# Chapter 3

# Perturbation theory

## 3.1 Motivation

In the previous chapter we were able to evaluate path integrals explicitly for examples such as the harmonic oscillator or (in the homework) a particle without potential. This was possible because the Lagrangian or Hamiltonian in these cases contained terms up to quadratic order in the relevant variables and then the integrals involved were Gauss or Fresnel integrals (or simpler). However when they are terms of higher order than quadratic this is no longer possible. An approach that can treat this very frequent situation is provided by perturbation theory. Considering the Lagrangian version of path integrals for now, perturbation theory works well if the Lagrangian can be written as a term that contains contributions of at most quadratic order in $\boldsymbol{r}$ and $\dot{\boldsymbol{r}}$, plus a small additional term (normally in the potential) that contains perturbations of cubic or higher order. We then have

$$L(\boldsymbol{r},\dot{\boldsymbol{r}}) = \underbrace{L_0(\boldsymbol{r},\dot{\boldsymbol{r}})}_{\text{quadratic}} + \epsilon L_1(\boldsymbol{r},\dot{\boldsymbol{r}}).$$

Here $\epsilon$ is a small parameter, and the perturbation to the Lagrangian is given by $\epsilon L_1$. For example we can consider $L_1 = \boldsymbol{r}^4$. Now we can plug this Lagrangian into the path integral, leading to

$$\int D[\boldsymbol{r}] e^{\frac{i}{\hbar}\int L dt'} = \int D[\boldsymbol{r}] e^{\frac{i}{\hbar}\int L_0 dt'} e^{\frac{i\epsilon}{\hbar}\int L_1 dt'},$$

and we can Taylor expand the second exponential for small $\epsilon$. If we go up to linear order in $\epsilon$ we obtain

$$e^{\frac{i\epsilon}{\hbar}\int L_1 dt'} \approx 1 + \frac{i\epsilon}{\hbar}\int L_1 dt'.$$

The path integral thus obtains a leading contribution that is just the same as without perturbation, and the additional summand

$$\frac{i\epsilon}{\hbar}\int D[\boldsymbol{r}]\left(\int L_1 dt'\right) e^{\frac{i}{\hbar}\int L_0 dt'}.$$

Evaluating this summand will lead to a **Fresnel integral**, as $L_0$ is quadratic, but with an a **prefactor in front of the exponential**, e.g. involving $L_1 = \boldsymbol{r}^4$. In order to be able to evaluate path integrals with terms beyond quadratic order we thus have to be learn how to evaluate Fresnel integrals with prefactors. Further expressions of this type arise if we go beyond linear order in expanding the exponential.

**Similar problems.** There are many situations leading to the same problem, sometimes with Gaussians instead of Fresnel integrals:

- The simplest integrals of a similar type do not involve any paths, just a Gaussian or Fresnel integral with further factors outside the exponent, e.g.

$$\int x_{k_1} x_{k_2} \ldots e^{-\frac{1}{2}\boldsymbol{x}\cdot A\boldsymbol{x}} d^n x$$

  where $A$ is a matrix and $\boldsymbol{x}$ is a vector. We will look at these examples first. They illustrate the use of perturbation theory in the setting of matrices and vectors with discrete parameters, which is relevant for example in Random Matrix Theory and Quantum Information.

- If we look for partition functions of systems with quadratic and higher-order contributions to the potential we can split off the higher order contribution similarly to as for the propagator. The formulas will be analogous apart from the replacement $\frac{i}{\hbar}t \to \beta$ discussed before, and instead of the Fresnel integral we have a Gaussian integral.

- In Statistical Mechanics we could also be interested in evaluating statistical averages of some quantities, so even if the kinetic and potential energy are quadratic we could have a quantity in front of the Gaussian that we would like to average.

- In quantum field theory and particle physics so called correlation functions play an important role. These lead to path integrals of the type

$$\int D[x] x(t_1) x(t_2) e^{\frac{i}{\hbar}\int L dt'}$$

  which also require to consider Fresnel integrals with a prefactor even in case the Lagrangian involves only quadratic terms.

## 3.2 Wick's theorem

We want to start by considering integrals of the form

$$\int x_{k_1} x_{k_2} \ldots \exp\left(-\frac{1}{2}\boldsymbol{x}^T A \boldsymbol{x}\right) d^n x.$$

where $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)$ is an $n$-dimensional real vector and $A$ is an $n \times n$ real symmetrix matrix. For the integral to converge we require $A$ to be positive definite. This means that $\boldsymbol{x}^T A \boldsymbol{x}$ must be positive for all $\boldsymbol{x} \neq 0$, or equivalently all eigenvalues of $A$ must be positive.

We start by evaluating the Gaussian integral without prefactors.

**Lemma.**

$$\int_{\mathbb{R}^n} \exp\left(-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x}\right) = \frac{(2\pi)^{n/2}}{\sqrt{\det A}} \equiv c \tag{3.1}$$

This generalises the one-dimensional Gaussian integral $\int \exp\left(-\frac{1}{2}ax^2\right) dx = \sqrt{\frac{2\pi}{a}}$.

**Proof.** We start be showing the proposition for the case that $A$ is a diagonal matrix with diagonal elements $a_1, a_2, \ldots, a_n$. We then have

$$\int \exp\left(-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x}\right) d^n x = \int \exp\left(-\frac{1}{2}\sum_{k=1}^{n} a_k x_k^2\right) d^n x = \prod_{k=1}^{n}\sqrt{\frac{2\pi}{a_k}} = \frac{(2\pi)^{n/2}}{\sqrt{\det A}}.$$

Here we have evaluated the one-dimensional Gauss integrals for each $k$ and then used that the determinant of a diagonal matrix is the product of its diagonal elements.

For the general case we use that every real symmetric matrix can be written as

$$A = \mathcal{O}^T \underbrace{\begin{pmatrix} a_1 & & \\ & \ddots & \\ & & a_n \end{pmatrix}}_{D} \mathcal{O}$$

where $\mathcal{O}$ is an orthogonal matrix with $\mathcal{O}^T = \mathcal{O}^{-1}$ and $a_1, \ldots, a_n$ are the eigenvalues forming a diagonal matrix $D$. With this representation of $A$ the integral can be written as

$$\int \exp\left(-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x}\right) d^n x = \int \exp\left(-\frac{1}{2}\boldsymbol{x}^T \mathcal{O}^T D\mathcal{O}\boldsymbol{x}\right) d^n x$$
$$= \int \exp\left(-\boldsymbol{y}^T D\boldsymbol{y}\right) d^n y = \frac{(2\pi)^{n/2}}{\sqrt{\det D}} = \frac{(2\pi)^{n/2}}{\sqrt{\det A}}$$

Here we defined $\boldsymbol{y} = \mathcal{O}\boldsymbol{x}$ and transformed the integral into an integral over $\boldsymbol{y}$. The Jacobian matrix of this transformation is $\mathcal{O}$ which as an orthogonal matrix has a determinant with absolute value 1. Finally we used that the $\det D$ is the product of the eigenvalues $a_1, \ldots, a_n$ and hence equal to $\det A$.

**Notation.** In the following we will consider the normalised Gaussian

$$\frac{1}{c}\exp\left(-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x}\right)$$

and we define $\langle \ldots \rangle$ as the average

$$\langle \ldots \rangle = \frac{1}{c}\int \exp\left(-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x}\right) \ldots d^n x.$$

Here $\ldots$ represents an arbitrary expression depending on $\boldsymbol{x}$ that can be averaged. As the Gaussian with the prefactor above is normalised we immediately have

$$\langle 1 \rangle = 1.$$

**Gaussian averages of products.** We are now interested in averages of the type $\langle x_{k_1} x_{k_2} \ldots \rangle$. A first result about these is the following:

We have

$$\langle x_{k_1} x_{k_2} \ldots \rangle = 0$$

if the number of factors is odd.

This follows immediately from the fact that in case of an odd number of factors the integrand flips sign if we replace $\boldsymbol{x}$ by $-\boldsymbol{x}$. Hence the contribution of any $\boldsymbol{x}$ to the integral is compensated by the contribution of $-\boldsymbol{x}$.

In order to evaluate averages with an even number of factors as well we first determine $\langle e^{\boldsymbol{j}^T \boldsymbol{x}} \rangle$. This quantity is called the **generating function** and the parameter $\boldsymbol{j} \in \mathbb{R}^n$ is called the **source**. The advantage of this generating function is that we can generate any average $\langle x_{k_1} x_{k_2} \ldots \rangle$ by taking derivatives of the generating function w.r.t. suitable components of $\boldsymbol{j}$, and then setting $\boldsymbol{j} = 0$.

**Lemma.**

$$\left\langle \exp\left(\boldsymbol{j}^T \boldsymbol{x}\right) \right\rangle = \exp\left(\frac{1}{2} \boldsymbol{j}^T A^{-1} \boldsymbol{j}\right) \tag{3.2}$$

**Proof.** The average above can be written as the shifted Gaussian integral

$$\left\langle \exp\left(\boldsymbol{j}^T \boldsymbol{x}\right) \right\rangle \quad = \quad c^{-1} \int \exp\left(-\frac{1}{2} \boldsymbol{x}^T A \boldsymbol{x} + \boldsymbol{j}^T \boldsymbol{x}\right) d^n x$$

We now try to remove the linear term by making a variable transformation the variable transformation $\boldsymbol{x} = \boldsymbol{z} + A^{-1} \boldsymbol{j}$. As this is just a constant shift the Jacobian determinant of this transformation is 1. We thus obtain

$$\left\langle \exp\left(\boldsymbol{j}^T \boldsymbol{x}\right) \right\rangle \quad = \quad c^{-1} \int \exp\left(-\frac{1}{2} \underbrace{(\boldsymbol{z} + A^{-1} \boldsymbol{j})^T}_{\boldsymbol{z}^T + \boldsymbol{j}^T A^{-1}} A (\boldsymbol{z} + A^{-1} \boldsymbol{j}) + \boldsymbol{j}^T (\boldsymbol{z} + A^{-1} \boldsymbol{j})\right) d^n z$$

where we used that if $A$ is symmetric the same applies to $A^{-1}$ and hence $(A^{-1})^T = A^{-1}$. If we expand the brackets we now obtain

$$\begin{aligned} & \left\langle \exp\left(\boldsymbol{j}^T \boldsymbol{x}\right) \right\rangle \\ = \quad & c^{-1} \int \exp\left(-\frac{1}{2} \boldsymbol{z}^T A \boldsymbol{z} - \cancel{\frac{1}{2} \boldsymbol{j}^T \boldsymbol{z}} - \cancel{\frac{1}{2} \boldsymbol{z}^T \boldsymbol{j}} - \frac{1}{2} \boldsymbol{j}^T A^{-1} \boldsymbol{j} + \cancel{\boldsymbol{j}^T \boldsymbol{z}} + \boldsymbol{j}^T A^{-1} \boldsymbol{j}\right) d^n z \\ = \quad & c^{-1} \int \exp\left(-\frac{1}{2} \boldsymbol{z}^T A \boldsymbol{z}\right) d^n z \exp\left(\frac{1}{2} \boldsymbol{j}^T A^{-1} \boldsymbol{j}\right) \\ = \quad & \exp\left(\frac{1}{2} \boldsymbol{j}^T A^{-1} \boldsymbol{j}\right) \end{aligned}$$

where we have split off the part of the exponent independent of $\boldsymbol{z}$ and we used (3.1).

Using (3.2) we now consider the case of two prefactors:

> **Lemma.**
> $$\langle x_k x_{k'} \rangle = (A^{-1})_{kk'}$$

**Proof.** We can produce two factors $x_k$, $x_{k'}$ by taking derivatives of the generating function w.r.t. the corresponding components of the source. Afterwards the remaining exponential can be turned into 1 by setting $\boldsymbol{j} = 0$. We thus get

$$\langle x_k x_{k'} \rangle = \frac{\partial}{\partial j_k} \frac{\partial}{\partial j_{k'}} \left\langle \exp\left(\boldsymbol{j}^T \boldsymbol{x}\right) \right\rangle \Big|_{\boldsymbol{j}=0} = \frac{\partial}{\partial j_k} \frac{\partial}{\partial j_{k'}} \exp\left(\frac{1}{2} \boldsymbol{j}^T A^{-1} \boldsymbol{j}\right) \Big|_{\boldsymbol{j}=0}.$$

Now we use the following result for the derivative of quadratic expressions as arising above

$$\frac{\partial}{\partial j_k} \left(\frac{1}{2} \boldsymbol{j}^T A^{-1} \boldsymbol{j}\right) = (A^{-1} \boldsymbol{j})_k = \sum_n (A^{-1})_{kn} j_n.$$

This can be checked easily using Kronecker deltas and the symmetry of $A^{-1}$ (actually $A^{-1}$ could have been replaced by any symmetric matrix). Inserting this result in the preceding formula we obtain

$$\begin{aligned} \langle x_k x_{k'} \rangle &= \frac{\partial}{\partial j_{k'}} \sum_n (A^{-1})_{kn} j_n \exp\left(\frac{1}{2} \boldsymbol{j}^T A^{-1} \boldsymbol{j}\right) \Big|_{\boldsymbol{j}=0} \\ &= \sum_n (A^{-1})_{kn} \delta_{nk'} \\ &= (A^{-1})_{kk'} \end{aligned}$$

Here we have first taken the derivative w.r.t. $j_k$. Then the derivative w.r.t. $j_{k'}$ can act on the factor $j_n$ or on the exponential. However the term where it acts on the exponential will vanish because it still has the factor $j_n$ which is set equal to zero. The remaining steps follow using $\frac{\partial j_n}{\partial j_{k'}} = \delta_{nk'}$.

We now generalise this result to arbitrary products.

> **Wick's theorem.** Any average $\langle x_{k_1} x_{k_2} x_{k_3} \ldots \rangle$ can be obtained by summing over all ways of connecting the factors pairwise by **contraction lines** as in
>
> $$\langle \overline{x_{k_1} x_{k_2}}\, \overline{x_{k_3} x_{k_4}} \rangle$$
>
> The contribution of each way of drawing these lines is a product of factors
>
> $$(A^{-1})_{k_i, k_l}$$
>
> arising from each contraction line connecting $x_{k_i}$ and $x_{k_l}$.

This means that the average over the contracted factors is evaluated **as if the rest of the integrand were absent**.

**Example.** If we have only two factors there is only one way of connecting the factors pairwise and we have

$$\langle x_{k_1} x_{k_2} \rangle = \langle \overline{x_{k_1} x_{k_2}} \rangle = (A^{-1})_{k_1, k_2}$$

as before. For four factors there are three ways of drawing contraction lines

$$\langle x_{k_1} x_{k_2} x_{k_3} x_{k_4}\rangle = \langle \wick{\c1 x_{k_1} \c1 x_{k_2} \c1 x_{k_3} \c1 x_{k_4}}\rangle + \langle \wick{\c1 x_{k_1} \c2 x_{k_2} \c1 x_{k_3} \c2 x_{k_4}}\rangle + \langle \wick{\c1 x_{k_1} \c2 x_{k_2} \c2 x_{k_3} \c1 x_{k_4}}\rangle.$$

According to Wick's theorem this leads to

$$\langle x_{k_1} x_{k_2} x_{k_3} x_{k_4}\rangle = (A^{-1})_{k_1,k_2}(A^{-1})_{k_3,k_4} + (A^{-1})_{k_1,k_3}(A^{-1})_{k_2,k_4} + (A^{-1})_{k_1,k_4}(A^{-1})_{k_2,k_3}.$$

**Proof.** The proof generalises the one for products of two factors. The average can be obtained from the generating function via

$$\begin{aligned}\langle x_{k_1} x_{k_2} x_{k_3}\ldots\rangle &= \frac{\partial}{\partial j_{k_1}}\frac{\partial}{\partial j_{k_2}}\frac{\partial}{\partial j_{k_3}}\ldots\left\langle \exp\left(\boldsymbol{j}^T\boldsymbol{x}\right)\right\rangle\Big|_{\boldsymbol{j}=0}\\ &= \frac{\partial}{\partial j_{k_1}}\frac{\partial}{\partial j_{k_2}}\frac{\partial}{\partial j_{k_3}}\ldots\exp\left(\frac{1}{2}\boldsymbol{j}^T A^{-1}\boldsymbol{j}\right)\Big|_{\boldsymbol{j}=0}.\end{aligned}$$

Now every derivative $\frac{\partial}{\partial j_{k_i}}$ acting on the exponential produces a factor

$$\sum_n (A^{-1})_{k_i,n} j_n$$

However we later set $\boldsymbol{j}=0$. So for any summand $n$ a contribution arises only if the factor $j_n$ is removed by one of the later derivatives $\frac{\partial}{\partial j_{k_l}}$. This requires $k_l = n$. As we need this derivative to remove the factor $j_n$ the term where it acts on the exponential is irrelevant. If we have a pair of derivatives $\frac{\partial}{\partial j_{k_i}}$, $\frac{\partial}{\partial j_{k_l}}$ where one derivative acts on the exponential and the other one removes a component of $\boldsymbol{j}$ this altogether leads to a factor

$$(A^{-1})_{k_i,k_l}.$$

We only get a non-vanishing contribution if all derivatives $\frac{\partial}{\partial j_{k_1}}, \frac{\partial}{\partial j_{k_2}}, \frac{\partial}{\partial j_{k_3}}, \ldots$ are paired up in this way. All ways of pairing them up have to be taken into account. A helpful notation for keeping track of these pairings is to consider the product $\langle x_{k_1} x_{k_2} x_{k_3}\ldots\rangle$. Then we draw contraction lines between $x_{k_i}$ and $x_{k_l}$ if the corresponding derivatives $\frac{\partial}{\partial j_{k_i}}$, $\frac{\partial}{\partial j_{k_l}}$ are paired up. This completes the proof.

**Example: One-dimensional integrals.** We consider the one-dimensional Gaussian averages with $A = 1$,

$$\langle\ldots\rangle = \int_{-\infty}^{\infty}\sqrt{2\pi}e^{-\frac{1}{2}x^2}\ldots dx\,.$$

We obtain $\langle x\rangle = 0$, $\langle x^3\rangle = 0$, etc because the integrand is odd in $x$ or, equivalently, because an odd number of factors can't be grouped into pairs so there are no permissible ways of drawing contraction lines. Furthermore we have, following on from our earlier example,

$$\langle x^2\rangle = \langle \wick{\c1 x \c1 x}\rangle = 1$$

and

$$\langle x^4\rangle = \langle \wick{\c1 x \c1 x \c1 x \c1 x}\rangle + \langle \wick{\c1 x \c2 x \c1 x \c2 x}\rangle + \langle \wick{\c1 x \c2 x \c2 x \c1 x}\rangle = 3.$$

In general for $\langle x^{2n}\rangle$ we start with a contraction involving the first factor $x$. There are $2n-1$ choices for the factor it is contracted with. Afterwards $2n-2$ uncontracted factors are left. If we draw a contraction line involving the first of these factors we have $2n-3$ choices for the factor it is contracted with. Due to $A=1$ each way of drawing contraction lines just contributes 1 to the result. Continuing like this we obtain

$$\langle x^{2n}\rangle = (2n-1)(2n-3)(2n-5)\dots$$

which is often denoted by the double factorial

$$\langle x^{2n}\rangle = (2n-1)!!\ .$$

For example we have

$$\langle x^6\rangle = 5\cdot 3\cdot 1 = 15$$

and

$$\langle x^8\rangle = 7\cdot 5\cdot 3\cdot 1 = 105.$$

**Wick's theorem for Fresnel integrals.** We now consider Fresnel integrals, with $e^{-\frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x}}$ replaced by

$$e^{\frac{i}{2}\boldsymbol{x}^T A\boldsymbol{x}}. \tag{3.3}$$

We again require $A$ to be symmetric. There is no longer a reason to require $A$ to be positive definite, but we still assume it has no vanishing eigenvalues and is therefore invertible. We will see that all that changes in this case is **an extra factor $i$ in Wick's theorem**.

To show this we note that the one dimensional Gauss integral is turned into the one dimensional Fresnel integral seen in section 2.1,

$$\int_{-\infty}^{\infty} e^{\frac{i}{2}ax^2} = \sqrt{\frac{2\pi}{|a|}}e^{i\frac{\pi}{4}\operatorname{sgn} a}$$

The analogous formula in $n$ dimensions is

$$\int_{\mathbb{R}^n} e^{\frac{i}{2}\boldsymbol{x}^T A\boldsymbol{x}} d^n x = \frac{(2\pi)^{n/2}}{\sqrt{\det A}}e^{i\nu\frac{\pi}{4}} \equiv c$$

where $\nu$ is the difference between the number of positive eigenvalues of $A$ and the number of negative eigenvalues. $\nu$ is thus the appropriate generalisation of $\operatorname{sgn} a$. We are now interested in the average

$$\langle \dots\rangle = \frac{1}{c}\int e^{\frac{i}{2}\boldsymbol{x}^T A\boldsymbol{x}} \dots\ .$$

As before the averages of products $\langle x_{k_1}x_{k_2}\dots\rangle$ can be obtained by taking derivatives of a suitably defined generating function. As in (3.3) we flipped the signs and inserted a factor $i$ compared to the Gaussian case, we make the same change in the generating function and write

$$\langle e^{-i\boldsymbol{j}^T\boldsymbol{x}}\rangle = e^{-\frac{i}{2}\boldsymbol{j}^T A^{-1}\boldsymbol{j}}.$$

We then obtain

$$\langle x_k x_{k'} \rangle = -\frac{\partial}{\partial j_k}\frac{\partial}{\partial j_{k'}}\langle e^{-i\boldsymbol{j}^T\boldsymbol{x}}\rangle\big|_{\boldsymbol{j}=0} = -\frac{\partial}{\partial j_k}\frac{\partial}{\partial j_{k'}}e^{-\frac{i}{2}\boldsymbol{j}^T A^{-1}\boldsymbol{j}}\big|_{\boldsymbol{j}=0}$$

and the same calculation as for the Gauss integral leads to

$$\langle x_k x_{k'} \rangle = i(A^{-1})_{kk'}.$$

An analogous factor arises in Wick's theorem as the contribution of each contraction. This is the change one would have expected naively by realising that $e^{\frac{i}{2}\boldsymbol{x}^T A\boldsymbol{x}}$ is obtained from the previous Gaussian via the replacement $A \to -iA$ which implies $A^{-1} \to iA^{-1}$.

## 3.3 Anharmonic oscillator

We now apply Wick's theorem to path integrals. As an example we consider the anharmonic or perturbed harmonic oscillator. This is just the harmonic oscillator with a small perturbation $\epsilon x^4$ (with $\epsilon \ll 1$) added to the potential, leading to the Lagrangian

$$L = T - U = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}m\omega^2 x^2 - \epsilon x^4.$$

Our aim will be to evaluate the path integral for the propagator $K(0,0,t)$ describing motion from $x_0 = 0$ to $x_f = 0$, and to extract the ground state energy from this result using the procedure from section 2.5. The main technical challenge will be to go from the version of Wick's theorem with discrete indices to a situation where time appears as a continuous parameter. This will be done by making the 'natural' replacements, with sums replaced by integrals, vectors by functions, matrices by operators. (These replacements could be justified formally but we will sometimes appeal to intuition about what is the natural continuous generalisation of a discrete object.) The path integral for the anharmonic oscillator is

$$K(0,0,t) = \int_{x(0)=x(t)=0} D[x]\exp\left(\frac{i}{\hbar}\int_0^t\left[\frac{1}{2}m\dot{x}(t')^2 - \frac{1}{2}m\omega^2 x(t')^2 - \frac{\epsilon}{x}(t')^4\right]dt'\right).$$

**Comparison to the discrete case.** Here the function $x(t')$ is the continuous analogue of the vector $\boldsymbol{x} = (x_1, x_2, \ldots)$ considered earlier. The analogue of the quadratic term $\frac{i}{2}\boldsymbol{x}^T A\boldsymbol{x}$ involves the quadratic parts of the action, associated to the harmonic oscillator. They can be written as

$$\frac{i}{\hbar}S_0 = \frac{i}{\hbar}\int_0^t\left[\frac{1}{2}m\dot{x}(t')^2 - \frac{1}{2}m\omega^2 x(t')^2\right]dt'$$

where $S_0$ indicates the action of the harmonic oscillator. The integral here is obviously quadratic but it would be closer to $\frac{i}{2}\boldsymbol{x}^T A\boldsymbol{x}$ if we could write the integrand with $x(t')$ on the left and on the right and an operator in between. To bring it into this form we integrate by parts,

$$\int_0^t \dot{x}(t')^2 dt' = \underbrace{x(t')\dot{x}(t')\big|_0^t}_{=0} - \int_0^t x(t')\ddot{x}(t')dt' = -\int_0^t x(t')\frac{\partial^2}{\partial t'^2}x(t')dt'$$

leading to

$$\frac{i}{\hbar}S_0 = \frac{i}{2}\int_0^t x(t')\left(-\frac{m}{\hbar}\right)\left(\frac{\partial^2}{\partial t'^2} + \omega^2\right)x(t').$$

Hence the operator

$$A = \left(-\frac{m}{\hbar}\right)\left(\frac{\partial^2}{\partial t'^2} + \omega^2\right)$$

is the analogue of the matrix $A$ appearing in the discrete version of Wick's theorem. This replacement is natural as differential (and other) operators act on functions in a similar way as matrices act on vectors.

**Inverse of $A$.** For Wick's theorem we need the inverse of $A$ which should be an operator as well. We now assume that $A^{-1}$ is an operator whose application to a function $x(t')$ can be written in the form

$$(A^{-1}x)(t') = \int_0^t G(t', t'')x(t'')dt'' \tag{3.4}$$

where the parameters $t', t''$ take a role similar to indices of matrices an vectors. $G(t', t'')$ is called the integral kernel of $A^{-1}$. To determine $A^{-1}$ and $G(t', t'')$ we use that $AA^{-1}$ has to be the identity. This implies that for all functions $x(t')$ we must have

$$x(t') = AA^{-1}x(t') = A\int_0^t G(t', t'')x(t'')dt'' = \int_0^t AG(t', t'')x(t'')dt''.$$

Now comparing the first and the final expressions in this line we see that $G(t', t'')$ has to satisfy

$$AG(t', t'') = \delta(t' - t'')$$

which is the differential equation

$$\left(-\frac{m}{\hbar}\right)\left(\frac{\partial^2}{\partial t'^2} + \omega^2\right)G(t', t'') = \delta(t' - t''). \tag{3.5}$$

In addition, when considering operators acting on functions it is important to consider the precise space of functions they are acting on. In the present problems we are interested in functions $x(t')$ that satisfy $x(0) = x(t) = 0$. Hence application of $A$ according to (3.4) to a function satisfying these requirements should return another function satisfying them. This leads to the conditions

$$G(0, t'') = G(t, t'') = 0 \tag{3.6}$$

guaranteeing that $\int_0^t G(t',t'')x(t'')dt''$ vanishes for $t'=0$ or $t'=t$. We could now use (3.5) and (3.6) to determine $G(t',t'')$ by calculation but it will be slightly easier to just state the result and prove that it's true.

**Proposition.** The solution $G(t',t'')$ subject to the requirements (3.5) and (3.6) is

$$G(t',t'') = -\frac{\hbar}{m\omega\sin\omega t}\begin{cases}\sin\omega t'\sin\omega(t''-t) & \text{for } t'\leq t'' \\ \sin\omega t''\sin\omega(t'-t) & \text{for } t'>t''.\end{cases}$$

Note that in spite of the case distinction $G(t',t'')$ is continuous, and the lower formula would give the same result for $G(t',t')$ as the upper one. However crucially we will see that the first derivative makes a jump at $t'=t''$.

**Proof.** The boundary conditions (3.6) are satisfied because for $t'=0$ we are in the first case and the vanishes result vanishes due to $\sin\omega t'=0$. For $t'=t$ we are in the second case and the result vanishes due to $\sin\omega(t'-t)=0$. For $t'\neq t''$ the differential equation (3.5) simply boils down to the oscillator equation

$$\left(\frac{\partial^2}{\partial t'^2}+\omega^2\right)G(t',t'')=0.$$

which is satisfied due to the terms $\sin\omega t'$ and $\sin\omega(t'-t)$. The tricky part is to show that in (3.5) the delta function arises for $t'=t''$. To show this we evaluate the first derivative

$$\frac{\partial}{\partial t'}G(t',t'') = -\frac{\hbar\omega}{m\omega\sin\omega t}\begin{cases}\cos\omega t'\sin\omega(t''-t) & \text{for } t'<t'' \\ \sin\omega t''\cos\omega(t'-t) & \text{for } t'>t''.\end{cases}$$

Crucially this result has a jump at $t'=t''$. Now using the Heaviside function

$$\Theta(x) = \begin{cases}1 & \text{for } x>0 \\ 0 & \text{for } x<0\end{cases}$$

we can rewrite our result as

$$\begin{aligned}\frac{\partial}{\partial t'}G(t',t'') &= -\frac{\hbar\omega}{m\omega\sin\omega t}[\cos\omega t'\sin\omega(t''-t) \\ &\quad +\Theta(t'-t'')(\sin\omega t''\cos\omega(t'-t)-\cos\omega t'\sin\omega(t''-t))].\end{aligned}$$

If we then apply $\frac{\partial}{\partial t'}$ for a second time, the application to the trigonometric functions will only give terms that we already know will be compensated by $\omega^2 G(t',t'')$. However in addition to these we have to take into account the term where $\frac{\partial}{\partial t'}$ acts on $\Theta(t'-t'')$. To evaluate this term we use that the derivative of the Heaviside function is the delta function. We thus obtain

$$\left(\frac{\partial^2}{\partial t'^2}+\omega^2\right)G(t',t'') = -\frac{\hbar\omega}{m\omega\sin\omega t}\delta(t'-t'')(\sin\omega t''\cos\omega(t'-t)-\cos\omega t'\sin\omega(t''-t))$$

Now in the factor following the delta function we can replace $t''$ by $t'$ as this factor only contributes if the argument of the delta function is zero. Then we can use a trigonometric identity to simplify

$$\sin\omega t'\cos\omega(t'-t)-\cos\omega t'\sin\omega(t'-t)=\sin(\omega t'-\omega(t'-t))=\sin\omega t$$

and we obtain

$$\left(\frac{\partial^2}{\partial t'^2}+\omega^2\right)G(t',t'')=-\frac{\hbar}{m}\delta(t'-t'')$$

which implies (3.5).

**Propagator.** We now return to the path integral for the propagator. For the anharmonic oscillator we have

$$\begin{aligned}K_{\text{anh}}(0,0,t) &= \int_{x(0)=x(t)=0} D[x]\exp\left(\frac{i}{\hbar}\int_0^t\left[\frac{1}{2}m\dot{x}(t')^2-\frac{1}{2}m\omega^2x(t')^2-\epsilon x(t')^4\right]dt'\right)\\ &= \int_{x(0)=x(t)=0} D[x]\exp\left(\frac{i}{\hbar}\int_0^t\left[\frac{1}{2}m\dot{x}(t')^2-\frac{1}{2}m\omega^2x(t')^2\right]dt'\right)\exp\left(-\frac{i\epsilon}{\hbar}\int_0^t x(t')^4dt'\right).\end{aligned}$$

We first have to translate this into our notation with averages $\langle\ldots\rangle$. We have

$$\langle\ldots\rangle=\frac{1}{c}\int_{x(0)=x(t)=0} D[x]\exp\left(\frac{i}{\hbar}\int_0^t\left[\frac{1}{2}m\dot{x}(t')^2-\frac{1}{2}m\omega^2x(t')^2\right]dt'\right)\ldots$$

where $c$ is the integral involving only the quadratic terms. In the present case this is just the propagator of the harmonic oscillator,

$$c=K_{\text{harm}}(0,0,t)=\int_{x(0)=x(t)=0} D[x]\exp\left(\frac{i}{\hbar}\int_0^t\left[\frac{1}{2}m\dot{x}(t')^2-\frac{1}{2}m\omega^2x(t')^2\right]dt'\right).$$

In this notation the propagator of the anharmonic oscillator can be written as

$$K_{\text{anh}}(0,0,t)=K_{\text{harm}}(0,0,t)\left\langle\exp\left(-\frac{i\epsilon}{\hbar}\int_0^t x(t')^4dt'\right)\right\rangle. \tag{3.7}$$

As $\epsilon$ is small we can expand the exponential in a Taylor series. If we go up to quadratic order we obtain

$$\begin{aligned}K_{\text{anh}}(0,0,t) &= K_{\text{harm}}(0,0,t)\Bigg(1-\frac{i\epsilon}{\hbar}\int_0^t dt'\langle x(t')^4\rangle\\ &\quad+\frac{1}{2}\left(-\frac{i\epsilon}{\hbar}\right)^2\int_0^t dt'\int_0^t dt''\langle x(t')^4x(t'')^4\rangle+O(\epsilon^3)\Bigg)\end{aligned}$$

where we have interchanged the time integral and the average, and we renamed one of the integration variables in the squared integral into $t''$.

We now consider the term linear in $\epsilon$, and use Wick's theorem to evaluate the average $\langle x(t')^4\rangle$ involved in it. The factors $x(t')$ here are the continuous analogues of the factors $x_k$ we had in the discrete formulation of Wick's theorem. If we contract the $x(t')$'s as we did with the $x_k$'s we obtain

$$\langle x(t')^4\rangle=\langle x(t')x(t')x(t')x(t')\rangle+\langle x(t')x(t')x(t')x(t')\rangle+\langle x(t')x(t')x(t')x(t')\rangle.$$

Now in the discrete case (with Fresnel integrals) every contraction line between $x_{k_i}$ and $x_{k_l}$ gave a contribution $i(A^{-1})_{k_i,k_l}$. In the continuous case this means that contractions between $x(t')$ and $x(t'')$ should lead to give $iA^{-1}$ evaluated at the times $t'$ and $t''$. The obvious interpretation of this is to take the kernel of $A^{-1}$ and write $iG(t',t'')$. In the formula above all contractions hence give factors $iG(t',t')$ and we obtain

$$\langle x(t')^4\rangle = 3(iG(t',t'))^2.$$

With

$$G(t',t') = -\frac{\hbar \sin\omega t' \sin\omega(t'-t)}{m\omega \sin\omega t}. \tag{3.8}$$

we thus obtain

$$K_{\text{anh}}(0,0,t) = K_{\text{harm}}(0,0,t)\left(1 + \frac{3i\epsilon}{\hbar}\int_0^t G(t',t')^2 dt' + O(\epsilon^2)\right) \tag{3.9}$$

where we have neglected all higher-order terms, including the quadratic terms still written above.

**Ground state energy.** We now use our previous result to study how the ground state energy of the harmonic oscillator is changed by the perturbation. Hence we replace $\frac{i}{\hbar}t \to \beta$, $\frac{i}{\hbar}t' \to \beta'$ as in section 2.5; this leads to $\langle 0|e^{-\beta\hat{H}_{\text{anh}}}|0\rangle$ which should be proportional to $e^{-\beta E_0}$ in the limit $\beta \to \infty$. (We stress that here 0 indicates the initial and final position at the origin, this should not be confused with the notation $|0\rangle$ sometimes used for the ground state.) Approximating $\langle 0|e^{-\beta\hat{H}_{\text{anh}}}|0\rangle$ in our limit thus allows to read off the ground state energy $E_0$.

The replacement $\frac{i}{\hbar}t \to \beta$ leads to

$$\langle 0|e^{-\beta\hat{H}_{\text{anh}}}|0\rangle = \langle 0|e^{-\beta\hat{H}_{\text{harm}}}|0\rangle\left(1 + 3\epsilon\int_0^\beta G\left(\frac{\hbar}{i}\beta', \frac{\hbar}{i}\beta'\right)^2 d\beta' + O(\epsilon^2)\right) \tag{3.10}$$

where we have

$$G\left(\frac{\hbar}{i}\beta', \frac{\hbar}{i}\beta'\right) = -\frac{\hbar \sin\left(\omega\frac{\hbar}{i}\beta'\right)\sin\left(\omega\frac{\hbar}{i}(\beta'-\beta)\right)}{m\omega\sin\left(\omega\frac{\hbar}{i}\beta\right)}. \tag{3.11}$$

For large $\beta$ we can approximate

$$\sin\left(\omega\frac{\hbar}{i}\beta\right) = \frac{1}{2i}\left(e^{\omega\hbar\beta} - e^{-\omega\hbar\beta}\right) \approx \frac{1}{2i}e^{\omega\hbar\beta}.$$

and analogously we obtain for large $\beta'$

$$\sin\left(\omega\frac{\hbar}{i}\beta'\right) \approx \frac{1}{2i}e^{\omega\hbar\beta'}.$$

Note that we have $0 \le \beta' \le \beta$ so $\beta'$ is not large in the beginning of the integration interval but it is large for more and more of the integration interval the larger $\beta$ gets, so substituting the above approximation in the integral indeed gives a good approximation. With

$$-\sin\left(\omega\frac{\hbar}{i}(\beta'-\beta)\right) = \sin\left(\omega\frac{\hbar}{i}(\beta-\beta')\right) \approx \frac{1}{2i}e^{\omega\hbar(\beta-\beta')}$$

we obtain

$$G\left(\frac{\hbar}{i}\beta', \frac{\hbar}{i}\beta'\right) \approx \frac{\hbar}{2im\omega}$$

which means that for large $\beta$ all exponentials in the integrand cancel. Substitution into (3.10) and integration now yields the following result for large $\beta$

$$\langle 0|e^{-\beta \hat{H}_{\rm anh}}|0\rangle \approx \langle 0|e^{-\beta \hat{H}_{\rm harm}}|0\rangle \left(1 - \frac{3}{4}\epsilon\left(\frac{\hbar}{m\omega}\right)^2 \beta + O(\epsilon^2)\right).$$

We now use the result from section 2.5 for the first factor, and we write the second factor as an exponential using that $\epsilon$ is small. This gives the following proportionality for small $\epsilon$ and large $\beta$

$$\langle 0|e^{-\beta \hat{H}_{\rm anh}}|0\rangle \propto e^{-\beta\frac{1}{2}\hbar\omega} e^{-\frac{3}{4}\epsilon\left(\frac{\hbar}{m\omega}\right)^2\beta} = e^{-\beta\left[\frac{1}{2}\hbar\omega + \frac{3}{4}\epsilon\left(\frac{\hbar}{m\omega}\right)^2\right]}.$$

We thus conclude that, considering only the linear order in $\epsilon$, the perturbation changes the ground state energy into

$$E_0 = \frac{1}{2}\hbar\omega + \frac{3}{4}\epsilon\left(\frac{\hbar}{m\omega}\right)^2.$$

**Feynman diagrams.** We now introduce a helpful notation for writing down contractions like the ones we considered for $\langle x(t')^4\rangle$. We also allow for contractions between $x$ with different time arguments. In the new notation any contraction line

$$\overbrace{x(t')x(t'')}$$

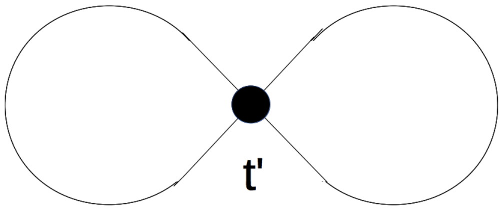
is indicated by a line connecting vertices that represent $t'$ and $t''$. According to Wick's theorem the contribution of this line is $iG(t',t'')$. Each time argument appearing in the problem is denoted only by a single vertex, hence a contraction line involving identical time arguments like

$$\overbrace{x(t')x(t')}$$

is represented by a loop starting and ending at the same vertex $t'$. The usual convention also requires that any time vertex that has more than one end of a line attached is automatically integrated over[1]. With this convention each of the three ways of contracting $x(t')$ in

$$\int_0^t dt' \langle x(t')^4\rangle$$

is denoted by




As there are three choices of contractions one says that this diagram has multiplicity 3 and $\int_0^t dt' \langle x(t')^4\rangle$ yields 3 times the diagram depicted.

**$\epsilon^2$ contribution.** To illustrate these diagrams further we also consider the $\epsilon^2$ contribution to $K(0,0,t)$ which is proportional to

$$\int_0^t dt' \int_0^t dt'' \langle x(t')^4 x(t'')^4\rangle. \tag{3.12}$$

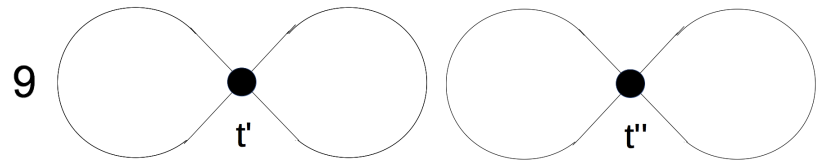
The associated diagrams are similar to the discrete example from the problem class:

- First we consider the case that all contraction lines connect $x$ with the same argument, e.g.

$$\begin{aligned} &\int_0^t dt' \int_0^t dt'' \langle \overbrace{x(t')x(t')}\,\overbrace{x(t')x(t')}\,\overbrace{x(t'')\overbrace{x(t'')x(t'')}x(t'')}\rangle \\ = &\int_0^t dt' \int_0^t dt'' (iG(t',t'))^2 (iG(t'',t''))^2 \end{aligned}$$

[1] We did not follow this convention in the problem class where we considered a discrete example, as in this case the vertices were just associated to indices 1 and 2.

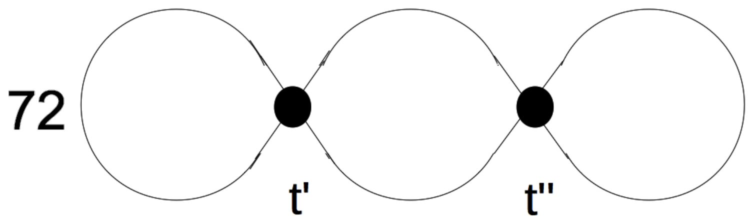
There are 9 contributions of this type as there are 3 choices for contracting the $x(t')$ among themselves and 3 choices for contracting the $x(t'')$ among themselves. The overall contribution to (3.12) can thus be written as



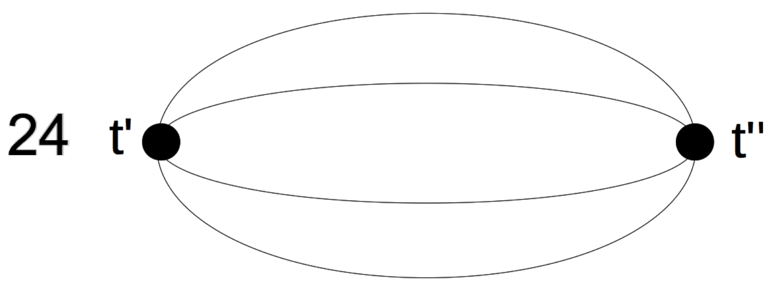

- Next we assume that there are two contractions between $x(t')$ and $x(t'')$ and one contraction each among the $x(t')$ and among the $x(t'')$, as for example in

$$\begin{aligned} & \int_0^t dt' \int_0^t dt'' \langle x(t')x(t')x(t')x(t')x(t'')x(t'')x(t'')x(t'')\rangle \\ = & \int_0^t dt' \int_0^t dt'' (iG(t',t''))^2 iG(t',t') iG(t'',t'') \end{aligned}$$

The corresponding diagram has multiplicity 72. To understand this note that there are $\binom{4}{2} = 6$ ways of grouping the four factors $x(t')$ into two factors to be contracted with each other and two factors to be contracted with $x(t'')$. An analogous 6 choices arise from grouping the $x(t'')$ in a similar way. Then there are two ways in which we can draw the required contractions lines between $x(t')$ and $x(t'')$. The contribution to (3.12) is therefore




- Finally all contractions could be between $x(t')$ and $x(t'')$. In this case the first $x(t')$ can be contracted with four possible $x(t'')$, for the next $x(t')$ there are three $x(t'')$ left, and then there are two and finally only one. The multiplicity is thus $4! = 24$ and we obtain




The multiplicities sum to $105 = 7!!$ which is the overall number of possibilities to contract eight factors pairwise.

Performing the integrals we could now determine the $\epsilon^2$ contribution to $K(0,0,t)$. This would give an even better description of wave propagation for the anharmonic oscillator than (3.9). In addition after the substitution $\frac{i}{\hbar}t \to \beta$ we can get $\langle 0|e^{-\beta\hat{H}}|0\rangle$ up to order $\epsilon^2$ which allows to determine $E_0$ up to order $\epsilon^2$. However these calculations will be omitted here.