Lecture notes FY8305

August, 2019

Digitialized from "FAG 74986 Funksjonal-integral metoder HØST 1996". Used as lecture notes for self-study in the course "FY8305 - Functional Integral Methods in Condensed Matter Physics". **Link to course page**

Contributors to the project

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Contents

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 (9.28).
- The limits in (10.8) 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

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

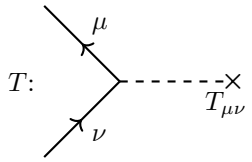


Figure 1: Scattering from an external potential $v_{\mu\nu}c_\mu^\dagger c_\nu$

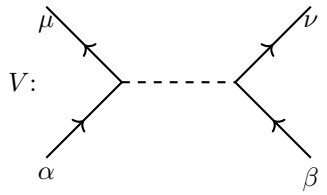


Figure 2: Exchange interaction between two particles.

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:

3.1.1 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.**

3.1.2 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

3.2.1 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.

3.2.2 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

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

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

3.2.3 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.

3.2.4 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".

3.2.5 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 $|\phi\rangle$

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

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

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

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

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

4.2.1 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:

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

4.2.2 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

5.2.1 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.

5.2.2 Overlap

The overlap between two coherent fermion states:

$$\begin{aligned}\langle\psi|\psi'\rangle &= \langle 0|\prod_{\mu,\nu}\left(1+\xi_\nu^* c_\nu\right)\left(1-\xi_\mu c_\mu^\dagger\right)|0\rangle \\ &= \prod_{\mu,\nu}\langle 0|\left(1+\xi_\nu^* c_\nu \xi_\mu c_\mu^\dagger\right)|0\rangle \\ &= \prod_{\nu\neq\mu}\cdot 1 \prod_\mu\left(1+\xi_\mu^*\xi_\mu\right) \\ &= \prod_\mu\left(1+\xi_\mu^*\xi_\mu\right) \\ \text{Re-exponentiation} \implies \langle\psi|\psi'\rangle &= \mathrm{e}^{\sum_\mu \xi_\mu^*\xi_\mu}.\end{aligned}$$

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

5.2.3 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 therefor 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:

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

Fermions:

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

Common notation:

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

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 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

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

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 $\ln\left(\partial_\tau + \varepsilon_k\right)$

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

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

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

such that

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

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.

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

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

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

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

$$= \mathrm{e}^{\sum_{k,\sigma} \sum_{\omega_n} \ln(-i\omega_n+\varepsilon_k)} \tag{9.17}$$

$$= \prod_{k,\sigma} \mathrm{e}^{\sum_{\omega_n} \ln(-i\omega_n+\varepsilon_k)}. \tag{9.18}$$

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

$$f(z) = \frac{1}{1+\mathrm{e}^{\beta z}} \tag{9.19}$$

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

$$\oint \mathrm{d}z\, g(z) = 2\pi i \,\mathrm{Res}\left[g(z_0)\right] \tag{9.20}$$

$$\mathrm{Res}\left[g(z_0)\right] = \lim_{z\to z_0}\left[(z-z_0)g(z)\right] \tag{9.21}$$

So for the Fermi distribution in (9.19), we get

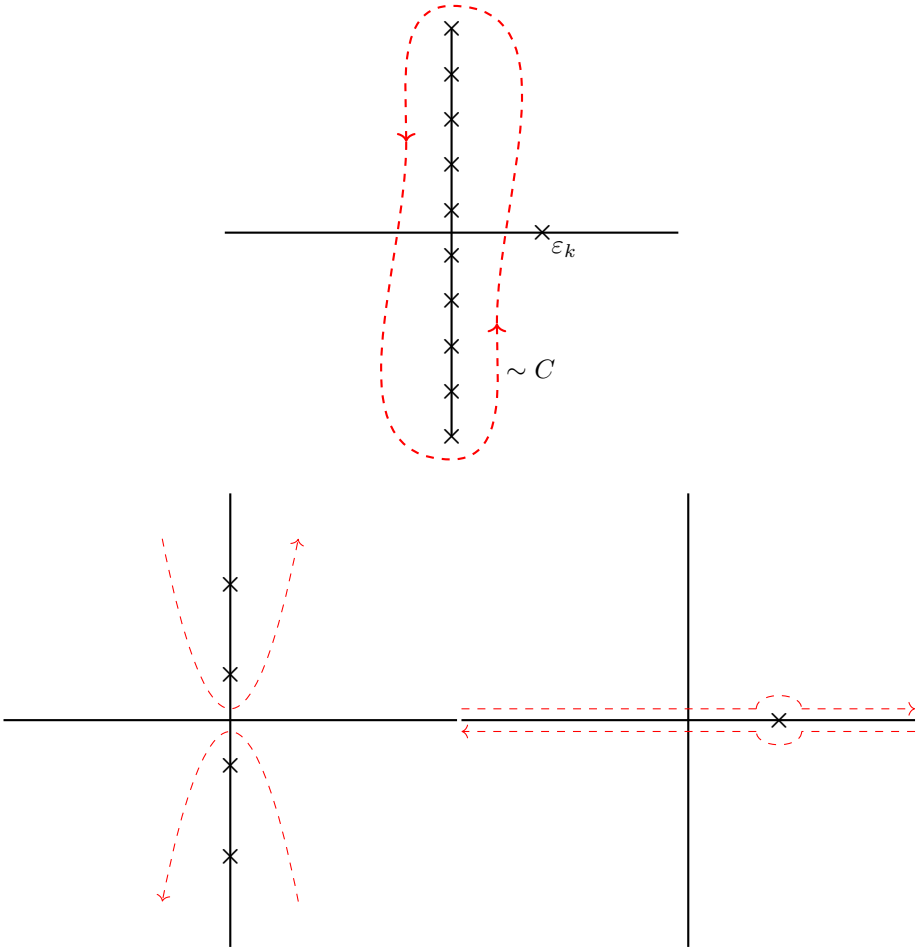
$$\begin{aligned}
\mathrm{Res}\left[f(i\omega_n)\right] &= \lim_{z\to i\omega_n}\left[(z-i\omega_n)f(z)\right] \\
\lim_{z\to i\omega_n} &= \lim_{z\to i\omega_n} \frac{1}{1+\mathrm{e}^{\beta(z-i\omega_n+i\omega_n)}} \\
&= \lim_{z\to i\omega_n} \frac{1}{1-\mathrm{e}^{\beta(z-i\omega_n)}} \\
&= \frac{1}{1-1-\beta(z-i\omega_n)+\ldots} \\
&= -\frac{1}{\beta}\frac{1}{z-i\omega_n} \implies \\
\mathrm{Res}\left[f(i\omega_n)\right] &= -\frac{1}{\beta}
\end{aligned} \tag{9.22}$$

We then have

$$\oint \mathrm{d}z\, f(z) = 2\pi i \,\mathrm{Res}\, f(z_0) \tag{9.23}$$

$$= -\frac{2\pi i}{\beta} \implies \tag{9.24}$$

$$\sum_{\substack{i\omega_n \\ \omega_n \mathrm{odd}}} g(i\omega_n) = -\frac{\beta}{2\pi i}\oint \mathrm{d}z\, g(z)f(z) \equiv I \tag{9.25}$$



where the path encloses all simple poles of the Fermi distribution (9.19) and

$$g(i\omega_n) = \ln(-i\omega_n + \varepsilon_k) \tag{9.26}$$

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

$$\tilde{I} = \frac{\beta}{2\pi i} \int_{-\infty}^{\infty} \mathrm{d}\varepsilon \left[f(\varepsilon + i\delta) \ln\left(-\varepsilon - i\delta + \varepsilon_k\right) - f(\varepsilon - i\delta) \ln\left(-\varepsilon + i\delta + \varepsilon_k\right) \right]. \tag{9.27}$$

2

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

This is equal to

$$\tilde{I} = \frac{\beta}{2\pi i} \int_{-\infty}^{\infty} \mathrm{d}\varepsilon \, f(\varepsilon) \left[\ln(-\varepsilon - i\delta + \varepsilon_k) - \ln(-\varepsilon + i\delta + \varepsilon_k) \right]. \tag{9.28}$$

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.

$$\begin{aligned} &\ln(-\varepsilon - i\delta + \varepsilon_k) - \ln(-\varepsilon + i\delta + \varepsilon_k) \\ &= \ln|-\varepsilon + \varepsilon_k| + i\pi^- - \ln|-\varepsilon + \varepsilon_k| - i\pi^+ \\ &= i(\pi^- - \pi^+) = 0^3 \end{aligned} \tag{9.29}$$

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.

$$\begin{aligned} &\ln(-\varepsilon - i\delta + \varepsilon_k) - \ln(-\varepsilon + i\delta + \varepsilon_k) \\ &= \ln|-\varepsilon + \varepsilon_k| - \ln|-\varepsilon + \varepsilon_k| + i \cdot 0 - 2\pi i = -2\pi i \end{aligned} \tag{9.30}$$

Now we can return to the integral

$$\tilde{I} = -\frac{2\pi i}{2\pi i}\beta \int_{\varepsilon_k}^{\infty} \mathrm{d}\varepsilon \, f(\varepsilon) \tag{9.31}$$

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

$$= -\beta \int_{\varepsilon_k}^{\infty} \mathrm{d}\varepsilon \, \frac{\mathrm{e}^{-\beta\varepsilon}}{1 + \mathrm{e}^{-\beta\varepsilon}} \tag{9.33}$$

$$= \int_{\varepsilon_k}^{\infty} \mathrm{d}\varepsilon \, \frac{\mathrm{d}}{\mathrm{d}\varepsilon} \ln\left(1 + \mathrm{e}^{-\beta\varepsilon}\right) \tag{9.34}$$

$$= -\ln\left(1 + \mathrm{e}^{-\beta\varepsilon_k}\right). \tag{9.35}$$

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

$$I = \sum_{\omega_n} \ln(-i\omega_n + \varepsilon_k) = \ln\left(1 + \mathrm{e}^{-\beta\varepsilon_k}\right). \tag{9.36}$$

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

$$\begin{aligned} \mathcal{Z} &= \mathrm{e}^{\sum_{k\sigma}\sum_{\omega_n}\ln(-i\omega_n+\varepsilon_k)} = \mathrm{e}^{\sum_{k\sigma}\ln\left(1+\mathrm{e}^{-\beta\varepsilon_k}\right)} \\ &= \prod_{k,\sigma}\left(1 + \mathrm{e}^{-\beta\varepsilon_k}\right). \end{aligned} \tag{9.37}$$

Equation (9.37) is a well known result for fermions. This is the partition function for a free fermion gas with Hamiltonian

$$\mathcal{H} = \sum_{k,\sigma} \varepsilon_k c^\dagger_{k\sigma} c_{k\sigma}. \tag{9.38}$$

10 Free Boson gas

Page 85 in the pdf (63 in notes).

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

$$\mathcal{H} = \sum_q \omega_q a_q^\dagger a_q \tag{10.1}$$

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

$$\mathcal{Z} = \int \mathcal{D}\left[\varphi^*(\tau)\right] \mathcal{D}\left[\varphi(\tau)\right] \mathrm{e}^{\mathcal{S}}. \tag{10.2}$$

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

$$\mathcal{S} = -\sum_q \int_0^\beta \mathrm{d}\tau\, \varphi_q^*(\tau) \left(\partial_\tau + \omega_q\right) \varphi_q(\tau) \tag{10.3}$$

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

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

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

We thus have to find a local expression for

$$\ln(\partial_\tau + \omega_q). \tag{10.4}$$

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

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

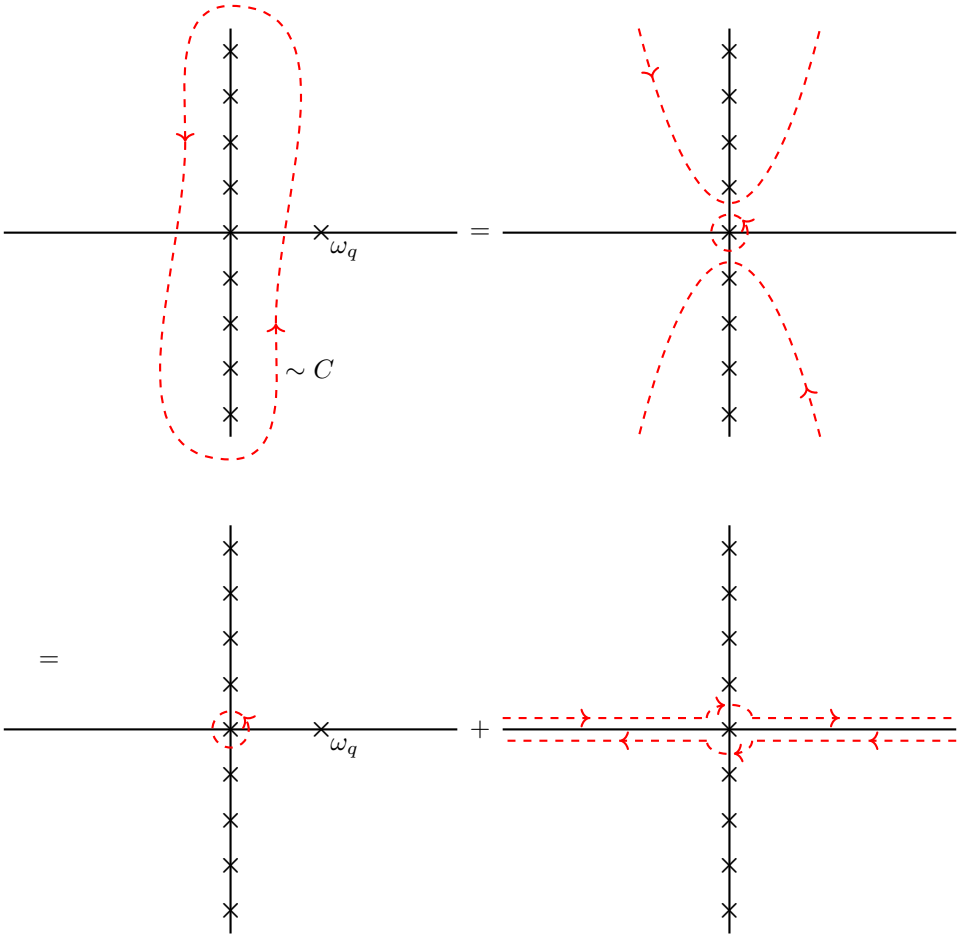
$$\omega_\nu = \frac{2\nu\pi}{\beta}$$

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

$$\mathcal{Z} = \mathrm{e}^{-\sum_q \sum_{\omega_\nu} \ln(-i\omega_\nu + \omega_q)} \tag{10.5}$$



To compute (10.5), we need a result for

$$\sum_{\omega_\nu} \ln(-i\omega_\nu + \omega_q). \tag{10.6}$$

Using the same technique as we did in section 9, we observe that $i\omega_\nu$ are poles in the Bose-Einstein distribution

$$b(z) = \frac{1}{\mathrm{e}^{\beta z} - 1}, \tag{10.7}$$

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 $g(i\omega_\nu) = \ln(-i\omega_\nu + \omega_q)$

$$\begin{aligned}\sum_{\omega_\nu} g(i\omega_\nu) &= +\frac{\beta}{2\pi i}\oint_{\mathcal{C}} \mathrm{d}z\, g(z)b(z) \\ &= \frac{\beta}{2\pi i}\int_{-\infty}^{0^-} \mathrm{d}\varepsilon\, b(\varepsilon)\left[\ln(-\varepsilon - i\delta + \omega_q) - \ln(-\varepsilon + i\delta + \omega_q)\right] \\ &+ \frac{\beta}{2\pi i}\int_{0^+}^{\omega_q} \mathrm{d}\varepsilon\, b(\varepsilon)\left[\ln(-\varepsilon - i\delta + \omega_q) - \ln(-\varepsilon + i\delta + \omega_q)\right] \\ &= \beta\int_{\omega_q}^{\infty} \mathrm{d}\varepsilon\, b(\varepsilon)\left[\ln(-\varepsilon - i\delta + \omega_q) - \ln(-\varepsilon + i\delta + \omega_q)\right] \qquad (10.8)\end{aligned}$$

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 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

$$\begin{aligned}\mathcal{Z} &= \mathrm{e}^{-\sum_q \sum_{\omega_\nu} \ln(-i\omega_\nu+\omega_q)} \\ &= \mathrm{e}^{-\sum_q \ln\left(1-\mathrm{e}^{-\beta\omega_q}\right)} \\ &= \prod_q \frac{1}{1-\mathrm{e}^{-\beta\omega_q}} \qquad (10.9) \\ &= \mathrm{e}^{-\beta F}.\end{aligned}$$

We recognize (10.9) as the partition function for a free boson gas, with free energy

$$F = \frac{1}{\beta}\sum_q \ln\left(1-\mathrm{e}^{-\beta\omega_q}\right). \qquad (10.10)$$

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 $\mathrm{Tr}\, A(\partial_\tau)$. In addition, the methods are familiar for interacting problems, which we will consider later.

11 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

$$A = \begin{pmatrix} \delta a^\dagger \\ \delta a \end{pmatrix}, A^\dagger = \begin{pmatrix} \delta a & \delta a^\dagger \end{pmatrix} \tag{11.1}$$

$$\begin{aligned} \mathcal{S}_{\text{eff}} &\simeq \mathcal{S}_{\text{MF}} - \sum_q A^\dagger D^{-1}(q) A \\ \mathcal{Z} &\simeq \mathrm{e}^{\mathcal{S}_{\text{MF}}} \int \mathcal{D}A^\dagger \mathcal{D}A \mathrm{e}^{-\sum_q A^\dagger D^{-1} A} \\ \mathcal{Z} &= \mathrm{e}^{\mathcal{S}_{\text{MF}}} \mathrm{e}^{-\operatorname{Tr}\ln D^{-1}} \end{aligned} \tag{11.2}$$

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

$$F = F_{\text{MF}} + \frac{1}{\beta} \operatorname{Tr}\ln D^{-1}. \tag{11.3}$$

We can now correct the mean field values for $a, a^\dagger$ by minimizing (11.3) with respect to $a, a^\dagger$.

$$\frac{\partial F}{\partial a} = 0 = \frac{\partial F_{\text{MF}}}{\partial a} + \underbrace{\frac{\partial}{\partial a}\left(\frac{1}{\beta} \operatorname{Tr}\ln D^{-1}\right)}_{\text{Correction term}}. \tag{11.4}$$

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.

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

Consider the Hamiltonian

$$\mathcal{H} = -\sum_{i,j} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} - \mu \sum_{i,\sigma} n_{i\sigma}. \tag{12.1}$$

At $\underline{U = 0}$, the Hamiltonian (12.1) transforms to

$$\mathcal{H} = \sum_{k,\sigma} (\varepsilon_k - \mu)\, c^\dagger_{k\sigma} c_{k\sigma} \tag{12.2}$$

with nearest neighbour hopping

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

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

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

$$\mathcal{H} = -\sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} \tag{12.3}$$

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

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

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

12.1 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

$$X_i^{\alpha\beta} = |\alpha, i\rangle\langle\beta, i|\,. \tag{12.4}$$

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

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 (12.1) that we can drop the operators involving doubly occupied states $X_i^{-\sigma 2}, X_i^{2-\sigma}$ such that we can write[5]

$$c_{i\sigma} = X_i^{0\sigma} \tag{12.5}$$

$$c_{j\sigma}^\dagger = X_j^{\sigma 0} \tag{12.6}$$

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

$$\mathcal{H} = -t \sum_{i,j,\sigma} X_i^{\sigma 0} X_j^{0\sigma} \tag{12.7}$$

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 (12.4), these are

$$\begin{aligned} \left[X_i^{\alpha\beta}, X_j^{\gamma\eta} \right]_\pm &= |\alpha i\rangle \langle \beta i | \gamma j \rangle \langle \eta j | \pm | \gamma j \rangle \langle \eta j | \alpha i \rangle \langle \beta i | \\ &= \delta_{ij} \delta_{\beta\gamma} X_i^{\alpha\eta} \pm \delta_{ij} \delta_{\eta\alpha} X_j^{\gamma\beta} \\ &= \delta_{ij} \left[\delta_{\beta\gamma} X_i^{\alpha\eta} \pm \delta_{\eta\alpha} X_i^{\gamma\beta} \right] \end{aligned} \tag{12.8}$$

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.

$$\begin{aligned}\left[X_i^{0\sigma}, X_i^{\sigma' 0}\right]_+ &= X_i^{0\sigma} X_i^{\sigma' 0} + X_i^{\sigma' 0} X_i^{0\sigma} \\ &= \delta_{\sigma\sigma'} X_i^{00} + X_i^{\sigma'\sigma} \\ &= \delta_{\sigma\sigma'} b_i^\dagger b_i + f_{i\sigma}^\dagger f_{i\sigma'}\end{aligned} \tag{12.9}$$

Or,using the representations directly:

$$\begin{aligned}\left[b_i^\dagger f_{i\sigma}, f_{i\sigma'}^\dagger b_i\right]_+ &= f_{i\sigma'}^\dagger f_{i\sigma}\left(1 + b_i^\dagger b_i\right) + b_i^\dagger b_i\left(\delta_{\sigma\sigma'} - f_{i\sigma'}^\dagger f_{i\sigma}\right) \\ &= \delta_{\sigma\sigma'} b_i^\dagger b_i + f_{i\sigma'}^\dagger f_{i\sigma} \\ &= \delta_{\sigma\sigma'} X_i^{00} + X_i^{\sigma'\sigma}.\end{aligned} \tag{12.10}$$

We see that (12.9) and (12.10) are equal and thus this representation gives the correct commutation relations. We still have the completeness relation

$$\begin{aligned}1 &= \sum_\alpha |\alpha i\rangle\langle\alpha i| \\ &= X_i^{00} + \sum_\sigma X_i^{\sigma\sigma} \\ &= b_i^\dagger b_i + \sum_\sigma f_{i\sigma}^\dagger f_{i\sigma}\end{aligned} \tag{12.11}$$

12.2 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 (12.5), $c_{i\sigma}^\dagger = X_i^{\sigma 0} \Leftrightarrow f_{i\sigma}^\dagger b_i$ 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

$$b_i^\dagger b_i + \sum_\sigma f_{i\sigma}^\dagger f_{i\sigma} = 1, \tag{12.12}$$

which is now a leading constraint expressed with an equality.

The Hamiltonian (12.7)of the problem is written on the form

$$\mathcal{H} = -\sum_{i,j,\sigma} t_{ij} f_{i\sigma}^\dagger b_i b_j^\dagger f_{j\sigma}. \tag{12.13}$$

Equations (12.12) and (12.13) define our problem, which we are to solve. Define

$$Q_i \equiv \sum_\sigma f_{i\sigma}^\dagger f_{i\sigma} + b_i^\dagger b_i \tag{12.14}$$

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

$$\prod_{i,\tau} \int_{-\pi}^{\pi} \frac{\mathrm{d}\lambda_i}{2\pi} \mathrm{e}^{-i\int_0^\beta \lambda_i(\tau)(Q_i-1)\mathrm{d}\tau} = \prod_{i,\tau} \delta_{Q_i,1} \tag{12.15}$$

The partition function is given by

$$\mathcal{Z} = \int \mathcal{D}\varphi^* \mathcal{D}\varphi \mathcal{D}b^* \mathcal{D}b \left(\prod_i \prod_\tau \delta_{Q_i,1} \right) \mathrm{e}^{\mathcal{S}} \tag{12.16}$$

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

$$\begin{aligned} \mathcal{S} = &- \sum_{i,\sigma} \int_0^\beta \mathrm{d}\tau \left[\underbrace{b_i^* \frac{\partial b_i}{\partial \tau}}_{\text{NB!}} + \varphi_{i\sigma}^* \frac{\partial \varphi_{i\sigma}}{\partial \tau} \right] \\ &+ \sum_{i,j,\sigma} \int_0^\beta \mathrm{d}\tau\, \varphi_{i\sigma}^*(\tau) b_i(\tau) t_{ij} b_j^*(\tau) \varphi_{j\sigma}(\tau) \end{aligned} \tag{12.17}$$

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 (12.17) as

$$\begin{aligned} \mathcal{S} = &- \sum_i \int_0^\beta \mathrm{d}\tau\, b_i^* \frac{\partial b_i}{\partial \tau} \\ &- \sum_{i,j,\sigma} \int_0^\beta \mathrm{d}\tau\, \varphi_{i\sigma}^* \left(\partial_\tau \delta_{ij} - t_{ij} b_i b_j^* \right) \varphi_{j\sigma}. \end{aligned} \tag{12.18}$$

Now introduce Abrikosov's trick

$$\mathcal{Z} = \int \mathcal{D}\varphi^* \mathcal{D}\varphi \mathcal{D}b^* \mathcal{D}b \mathcal{D}\lambda\, \mathrm{e}^{\tilde{\mathcal{S}}} \tag{12.19}$$

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

[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!

$$\mathcal{Z} = \int \mathcal{D}b^\dagger \mathcal{D}b \mathcal{D}\lambda \mathrm{e}^{\mathcal{S}_{\mathrm{eff}}[b^\dagger, b, \lambda]}, \tag{12.20}$$

with

$$\begin{aligned} \mathcal{S}_{\mathrm{eff}} = &- \sum_i \int_0^\beta \mathrm{d}\tau \, b_i^\dagger \left(\partial_\tau + i\lambda\right) b_i + i \sum_i \int_0^\beta \mathrm{d}\tau \, \lambda_i \\ &+ \mathrm{Tr} \ln \mathcal{G}^{-1} \end{aligned} \tag{12.21}$$

$$\mathcal{G}^{-1} = \left(\partial_\tau + i\lambda_i\right) \delta_{ij} - t_{ij} b_i b_i^\dagger \tag{12.22}$$

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).

$$\mathcal{G}^{-1} = (\partial_\tau + \lambda)\delta_{ij} - |b|^2 t_{ij}. \tag{12.23}$$

To compute (12.23), 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

$$\mathrm{Tr} \ln \mathcal{G}^{-1} = \frac{1}{\beta} \sum_{k, \omega_n} \ln(-i\omega_n + \varepsilon_k) \tag{12.24}$$

$$= \frac{1}{\beta} \sum_{k, \omega_n} \ln(i\omega_n - \varepsilon_k), \tag{12.25}$$

$$\varepsilon_k = -2tb^2 \sum_i \cos(k_i) + \lambda, \tag{12.26}$$

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

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

12.3 Mean-field

$$\mathcal{G}^{-1} = -i\omega_n + \varepsilon_k \tag{12.27}$$

$$\mathcal{G}_F(k, i\omega) = \frac{1}{i\omega - \varepsilon_k} = -\left\langle \varphi\varphi^\dagger \right\rangle \tag{12.28}$$

where

$$\varepsilon_k = -2tb^2\gamma_k - (\mu + \lambda). \tag{12.29}$$

$\mathcal{G}_F(k, i\omega)$: 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".