Chapter 5

Path integrals in second quantisation

5.1 Bosons

We now want to discuss how to write down path integrals for many-particle systems in second quantisation. For technical reasons we will not consider the full propagator, i.e. arbitrary matrix elements of the time evolution operator $e^{-\frac{i}{\hbar}\hat{H}t}$, but only its **trace**. We will start by discussing this trace in standard single-particle quantum mechanics, where it can be obtained by integrating as in

$$\text{tr } e^{-\frac{i}{\hbar}\hat{H}t} = \int d^n r \left\langle \boldsymbol{r} \middle| e^{-\frac{i}{\hbar}\hat{H}t} \middle| \boldsymbol{r} \right\rangle = \int d^n r K(\boldsymbol{r}, \boldsymbol{r}, t).$$

If we were using a discrete basis we would instead compute the trace by summing over diagonal elements labelled by integers; here we are using a continuous basis and hence the sum has to be replaced by an integral.

Motivation. To illustrate that the trace of the time-evolution operator is a natural quantity to look at we give two examples:

- We have seen that in *Statistical Mechanics* the partition function (for the canonical ensemble)
$$\text{tr } e^{-\beta\hat{H}}$$
plays an important role, and that the corresponding matrix elements can be accessed from the propagator through the replacement
$$\frac{i}{\hbar}t \to \beta$$
For consistency with the treatment of the propagator we then continued to study the matrix elements but instead we could have looked at the trace.
- In *Quantum Chaos* the level density $d(E) = \sum_j \delta(E - E_j)$ is obtained from the propagator through a series of steps that involves taking a trace.

Phase-space path integral for the trace. We have previously derived the Hamiltonian mechanics version of the path integral

$$\left\langle \boldsymbol{r}_f \middle| e^{-\frac{i}{\hbar}\hat{H}t} \middle| \boldsymbol{r}_0 \right\rangle = \int D[\boldsymbol{r}]D[\boldsymbol{p}] \exp\left[\frac{i}{\hbar}\int_0^t dt' \left(\boldsymbol{p}(t')\cdot\dot{\boldsymbol{r}}(t') - H(\boldsymbol{r}(t'),\boldsymbol{p}(t'))\right)\right]$$

where $\boldsymbol{r}(0)=\boldsymbol{r}_0, \boldsymbol{r}(t)=\boldsymbol{r}_f$. Here the integration measure was defined by

$$\int D[\boldsymbol{r}]D[\boldsymbol{p}]\ldots = \lim_{N\to\infty}\frac{1}{(2\pi\hbar)^{nN}}\int d^n r_1 \ldots d^n r_{N-1} d^n p_0 \ldots d^n p_{N-1}\ldots$$

To take the trace we have to identify $\boldsymbol{r}_0$ and $\boldsymbol{r}_f$ and integrate over this variable as well. This leads to

$$\text{tr } e^{-\frac{i}{\hbar}\hat{H}t} = \int d^n r_0 \left\langle \boldsymbol{r}_0 \middle| e^{-\frac{i}{\hbar}\hat{H}t} \middle| \boldsymbol{r}_0 \right\rangle$$

and thus

$$\text{tr } e^{-\frac{i}{\hbar}\hat{H}t} = \int \tilde{D}[\boldsymbol{r}]\tilde{D}[\boldsymbol{p}] \exp\left[\frac{i}{\hbar}\int_0^t dt' \left(\boldsymbol{p}(t')\cdot\dot{\boldsymbol{r}}(t') - H(\boldsymbol{r}(t'),\boldsymbol{p}(t'))\right)\right]. \qquad (5.1)$$

Here the integration measure has changed because we have absorbed the integral over $\boldsymbol{r}_0$ into it. We now have

$$\int \tilde{D}[\boldsymbol{r}]\tilde{D}[\boldsymbol{p}]\ldots = \lim_{N\to\infty}\frac{1}{(2\pi\hbar)^{nN}}\int d^n r_0 \ldots d^n r_{N-1} d^n p_0 \ldots d^n p_{N-1}\ldots .$$

As we have identified $\boldsymbol{r}_0$ and $\boldsymbol{r}_f = \boldsymbol{r}_N$ the path integral is taken over all functions $\boldsymbol{r}(t')$ with $\boldsymbol{r}(0)=\boldsymbol{r}(t)$. One can show that it is permissible to also take the momenta as periodic with $\boldsymbol{p}(t)=\boldsymbol{p}(0)$.[1]

As before the classical Hamiltonian $H(\boldsymbol{r},\boldsymbol{p})$ used in the path integral is obtained from the quantum Hamiltonian by replacing the position and momentum operators $\hat{\boldsymbol{r}}$, $\hat{\boldsymbol{p}}$ by the classical variables $\boldsymbol{r}$, $\boldsymbol{p}$.

Second quantisation. In second quantisation the Hamiltonian is written in terms of creation and annihilation operators $a_j^\dagger$ and a_j. It is hence natural to assume that a path integral can be written down for such Hamiltonians as well, and that this will involve replacing $a_j^\dagger$ and a_j by analogues of classical variables. This is indeed correct, and in the case of bosonic systems the analogues of the classical variables are complex numbers that are mutually complex conjugate instead of adjoint. As we omitted writing hats above the creation and annihilation operator the variable replacing a_j will be just denoted by a_j as well but it is now a complex number. The creation operator $a_j^\dagger$ is replaced by the complex conjugate $a_j^* \in \mathbb{C}$.

We now expect an expression as in (5.1) where the Hamiltonian H inside the path integral has the creation and annilation operators replaced by the corresponding

[1] We can simply define $\boldsymbol{p}_N = \boldsymbol{p}_0$. Imposing such a definition would affect how time derivatives of $\boldsymbol{p}$ look in a discretised formula but it is ok here as no such time derivatives enter the action.

complex variables. The only thing that is not immediately clear is what will happen with the integral over $\boldsymbol{p}(t') \cdot \dot{\boldsymbol{r}}(t')$. With the appropriate choice replacement for $\boldsymbol{p}(t') \cdot \dot{\boldsymbol{r}}(t')$ the path integral turns into

$$\begin{aligned} \text{tr } e^{-\frac{i}{\hbar}\hat{H}t} &= \int D[a_1, a_2, \ldots] \exp\Big[\int_0^t dt' \Big(-\sum_j a_j^*(t')\dot{a}_j(t') \\ &\quad -\frac{i}{\hbar} H(a_1(t'), a_2(t'), \ldots, a_1^*(t'), a_2^*(t'), \ldots)\Big)\Big] \end{aligned} \tag{5.2}$$

Here we integrate over all complex functions $a_j(t')$ subject to the condition $a_j(t) = a_j(0)$. These $a_j(t')$ take the role of $\boldsymbol{r}(t')$, $\boldsymbol{p}(t')$ in (5.1).

Motivation. We have already given a heuristic happened to the term $\boldsymbol{p}(t') \cdot \dot{\boldsymbol{r}}(t')$ looks less mysterious if we remember that the creation and annihilation operators are very similar to the ladder operators used when studying the harmonic oscillator in 3rd year quantum mechanics. These operators were related to position and momentum operators. If we assume that the same relation holds between $a_j(t'), a_j^*(t')$ and fictitious coordinates $r_j(t')$ and momenta $p_j(t')$ we have

$$\begin{aligned} a_j(t') &= \frac{1}{\sqrt{2\hbar}}(r_j(t') + ip_j(t')) \\ a_j^*(t') &= \frac{1}{\sqrt{2\hbar}}(r_j(t') - ip_j(t')) \end{aligned}$$

(Compared to the formula in 3rd year quantum mechanics we have here set the m and ω equal to 1.) If we solve these equations for $r_j(t')$ and $p_j(t')$ we obtain

$$\begin{aligned} r_j(t') &= \sqrt{\frac{\hbar}{2}}(a_j(t') + a_j^*(t')) \\ p_j(t') &= \sqrt{\frac{\hbar}{2}}\frac{1}{i}(a_j(t') - a_j^*(t')). \end{aligned}$$

Integration by parts then leads to the replacement

$$\frac{i}{\hbar}\int_0^t dt' p_j(t')\dot{r}_j(t') = \int_0^t dt' \frac{1}{2}(a_j(t') - a_j^*(t'))(\dot{a}_j(t') + \dot{a}_j^*(t')) = -\int_0^t dt' a_j^*(t')\dot{a}_j(t') \tag{5.3}$$

for each summand j.

Derivation. A full derivation of (5.5) is given e.g. in the Altland & Simons book. It makes use of coherent states which we are not covering here.

Continuum limit. Similarly to section 2.4, if one takes a continuum limit of path integrals as here one obtains path integrals over $a(x, t')$ with x replacing the discrete

index j. This also applies if the system is naturally a continuous one and taking the continuum limit just means avoiding a discrete approximation. For example for a one dimensional system without interaction we would get

$$\operatorname{tr} e^{-\frac{i}{\hbar}\hat{H}t} = \int_{a(x,t') \text{ with } a(x,0)=a(x,t)} D[a] \exp\left[-\int_0^t dt' \int dx\; a^*(x,t')\dot{a}(x,t') \right.$$
$$\left. -\frac{i}{\hbar}\int_0^t dt' \int dx\; a^*(x,t') \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + U(x) \right) a(x,t') \right]$$

Here the first term in the exponent is what we get from (5.3) in the continuum limit. The second term is what we get from the time integral over the Hamiltonian if we insert the noninteracting part of $\hat{H}_{\text{mult}}$ given in the very end of section 4.5.

Operator ordering. In the derivation of the path integral in second quantisation one has to pay attention at operator ordering. In general there are different ways to write the same operator, e.g. $a_i^\dagger a_j^\dagger a_j a_i$ and $a_i^\dagger a_i (a_j^\dagger a_j - \delta_{ij})$, and these will lead to different expressions if we replace all operators by complex numbers. Indeed there are different conventions that one can follow when deriving the path integral. The version in the Altland & Simons book assumes normal ordering, i.e. all $a^\dagger$'s have to be placed before the a's. Then one obtains the integral as stated above, and when the action is written in discretised form the integral over the Hamiltonian turns into a sum whose terms combine the a from each discretisation step with the a^* from the following step. This difference is not visible in the continuous form of the path integral.

Applications. The applications of path integrals in second quantisation are similar to those for single particle systems.

- Path integral are a convenient starting point for **perturbation theory.** For example the path integral for the Bose-Hubbard model with two sites can be written as

$$\int D[a_1, a_2, \ldots] \exp\left(- \int_0^t dt' \sum_j a_j^*(t') \dot{a}_j(t') \right.$$
$$\left. - \frac{i}{\hbar} \left(-a_1^*(t') a_2(t') - a_1^*(t') a_2(t') + \frac{U^{\text{int}}}{2} \sum_j a_j(t')^{*2} a_j(t')^2 \right) \right).$$

  If U^{int} is small we can employ perturbation theory with a quadratic term composed of the leading summands and the interaction as a quartic perturbation.

- We can also look for contributions for which the **action is stationary**, as these play a role analogous to classical trajectories in single body quantum mechanics. For the Bose-Hubbard model we can write the exponential as

$$e^{\frac{i}{\hbar} \int dt' f}$$

  where the integrand

$$f = -\frac{\hbar}{i} \sum_j a_j^* \dot{a}_j + a_1^* a_2 + a_1^* a_2 - \frac{U^{\text{int}}}{2} \sum_j a_j^{*2} a_j^2$$

  plays a role analogous to the Lagrangian. The action is stationary if the corresponding Euler-Lagrange equations are satisfied. Let us assume that these can be written down as if a_j, a_j^* were independent variables (this requires a proof). Then we obtain

$$\frac{\partial f}{\partial a_j} = \frac{d}{dt'} \frac{\partial f}{\partial \dot{a}_j}, \qquad \frac{\partial f}{\partial a_j^*} = \frac{d}{dt'} \frac{\partial f}{\partial \dot{a}_j^*}.$$

  The second of these equation now boils down to

$$-\frac{\hbar}{i} \dot{a}_j + a_{j\pm1} - U^{\text{int}} a_j^{*2} a_j = 0$$

which can be rewritten as

$$i\hbar\dot{a}_j = -a_{j\pm1} + U^{\text{int}}|a_j|^2 a_j.$$

The first equation simply turns into the complex conjugate of this result. As the a_j arose from replacing the wavefunction by an operator, and then replacing the operator again by a wavefunction, it is natural to compare their behaviour to that of a wavefunction. Without interaction the above equation would indeed turn into the Schrödinger equation for the Bose-Hubbard model with a single particle. With the interaction we obtain a similar equation where the interaction term gives a nonlinear contribution. It is called the **nonlinear Schrödinger equation** or **Gross-Pitaevski equation**. We will not consider this equation further, but we note that its general variant plays an important role e.g. in the theory of Bose-Einstein condensation.

5.2 Fermions

This subsection is not examinable.

We now want to generalise the preceding results and write down a path integral for fermionic second quantised systems. To do so we should again replace the creation and annihilation operators by numbers. However this time we face the challenge that the annihilation and creation operators anticommute (apart from the case $[a_i, a_i^\dagger]_+ = 1$). In the bosonic case these operators commuted (with an analogous exception) and it was therefore natural to replace them by complex numbers which also commute. In contrast for fermions we should use 'numbers' that anticommute. Such numbers have indeed been defined, and there are known as Grassmann variables or simply Grassmannians.

Definition. $\eta_1, \eta_2, \dots \eta_N$ are called Grassmann variables if they satisfy the commutation relation

$$[\eta_i, \eta_j]_+ = 0$$

for all $i, j = 1, 2, \dots, N$ or equivalently

$$\eta_i \eta_j = -\eta_j \eta_i.$$

Here we simply introduce variables defined to have these properties, we don't require any particular representation e.g. through matrices. When applying these variables in the context of creation and annihilation operators we also have to talk about complex conjugation of Grassmannians, this issue will be postponed until later.

Corollary. As a consequence of our definition we have

$$\eta_i \eta_i + \eta_i \eta_i = 0$$

i.e.

$$\eta_i^2 = 0$$

for all i.

Functions. As Grassmannians square to 0, all higher powers have to vanish as well. Hence if we consider general function of a single Grassmannian η_i its Taylor expansion will only involve the constant and linear terms,

$$f(\eta_i) = a + b\eta_i.$$

For two Grassmannians we have the constant term, linear terms in both of them, and a quadratic term involving their product,

$$g(\eta_i, \eta_j) = a + b\eta_i + c\eta_j + d\eta_i\eta_j.$$

For N variables we have 2^N terms, each of which is either independent of or linear in each of the N Grassmannians.

In the language of Pure Mathematics, all possible functions of η_i, η_j (with coefficients in either $\mathbb{R}$ or $\mathbb{C}$) form an *associative algebra* and the Grassmannians are the *generators* of this algebra. There is also a close link to the properties of *differential forms* studied in the Differentiable Manifolds course.

Derivatives. Derivatives of these functions are easy to define as we just have to deal with the constant and linear cases, but we have to note that the differential operator now anticommutes as well.

Definition. The derivative $\frac{\partial}{\partial\eta_i}$ is defined such that

- $\frac{\partial}{\partial\eta_i}\eta_i = 1$,
- $\frac{\partial}{\partial\eta_i}$ applied to a term independent of η_i gives 0,
- $\frac{\partial}{\partial\eta_i}$ anticommutes with Grassmannian variables and other derivatives.

To realise why the anticommutation relation is required for consistency consider the following derivative (for $i \neq j$)

$$\frac{\partial}{\partial\eta_i}\eta_j\eta_i = -\frac{\partial}{\partial\eta_i}\eta_i\eta_j = -\eta_j.$$

Here we did not move the differential operator but we exchanged the two Grassmannians in order to be able to apply the operator directly to η_i. However if we want to move $\frac{\partial}{\partial\eta_i}$ to the right instead we will obtain the same result only if it anticommutes with η_j.

Integrals. The definition of the integral is surprising at first.

Definition. The integral $\int d\eta_i$ is defined to coincide with the corresponding derivative, i.e.

- $\int d\eta_i \eta_i = 1$,
- $\int d\eta_i$ applied to a term independent of η_i gives 0,
- $\int d\eta_i$ anticommutes with Grassmannian variables and other derivatives/integrals.

We note that this integral does not have limits and should just be identified with a definite integral such as an integral from $-\infty$ to ∞. There are no integrals with different integration limits in the Grassmannian context, and we should not expect differentiation and integration to be inverses of each other. To motivate why this definition is natural we note that

- the result of the integral is independent of the integration variable, as expected for a definite integral,
- and the result of Gaussian integrals is closely related to its conventional analogue.

We'll now move on to compute the Gaussian integrals but first we need some more preparations.

Products of Grassmannians. Products of two Grassmannians commute with other Grassmannians. This follows from

$$(\eta_i \eta_j)\eta_k = -\eta_i \eta_k \eta_j = \eta_k (\eta_i \eta_j)$$

where two minus signs cancelled, and it carries though immediately to products with an even number of factors.

Complex conjugation. One often has to apply Grassmannians in a context where the corresponing commuting variables are complex. In this case it is helpful to introduce complex conjugation of Grassmannians. This is done by defining η_i and η_i^*, but simply regarding them as independent Grassmannian variables.

(The conventions for this vary in the literature, and some authors refuse to use complex notation for Grassmannians as there is no genuine complex structure. Some authors define $(\eta_i^*)^* = -\eta_i$ for reasons that we will not discuss here.)

One-dimensional Gauss integral. Using 'complex' Grassmannians the Gauss integral can be evaluated as

$$\begin{aligned} & \int d\eta^* \int d\eta e^{-a\eta^*\eta} \\ = & \int d\eta^* \int d\eta \Big(1 - a\eta^*\eta + \underbrace{\frac{1}{2}(a\eta^*\eta)^2 + \dots}_{=0}\Big) \\ = & \underbrace{\int d\eta^* \int d\eta\, 1}_{=0} + a \int d\eta^* \underbrace{\int d\eta\, \eta}_{=1} \eta^* \\ = & \ a. \end{aligned}$$

Here we Taylor expanded, used that powers of Grassmannians are zero and the integral of 1 is zero, then used the the anticommutation relation of η and η^*, and finally the definition of the integral for linear terms. To compare this result to the case of commuting complex variables we recall that (see problem sheet 3, question 1)

$$\int \underbrace{\frac{d\mathrm{Re}z\, d\mathrm{Im}z}{\pi}}_{=dz^*dz} e^{-a|z|^2} = \frac{1}{\pi}\sqrt{\frac{\pi}{a}}\sqrt{\frac{\pi}{a}} = \frac{1}{a}$$

where we used twice the result for a real Gauss integral. With the formal definition of dz^*dz given here the results for the two cases are inverses of each other.

Multi-dimensional Gaussian integral. This observation carries over to the multi-dimensional case where we have, for commuting complex numbers

$$\int dz_1^* dz_1 \dots dz_N^* dz_N e^{-\boldsymbol{z}^\dagger A \boldsymbol{z}} = \frac{1}{\det A}.$$

We will show that the corresponding Grassmannian integral is

$$I = \int d\eta_1^* d\eta_1 \dots d\eta_N^* d\eta_N \exp\left(-\boldsymbol{\eta}^\dagger A \boldsymbol{\eta}\right) = \det A,$$

for arbitrary matrices A.

Proof: Writing the exponent in components we obtain

$$I = \int d\eta_1^* d\eta_1 \dots d\eta_N^* d\eta_N \exp\left(-\sum_{ij} \eta_i^* A_{ij} \eta_j\right)$$

Here non-vanishing contributions can arise only from terms where each of the $2N$ Grassmannian variables appears once in the integrand. These terms form part of the N-th term in the Taylor expansion, which means that we have

$$I = \int d\eta_1^* d\eta_1 \dots d\eta_N^* d\eta_N \frac{1}{N!}\left(-\sum_{ij} \eta_i^* A_{ij} \eta_j\right)^N.$$

We can get rid of the minus sign if we exchange the η^*, η in the integration measure in a way that produces a compensating factor $(-1)^N$. This leads to

$$I = \int d\eta_1 d\eta_1^* \dots d\eta_N d\eta_N^* \frac{1}{N!} \left(\sum_{ij} \eta_i^* A_{ij} \eta_j \right)^N$$

Still a non-vanishing result will only occur for terms where each η_i^* appears only once. For these terms it is natural to take the N factors and then reorder them with increasing i. As the factors each involve two Grassmannians they commute. But we have to take into account that each term with i written in increasing order arises from $N!$ terms in the line above. This compensates the divisor $N!$ and we obtain

$$I = \int d\eta_1 d\eta_1^* \dots d\eta_N d\eta_N^* \sum_\pi \prod_{i=1}^N \eta_i^* A_{i\pi(i)} \eta_{\pi(i)}$$

where we brought in a summation over permutations π that still has to be explained. To obtain a non-vanishing contribution also all choices of η_j have to be different. As both the i and j must exhaust all integers from 1 to N they must be mapped to each other by a permutation π. Hence we can replace j by $\pi(i)$ if we take a sum over permutations π.

Finally we have to reorder the factors $\eta_{\pi(i)}$ such that they appear in increasing order as well. This can be done by exchanging η^* factors between subsequent products $\eta_i^* A_{i\pi(i)} \eta_{\pi(i)}$. Each such exchange can be seen as a transposition, and it brings in a minus sign, as seen in the following example:

$$\eta_1^* \eta_2 \eta_2^* \eta_1 = \eta_1^* \eta_1 \eta_2 \eta_2^* = -\eta_1^* \eta_1 \eta_2^* \eta_2$$

Hence reordering the factors η leads to multiplication with the sign of π and we obtain

$$I = \int d\eta_1 d\eta_1^* \dots d\eta_N d\eta_N^* \sum_\pi \operatorname{sgn} \pi \prod_{i=1}^N \eta_i^* A_{i\pi(i)} \eta_i.$$

Performing the integrals as in

$$\int d\eta_i d\eta_i^* \eta_i^* \eta_i = 1$$

this leads to

$$I = \sum_\pi \prod_{i=1}^N A_{i\pi(i)} = \det A$$

as desired.

Perturbation theory. We can now perform Gaussian averages in a way similar to commuting variables. A Gaussian average for Grassmannian variables should be defined by

$$\langle \dots \rangle = \frac{1}{c} \int d\eta_1^* d\eta_1 \dots d\eta_N^* d\eta_n e^{-\boldsymbol{\eta}^\dagger A \boldsymbol{\eta}} \dots$$

where $c = \det A$. We'll just explicitly calculate the quadratic averages for the one dimension ($A = a$), to practice Grassmannian integration. We have

$$\langle \eta\eta^* \rangle = \frac{1}{a}\int d\eta^* d\eta\, \eta\, \eta^* e^{-a\eta^*\eta} = \frac{1}{a}\int d\eta^* d\eta\, \eta\, \eta^* = \frac{1}{a}$$

where we only needed the constant term in the exponential as all later terms combine with the prefactor to quadratic or higher powers of the integration variables. In addition we have

$$\langle \eta\eta \rangle = \langle \eta^*\eta^* \rangle = 0$$

which follows immediately from the fact that the integrands are zero.

These examples motivate the following variant of Wick's theorem (which we will not prove):

Wick's theorem for Grassmannian variables. Averaged products of Grassmannians η_i, η_i^* can be evaluated as follows:

- Sum over all ways to contract the η's and η^*'s pairwise.
- Reorder the factors such that contracted elements appear next to each other in the form $\overbrace{\eta_j \eta_k^*}$ (this may lead to sign factors from the anticommutation relation).
- Assign to each contraction line $\overbrace{\eta_j \eta_k^*}$ a factor $(A^{-1})_{jk}$.

As an example we have

$$\begin{aligned}\langle \eta_{j_1}\eta_{j_2}^*\eta_{j_3}^*\eta_{j_4}\rangle &= \langle \overbrace{\eta_{j_1}\eta_{j_2}^*}\,\overbrace{\eta_{j_3}^*\eta_{j_4}}\rangle + \langle \overbrace{\eta_{j_1}\eta_{j_2}^*\eta_{j_3}^*}\,\eta_{j_4}\rangle = -\langle \overbrace{\eta_{j_1}\eta_{j_2}^*}\,\overbrace{\eta_{j_4}\eta_{j_3}^*}\rangle + \langle \overbrace{\eta_{j_1}\eta_{j_3}^*}\,\overbrace{\eta_{j_4}\eta_{j_2}^*}\rangle \\ &= -(A^{-1})_{j_1 j_2}(A^{-1})_{j_4 j_3} + (A^{-1})_{j_1 j_3}(A^{-1})_{j_4 j_2}.\end{aligned}$$

Path integral. We are now ready to formulate a path integral for fermionic systems. In analogy to the bosonic case we have

$$\begin{aligned}\mathrm{tr}\; e^{-\frac{i}{\hbar}\hat{H}t} &= \int D[a_1, a_2, \ldots] \exp\Big[\int_0^t dt' \Big(-\sum_j a_j^*(t')\dot{a}_j(t') \\ &\quad -\frac{i}{\hbar} H(a_1(t'), a_2(t'), \ldots, a_1^*(t'), a_2^*(t'), \ldots)\Big)\Big]. \qquad (5.4)\end{aligned}$$

Here the fermionic creation and annihilation operators have been replaced by (time-dependent) Grassmannians a_j^*, a_j. These are now subject to the condition

$$a_j(t) = -a_j(0), \qquad a^*(t) = -a^*(0).$$

In the derivation with coherent states (see Altland & Simons) this condition arises from the way the trace is written in terms of these states. The integration measure

is given by

$$\int D[a_1, a_2, \ldots] \ldots = \lim_{N\to\infty} \prod_j \prod_{k=0}^{N-1} \int da_{jk}^* da_{jk} \ldots$$

where the index j runs over single particle states e.g. associated to sites and the index $k = 0, \ldots, N-1$ runs over discretisation steps in time. All a_{jk}^*, a_{jk} are independent Grassmannian variables.

Example. As an example we want to treat the **fermionic harmonic oscillator**. This is just to illustrate the method, as we will see in the end for this simple system the result can be obtained much faster through direct computation. The Hamiltonian of the fermionic harmonic oscillator can be written as

$$\hat{H} = \hbar\omega a^\dagger a$$

where $a^\dagger, a$ are fermionic creation and annihilation operators. Here we did not include a ground state energy. The path integral now turns into

$$I = \operatorname{tr} e^{-\frac{i}{\hbar}\hat{H}t} \quad = \quad \int D[a] \exp\Big[\int_0^t dt' \Big(- a^*(t')\dot{a}(t') - \frac{i}{\hbar}\hbar\omega a^*(t')a(t')\Big)\Big].$$

We will use the discretised form of this integral

$$I = \lim_{N\to\infty} \int da_0^* da_0 \ldots \exp\left(- \sum_{k=0}^{N-1} a_{k+1}^* \frac{a_{k+1} - a_k}{\tau}\tau - i\omega \sum_{k=0}^{N-1} a_{k+1}^* a_k \tau \right).$$

Here $\tau = \frac{t}{N}$ is the width of the timesteps, and we wrote the Hamiltonian with the a^* at a later point in time than the a, in line with the earlier remark about operator ordering. The antiperiodic boundary conditions in time entail $a_N = -a_0$ and $a_N^* = -a_0^*$. The above expression can be rearranged as

$$\begin{aligned} I &= \lim_{N\to\infty} \int da_0^* da_0 \ldots \exp\left(- \sum_{k=0}^{N-1} a_{k+1}^* a_{k+1} + (1 - i\omega\tau) \sum_{k=0}^{N-1} a_{k+1}^* a_k \right) \\ &= \lim_{N\to\infty} \int da_0^* da_0 \ldots \exp\left(\sum_{k=0}^{N-1} a_k a_k^* + (1 - i\omega\tau) \sum_{k=0}^{N-1} a_{k+1}^* a_k \right). \end{aligned}$$

If we write a separate exponential for each summand and use that their Taylor expansion stops after the linear term we obtain

$$I = \lim_{N\to\infty} \int da_0^* da_0 \ldots \prod_{k=0}^{N-1} (1 + a_k a_k^*) \prod_{k=0}^{N-1} (1 + (1 - i\omega\tau) a_{k+1}^* a_k).$$

Now we will get a non-vanishing contribution only from terms where each a_k and a_k^* appears as a factor exactly once. This is only possible if we either combine all linear terms from the first product or all linear terms from the second product, otherwise we would always miss a Grassmannian or have a Grassmannian appear twice. Hence I can be written as

$$I = I_1 + I_2$$

where

$$I_1 = \lim_{N\to\infty} \int da_0^* da_0 \dots \prod_{k=0}^{N-1} a_k a_k^* = 1$$

and

$$I_2 = \lim_{N\to\infty} \int da_0^* da_0 da_1^* da_1 \dots da_{N-1}^* da_{N-1} \prod_{k=0}^{N-1} (1 - i\omega\tau) a_{k+1}^* a_k.$$

To evaluate this integral it is helpful to permute da_0^* thr

ough to the end, and compensate the arising sign factor by writing da_N^*. This leads to

$$I_2 = \lim_{N\to\infty} \int (da_0 da_1^*) da_1 \dots da_{N-1}^* (da_{N-1} da_N^*) \prod_{k=0}^{N-1} (1 - i\omega\tau) a_{k+1}^* a_k$$

where the arrangement of the integration variables mirrors that of the factors. This allows us to evaluate the integral as

$$I_2 = \lim_{N\to\infty} (1 - i\omega\tau)^N = \lim_{N\to\infty} \left(1 - \frac{i\omega t}{N}\right)^N = e^{-i\omega t}$$

leading to

$$I = \operatorname{tr} e^{-\frac{i}{\hbar}\hat{H}t} = 1 + e^{-i\omega t}.$$

This result can be checked immediately by direct calculation. The eigenstates of the fermionic harmonic oscillator are $|0\rangle$ and $|1\rangle$ with

$$\hbar\omega a^\dagger a|0\rangle = 0, \qquad \hbar\omega a^\dagger a|1\rangle = \hbar\omega|1\rangle.$$

This leads to the trace

$$\operatorname{tr} e^{-\frac{i}{\hbar}\hat{H}t} = e^{-\frac{i}{\hbar}E_1 t} + e^{-\frac{i}{\hbar}E_2 t} = 1 + e^{-i\omega t}$$

in agreement with the path integral result.

Problems. As the material from subsection 5.2 is not examinable it will not be covered in a problem sheet but here are two short exercise questions. They don't have to be handed in. Answers will appear on the course page.

1. Evaluate the integral

$$\int \prod_{j=1}^{3} (d\eta_j^* d\eta_j)(\eta_1^* + \eta_2^* + \eta_3^*)^2 (\eta_1 + \eta_2 + \eta_3)^2 \exp(2i\eta_1^*\eta_2 - 2i\eta_2^*\eta_1 + \eta_3^*\eta_3)$$

   where η_j, η_j^* are Grassmannians.

2. Derive a formula for $\operatorname{tr}(\lambda I - A)^{-1}$ (where A is a hermitian matrix) involving a complex integral, a Grassmannian integral, and a derivative w.r.t. λ. This problem can be solved by using $\det = \exp\operatorname{tr}\ln$ as well as the Gaussian integrals for complex numbers and Grassmannians. It is useful as a starting point if one wants to compute averages of such traces.