagger F_m \leq 1, \tag{17.28}$$

i.e. we have no double occupancy. As we did for the Hubbard model at $U = \infty$, wee introduce b-bosons.

$$\begin{aligned} F_m^\dagger &= f_m^\dagger b \\ F_m &= f_m b^\dagger \\ \sum_m & f_m^\dagger f_m + b^\dagger b = 1 \end{aligned}$$

$F_m, F_m^\dagger$ are Hubbard operators, and does not satisfy simple commutation relations. When this restriction is satisfied, we have

$$\mathcal{H} = E_0 \sum_m f_m^\dagger f_m + \sum_{k,\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + V \sum_{k,\sigma} \left(f_\sigma^\dagger b c_{k\sigma} + c_{k\sigma}^\dagger b^\dagger f_\sigma \right) \tag{17.29}$$

with the restriction

$$\sum_m f_m^\dagger f_m + b^\dagger b = 1 \equiv Q. \tag{17.30}$$

As we did for $U = \infty$ Hubbard:

$$\mathcal{Z} = \int \mathcal{D}c^\dagger \mathcal{D}c \mathcal{D}f^\dagger \mathcal{D}f \mathcal{D}b^\dagger \mathcal{D}b \, \mathrm{e}^{\mathcal{S}} \delta_{Q,1} \tag{17.31}$$

$$\begin{aligned} \mathcal{S} = &- \sum_m \int_0^\beta \mathrm{d}\tau \, f_m^\dagger \left(\partial_\tau + E_0 \right) f_m - \sum_{k,\sigma} \int_0^\beta \mathrm{d}\tau \, c_{k\sigma} \left(\partial_\tau + \varepsilon_k \right) c_{k\sigma}) \\ &- \int_0^\beta \mathrm{d}\tau \, b^\dagger \partial_\tau b - V \sum_{k,\sigma} \int_0^\beta \mathrm{d}\tau \left(c_{k\sigma}^\dagger b^\dagger f_\sigma + f_\sigma^\dagger b c_{k\sigma} \right). \end{aligned} \tag{17.32}$$

Again, we use Abrikosov's trick, that for each value of τ use that

$$\delta_{Q,1} = \int_{-\pi}^{\pi} \frac{\mathrm{d}\lambda}{2\pi} \mathrm{e}^{-i\lambda(Q-1)} \tag{17.33}$$

$$\Rightarrow \mathcal{Z} = \int_{-\pi}^{\pi} \frac{\mathrm{d}\lambda}{2\pi} \int \mathcal{D}c^\dagger \mathcal{D}c \mathcal{D}f^\dagger \mathcal{D}f \mathcal{D}b^\dagger \mathcal{D}b \, \mathrm{e}^{\tilde{\mathcal{S}}} \tag{17.34}$$

$$\begin{aligned} \tilde{\mathcal{S}} = &- \sum_m \int_0^\beta \mathrm{d}\tau \, f_m^\dagger \left(\partial_\tau + E_0 + i\lambda\right) f_m - \sum_{k,\sigma} \int_0^\beta \mathrm{d}\tau \, c_{k\sigma} \left(\partial_\tau + \varepsilon_k\right) c_{k\sigma}) \\ &- \int_0^\beta \mathrm{d}\tau \, b^\dagger \left(\partial_\tau + i\lambda\right) b - V \sum_{k,\sigma} \int_0^\beta \mathrm{d}\tau \left(c_{k\sigma}^\dagger b^\dagger f_\sigma + f_\sigma^\dagger b c_{k\sigma} \right) + i \int_0^\beta \mathrm{d}\tau \, \lambda \end{aligned} \tag{17.35}$$

Again we introduce $\mathcal{G}_0 = \partial_\tau + \varepsilon_k$, and make a shift of the c-fields:

$$\begin{aligned} &\sum_{k\sigma} \left[c_{k\sigma}^\dagger \mathcal{G}_0^{-1} c_{k\sigma} + V \left(c_{k\sigma}^\dagger b^\dagger f_\sigma + f_\sigma^\dagger b c_{k\sigma} \right) \right] \\ &\quad = \sum_{k,\sigma} \underbrace{\left(c_{k\sigma}^\dagger + V f_\sigma^\dagger b \mathcal{G}_0 \right)}_{\tilde{c}^\dagger} \mathcal{G}_0^{-1} \left(c_{k\sigma} + V \mathcal{G}_0 b^\dagger f_\sigma \right) \\ &\qquad - V^2 \sum_\sigma f_\sigma^\dagger b \left(\sum_k \mathcal{G}_0 \right) b^\dagger f_\sigma \end{aligned}$$

Now, do the functional integrals $\int \mathcal{D}\tilde{c}^\dagger \mathcal{D}\tilde{c}$ such that $\mathcal{Z} = \mathcal{Z}_0 \cdot \tilde{\mathcal{Z}}$ with

$$\mathcal{Z}_0 = \mathrm{e}^{\mathrm{Tr} \ln \mathcal{G}_0^{-1}}$$

and

$$\tilde{\mathcal{Z}} = \int_{-\pi}^{\pi} \frac{\mathrm{d}\lambda}{2\pi} \int \mathcal{D}f^\dagger \mathcal{D}f \mathcal{D}b^\dagger \mathcal{D}b \, \mathrm{e}^{\mathcal{S}_{\mathrm{eff}}},$$

where

$$\begin{aligned} \mathcal{S}_{\mathrm{eff}} = \int_0^\beta \mathrm{d}\tau \, [&- b^\dagger \left(\partial_\tau + i\lambda\right) b - \sum_m f_m^\dagger \left(\partial_\tau + E_0 + i\lambda\right) f_m \\ &+ \sum_m f_m^\dagger V^2 b \left(\sum_k \mathcal{G}_0 \right) b^\dagger f_m \\ &+ i\lambda] \end{aligned}$$

We can now do the $\int \mathcal{D}f^\dagger \mathcal{D}f$-integration:

$$\tilde{\mathcal{Z}} = \int_{-\pi}^{\pi} \frac{\mathrm{d}\lambda}{2\pi} \int \mathcal{D}b^\dagger \mathcal{D}b \, \mathrm{e}^{\tilde{\mathcal{S}}_{\mathrm{eff}}[b^\dagger, b, \lambda]}. \tag{17.36}$$

The theory is now bosonized, with

$$\tilde{\mathcal{S}}_{\text{eff}}[b^\dagger, b, \lambda] = -\int_0^\beta \mathrm{d}\tau \left(b^\dagger \left(\partial_\tau + i\lambda \right) b + i\lambda \right) + \mathrm{Tr} \ln \left(\mathcal{G}_f^{-1}[b^\dagger, b, \lambda] \right) \tag{17.37}$$

$$\mathcal{G}_f^{-1} = \partial_\tau + E_0 + i\lambda - V^2 b^\dagger \left(\sum_k \frac{1}{\partial_\tau + \varepsilon_k} \right) b \tag{17.38}$$

Remembering the results (17.16) for $U = 0$, we see that $U = \infty$ has two effects:

i Shift of E_0

ii Renormalized hybridisation

Again, the resulting effective action is to complicated to be calculated exactly. Let us therefore introduce a saddle point approximation by

$$\begin{aligned} b(\tau) &= b \\ i\lambda &= \lambda. \end{aligned}$$

$$\begin{aligned} \tilde{\mathcal{S}}_{\text{eff}} &= -\beta\lambda(b^2 - 1) + \mathrm{Tr} \ln \left(\partial_\tau + E_0 + \lambda - V^2 b^2 \sum_k \mathcal{G}_0 \right) \\ &= -\beta\lambda(b^2 - 1) + \sum_\sigma \sum_{\omega_n} \ln \left(-i\omega_n + \varepsilon_f + s_0^2 \sum_k \frac{1}{i\omega_n - \varepsilon_k} \right) \\ &= -\beta\lambda(b^2 - 1) + 2 \sum_{\omega_n} \ln \left(-\omega_n + \varepsilon_f - i\Delta \mathrm{sgn}(\omega_n) \right) \\ &= -\beta\lambda(b^2 - 1) + 2\beta \int_{-D}^{D} \frac{\mathrm{d}\varepsilon}{\pi} f(\varepsilon) \tan^{-1} \left(\frac{\Delta}{\varepsilon_f - \varepsilon} \right), \end{aligned} \tag{17.39}$$

where we introduced $s_0 \equiv bV, \Delta \equiv \pi\rho_0 s_0^2$ and followed the same derivation as (17.24) with the appropriate changes. If we compare (17.39) with the effective action from the $U = 0$ -case,

$$\mathcal{S}_{\text{eff},U=0} = 2\beta \int_{-D}^{D} \frac{\mathrm{d}\varepsilon}{\pi} f(\varepsilon) \tan^{-1} \left(\frac{\Delta_0}{E_0 - \varepsilon} \right), \tag{17.40}$$

we have for $U = \infty$ a shift in the scattering resonance at $\varepsilon_f = E_0 + \lambda$. As we will now see, ε_f is "nailed" to the Fermi-level, such that even if E_0 is far outside the conduction band, ε_f is practically on the Fermi level. Thus, impurities always affect the physics at the Fermi level. This permanent nailing is the origin of the Kondo-effect and heavy-fermion behaviour. **This is thus a correlation effect.** We will now minimize the effective action with respect to b^2 and λ. $\varepsilon_f = E_0 + \lambda \Rightarrow \lambda = \varepsilon_f - E_0$, and $s_0 = bV \rightarrow b^2 = s_0^2/(\ V^2)$. Then

$$\tilde{\mathcal{S}}_{\text{eff}} = -\beta\left(\varepsilon_f - E_0\right)\left(\frac{s_0^2}{V^2} - 1\right) \tag{17.41}$$

$$+ 2\beta \int_{-D}^{D} \frac{\mathrm{d}\varepsilon}{\pi} f(\varepsilon) \tan^{-1}\left(\frac{\Delta}{\varepsilon_f - \varepsilon}\right) \tag{17.42}$$

$$\frac{\partial \tilde{\mathcal{S}}_{\text{eff}}}{\partial \varepsilon_f} = 0 \tag{17.43}$$

$$\frac{\partial \tilde{\mathcal{S}}_{\text{eff}}}{\partial s_0} = 0 \tag{17.44}$$

Eqs. (17.43),(17.44) are self consistent equations for deciding ε_f, s_0.

Notice also that for $T = 0$, the effective action is well defined. The method therefore gives a well defined description of the low-T physics. Consider the $T = 0$ case:

$$\tilde{\mathcal{S}}_{\text{eff}} = -\beta\left(\varepsilon_f - E_0\right)\left(\frac{s_0^2}{V^2} - 1\right) \tag{17.45}$$

$$+ 2\beta \int_{-D}^{0} \frac{\mathrm{d}\varepsilon}{\pi} \tan^{-1}\left(\frac{\Delta}{\varepsilon_f - \varepsilon}\right) \tag{17.46}$$

$$\tan^{-1}(x) = \frac{-i}{2} \ln\left(\frac{1+ix}{1-ix}\right) \tag{17.47}$$

And the quantity

$$\begin{aligned}
\int_{-D}^{0} \frac{\mathrm{d}\varepsilon}{\pi} \tan^{-1}\left(\frac{\Delta}{\varepsilon_f - \varepsilon}\right) &= \int_{0}^{D} \frac{\mathrm{d}\varepsilon}{\pi} \tan^{-1}\left(\frac{\Delta}{\varepsilon_f + \varepsilon}\right) \\
&= \int_{\varepsilon_f}^{D+\varepsilon_f} \frac{\mathrm{d}x}{\pi} \tan^{-1}\left(\frac{\Delta}{x}\right) \\
&= \frac{1}{\pi}\Big|_{\varepsilon_f}^{D+\varepsilon_f} x \tan^{-1}\left(\frac{\Delta}{x}\right) - \frac{1}{\pi}\int_{\varepsilon_f}^{D+\varepsilon_f} \mathrm{d}x \, \frac{x}{1+\frac{\Delta^2}{x^2}}\left(\frac{-\Delta}{x^2}\right) \\
&= \frac{1}{\pi}\left[(D+\varepsilon_f)\tan^{-1}\left(\frac{\Delta}{D+\varepsilon_f}\right) - \varepsilon_f \tan^{-1}\left(\frac{\Delta}{\varepsilon_f}\right)\right] \\
&\quad + \frac{\Delta}{2\pi}\ln\left(\frac{(D+\varepsilon_f)^2 + \Delta^2}{\varepsilon_f^2 + \Delta^2}\right) \\
&\overset{D>>(\Delta,\varepsilon_f)}{\simeq} \frac{-\varepsilon_f}{\pi}\tan^{-1}\left(\frac{\Delta}{\varepsilon_f}\right) - \frac{\Delta}{2\pi}\ln\left(\frac{\varepsilon_f^2+\Delta^2}{D^2}\right) \\
&\quad + \frac{D+\varepsilon_f}{\pi}\tan^{-1}\left(\frac{\Delta}{D+\varepsilon_f}\right)
\end{aligned}$$

Now $\varepsilon_f + D >> (\Delta, \varepsilon_f) \Rightarrow \tan^{-1}(\Delta/(\varepsilon_f + D)) \simeq \Delta/(\varepsilon_f + D)$ which implies

$$\begin{aligned}
&\frac{\Delta}{\pi} - \frac{\varepsilon_f}{\pi}\tan^{-1}(\Delta/(\varepsilon_f)) - \frac{\Delta}{2\pi}\ln\left(\frac{\varepsilon_f^2+\Delta^2}{D^2}\right) \\
&\simeq \int_{-D}^{0} \mathrm{d}\varepsilon \tan^{-1}\left(\frac{\Delta}{\varepsilon_f - \varepsilon}\right)
\end{aligned}$$

$$\begin{aligned}
\tilde{\mathcal{S}}_{\text{eff}} &= -\beta(\varepsilon_f - E_0)\left(\frac{\Delta}{\Delta_0} - 1\right) \\
&+ 2\beta\left(\frac{\Delta}{\pi} - \frac{\varepsilon_f}{\pi}\tan^{-1}\left(\frac{\Delta}{\varepsilon_f}\right) - \frac{\Delta}{2\pi}\ln\left(\frac{\varepsilon_f^2+\Delta^2}{D^2}\right)\right) = -\beta\tilde{U}_{\text{eff}},
\end{aligned} \tag{17.48}$$

at $T = 0$. $s_0^2/V^2 = \Delta/\Delta_0$ with $\Delta = \pi\rho_0 s_0^2, \Delta = \pi\rho_0 V^2$. The equations to evaluate are

$$\frac{\partial \tilde{U}_{\text{eff}}}{\partial \Delta} = 0 \qquad\qquad \frac{\partial \tilde{U}_{\text{eff}}}{\partial \varepsilon_f} = 0$$

$$\begin{aligned}
\frac{\partial \tilde{U}_{\text{eff}}}{\partial \Delta} = 0 &= \frac{1}{\Delta_0}(\varepsilon_f - E_0) - \frac{2}{\pi} + \frac{2\varepsilon_f}{\pi}\frac{1}{1+\frac{\Delta^2}{\varepsilon_f^2}}\frac{1}{\varepsilon_f} \\
&\quad + \frac{1}{\pi}\ln\left(\frac{\varepsilon_f^2+\Delta^2}{D^2}\right) + \frac{\Delta}{\pi}\frac{2\Delta}{\varepsilon_f^2+\Delta^2} \\
&= \frac{1}{\Delta_0}(\varepsilon_f - E_0) - \frac{2}{\pi} + \frac{2}{\pi}\left(\frac{\varepsilon_f^2+\Delta^2}{\varepsilon_f^2+\Delta^2}\right) + \frac{1}{\pi}\ln\left(\frac{\varepsilon_f^2+\Delta^2}{D^2}\right) = 0 \\
\Rightarrow &\frac{\Delta_0}{\pi}\ln\left(\frac{\varepsilon_f^2+\Delta^2}{D^2}\right) = E_0 - \varepsilon_f \\
\frac{\partial \tilde{\mathcal{S}}_{\text{eff}}}{\partial \varepsilon_f} = 0 &= \frac{\Delta}{\Delta_0} - 1 + \frac{2}{\pi}\tan^{-1}\left(\frac{\Delta}{\varepsilon_f}\right) \\
\Rightarrow &\frac{2}{\pi}\tan^{-1}\left(\frac{\Delta}{\varepsilon_f}\right) = 1 - \frac{\Delta}{\Delta_0} \equiv \sum_m \langle f_m^\dagger f_m\rangle = n_f
\end{aligned}$$

$$\begin{aligned}\frac{\partial \tilde{\mathcal{S}}_{\text{eff}}}{\partial \varepsilon_f} &= 0 \\ &= \frac{\Delta}{\Delta_0} - 1 + \frac{2}{\pi}\tan^{-1}\left(\frac{\Delta}{\varepsilon_f}\right) \\ &+ \frac{2\varepsilon_f}{\pi}\frac{1}{1+\frac{\Delta^2}{\varepsilon_f^2}}\left(\frac{-\Delta}{\varepsilon_f^2}\right) \\ &+ \frac{2\Delta}{2\pi}\frac{2\varepsilon_f}{\varepsilon_f^2+\Delta^2} \\ &= \frac{\Delta}{\Delta_0} - 1 + \frac{2}{\pi}\tan^{-1}\left(\frac{\Delta}{\varepsilon_f}\right) = 0\end{aligned}$$

Now assume E_0 is large and negative, $|E_0| >> D$, then $n_f \simeq 1$ which implies

$$\frac{\Delta_0}{\varepsilon_f}\ln\left(\frac{\varepsilon_f^2+\Delta^2}{D^2}\right) \simeq E_0$$

Define

$$k_b T_a \equiv \sqrt{\varepsilon_f^2+\Delta^2}, \tag{17.49}$$

a typical energy for resonance. Then

$$\begin{aligned}\frac{2\Delta_0}{\pi}\ln\left(\frac{k_B T_A}{D}\right) &= -|E_0| \\ k_B T_A &\simeq D\mathrm{e}^{\frac{-\pi|E_0|}{2\Delta_0}}\end{aligned}$$

$D : 10^4\text{K}$. $k_B T_A : 1\text{K}$ when $|E_0|$ is large. $\varepsilon \simeq k_B T_K$.

If $U = 0$:

$$U_{\text{eff}} = -\frac{2\Delta_0}{\pi} + \frac{2E_0}{\pi}\tan^{-1}\left(\frac{\Delta_0}{E_0}\right) \tag{17.50}$$

$$+ \frac{2\Delta_0}{\pi}\ln\left(\frac{E_0^2+\Delta_0^2}{D^2}\right) \tag{17.51}$$

$\Rightarrow k_B T_k \sim E_0$. Thus, not a small scale. When $|E_0|$ is moderate, $n_f = 1 - \Delta/\Delta_0 < 1$. This means that we have valence-fluctuations on the magnetic impurity. (Valence-fluctuations = charge- and spin-fluctuations) When $|E_0| >> D \Rightarrow n_f \Rightarrow 1$, no longer any valence fluctuations.(Valence-fluctuations = charge fluctuations) What fluctuations are we left with in this limit? The answer is spin fluctuations. The physics is that a local impurity spin causes the spin of a passing conduction band electron to flip. A model that describes such a scattering is the Kondo model:

$$\mathcal{H}_K = \sum_{k,\sigma}\varepsilon_k c_{k\sigma}^\dagger c_{k\sigma} + J\sum_{\substack{k,k'\\ \sigma,\sigma'}}\mathbf{S}\cdot c_{k\sigma}^\dagger \tau_{\sigma\sigma'} c_{k'\sigma'}, \tag{17.52}$$

where the $\tau_{\sigma\sigma'}$ are Pauli-matrices and $\mathbf{S}$ is a localized impurity-spin. Since this modell described the physics of the Anderson-model in the limit $|E_0| >> D$ (called the Kondo-limit), we should be able to derive $\mathcal{H}_K$ from the Anderson-model in this limit. This is show as follows: $|E_0| >> D \implies$ the magnetic impurity is virtually unoccupied.

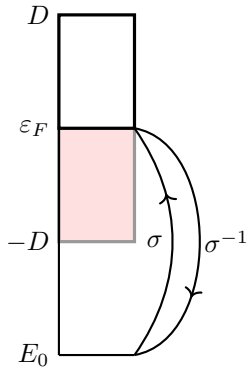


Figure 9: Effect of the coupling

The effect of the coupling V can be taken to the second order in perturbation theory:

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_0 + \mathcal{H}_I \\ \mathcal{H}_0 &= \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + E_0 \sum_\sigma F^\dagger_\sigma F_\sigma \\ \mathcal{H}_I &= V \sum_{k,\sigma} \left(F^\dagger_\sigma c_{k\sigma} + h.c. \right) \end{aligned} \tag{17.53}$$

The second order process in Figure 9 is described by

$$\begin{aligned} -\frac{V^2}{-E_0 + \varepsilon_F} \sum_{k,\sigma} c^\dagger_{k\sigma} F_\sigma \sum_{k',\sigma'} F^\dagger_{\sigma'} c_{k'\sigma'} & \\ = +\frac{V^2}{|E_0|} \sum_{\substack{k,k' \\ \sigma,\sigma'}} F^\dagger_{\sigma'} F_\sigma c^\dagger_{k\sigma} c_{k'\sigma'} & \\ = J \sum_{\substack{k,k' \\ \sigma,\sigma'}} F^\dagger_{\sigma'} F_\sigma c^\dagger_{k\sigma} c_{k'\sigma'} & \\ J = \frac{V^2}{|E_0|} & \end{aligned} \tag{17.54}$$

This will include the spin-flip-process in some way. We will explicitly show that for the $s = 1/2$ case, this has the same form as in the Kondo-model.

$$\begin{aligned}\sum_{\sigma,\sigma'} F^\dagger_{\sigma'} F_\sigma c^\dagger_{k\sigma} c_{k'\sigma'} = &\underbrace{\uparrow\ \uparrow}\cdot\underbrace{\uparrow\ \uparrow}\\ &+\underbrace{\downarrow\ \uparrow}\cdot\underbrace{\downarrow\ \uparrow}\\ &+\underbrace{\uparrow\ \downarrow}\cdot\underbrace{\uparrow\ \downarrow}\\ &+\underbrace{\downarrow\ \downarrow}_{F}\cdot\underbrace{\downarrow\ \downarrow}_{c}\end{aligned}$$

Spin states:

$$|\uparrow\rangle = \begin{pmatrix}1\\0\end{pmatrix} \quad ; \quad |\downarrow\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

The following expression holds, and also correspondingly for the F-sector:

$$\begin{aligned}c^\dagger_\uparrow c_\uparrow |\uparrow\rangle &= |\uparrow\rangle\\ c^\dagger_\uparrow c_\uparrow |\downarrow\rangle &= 0\\ c^\dagger_\downarrow c_\downarrow |\uparrow\rangle &= 0\\ c^\dagger_\downarrow c_\downarrow |\downarrow\rangle &= |\downarrow\rangle\\ c^\dagger_\uparrow c_\downarrow |\uparrow\rangle &= 0\\ c^\dagger_\uparrow c_\downarrow |\uparrow\rangle &= |\uparrow\rangle\\ c^\dagger_\downarrow c_\uparrow |\uparrow\rangle &= |\downarrow\rangle\\ c^\dagger_\downarrow c_\uparrow |\downarrow\rangle &= 0\end{aligned}$$

We can rewrite these expressions as

$$\begin{aligned}c^\dagger_\uparrow c_\uparrow &= \begin{pmatrix}1&0\\0&0\end{pmatrix} = \frac{1}{2}(1+\tau_z)\\ c^\dagger_\downarrow c_\downarrow &= \begin{pmatrix}0&0\\0&1\end{pmatrix} = \frac{1}{2}(1-\tau_z)\\ c^\dagger_\uparrow c_\downarrow &= \begin{pmatrix}0&1\\0&0\end{pmatrix} = \frac{1}{2}(\tau_x + i\tau_y)\\ c^\dagger_\downarrow c_\uparrow &= \begin{pmatrix}0&0\\1&0\end{pmatrix} = \frac{1}{2}(\tau_x - i\tau_y)\end{aligned}$$

$$\begin{aligned}\implies J\sum_{\substack{k,k'\\ \sigma,\sigma'}}\Big[&F^\dagger_{\sigma'}\frac{1}{2}\left(\delta_{\sigma'\sigma}+\tau^z_{\sigma'\sigma}\right)F_\sigma c^\dagger_{k\sigma}\frac{1}{2}\left(\delta_{\sigma\sigma'}+\tau^z_{\sigma\sigma'}\right)c_{k'\sigma'}\\ &+F^\dagger_{\sigma'}\tau^-_{\sigma'\sigma}F_\sigma c^\dagger_{k\sigma}\tau^+_{\sigma\sigma'}c_{k'\sigma'}+F^\dagger_{\sigma'}\tau^+_{\sigma'\sigma}F_\sigma c^\dagger_{k\sigma}\tau^-_{\sigma\sigma'}c_{k'\sigma'}\\ &+F^\dagger_{\sigma'}\frac{1}{2}\left(\delta_{\sigma'\sigma}-\tau^z_{\sigma'\sigma}\right)F_\sigma c^\dagger_{k\sigma}\frac{1}{2}\left(\delta_{\sigma\sigma'}-\tau^z_{\sigma\sigma'}\right)c_{k'\sigma'}\Big]\end{aligned}$$

The terms with $\delta_{\sigma\sigma'}$ are potential scattering, we can ignore these terms.

$$\implies J\sum_{\substack{k,k'\\ \sigma,\sigma'}}\underbrace{F^\dagger_{\sigma'}\vec{\tau}_{\sigma'\sigma}F_\sigma}_{\text{Impurity-spin}}\cdot\underbrace{c^\dagger_{k\sigma}\vec{\tau}_{\sigma\sigma'}c_{k'\sigma'}}_{\text{Electron spin}} \tag{17.55}$$

$J\mathbf{S}\cdot\mathbf{s}$; $\underline{J>0}$. We have an antiferromagnetic coupling. Below T_K, the spin of the conducting electron binds in a singlet state with the impurity spin (in the Kondo-limit) and creates a scattering resonance on the Fermi level. The impurity spin is compensated by the spin in the conducting band. I.e. the conduction band electron screens the impurity spin. When there are few impurity spins relative to the number of electrons within an energy $\sim T_K$ from ε_F, all the impurity spins are screened. The ground state is <u>not</u> magnetically ordered. We instead get a (renormalized) Fermi-liquid. To summarize:

$\underline{T > T_K}$: The conduction band electrons are entirely decoupled from the impurity spins. Weak coupling regime.

$\underline{T < T_K}$: The electron spin and impurity spin coupled in a spin-singlet. Scattering resonance. Strong coupling regime.

18 Anderson lattice-model and Heavy Fermion systems

Assume a metal where we have introduced so many magnetic impurities that we cannon treat them as isolated impurities anymore. We are therefore looking at a itinerant electron-system, coupled to a lattice of Kondo-type impurities, similar to the impurities in the last section. The system is then described by the Anderson lattice-model:

$$H = \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} + E_0 \sum_{i\sigma} F^\dagger_{i\sigma} F_{i\sigma} + U \sum_i F^\dagger_{i\uparrow} F_{i\uparrow} F^\dagger_{i\downarrow} F_{i\downarrow} + \sum_{ik\sigma} V_{k\sigma i} \left(c^\dagger_{k\sigma} F_{i\sigma} + F^\dagger_{i\sigma} c_{k\sigma} \right)$$

this is also a complicated problem, due to the U-term. We set $U = \infty$, as we did before, which means no-double occupancy constraint on each lattice site i. The number of lattice sites are constant, whereas the number of occupants can vary. We define new fermionic and bosonic operators, similarly to what we did before

$$F^\dagger_{i\sigma} = f^\dagger_{i\sigma} b_i$$
$$F_{i\sigma} = f_{i\sigma} b^\dagger_i.$$

We therefore have an extra boson-field, b_i, similar to what we had in the impurity problem, but now for each lattice site i. From this, we get

$$\sum_\sigma F^\dagger_{i\sigma} F_{i\sigma} \leq 1$$
$$\implies Q_i \equiv \sum_\sigma f^\dagger_{i\sigma} f_{i\sigma} + b^\dagger_i b_i = 1.$$

The partition function for $U = \infty$:

$$Z = \int \mathcal{D}c^\dagger \mathcal{D}c \mathcal{D}f^\dagger \mathcal{D}f \mathcal{D}b^\dagger \mathcal{D}b \left(\prod_{i\tau} \delta_{Q_i,1} \right) \mathrm{e}^S$$
$$S = -\sum_{i\sigma} \int_0^\beta \mathrm{d}\tau \left[b^\dagger_i \frac{\partial b_i}{\partial \tau} + f^\dagger_{i\sigma} (\partial_\tau + E_0) f_{i\sigma} \right] - \sum_{k\sigma} \int_0^\beta \mathrm{d}\tau c^\dagger_{k\sigma} (\partial_\tau + \varepsilon_k) c_{k\sigma} - \sum_{k\sigma i} \int_0^\beta \mathrm{d}\tau V_{k\sigma i} \left(c^\dagger_{k\sigma} b^\dagger_i f_{i\sigma} + f^\dagger_{i\sigma} c_{k\sigma} b_i \right)$$

where we have imposed the constraint on both imaginary time τ and the lattice points i.

$$\prod_{i\tau}\delta_{Q_i,1}=\prod_{i\tau}\int_{-\pi}^{\pi}\frac{\mathrm{d}\lambda_i}{2\pi}\mathrm{e}^{-i\sum_i\int_0^\beta \mathrm{d}\tau\lambda_i(Q_i-1)}.$$

Thus we get, as in the impurity problem, an un-constrained partition function,

$$Z=\int\mathcal{D}c^\dagger\mathcal{D}c\mathcal{D}f^\dagger\mathcal{D}f\mathcal{D}b^\dagger\mathcal{D}b\mathcal{D}\lambda\mathrm{e}^{\tilde{S}}$$

$$\begin{aligned}\tilde{S}=&-\sum_{i\sigma}\int_0^\beta\mathrm{d}\tau\left[b_i^\dagger\frac{\partial b_i}{\partial\tau}+f_{i\sigma}^\dagger(\partial_\tau+E_0)f_{i\sigma}\right]-\sum_{k\sigma}\int_0^\beta\mathrm{d}\tau c_{k\sigma}^\dagger(\partial_\tau+\varepsilon_k)c_{k\sigma}\\&-\sum_{k\sigma i}\int_0^\beta\mathrm{d}\tau V_{k\sigma i}\left(c_{k\sigma}^\dagger b_i^\dagger f_{i\sigma}+f_{i\sigma}^\dagger c_{k\sigma}b_i\right)-\sum_i\int_0^\beta\mathrm{d}\tau i\lambda_i\left(\sum_\sigma f_{i\sigma}^\dagger f_{i\sigma}+b_i^\dagger b_i-1\right)\\=&\sum_i\int_0^\beta\mathrm{d}\tau i\lambda_i-\sum_{i\sigma}\int_0^\beta\mathrm{d}\tau\left[b_i^\dagger(\partial_\tau+i\lambda_i)b_i+f_{i\sigma}^\dagger(\partial_\tau+E_0+i\lambda_i)f_{i\sigma}\right]\\&-\sum_{k\sigma}\int_0^\beta\mathrm{d}\tau c_{k\sigma}^\dagger(\partial_\tau+\varepsilon_k)c_{k\sigma}-\sum_{k\sigma i}\int_0^\beta\mathrm{d}\tau V_{k\sigma i}\left(c_{k\sigma}^\dagger b_i^\dagger f_{i\sigma}+f_{i\sigma}^\dagger c_{k\sigma}b_i\right).\end{aligned}$$

Mean field:

$$i\lambda_i\to\lambda\qquad b_i\to b\qquad E_o+i\lambda\to E_0+\lambda\equiv\varepsilon_f$$

The the action becomes

$$\begin{aligned}\tilde{S}=N\beta\lambda-N\beta\lambda b^2-\sum_{i\sigma}\int_0^\beta\mathrm{d}\tau f_{i\sigma}^\dagger(\partial_\tau+\varepsilon_f)f_{i\sigma}-\sum_{k\sigma}\int_0^\beta\mathrm{d}\tau c_{k\sigma}^\dagger(\partial_\tau+\varepsilon_k)c_{k\sigma}\\-\sum_{k\sigma i}\int_0^\beta\mathrm{d}\tau V_{k\sigma i}b\left(c_{k\sigma}^\dagger f_{i\sigma}+f_{i\sigma}^\dagger c_{k\sigma}\right),\end{aligned}$$

where N is the volume, i.e. the number of impurity lattice sites, of the system. Now we approximate the coupling term and Fourier transform the k-part of the f-sector

$$\begin{aligned}\sum_{i\sigma}\int_0^\beta\mathrm{d}\tau f_{i\sigma}^\dagger(\partial_\tau+\varepsilon_f)f_{i\sigma}\to\sum_{k\sigma}\int_0^\beta\mathrm{d}\tau f_{k\sigma}^\dagger(\partial_\tau+\varepsilon_f)f_{k\sigma}\\-\sum_{k\sigma i}\int_0^\beta\mathrm{d}\tau V_{k\sigma i}b\left(c_{k\sigma}^\dagger f_{i\sigma}+f_{i\sigma}^\dagger c_{k\sigma}\right)\to-\sum_{k\sigma}\int_0^\beta\mathrm{d}\tau Vb\left(c_{k\sigma}^\dagger f_{k\sigma}+f_{k\sigma}^\dagger c_{k\sigma}\right).\end{aligned}$$

When we write the model like this, it is essentially a Fourier transformed real-space model with unit cells consisting of $c-$ and $f-$electron orbitals. The

$c-$electrons can jump, whereas the $f-$ electrons cannot, since they are dispersionless. They become mobile, since they are coupled to the $c-$electrons via the matrix element V.

$$\sum_{ij\sigma} t_{cc}^{ij} c_{i\sigma}^\dagger c_{j\sigma} \to \sum_{k\sigma} \varepsilon_k c_{k\sigma}^\dagger c_{k\sigma}$$
$$E_0 \sum_i F_{i\sigma}^\dagger F_{i\sigma} \to E_0 \sum_k F_{k\sigma}^\dagger F_{k\sigma}$$
$$V \sum_i \left(c_i^\dagger F_i + F_i^\dagger c_i \right) \to V \sum_{k\sigma} \left(c_{k\sigma}^\dagger F_{k\sigma} + F_{k\sigma}^\dagger c_{k\sigma} \right)$$

and there are as many lattice sites for the electrons as there are for the impurities. Then we get, in mean field theory

$$Z = \mathrm{e}^{-N\beta\lambda(b^2-1)} \int \mathcal{D}\psi^\dagger \mathcal{D}\psi \mathrm{e}^{S_{MF}}$$
$$S_{MF} = -\sum_{k\sigma} \int_0^\beta \mathrm{d}\tau \psi_{k\sigma}^\dagger A \psi_{k\sigma}$$
$$\psi_{k\sigma} = \begin{pmatrix} c_{k\sigma} \\ f_{k\sigma} \end{pmatrix}$$
$$A = \begin{pmatrix} \partial_\tau + \varepsilon_k & Vb \\ Vb & \partial_\tau + \varepsilon_f \end{pmatrix}$$

$$Z = \mathrm{e}^{-N\beta\lambda(b^2-1)} \mathrm{e}^{\mathrm{Tr}\ln A}$$

$$\mathrm{Tr}\ln A = \sum_{k\sigma} \int_0^\beta \mathrm{d}\tau\, \mathrm{tr}\ln \begin{pmatrix} \partial_\tau + \varepsilon_k & Vb \\ Vb & \partial_\tau + \varepsilon_f \end{pmatrix}$$
$$= \frac{1}{\beta} \sum_{\omega_n} \sum_{k\sigma} \int_0^\beta \mathrm{d}\tau\, \mathrm{tr}\ln \begin{pmatrix} -i\omega_n + \varepsilon_k & Vb \\ Vb & -i\omega_n + \varepsilon_f \end{pmatrix}$$
$$= \sum_{\omega_n} \sum_{k\sigma} \ln\left(i\omega_n - E_k^+\right)\left(i\omega_n - E_k^-\right) = 2 \sum_k \ln\left[\left(1 + \mathrm{e}^{-\beta E_k^+}\right) \left(1 + \mathrm{e}^{-\beta E_k^-}\right) \right]$$
$$E_k^\pm = \frac{1}{2} \left(\varepsilon_k + \varepsilon_f \pm \sqrt{(\varepsilon_k - \varepsilon_f)^2 + 4V^2 b^2} \right)$$
$$f = N\lambda(b^2-1) - \frac{2}{\beta} \sum_k \left[\ln\left(1 + \mathrm{e}^{-\beta E_k^+}\right)\ \ln\left(1 + \mathrm{e}^{-\beta E_k^-}\right) \right]$$

Again this has the form of an electron gas plus a purely bosonic contribution.

We see that the dispersion relations close to the renormalized impurity-surface (ε_f) are very flat. This implies that the quasi-particles have a large

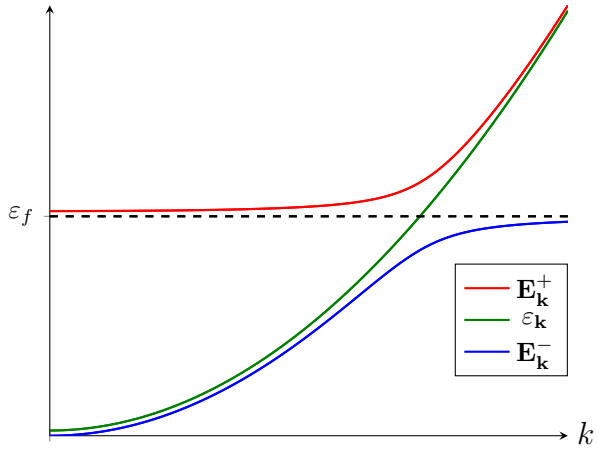


Figure 10: How the dispersion relation changes when $V \neq 0$. NB: All the energy levels relative the Fermi-level.

effective mass.

$$\begin{aligned} Z &= Z_b \cdot Z_f \\ Z_f &= \int \mathcal{D}\psi^\dagger \mathcal{D}\psi e^S \\ S &= -\sum_{k\sigma} \int_0^\beta \mathrm{d}\tau \psi_{k\sigma}^\dagger A \psi_{k\sigma} \end{aligned}$$

This partition function is an effective free-fermion theory with the Hamilton-operator

$$\begin{aligned} H &= \sum_{k\sigma} \psi_{k\sigma}^\dagger \begin{pmatrix} \varepsilon_k & Vb \\ Vb & \varepsilon_f \end{pmatrix} \psi_{k\sigma} \\ S &= -\int_0^\beta \mathrm{d}\tau \left[\sum_{k\sigma} \psi_{k\sigma}^\dagger \frac{\partial \psi_{k\sigma}^\dagger}{\partial \tau} + \psi_{k\sigma}^\dagger H \psi_{k\sigma} \right] \\ &= \sum_{k\sigma} \varphi_{k\sigma}^\dagger \frac{\partial \varphi_{k\sigma}^\dagger}{\partial \tau} + \varphi_{k\sigma}^\dagger D \varphi_{k\sigma} \\ H &= \sum_{k\sigma} E_k^+ \varphi_{k\sigma,+}^\dagger \varphi_{k\sigma,+} + E_k^- \varphi_{k\sigma,-}^\dagger \varphi_{k\sigma,-} \end{aligned}$$

$$\varphi_{k\sigma} = \begin{pmatrix} \varphi_{k\sigma,+} \\ \varphi_{k\sigma,-} \end{pmatrix} \quad D = \begin{pmatrix} E_k^+ & 0 \\ 0 & E_k^- \end{pmatrix}$$

Where we have diagonalized the Hamiltonian. Even when $U \to \infty$, the system is a renormalized free electron gas, maybe with heavy electrons!

In the last section, we proved that ε_f was nailed to the Fermi-surface

$$\varepsilon_f = D\mathrm{e}^{-\frac{\pi|E_0|}{2\Delta_0}} \quad \Delta_0 = \pi\rho_0 V^2.$$

Is this the case in this lattice model? To answer this question, we must solve the stationary point equation.

The physics of the system is determined at the Fermi-surface, or very near. If ε_f is nailed to the Fermi-surface in this case as well, the low-energy excitations (i.e. most important fluctuations) will have a large effective mass: $E_k^{\pm}$ is flat near ε_f. We get a heavy-fermion system from correlation effects, because $\varepsilon_f \approx \varepsilon_F$ when U is large.

Before moving on to the stationary point condition, we will have a look at the propagators of the system.

Fermion propagator:

$$\begin{aligned}
\psi_{k\sigma} &= \begin{pmatrix} c_{k\sigma} \\ f_{k\sigma} \end{pmatrix} \\
G(\tau, \varepsilon_k, \varepsilon_f) &= -\left\langle \psi_{k\sigma}\psi_{k\sigma}^\dagger \right\rangle \\
G^{-1}(\tau, \varepsilon_k, \varepsilon_f) = -A &= -\begin{pmatrix} \partial_\tau + \varepsilon_k & Vb \\ Vb & \partial_\tau + \varepsilon_f \end{pmatrix} \\
G^{-1}(k, i\omega_n) &= -\begin{pmatrix} -i\omega_n + \varepsilon_k & Vb \\ Vb & -i\omega_n + \varepsilon_f \end{pmatrix} \\
G(k, i\omega_n) &= \frac{1}{\det G^{-1}} \begin{pmatrix} i\omega_n - \varepsilon_k & Vb \\ Vb & i\omega_n - \varepsilon_f \end{pmatrix}
\end{aligned}$$

$$\begin{aligned}
\det G^{-1} &= (i\omega_n - \varepsilon_k)(i\omega_n - \varepsilon_f) - s_0^2 = (i\omega_n - E_k^+)(i\omega_n - E_k^-) \\
E_k^{\pm} &= \frac{1}{2}\left(\varepsilon_k + \varepsilon_f \pm \sqrt{(\varepsilon_k - \varepsilon_f)^2 + 4s_0^2}\right)
\end{aligned}$$

$$\begin{aligned}
G_{cc}(k, i\omega_n) &= -\left\langle c_{k\sigma}c_{k\sigma}^\dagger \right\rangle = \frac{i\omega_n - \varepsilon_f}{(i\omega_n - E_k^+)(i\omega_n - E_k^-)} \\
G_{ff}(k, i\omega_n) &= -\left\langle f_{k\sigma}f_{k\sigma}^\dagger \right\rangle = \frac{i\omega_n - \varepsilon_k}{(i\omega_n - E_k^+)(i\omega_n - E_k^-)}
\end{aligned}$$

$$G_{cf} = G_{fc} = -\left\langle c_{k\sigma} f^\dagger_{k\sigma} \right\rangle = \frac{s_0}{(i\omega_n - E^+_k)(i\omega_n - E^-_k)} = 0 \quad (V = 0).$$

When the hybridization term is 0, the vertices connecting $c-$ and $f-$field are 0, and hence the probability of a $c-$fermion changing to a $f-$fermion is 0.

$V = 0$:

$$G_{cc}(k, i\omega_n) = -\left\langle c_{k\sigma} c^\dagger_{k\sigma} \right\rangle = \frac{i\omega_n - \varepsilon_f}{(i\omega_n - \varepsilon_k)(i\omega_n - \varepsilon_f)} = \frac{1}{i\omega_n - \varepsilon_k}$$
$$G_{ff}(k, i\omega_n) = -\left\langle f_{k\sigma} f^\dagger_{k\sigma} \right\rangle = \frac{i\omega_n - \varepsilon_k}{(i\omega_n - \varepsilon_k)(i\omega_n - \varepsilon_f)} = \frac{1}{i\omega_n - \varepsilon_f}$$

In this case, the $f-$fermions are dispersionless, which means that they are localized, as expected. The effect of U is only present in G_{ff}: $E_0 \to \varepsilon_f$. We can write these propagators on Fermi-liquid form, even when $V \neq 0$. We show this looking at G_{cc}:

$$G_{cc}(k, i\omega_n) = -\left\langle c_{k\sigma} c^\dagger_{k\sigma} \right\rangle = \frac{i\omega_n - \varepsilon_f}{(i\omega_n - E^+_k)(i\omega_n - E^-_k)} = \frac{A}{i\omega_n - E^+_k} + \frac{B}{i\omega_n - E^-_k}$$
$$\implies (A + B)i\omega_n - (BE_k k + AE^-_k) = i\omega_n - \varepsilon_f.$$

By using $A + B = 1$, we get the following expressions for A and B using the equation above.

$$A = \frac{1}{2}\left(1 + \frac{\varepsilon_k - \varepsilon_f}{\sqrt{(\varepsilon_k - \varepsilon_f)^2 + 4s_0^2}}\right) \quad B = \frac{1}{2}\left(1 - \frac{\varepsilon_k - \varepsilon_f}{\sqrt{(\varepsilon_k - \varepsilon_f)^2 + 4s_0^2}}\right)$$

In the limit $s_0 \ll |\varepsilon_k - \varepsilon_f|$, we get $A \approx 1, B \approx 0$. And in the limit $s_0 \ll |\varepsilon_k - \varepsilon_f|, \varepsilon_k - \varepsilon_f < 0$, we get the opposite. In addition, $E^+_k \approx \varepsilon_k$ and $E^-_k \approx \varepsilon_f$ under these considerations, and we get the desired Fermi-liquid (simple pole) form in both cases

$$G_{cc}(k, i\omega_n) \approx \frac{1}{i\omega_n - \varepsilon_k} \quad G_{ff}(k, i\omega_n) \approx \frac{1}{i\omega_n - \varepsilon_f}, \quad \varepsilon_k - \varepsilon_f > 0$$
$$G_{cc}(k, i\omega_n) \approx \frac{1}{i\omega_n - \varepsilon_f} \quad G_{ff}(k, i\omega_n) \approx \frac{1}{i\omega_n - \varepsilon_k}, \quad \varepsilon_k - \varepsilon_f < 0.$$

Free energy per unit cell:

$$f = -\lambda(1 - b^2) - \frac{2}{\beta N}\sum_k \ln\left(1 + \mathrm{e}^{-\beta E^+_k}\right)\ln\left(1 + \mathrm{e}^{-\beta E^-_k}\right)$$
$$= -(\varepsilon_f - E_0)\left(1 - \frac{\Delta}{\Delta_0}\right) - \frac{2}{\beta N}\sum_k \ln\left(1 + \mathrm{e}^{-\beta E^+_k}\right)\ln\left(1 + \mathrm{e}^{-\beta E^-_k}\right),$$

where N is the number of unit cells/lattice points.

$$\frac{\partial f}{\partial \varepsilon_f} = 0 = -1 + \frac{\Delta}{\Delta_0} + \frac{2}{N}\sum_k \left[\frac{\partial E_k^-}{\partial \varepsilon_f} f(E_k^-) + \frac{\partial E_k^+}{\partial \varepsilon_f} f(E_k^+)\right]$$

$$\frac{\partial f}{\partial \Delta} = 0 = \frac{\varepsilon_f - E_0}{\Delta_0} + \frac{2}{N}\sum_k \left[\frac{\partial E_k^-}{\partial \Delta} f(E_k^-) + \frac{\partial E_k^+}{\partial \Delta} f(E_k^+)\right]$$

$$-\frac{\partial f}{\partial \mu} = \frac{2}{N}\sum_k \left[f(E_k^-) + f(E_k^+)\right] = n = n_f + n_c.$$

The Kondo limit:

$$n_f = 1 - \frac{\Delta}{\Delta_0} \approx 1$$

$$\frac{\varepsilon_f - E_0}{\Delta_0} + 2\sum_{k<k_F} \frac{-1}{\pi\rho_0} \frac{1}{\sqrt{(\varepsilon_k - \varepsilon_f)^2 + s_0^2}} = 0$$

$$\frac{\varepsilon_f - E_0}{\Delta_0} \approx \frac{-2}{2D}\int_{-D}^{\mu} \frac{\mathrm{d}\varepsilon}{\varepsilon - \varepsilon_f} = -\frac{1}{D}\ln\left(\frac{\mu - \varepsilon_f}{-D - \varepsilon_f}\right)$$

$$\approx -\frac{1}{D}\ln\left(\frac{\varepsilon_f - \mu}{D}\right) = -2\rho_0 \ln\left(\frac{\varepsilon_f - \mu}{D}\right)$$

$\varepsilon_f \ll E_0$:

$$-\frac{\pi|E_0|}{2\Delta_0} \approx \ln\left(\frac{T_K}{D}\right)$$

$$T_K = D\mathrm{e}^{-\frac{\pi|E_0|}{2\Delta_0}}$$

ε_f near the Fermi-level implies that the quasi-particles have a large effective mass, typically in the range $m^* \approx 1000m$ when $U \to \infty$.

From this analysis, we can conclude that the system is effectively an electron gas with strongly renormalized quasi-particles. The quasi-particles are a linear combination of $c-$ and $f-$ fermions. The larger the value of $|E_0|$, the smaller the difference $\varepsilon_f - \varepsilon_F$ becomes. Since the $f-$fermions originally were localized, i.e. effectively infinite mass, the quasi-particles become more and more heavy as $|E_0|$ increase. In the Kondo regime, the mass becomes extremely large, $m^* \approx 1000m$. Even tho the mass becomes so large, the Fermi-liquid picture survives in $d = 3$. If $U = 0$, this effect vanishes, because the renormalization of the f-level wouldn't have taken place.

In the past sections, we've looked at a few examples of what is known as bosonization of fermion-theories, some with weak attractive interactions and some with strong repulsive interactions.

- Weak attractive interactions: BCS-theory, unstable electron gass picture.

- Strong repulsive interactions between fermions: Hubbard model, Anderson model, Anderson models, Kondo model. In these cases, the systems renormalize to free electron gasses even in the limit $U \to \infty$. They are Fermi liquids. In the next sections, we will have a look bosonization of 1-dimensional systems. We will see that arbitratily small interactions in these cases will destroy the Fermi-picture. The systems becomes a new type of metallic system - a new renormalization fixpoint called Luttinger liquid! Here the fermionic, single-particle picture we are intuitively familiar with is completely altered into a picture dominated by effective bosons, rather than fermions. There are no single-particle excitations, only collective bosonic excitations.

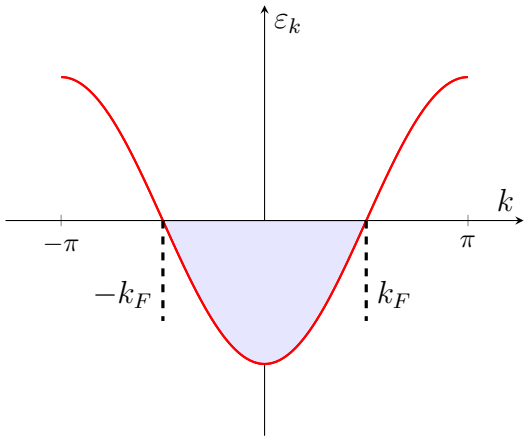


Figure 11: Dispersion relation. The fermi surface consists of two points

19 Interacting one-dimensional fermionic systems

19.1 1D interacting model

We model the system by $\mathcal{H} = H_0 + H_I$ as usual. Consider first H_0

$$\begin{aligned} \mathcal{H}_0 &= \sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} \\ &\Longrightarrow \sum_{k\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma} \end{aligned}$$

We are mainly interested in the low energy physics for this problem; We want to describe ε_k in the vicinity of the Fermi level. In this case, it is especially simple as it only consists of two points, as seen in Figure 11.

Right-moving: $k > 0$ and left-moving: $k < 0$. For both of which we have $\varepsilon_k \simeq V_F(|k| - k_F)$ and $|k - k_F| << k_F$. ε_k is here measured relative the Fermi level. For every electron spin σ we have one type of righ-moving and one type of left-moving fermions, seen in Figure 12.

$$\begin{aligned} \mathcal{H}_0 \simeq &\sum_{k,\sigma} V_F(k - k_F) c^\dagger_{1k\sigma} c_{1k\sigma} \\ &+ \sum_{k,\sigma} V_F(-k - k_F) c^\dagger_{2k\sigma} c_{2k\sigma}, \end{aligned} \tag{19.1}$$

where $c^\dagger_{1k\sigma}$ creates a right-moving fermion and $c^\dagger_{2k\sigma}$ creates a left-moving fermion

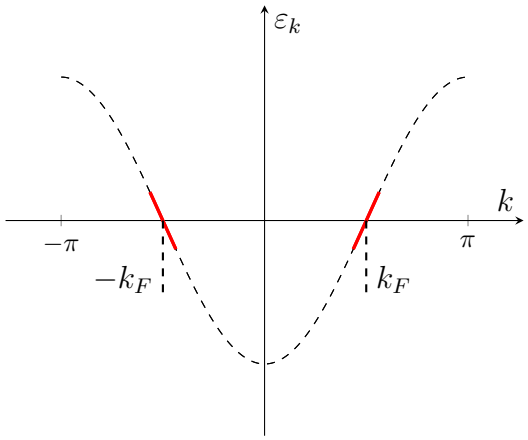


Figure 12: The right- and left-moving fermions of interest.

etc. NB: 19.1 is defined only at $|\pm k - k_F| << k_F$! We write this as

$$\mathcal{H} = \sum_{k,\sigma} \Big[\mathrm{e}^{-\alpha|k-k_F|} V_F(k-k_F) c^\dagger_{1k\sigma} c_{1k\sigma} + \mathrm{e}^{-\alpha|k-k_F|} V_F(-k-k_F) c^\dagger_{2k\sigma} c_{2k\sigma} \Big] . \tag{19.2}$$

Here, α is a cutoff-parameter to limit the k-summation to those who are close to Fermi level, but in such a way that we can sum over all k.

19.2 Free fermion propagators

19.3 Propagators in the interacting case

19.4 The phase factor

19.5 The bosonic excitation spectrum

19.6 Impulse distribution

19.7 "Summary"

20 Spin-charge separation of fermions

21 Appendix