# Introduction to Path Integrals

Stilianos Louca

May 29, 2010

---

## Contents

# 1 Introduction to the path integrals

Path integration, first developed by Feynman[4] in 1948, has come to be an elegant alternative to Schrödingers and Heißenbergs description of quantum theory. Its similarity to least-action principles in classical physics, provides with an intuitive interpretation of the nature of quantum processes. While classical trajectories in phase space extremize some sort of action $S$, quantum mechanical transition amplitudes can be described as an interference of *all possible* paths, weighted by a pure phase $e^{\frac{i}{\hbar}S}$. In this *sum*, the classical trajectory is only one of a multitude of possible trajectories, contributing to the evolution of the system.

Though lacking a mathematically solid foundation, the theory of path integration can readily be applied to several known quantum mechanical systems. Its power though, lies in its generalizability to field theories, thus constituting an alternative to the 2nd quantization approach. For more on the latter see any standard QFT book, for example Greiner[6].

This rather quick and dirty article is meant to provide with an introduction to one-parameter path integrals and its applications to various problems of non-relativistic quantum theory. It is based mainly on the books of Swanson[1] and Kleinert[2]. Thorough introductions can also be found in [3] and [5].

## 1.1 The canonical representation

We shall "derive" the path-integral formulation for $n$-dimensional Hamiltonians of the form

$$\hat{H}(t) = T(\hat{\mathbf{P}}, t) + V(\hat{\mathbf{X}}, t) \tag{1.1}$$

for transitions between the generalized eigenstates $|\mathbf{x}_\alpha\rangle$ of the position operator $\hat{\mathbf{X}}$. Let $\hat{U}(t, t_0)$ be the propagator of $\hat{H}$, then the transition probability from $|\mathbf{x}_\alpha\rangle$ to $|\mathbf{x}_\beta\rangle$ from time $t_\alpha$ to time $t_\beta$, is given by $\left|\langle\mathbf{x}_\beta|\,\hat{U}(t_\beta, t_\alpha)\,|\mathbf{x}_\alpha\rangle\right|^2$. The complex scalar

$$\langle\mathbf{x}_\beta, t_\beta\,|\mathbf{x}_\alpha, t_\alpha\rangle := \langle\mathbf{x}_\beta|\,\hat{U}(t_\beta, t_\alpha)\,|\mathbf{x}_\alpha\rangle \tag{1.2}$$

is called *transition amplitude*.

Now let $N \in \mathbb{N}$, *slice* the time span $[t_\alpha, t_\beta]$ into $N$ equidistant pieces of length $\varepsilon := (t_\beta - t_\alpha)/N$ and set $t_j := t_\alpha + j \cdot \varepsilon$. We may write (1.2) in the form

$$\begin{aligned}
\langle\mathbf{x}_\beta, t_\beta\,|\mathbf{x}_\alpha, t_\alpha\rangle &= \langle\mathbf{x}_\beta|\,\hat{U}(t_N, t_{N-1})\dots\hat{U}(t_1, t_0)\,|\mathbf{x}_\alpha\rangle \\
&= \int d^n\mathbf{x}_1 \dots d^n\mathbf{x}_{N-1}\;\; \langle\mathbf{x}_\beta|\,\hat{U}(t_N, t_{N-1})\,|\mathbf{x}_{N-1}\rangle\,\langle\mathbf{x}_{N-1}|\,\hat{U}(t_{N-1}, t_{N-2})\,|\mathbf{x}_{N-2}\rangle \dots \langle\mathbf{x}_1|\,\hat{U}(t_1, t_0)\,|\mathbf{x}_\alpha\rangle \\
&= \int d^n\mathbf{x}_1 \dots d^n\mathbf{x}_{N-1}\;\; \prod_{j=0}^{N-1}\langle\mathbf{x}_{j+1}|\,\hat{U}(t_{j+1}, t_j)\,|\mathbf{x}_j\rangle
\end{aligned} \tag{1.3}$$

whereas $\mathbf{x}_N := \mathbf{x}_\beta,\ \mathbf{x}_0 := \mathbf{x}_\alpha$. For mall enough time intervals $\varepsilon$ we may approximate

$$\hat{U}(t_{j+1}, t_j) \approx \exp\left[-\frac{i\varepsilon}{\hbar}\hat{H}(t_j)\right] \quad . \tag{1.4}$$

Using

$$\exp\Big[-\frac{i\varepsilon}{\hbar}\overbrace{\Big(T(\hat{\mathbf{P}}, t) + V(\hat{\mathbf{X}}, t)\Big)}^{H(\hat{\mathbf{P}}, \hat{\mathbf{X}}, t)}\Big] \overset{(A.5)}{=} \exp\left[-\frac{i\varepsilon}{\hbar}T(\hat{\mathbf{P}}, t)\right]\exp\left[-\frac{i\varepsilon}{\hbar}V(\hat{\mathbf{X}}, t)\right] + \mathcal{O}(\varepsilon^2) \quad , \tag{1.5}$$

we can write

$$\langle \mathbf{x}_{j+1}|\,\hat{U}(t_{j+1},t_j)\,|\mathbf{x}_j\rangle \overset{(1.4)\,\&(1.5)}{\approx} \int d^n\mathbf{p}_j\ \langle \mathbf{x}_{j+1}|\exp\left[-\frac{i\varepsilon}{\hbar}T(\hat{\mathbf{P}},t_j)\right]|\mathbf{p}_j\rangle\langle \mathbf{p}_j|\exp\left[-\frac{i\varepsilon}{\hbar}V(\hat{\mathbf{X}},t_j)\right]|\mathbf{x}_j\rangle$$

$$= \int d^n\mathbf{p}_j\ \exp\left[-\frac{i\varepsilon}{\hbar}\left(T(\mathbf{p}_j,t_j)+V(\mathbf{x}_j,t_j)\right)\right] \underbrace{\langle \mathbf{x}_{j+1}\,|\mathbf{p}_j\rangle}_{\frac{\exp[i\mathbf{p}_j\mathbf{x}_{j+1}/\hbar]}{(2\pi\hbar)^{\frac{n}{2}}}} \underbrace{\langle \mathbf{p}_j\,|\mathbf{x}_j\rangle}_{\frac{\exp[-i\mathbf{p}_j\mathbf{x}_j/\hbar]}{(2\pi\hbar)^{\frac{n}{2}}}}$$

$$= \int \frac{d^n\mathbf{p}_j}{(2\pi\hbar)^n}\ \exp\left[-\frac{i\varepsilon}{\hbar}H(\mathbf{x}_j,\mathbf{p}_j,t_j)\right]\cdot\exp\left[\frac{i}{\hbar}(\mathbf{x}_{j+1}-\mathbf{x}_j)\cdot\mathbf{p}_j\right] \tag{1.6}$$

and the transition amplitude (1.3) becomes

$$\langle \mathbf{x}_\beta,t_\beta\,|\mathbf{x}_\alpha,t_\alpha\rangle = \lim_{N\to\infty}\int d^n\mathbf{x}_1\dots d^n\mathbf{x}_{N-1}\int \frac{d^n\mathbf{p}_0}{(2\pi\hbar)^n}\cdots\frac{d^n\mathbf{p}_{N-1}}{(2\pi\hbar)^n}$$

$$\exp\left[\frac{i\varepsilon}{\hbar}\sum_{j=0}^{N-1}\left[\frac{1}{\varepsilon}(\mathbf{x}_{j+1}-\mathbf{x}_j)\cdot\mathbf{p}_j - H(\mathbf{x}_j,\mathbf{p}_j,t_j)\right]\right] \quad . \tag{1.7}$$

We interpret the value $\mathbf{x}_j$ as position and $\mathbf{p}_j$ as momentum of the particle at time $t_j := t_\alpha + j\cdot\varepsilon$ along a piecewise linear path (see fig. 1.1). The term $\dot{\mathbf{x}}_j := (\mathbf{x}_{j+1}-\mathbf{x}_j)/\varepsilon$ then becomes the approximate velocity of the particle between the times $t_j, t_{j+1}$. As $n\to\infty$ and $\varepsilon \sim \frac{1}{N}\to 0$, the sum in (1.7) goes over to the Riemann-integral

$$\int_{t_\alpha}^{t_\beta} \underbrace{[\dot{\mathbf{x}}(t)\cdot\mathbf{p}(t) - H(\mathbf{x}(t),\mathbf{p}(t),t)]}_{\mathcal{L}(\mathbf{x},\mathbf{p},t)}\ dt =: S[\mathbf{x},\mathbf{p}] \tag{1.8}$$

of the Lagrangian $\mathcal{L}$ along the path $\mathbf{x}(t),\mathbf{p}(t)$, described by the coordinates $\mathbf{x}_0,..,\mathbf{x}_N$ & $\mathbf{p}_0,..,\mathbf{p}_N$ at the more and more dense sample-times $t_0,..,t_N$. We write

$$\int_{(t_\alpha,\mathbf{x}_\alpha)}^{(t_\beta,\mathbf{x}_\beta)} D\mathbf{x}\ D\mathbf{p}\ \exp\left[\frac{i}{\hbar}S[\mathbf{x},\mathbf{p}]\right] := \lim_{N\to\infty}\int d^n\mathbf{x}_1\dots d^n\mathbf{x}_{N-1}\int\frac{d^n\mathbf{p}_0}{(2\pi\hbar)^n}\cdots\frac{d^n\mathbf{p}_{N-1}}{(2\pi\hbar)^n}$$

$$\exp\left[\frac{i\varepsilon}{\hbar}\sum_{j=0}^{N-1}\left[\frac{1}{\varepsilon}(\mathbf{x}_{j+1}-\mathbf{x}_j)\cdot\mathbf{p}_j - H(\mathbf{x}_j,\mathbf{p}_j,t_j)\right]\right] \tag{1.9}$$

and call $\int D\mathbf{x}\ D\mathbf{p}\ e^{S[\mathbf{x},\mathbf{p}]}$ a *path integral*. It can be interpreted as an integral over all possible paths $\mathbf{x}(t)$, $\mathbf{p}(t)$ connecting $\mathbf{x}_\alpha$ and $\mathbf{x}_\beta$ between the times $t_\alpha$ & $t_\beta$, weighted with the factor $e^{S[\mathbf{x},\mathbf{p}]}$, whereas $S[\mathbf{x},\mathbf{p}]$ is exactly the classical mechanical action of $\mathbf{x},\mathbf{p}$. Thus, the transition amplitude

$$\boxed{\langle \mathbf{x}_\beta|\,\hat{U}(t_\beta,t_\alpha)\,|\mathbf{x}_\alpha\rangle = \int_{(t_\alpha,\mathbf{x}_\alpha)}^{(t_\beta,\mathbf{x}_\beta)} D\mathbf{x}\ D\mathbf{p}\ \exp\left[\frac{i}{\hbar}\int_{t_\alpha}^{t_\beta}\mathcal{L}(\mathbf{x},\mathbf{p},t)\ dt\right]} \tag{1.10}$$

in a way results from a superposition of *all possible paths* of the particle, connecting $\mathbf{x}_\alpha$ and $\mathbf{x}_\beta$. While all paths contribute to the amplitude with the same weight, to each corresponds a different complex phase. Note how in (1.9), there is always one integration more for the particle momentum than position.

## 1.2 Path integrals over configuration space

In literature one often finds a somewhat different kind of path integral, where integration only covers paths in configuration space. For special kinds of Hamiltonians this is indeed equivalent to (1.10), as the momentum integrals can be evaluated right away. Suppose the Hamiltonian is of the form[1]

$$H(\mathbf{x},\mathbf{p},t) = \frac{1}{2}\mathbf{p}^T\mathbb{M}^{-1}\mathbf{p} + \mathbf{a}(\mathbf{x},t)\cdot\mathbf{p} + V(\mathbf{x},t) \quad , \tag{1.11}$$

with $\mathbb{M} \in \mathbb{R}^{n\times n}$ as symmetric, positive definite matrix and $\mathbf{a} : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n$. Then

$$\int \frac{d^n\mathbf{p}_j}{(2\pi\hbar)^n} \exp\left[\frac{i\varepsilon}{\hbar}\left[\frac{1}{\varepsilon}(\mathbf{x}_{j+1}-\mathbf{x}_j)\cdot\mathbf{p}_j - H(\mathbf{x}_j,\mathbf{p}_j,t_j)\right]\right] \qquad \Bigg| \qquad \mathbf{a}_j := \mathbf{a}(\mathbf{x}_j,t_j)$$

$$\overset{(1.11)}{=} \frac{e^{-\frac{i\varepsilon}{\hbar}V(\mathbf{x}_j,t_j)}}{(2\pi\hbar)^n}\cdot\int d^n\mathbf{p}_j\ \exp\left[-\frac{i\varepsilon}{2\hbar}\cdot\mathbf{p}_j^T\mathbb{M}^{-1}\mathbf{p}_j - \frac{i\varepsilon}{\hbar}\mathbf{a}_j\cdot\mathbf{p}_j + \frac{i}{\hbar}(\mathbf{x}_{j+1}-\mathbf{x}_j)\cdot\mathbf{p}_j\right]$$

$$\overset{(A.2)}{=} \sqrt{\frac{\det\mathbb{M}}{(2\pi\hbar i\varepsilon)^n}}\cdot\exp\left\{\frac{i\varepsilon}{\hbar}\left[\frac{1}{2\varepsilon^2}(\mathbf{x}_{j+1}-\mathbf{x}_j)^T\mathbb{M}(\mathbf{x}_{j+1}-\mathbf{x}_j) + \frac{1}{2}\mathbf{a}_j^T\mathbb{M}\mathbf{a}_j - \frac{1}{\varepsilon}(\mathbf{x}_{j+1}-\mathbf{x}_j)^T\mathbb{M}\mathbf{a}_j - V(\mathbf{x}_j)\right]\right\}$$

$$= \sqrt{\frac{\det\mathbb{M}}{(2\pi\hbar i\varepsilon)^n}}\cdot\exp\left[\frac{i\varepsilon}{\hbar}\cdot\mathcal{L}\left(\mathbf{x}_j,\ \frac{(\mathbf{x}_{j+1}-\mathbf{x}_j)}{\varepsilon},t_j\right)\right] \quad , \tag{1.12}$$

whereas

$$\mathcal{L}(\mathbf{x},\dot{\mathbf{x}},t) = \frac{1}{2}\dot{\mathbf{x}}^T\mathbb{M}\dot{\mathbf{x}} + \frac{1}{2}\mathbf{a}(\mathbf{x},t)^T\mathbb{M}\mathbf{a}(\mathbf{x},t) - \dot{\mathbf{x}}^T\mathbb{M}\mathbf{a}(\mathbf{x},t) - V(\mathbf{x},t) \tag{1.13}$$

is the classical Lagrangian corresponding to (1.11), this time as a function of $\mathbf{x},\dot{\mathbf{x}}$. We define

$$\int\limits_{(t_\alpha,\mathbf{x}_\alpha)}^{(t_\beta,\mathbf{x}_\beta)} \widetilde{D}\mathbf{x}\ \exp\left[\frac{i}{\hbar}S[\mathbf{x}]\right] := \lim_{N\to\infty}\left(\frac{\det\mathbb{M}}{(2\pi\hbar i\varepsilon)^n}\right)^{\frac{N}{2}}\int d^n\mathbf{x}_1\dots d^n\mathbf{x}_{N-1}\ \exp\left[\frac{i\varepsilon}{\hbar}\sum_{j=0}^{N-1}\mathcal{L}\left(\mathbf{x}_j,\ \frac{(\mathbf{x}_{j+1}-\mathbf{x}_j)}{\varepsilon},t_j\right)\right] \tag{1.14}$$

and notice that (1.10) becomes

$$\boxed{\langle\mathbf{x}_\beta|\,\hat{U}(t_\beta,t_\alpha)\,|\mathbf{x}_\alpha\rangle = \int\limits_{(t_\alpha,\mathbf{x}_\alpha)}^{(t_\beta,\mathbf{x}_\beta)}\widetilde{D}\mathbf{x}\ \exp\left[\frac{i}{\hbar}S[\mathbf{x}]\right] \quad ,} \tag{1.15}$$

with $S[\mathbf{x}] := \int\limits_{t_\alpha}^{t_\beta}\mathcal{L}(\mathbf{x},\dot{\mathbf{x}},t)\ dt$ as the classical action of the path $\mathbf{x}(t)$.

[1] Whereas we assume the path integral formulation to be generalizable beyond the standard form $H(\mathbf{x},\mathbf{p}) = T(\mathbf{p}) + V(\mathbf{x})$.

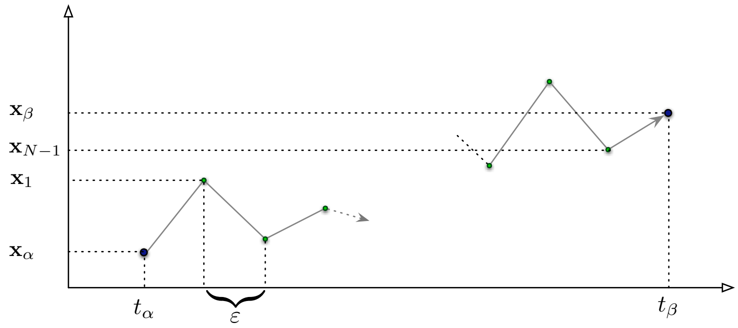


**Figure 1.1:** On the derivation of the path-integral formulation of transition amplitudes.

This path integral formulation, considering only paths in configuration space, was first introduced by Feynman[4].

## 1.3 The concept of quantum fluctuations

In the classical limit that the action $S[\mathbf{x},\mathbf{p}]$ takes on values much larger than $\hbar$, paths far away from the stationary one, lead to fast *oscillations* of the integrant in (1.10), thus canceling each other out. The leading order contributions to the transition amplitude $\langle \mathbf{x}_\beta | U(t_\beta,t_\alpha) | \mathbf{x}_\alpha \rangle$ then comes from nearly classical trajectories $\mathbf{x},\mathbf{p}$. On the other hand, approaching the quantum limit ($\hbar \approx S[\mathbf{x},\mathbf{p}]$) results in other classically impossible paths, so called *quantum fluctuations*, becoming relevant and contributing to the transition amplitude.

Let $\mathbf{x}_c(t),\mathbf{p}_c(t)$ be a classical trajectory for the Lagrangian $\mathcal{L}$, that is, extremizing the action $S[\mathbf{x}_c,\mathbf{p}_c] = \int_{t_\alpha}^{t_\beta} \mathcal{L}(\mathbf{x}_c,\mathbf{p}_c)\, dt$. For any other path $\mathbf{x}(t),\mathbf{p}(t)$, define the *path fluctuation* $\delta\mathbf{x} := \mathbf{x}-\mathbf{x}_c$ and $\delta\mathbf{p} := \mathbf{p}-\mathbf{p}_c$ with the constraint $\delta\mathbf{x}(t_\alpha) = \delta\mathbf{x}(t_\beta) = 0$. Then the action becomes[2]

$$S[\mathbf{x},\mathbf{p}] = S[\mathbf{x}_c,\mathbf{p}_c] + \left.\frac{dS}{d(\mathbf{x},\mathbf{p})}\right|_{(\mathbf{x}_c,\mathbf{p}_c)} (\delta\mathbf{x},\delta\mathbf{p}) + \frac{1}{2!}\left.\frac{d^2S}{d(\mathbf{x},\mathbf{p})^2}\right|_{(\mathbf{x}_c,\mathbf{p}_c)} (\delta\mathbf{x},\delta\mathbf{p})^2 + \mathcal{O}((\delta\mathbf{x},\delta\mathbf{p})^3) \quad . \tag{1.16}$$

Since $\mathbf{x}_c,\mathbf{p}_c$ extremizes the action $S$, the linear term in $(\delta\mathbf{x},\delta\mathbf{p})$ vanishes and we obtain the transition amplitude

$$\begin{aligned}\langle \mathbf{x}_\beta, t_\beta \,| \mathbf{x}_\alpha, t_\alpha\rangle &= e^{\frac{i}{\hbar}S[\mathbf{x}_c,\mathbf{p}_c]} \int_{(t_\alpha,0)}^{(t_\beta,0)} D\delta\mathbf{x}\; D\delta\mathbf{p}\; \exp\left[\frac{i}{2!\hbar}\left.\frac{d^2S}{d(\mathbf{x},\mathbf{p})^2}\right|_{\substack{\mathbf{x}_c\\ \mathbf{p}_c}} (\delta\mathbf{x},\delta\mathbf{p})^2 + \mathcal{O}((\delta\mathbf{x},\delta\mathbf{p})^3)\right] \\ &= e^{\frac{i}{\hbar}S[\mathbf{x}_c,\mathbf{p}_c]} \int_{(t_\alpha,0)}^{(t_\beta,0)} D\delta\mathbf{x}\; D\delta\mathbf{p}\; \exp\left[\frac{i}{2!\hbar}\int_{t_\alpha}^{t_\beta} (\delta\mathbf{x}(t),\delta\mathbf{p}(t))^T \left.\frac{\partial^2\mathcal{L}}{\partial(\mathbf{x},\mathbf{p})^2}\right|_{\substack{\mathbf{x}_c(t)\\ \mathbf{p}_c(t)}} (\delta\mathbf{x}(t),\delta\mathbf{p}(t)) + \mathcal{O}(\delta\mathbf{x}^3)\right] \\ &=: e^{\frac{i}{\hbar}S[\mathbf{x}_c,\mathbf{p}_c]} \cdot F(\mathbf{x}_\beta,t_\beta;\mathbf{x}_\alpha,t_\alpha) \quad ,\end{aligned} \tag{1.17}$$

with the so called *fluctuation factor* $F(\mathbf{x}_\beta,t_\beta;\mathbf{x}_\alpha,t_\alpha)$. If all derivatives of $\mathcal{L}$ higher than 2nd order vanish, then $\frac{\partial^2\mathcal{L}}{\partial(\mathbf{x},\mathbf{p})^2}$ does not depend on $\mathbf{x},\mathbf{p}$ and the fluctuation factor only depends on the times $t_\alpha,t_\beta$. In fact, if $\mathcal{L}$ is time-independent, then $F(t_\beta,t_\alpha) = F(t_\beta - t_\alpha)$.

Suppose for example a Lagrangian of the form[3]

$$\mathcal{L}(\mathbf{x},\dot{\mathbf{x}}) = \frac{1}{2}\dot{\mathbf{x}}^T\mathbb{M}\dot{\mathbf{x}} + \mathbf{x}^T\mathbb{A}\dot{\mathbf{x}} - \mathbf{x}^T\mathbb{V}\mathbf{x} - l(\mathbf{x},\dot{\mathbf{x}}) \tag{1.18}$$

[2]Where $\frac{dS}{d\mathbf{x}}$ is the derivative of the mapping $S:\Phi_q\times\Phi_p\to\mathbb{R}$ on the (assumed) Banach function spaces $\Phi_q,\Phi_p$ (configuration & momentum paths).

[3]Note that this is indeed the most general Lagrangian with vanishing 2nd derivatives.

with $\mathbb{M}, \mathbb{A}, \mathbb{V} \in \mathbb{R}^{n \times n}$ as real, symmetric matrices, $\mathbb{M}$ positive definite and $l : \mathbb{R}^n \to \mathbb{R}$ linear. Similarly to (1.17), it leads to the fluctuation factor[4]

$$F(t_\beta - t_\alpha) = \int\limits_{(t_\alpha,0)}^{(t_\beta,0)} \widetilde{D}\delta\mathbf{x} \ \exp\left[\frac{i}{2!\hbar}\int\limits_{t_\alpha}^{t_\beta} (\delta\mathbf{x}(t), \delta\dot{\mathbf{x}}(t))^T \frac{\partial^2 \mathcal{L}}{\partial(\mathbf{x}, \dot{\mathbf{x}})^2}\bigg|_{\substack{\mathbf{x}_c(t)\\ \dot{\mathbf{x}}_c(t)}} (\delta\mathbf{x}(t), \delta\dot{\mathbf{x}}(t))\right]$$

$$= \int\limits_{(t_\alpha,0)}^{(t_\beta,0)} \widetilde{D}\mathbf{x} \ \exp\left[\frac{i}{\hbar}\int\limits_{t_\alpha}^{t_\beta} \left[\frac{1}{2}\dot{\mathbf{x}}^T\mathbb{M}\dot{\mathbf{x}} + \dot{\mathbf{x}}^T\mathbb{A}\mathbf{x} - \mathbf{x}^T\mathbb{V}\mathbf{x}\right] \ dt\right]$$

$$\overset{(1.14)}{=} \lim_{N\to\infty} \left(\frac{\det \mathbb{M}}{(2\pi\hbar i\varepsilon)^n}\right)^{\frac{N+1}{2}} \int d^n\mathbf{x}_1 ... d^n\mathbf{x}_N$$

$$\exp\left[\frac{i\varepsilon}{\hbar}\sum_{j=0}^{N}\left[\frac{1}{2\varepsilon^2}(\mathbf{x}_{j+1} - \mathbf{x}_j)^T\mathbb{M}(\mathbf{x}_{j+1} - \mathbf{x}_j) + \frac{1}{\varepsilon}(\mathbf{x}_{j+1} - \mathbf{x}_j)^T\mathbb{A}\mathbf{x}_j - \mathbf{x}_j\mathbb{V}\mathbf{x}_j\right]\right]$$

$$= \lim_{N\to\infty} \left(\frac{\det \mathbb{M}}{(2\pi\hbar i\varepsilon)^n}\right)^{\frac{N+1}{2}} \int d^{nN}\mathbf{x} \ \exp\left[\frac{im}{2\hbar\varepsilon} \cdot \mathbf{x}^T\mathbb{L}^N\mathbf{x}\right] \qquad \bigg| \qquad m := \sqrt[n]{\det \mathbb{M}}$$

$$\overset{(A.3)}{=} \lim_{N\to\infty} \left[\frac{m}{2\pi\hbar i}\right]^{\frac{n}{2}} \cdot \frac{1}{\sqrt{\varepsilon^n \det \mathbb{L}^N}} \qquad \bigg| \qquad \varepsilon := \frac{(t_\beta - t_\alpha)}{N+1} \tag{1.19}$$

with the $N \times N$ matrix

$$\mathbb{L}^N := \frac{1}{m} \cdot \left(\begin{array}{c|c|c|c|c|c}
\substack{2\mathbb{M}-2\varepsilon\mathbb{A}\\ -2\varepsilon^2\mathbb{V}} & -\mathbb{M}+\varepsilon\mathbb{A} & 0 & 0 & & 0 \\ \hline
-\mathbb{M}+\varepsilon\mathbb{A} & \substack{2\mathbb{M}-2\varepsilon\mathbb{A}\\ -2\varepsilon^2\mathbb{V}} & -\mathbb{M}+\varepsilon\mathbb{A} & 0 & & 0 \\ \hline
0 & -\mathbb{M}+\varepsilon\mathbb{A} & \substack{2\mathbb{M}-2\varepsilon\mathbb{A}\\ -2\varepsilon^2\mathbb{V}} & -\mathbb{M}+\varepsilon\mathbb{A} & & 0 \\ \hline
0 & 0 & -\mathbb{M}+\varepsilon\mathbb{A} & \substack{2\mathbb{M}-2\varepsilon\mathbb{A}\\ -2\varepsilon^2\mathbb{V}} & \ddots & \\ \hline
 & & & & \ddots & \\ \hline
0 & 0 & 0 & 0 & \cdots & \substack{2\mathbb{M}-2\varepsilon\mathbb{A}\\ -2\varepsilon^2\mathbb{V}}
\end{array}\right) \tag{1.20}$$

and $m = \sqrt[n]{\det \mathbb{M}}$ as the *geometric mean mass* of the "particle".

## 1.4 Retrieving stationary states from transition amplitudes

Let $\{\Psi_E\}_E$ be the energy-eigenstates of the time-independent Hamiltonian $\hat{H}$ to the energy values $E$. We shall assume $\hat{H}$ to be non-degenerate. We can thus write

$$\langle\mathbf{x}_\beta|\,\hat{U}(t_\beta, t_\alpha)\,|\mathbf{x}_\alpha\rangle = \int dE \ \langle\mathbf{x}_\beta\,|\Psi_E\rangle\,\langle\Psi_E|\,U(t_\beta, t_\alpha)\,|\mathbf{x}_\alpha\rangle$$

$$= \int dE \ \Psi_E(\mathbf{x}_\beta)\Psi_E^*(\mathbf{x}_\alpha)e^{-\frac{i}{\hbar}(t_\beta - t_\alpha)} \quad . \tag{1.21}$$

[4]Note that (1.18) is of the type (1.13): Set

$$\mathbf{a}(\mathbf{x}) := \mathbb{M}^{-1}(\mathbb{A}\mathbf{x} + \mathbf{l}_2) \quad , \quad V(\mathbf{x}) := \mathbf{x}^T\mathbb{V}\mathbf{x} + \mathbf{l}_1 \cdot \mathbf{x} + \frac{1}{2}\mathbf{a}(\mathbf{x})^T\mathbb{M}\mathbf{a}(\mathbf{x}) \quad ,$$

whereas $l(\mathbf{x}, \dot{\mathbf{x}}) = \mathbf{l}_1 \cdot \mathbf{x} + \mathbf{l}_2 \cdot \dot{\mathbf{x}}$.

If $\tau_{\mathbf{x}_\beta,\mathbf{x}_\alpha}(E)$ is the Fourier-transformed of the transition amplitude, that is

$$\langle \mathbf{x}_\beta | \underbrace{\hat{U}(t_\beta, t_\alpha)}_{\hat{U}(t_\beta - t_\alpha)} | \mathbf{x}_\alpha \rangle = \int dE \; \tau_{\mathbf{x}_\beta,\mathbf{x}_\alpha}(E) \cdot e^{-\frac{i}{\hbar}E(t_\beta - t_\alpha)} \quad , \tag{1.22}$$

then a comparison with (1.21) yields

$$\Psi_E(\mathbf{x}_\beta)\Psi_E^*(\mathbf{x}_\alpha) = \tau_{\mathbf{x}_\beta,\mathbf{x}_\alpha}(E) \tag{1.23}$$

and thus (up to constant factors) the states $\Psi_E$. Thus, the transition amplitudes calculated by means of path-integrals, are indeed adequate to completely describe the stationary energy-states of a time-independent, non-degenerate quantum system.

# 2 Applications to quantum statistics

## 2.1 The quantum-mechanical partition function

As is known, for a quantum-mechanical system with fixed particle number in thermal equilibrium[5] with its environment, the canonical partition function[6]

$$Z(\beta) := \text{trace}\left(e^{-\beta \hat{H}}\right) \tag{2.1}$$

holds all thermodynamical information about the system[7]. By analytically extending the propagation operator $\hat{U}(t) := \exp\left[-\frac{i}{\hbar}t\hat{H}\right]$ to imaginary times and identifying $t := -i\hbar\beta$, one immediately obtains a connection to (2.1). Thus, to describe the thermodynamical equilibrium properties of the system, it suffices to study the trace of $\hat{U}$ and perform an analytical continuation to the imaginary time axis. This transition to imaginary times, is called a *Wick-rotation*, and allows the study of quantum-statistical problems by means of quantum-mechanical methods.

For an $n$-dimensional particle with Hamiltonian $\hat{H}(\hat{\mathbf{P}}, \hat{\mathbf{X}}) = T(\hat{\mathbf{P}}) + U(\hat{\mathbf{X}})$, we can write

$$Z(\beta) = \int d\mathbf{x}_\alpha \; \langle \mathbf{x}_\alpha | \hat{U}(-i\hbar\beta) | \mathbf{x}_\alpha \rangle \overset{(1.10)}{=} \int d\mathbf{x}_\alpha \int_{(0,\mathbf{x}_\alpha)}^{(-i\hbar\beta,\mathbf{x}_\alpha)} D\mathbf{x} \; D\mathbf{p} \; e^{\frac{i}{\hbar}S[\mathbf{x},\mathbf{p}]}$$

$$=: \oint_0^{-i\hbar\beta} D\mathbf{x} \; D\mathbf{p} \; e^{\frac{i}{\hbar}S[\mathbf{x},\mathbf{p}]} \tag{2.2}$$

where the "$\oint$" is to denote the periodic boundary conditions for the path integration performed. Whereas in classical statistical mechanics, the partition function

$$Z_{\text{cl}}(\beta) \sim \int d^n\mathbf{x} \; d^n\mathbf{p} \; e^{-\beta H(\mathbf{x},\mathbf{p})} \tag{2.3}$$

is constructed by weighting each microstate $(\mathbf{x}, \mathbf{p})$ with the factor $e^{-\beta H(\mathbf{x},\mathbf{p})}$, in quantum statistics each *path* $\mathbf{x}(t), \mathbf{p}(t)$ is weighted by the factor $e^{\frac{i}{\hbar}S[\mathbf{x},\mathbf{p}]}$, with the action $S[\mathbf{x}, \mathbf{p}]$ of a path replacing the energy $H(\mathbf{x}, \mathbf{p})$ of a state.

Expression (2.3) can also be written in a more direct form: By replacing $t = -i\tau$ and defining $\widetilde{\varepsilon} := \tau/N$, the

[5] That is, at fixed temperature. We shall assume $\hat{H}$ to be time-independent.
[6] With $\beta := 1/kT$ as *inverse temperature*.
[7] As an example, its free energy and entropy are given by $F = -kT \ln Z$ and $S = -\partial_T F$ respectively.

limit (1.9) takes the form

$$\int\limits_{(0,\mathbf{x}_\alpha)}^{(t,\mathbf{x}_\beta)} D\mathbf{x}\ D\mathbf{p}\ e^{\frac{i}{\hbar}S[\mathbf{x},\mathbf{p}]} = \lim_{N\to\infty}\int d^n\mathbf{x}_1\dots d^n\mathbf{x}_{N-1}\int\frac{d^n\mathbf{p}_0}{(2\pi\hbar)^n}\cdots\frac{d^n\mathbf{p}_{N-1}}{(2\pi\hbar)^n}$$

$$\exp\Bigg[\underbrace{-\frac{\widetilde{\varepsilon}}{\hbar}\sum_{j=0}^{N-1}\left[-\frac{i}{\widetilde{\varepsilon}}(\mathbf{x}_{j+1}-\mathbf{x}_j)\cdot\mathbf{p}_j+H(\mathbf{x}_j,\mathbf{p}_j)\right]}_{\overset{N\to\infty}{\longrightarrow}-\frac{1}{\hbar}\int\limits_0^\tau[-i\dot{\mathbf{x}}(\tau')\mathbf{p}(\tau')+H(\mathbf{x}(\tau'),\mathbf{p}(\tau'))]\ d\tau'}\Bigg]$$

$$= \int\limits_{(0,\mathbf{x}_\alpha)}^{(\tau,\mathbf{x}_\beta)} D\mathbf{x}\ D\mathbf{p}\ \exp\left[-\frac{1}{\hbar}S_e[\mathbf{x},\mathbf{p}]\right] \tag{2.4}$$

with

$$S_e[\mathbf{x},\mathbf{p}] := \int\limits_0^\tau [-i\dot{\mathbf{x}}(\tau')\mathbf{p}(\tau')+H(\mathbf{x}(\tau'),\mathbf{p}(\tau'))]\ d\tau' \tag{2.5}$$

as the so called *euclidean action* of the paths $\mathbf{x}(\tau'), \mathbf{p}(\tau')$. The canonical partition function can therefore be written as

$$Z(\beta) = \int d\mathbf{x}_\alpha \int_{(0,\mathbf{x}_\alpha)}^{(\beta\hbar,\mathbf{x}_\alpha)} D\mathbf{x}\ D\mathbf{p}\ e^{-\frac{1}{\hbar}S_e[\mathbf{x},\mathbf{p}]} = \oint_0^{\beta\hbar} D\mathbf{x}\ D\mathbf{p}\ \exp\left[-\frac{1}{\hbar}\int\limits_0^{\beta\hbar}[-i\dot{\mathbf{x}}\mathbf{p}+H(\mathbf{x},\mathbf{p})]\ d\tau'\right] \quad . \tag{2.6}$$

## 2.2 Particle density & classical limit

Consider a system in thermal equilibrium, with Hamiltonian $\hat{H}$. The density operator for the system is given by

$$\hat{\rho} = \frac{e^{-\beta\hat{H}}}{Z} \tag{2.7}$$

yielding the expected particle density

$$\rho(\mathbf{x}_\alpha) = \langle\mathbf{x}_\alpha|\,\hat{\rho}\,|\mathbf{x}_\alpha\rangle = Z^{-1}\int\limits_{(0,\mathbf{x}_\alpha)}^{(\beta\hbar,\mathbf{x}_\alpha)} D\mathbf{x}\ D\mathbf{p}\ e^{-\frac{1}{\hbar}S_e[\mathbf{x},\mathbf{p}]} \tag{2.8}$$

at position $\mathbf{x}_\alpha$.

Now suppose the Hamiltonian to be of the standard form $\hat{H} = \frac{\hat{\mathbf{P}}^2}{2m} + V(\hat{\mathbf{X}})$. Then, as is shown in Kleinert[2], in the high temperature limit $T\to\infty$, (2.8) goes (for sufficiently smooth potentials) over to the classical expression

$$\rho(\mathbf{x}_\alpha) \overset{T\to\infty}{\longrightarrow} \left[\int d^n\mathbf{x}\ e^{-V(\mathbf{x})/kT}\right]^{-1}\cdot e^{-V(\mathbf{x}_\alpha)/kT} = \rho_{\rm cl}(\mathbf{x}_\alpha) \quad . \tag{2.9}$$

# 3 Example: Harmonic oscillator

## 3.1 The fluctuation factor

Let us consider an $n$-dimensional harmonic oscillator within an harmonic potential, described by the real, diagonal matrix $\Omega \in \mathbb{R}^{n\times n}$, so that

$$\mathcal{L}(\mathbf{x},\dot{\mathbf{x}}) = \frac{m}{2}\dot{\mathbf{x}}^2 - \frac{m}{2}\mathbf{x}^T\Omega^2\mathbf{x} \quad , \quad \Omega = \mathrm{diag}(\omega_1,..,\omega_n) \quad . \tag{3.1}$$

Thus by section 1.3, the fluctuation factor becomes

$$F(t_\beta - t_\alpha) \overset{(1.19)}{=} \lim_{N\to\infty}\left[\frac{m}{2\pi\hbar i}\right]^{\frac{n}{2}} \cdot \frac{1}{\sqrt{\varepsilon^n \det \mathbb{L}^N}} = \lim_{N\to\infty}\left[\frac{m}{2\pi\hbar i}\right]^{\frac{n}{2}} \cdot \prod_{k=1}^{n} \frac{1}{\sqrt{\varepsilon \det \mathbb{L}_k^N}} \tag{3.2}$$

with $\mathbb{L}^N$ defined as in (1.20) with $\mathbb{M} := m\cdot\mathbb{1}$, $\mathbb{A} := 0$, $\mathbb{V} := m\Omega^2/2$ and

$$\mathbb{L}_k^N := \begin{pmatrix} 2-\varepsilon^2\omega_k^2 & -1 & 0 & 0 & \dots & 0 \\ -1 & 2-\varepsilon^2\omega_k^2 & -1 & 0 & & \\ 0 & -1 & 2-\varepsilon^2\omega_k^2 & -1 & & \\ 0 & 0 & -1 & 2-\varepsilon^2\omega_k^2 & & \\ \vdots & & & & \ddots & \\ 0 & & & & & 2-\varepsilon^2\omega_k^2 \end{pmatrix} \in \mathbb{R}^{N\times N} \quad . \tag{3.3}$$

Note how the decomposition of $\det \mathbb{L}^N$ into a product of $n$ determinants $\det \mathbb{L}_k^N$ corresponds to the separation of the $n$ coordinates[8]. The matrix $\frac{1}{\varepsilon^2}\mathbb{L}_k^N$ corresponds to the bilinear form

$$\frac{1}{\varepsilon^2}\mathbb{L}_k^N : \mathbf{x} \mapsto \sum_{j=1}^{N}\left[\frac{(x_{j+1}-x_j)^2}{\varepsilon^2} - \omega_k^2 x_j^2\right] \quad . \tag{3.4}$$

on $\mathbb{R}^N$. It can be interpreted as corresponding to the discrete version of[9] $(\partial_t^\dagger\partial_t - \omega_k^2)$, which instead of functions $f:[t_\alpha,t_\beta]\to\mathbb{R}$, operates on functions ($n$-tuples) $\mathbf{x}:\{1,..,n\}\to\mathbb{R}$.

We now show that the determinant of the $\mathbb{L}_k^N$ is generally[10] given by[11]

$$\det \mathbb{L}_k^N = \frac{\sin(\widetilde{\omega}_k\varepsilon(N+1))}{\sin(\widetilde{\omega}_k\varepsilon)} =: a_{N+1} \tag{3.5}$$

whereas

$$\sin\frac{\widetilde{\omega}_k\varepsilon}{2} := \frac{\omega_k\varepsilon}{2} \quad . \tag{3.6}$$

Note that by Leibnitz, from (3.3) one obtains the recursion formula

$$\det \mathbb{L}_k^N = (2-\varepsilon^2\omega_k^2)\cdot \det \mathbb{L}_k^{N-1} - \det \mathbb{L}_k^{N-2} \quad , \quad N\geq 2 \tag{3.7}$$

whereas

$$\det \mathbb{L}_k^0 := 1 \quad , \quad \det \mathbb{L}_k^1 = 2-\omega_k^2\varepsilon^2 \quad . \tag{3.8}$$

[8] Also see appendix A.4.

[9] Note that any operator $D:\mathcal{H}\to\mathcal{H}$ on a Hilbert-space $\mathcal{H}$, can be interpreted as a bilinear form by means of $f\mapsto\langle f, Df\rangle$, $f\in\mathcal{H}$.

[10] Without any connection assumed between $\varepsilon$ and $N$.

[11] For a justification of this ansatz see Kleinert[2].

By observing that $a_N$ also satisfies the recursion formula (3.7):

$$a_N = \frac{\sin(\widetilde{\omega}_k \varepsilon N)}{\sin(\widetilde{\omega}_k \varepsilon)} = \frac{\sin\left[\widetilde{\omega}_k \varepsilon (N-1)\right]\cos(\widetilde{\omega}_k \varepsilon) + \cos\left[\widetilde{\omega}_k \varepsilon (N-1)\right]\sin(\widetilde{\omega}_k \varepsilon)}{\sin(\widetilde{\omega}_k \varepsilon)}$$

$$= \frac{2\sin\left[\widetilde{\omega}_k \varepsilon (N-1)\right]\overbrace{\left[1 - 2\sin^2\frac{\widetilde{\omega}_k \varepsilon}{2}\right]}^{\cos(\widetilde{\omega}_k \varepsilon)} - \left[\sin\left[\widetilde{\omega}_k \varepsilon (N-1)\right]\cos(\widetilde{\omega}_k \varepsilon) - \cos\left[\widetilde{\omega}_k \varepsilon (N-1)\right]\sin(\widetilde{\omega}_k \varepsilon)\right]}{\sin(\widetilde{\omega}_k \varepsilon)}$$

$$\stackrel{(3.6)}{=} \frac{2\sin\left[\widetilde{\omega}_k \varepsilon (N-1)\right]\left(1 - \frac{\omega_k^2 \varepsilon^2}{2}\right) - \sin\left[\widetilde{\omega}_k \varepsilon (N-2)\right]}{\sin(\widetilde{\omega}_k \varepsilon)} = a_{N-1} \cdot (2 - \omega_k^2 \varepsilon^2) - a_{N-2} \tag{3.9}$$

and the initial conditions (3.15):

$$a_1 = 1 \quad , \quad a_2 = \frac{\sin(2\widetilde{\omega}_k \varepsilon)}{\sin(\widetilde{\omega}_k \varepsilon)} = 2\cos(\widetilde{\omega}_k \varepsilon) = 2\left(1 - 2\sin^2\frac{\widetilde{\omega}_k \varepsilon}{2}\right) \stackrel{(3.6)}{=} 2 - \omega_k^2 \varepsilon^2 \tag{3.10}$$

we conclude that indeed $\det \mathbb{L}_k^N = a_{N+1}$.

Thus, expression (3.2) evaluates to

$$F(t_\beta - t_\alpha) \stackrel{(3.5)}{=} \lim_{N\to\infty} \left[\frac{m}{2\pi\hbar i}\right]^{\frac{n}{2}} \cdot \prod_{k=1}^{n} \sqrt{\frac{\sin(\widetilde{\omega}_k \varepsilon)}{\varepsilon \sin\left[\widetilde{\omega}_k \varepsilon (N+1)\right]}} \quad . \tag{3.11}$$

Recall that $\varepsilon = (t_\beta - t_\alpha)/(N+1)$ and notice how $\widetilde{\omega}_k \stackrel{\varepsilon\to 0}{\longrightarrow} \omega_k$. Hence (3.11) yields the fluctuation factor:

$$\boxed{F(t_\beta - t_\alpha) = \left[\frac{m}{2\pi\hbar i}\right]^{\frac{n}{2}} \cdot \prod_{k=1}^{n} \sqrt{\frac{\omega_k}{\sin\left[\omega_k (t_\beta - t_\alpha)\right]}}} \tag{3.12}$$

for the $n$-dimensional harmonic oscillator. In the special case of a free particle ($\Omega \to 0$) the fluctuation factor becomes

$$\boxed{F(t_\beta - t_\alpha) = \left[\frac{m}{2\pi\hbar i (t_\beta - t_\alpha)}\right]^{\frac{n}{2}} \quad .} \tag{3.13}$$

From (3.5) one sees that, $\det \mathbb{L}_k^N$ is only then positive definite, when $|\widetilde{\omega}_k (t_\beta - t_\alpha)| < \pi$. For larger time intervals, the Fresnel-integral (1.19) would no longer evaluate as (A.3), but differ by phase factors $e^{\frac{i\pi}{2}\varkappa}$, $\varkappa \in \mathbb{Z}$ from (3.13), depending on the actual length $|t_\beta - t_\alpha|$. See Kleinert[2] for a more thorough elaboration on the issue.

The actual transition amplitude (1.15) is obtained by multiplying the fluctuation factor by $e^{\frac{i}{\hbar}S[\mathbf{x}_c]}$, with $S[\mathbf{x}_c]$ as the action of the classical trajectory $\mathbf{x}_c(t)$. It is straightforward to calculate the classical trajectory $\mathbf{x}_c$ connecting the points $\mathbf{x}_\alpha, \mathbf{x}_\beta$ at respective times $t_\alpha, t_\beta$ for the harmonic oscillator and obtain

$$S[\mathbf{x}_c] = \sum_{k=1}^{n} \frac{m\omega_k}{2\sin\left[\omega_k (t_\beta - t_\alpha)\right]} \cdot \left[((x_\alpha^k)^2 + (x_\beta^k)^2)\cos\left[\omega_k (t_\beta - t_\alpha)\right] - 2x_\alpha^k x_\beta^k\right] \tag{3.14}$$

**Note**

The results in section 1.3 and in particular example 3 indicate that, the problem of calculating the fluctuation factor for a given Lagrangian, often lies in finding the determinant of the Bilinear form $\mathbb{L}^N$ appearing in the lattice-version of the action and performing a meaningful limiting procedure. Back to the above example, let us consider w.l.o.g. the one-dimensional case ($\omega := \omega_1$). Let $\varepsilon > 0$ be fixed and define $D^N := \det \mathbb{L}_1^N$, then recursion formula 3.7 can be rewritten in the form

$$\frac{1}{\varepsilon}\left[\frac{1}{\varepsilon}\left(D^N - D^{N-1}\right) - \frac{1}{\varepsilon}\left(D^{N-1} - D^{N-2}\right)\right] + \omega^2 D^{N-1} = 0 \quad , \quad N = 2, 3, .. \tag{3.15}$$

If we interpret $\mathbf{D} := \left(D^N\right)_{N=0}^{N=\infty}$ as a function of $N$ (or $n \times \infty$-*matrix*) and introduce the *differential* operators

$$\nabla^l \mathbf{D}(N) := \frac{1}{\varepsilon}\left(D^N - D^{N-1}\right) \quad , \quad \nabla^r \mathbf{D}(N) := \frac{1}{\varepsilon}\left(D^{N+1} - D^N\right) \tag{3.16}$$

acting on the index-parameter $N$, then (3.15) takes the form

$$\boxed{\left[\nabla^l \nabla^r + \omega^2\right]\mathbf{D} = 0 \ .} \tag{3.17}$$

This is a special case of the so called *Gelfand-Yaglom-Formula*, which can be regarded as an equation of motion for the determinant $\mathbf{D}(N)$ as a function of $N$ on the discrete time-lattice. The start values are in view of (3.15), taken to be $D^0 := 1$ and $D^1 := 2 - \varepsilon^2\omega^2$. See Kleinert[2] for a more elaborate treatise of such equations of motion.

### 3.2 The partition function for harmonic oscillators

As an example, consider a system of $n$ uncoupled, identical harmonic oscillators. It is described by the Hamiltonian

$$H(\mathbf{x},\mathbf{p}) = \frac{\mathbf{p}^2}{2m} + \frac{m}{2}\omega^2\mathbf{x}^2 \quad , \quad \mathbf{x},\mathbf{p} \in \mathbb{R}^n \tag{3.18}$$

and by (3) has transition amplitude

$$\langle \mathbf{x}_\beta | \hat{U}(t) | \mathbf{x}_\alpha \rangle = \left[\frac{m\omega}{i2\pi\hbar\sin(\omega t)}\right]^{\frac{n}{2}} \cdot \exp\left[\frac{im\omega}{2\hbar\sin(\omega t)} \cdot \left[(\mathbf{x}_\alpha^2 + \mathbf{x}_\beta^2)\cos(\omega t) - 2\mathbf{x}_\alpha\mathbf{x}_\beta\right]\right] \ . \tag{3.19}$$

Hence in view of (2.2), the canonical partition function is given by

$$\begin{aligned} Z(\beta) &= \left[\frac{m\omega}{i2\pi\hbar\sin(\omega t)}\right]^{\frac{n}{2}} \cdot \int \mathbf{x}_\alpha \ \exp\left[\frac{im\omega\mathbf{x}_\alpha^2}{\hbar\sin(\omega t)} \cdot \left[\cos(\omega t) - 1\right]\right] \quad \Bigg| \quad t := -i\hbar\beta \\ &= \frac{1}{\left[2\cos(\omega t) - 2\right]^{\frac{n}{2}}} = \frac{1}{\left[2\sinh\left(\frac{\omega\hbar\beta}{2}\right)\right]^n} \end{aligned} \tag{3.20}$$

as expected[2].

# 4 Charged particles in magnetic fields

Using the results from section 1, we shall calculate the transition elements of a non-relativistic charged particle within an electromagnetic field. Though in principle, the Lagrangian is of the form (1.18), the techniques developed in sections 1.2 and 1.3 turn out to be impractical. We shall thus employ a more direct, brute force method[2] for evaluating the resulting path integral.

### 4.1 Action & gauge invariance

Consider a non-relativistic particle of mass $m$ and charge $q$ within an electromagnetic field, described by[12] the vector potential $\mathbf{A}(\mathbf{x})$ and scalar field $\Phi(\mathbf{x})$. Its Hamiltonian is given by

$$H(\mathbf{x},\mathbf{p}) = \frac{1}{2m}\left(\mathbf{p} - q\mathbf{A}(\mathbf{x})\right)^2 + q\Phi(\mathbf{x}) \tag{4.1}$$

[12] So that $\mathbf{B} = \nabla \times \mathbf{A}$ and $\mathbf{E} = -\nabla\Phi - \dot{\mathbf{A}}$.

which implies the action

$$S[\mathbf{x},\mathbf{p}] = \int_{t_\alpha}^{t_\beta} \underbrace{\left[\mathbf{p}\dot{\mathbf{x}} - \frac{1}{2m}\left(\mathbf{p} - q\mathbf{A}(\mathbf{x})\right)^2 - q\Phi(\mathbf{x})\right]}_{\mathcal{L}(\mathbf{x},\mathbf{p})} \, dt \tag{4.2}$$

for any path $(\mathbf{x},\mathbf{p})$ within times $t_\alpha, t_\beta$.

Alternatively, the action can be written as

$$S[\mathbf{x}] = \int_{t_\alpha}^{t_\beta} \underbrace{\left[\frac{m}{2}\dot{\mathbf{x}}^2 + q\dot{\mathbf{x}}\mathbf{A}(\mathbf{x}) - q\Phi(\mathbf{x})\right]}_{\mathcal{L}(\mathbf{x},\dot{\mathbf{x}})} \, dt \quad . \tag{4.3}$$

Now consider any arbitrary gauge transformation $\mathbf{A}' := \mathbf{A} + \nabla f,\ \Phi' := \Phi - \partial_t f$, then the Lagrangian becomes

$$\mathcal{L}'(\mathbf{x},\dot{\mathbf{x}}) = \mathcal{L}(\mathbf{x},\dot{\mathbf{x}}) + (\dot{\mathbf{x}}\nabla f + \partial_t f) = \mathcal{L}(\mathbf{x},\dot{\mathbf{x}}) + \frac{d}{dt} f(\mathbf{x}(t)) \tag{4.4}$$

which in turn induces the action

$$S'[\mathbf{x}] = \int_{t_\alpha}^{t_\beta} \mathcal{L}'(\mathbf{x},\dot{\mathbf{x}}) \, dt = S[\mathbf{x}] + q \cdot [f(\mathbf{x}_\beta) - f(\mathbf{x}_\alpha)] \tag{4.5}$$

The boundary term $S_{\text{bd}} := q\,[f(\mathbf{x}_\beta) - f(\mathbf{x}_\alpha)]$ corresponds to an additional phase factor in the transition amplitude $\langle \mathbf{x}_\beta, t \,|\mathbf{x}_\alpha, 0\rangle'$ and has no effect on the diagonal elements $\langle \mathbf{x}_\alpha, t \,|\mathbf{x}_\alpha, 0\rangle'$. In particular, the canonical partition function $Z(\beta)$ and expected particle density $\rho(\mathbf{x}_\alpha) = \langle \mathbf{x}_\alpha, -i\beta\hbar \,|\mathbf{x}_\alpha, 0\rangle / Z(\beta)$ are left unchanged.

## 4.2 Example: Homogeneous B-field

Suppose now that $\mathbf{A}(\mathbf{x}) = (0, xB, 0)$ (magnetic field along $z$ axis) and $\Phi = 0$. Then the transition amplitude from $\mathbf{x}_\alpha$ to $\mathbf{x}_\beta$ within time $t$ is given by

$$\langle \mathbf{x}_\beta | \hat{U}(t) | \mathbf{x}_\alpha \rangle = \lim_{N\to\infty} \int d^3\mathbf{x}_1 \dots d^3\mathbf{x}_N \int \frac{d^3\mathbf{p}_0}{(2\pi\hbar)^3} \cdots \frac{d^3\mathbf{p}_N}{(2\pi\hbar)^3}$$

$$\exp\left[\frac{i\varepsilon}{\hbar}\sum_{j=0}^{N}\left[\frac{1}{\varepsilon}(\mathbf{x}_{j+1}-\mathbf{x}_j)\cdot\mathbf{p}_j - \frac{1}{2m}(\mathbf{p}_j - q\mathbf{A}(\mathbf{x}))^2\right]\right] \quad \Big| \quad \varepsilon := \frac{t}{(N+1)}$$

$$= \int dx^1..dx^N \; \frac{d^3\mathbf{p}_0}{(2\pi\hbar)^3}..\frac{d^3\mathbf{p}_N}{(2\pi\hbar)^3} \; \exp\left[\frac{i\varepsilon}{\hbar}\sum_{j=0}^{N}\left[\frac{1}{\varepsilon}(x_{j+1}-x_j)p_j^x - \frac{1}{2m}\left[(p_j^x)^2 + (p_j^y - qx_jB)^2 + (p_j^z)^2\right]\right]\right]$$

$$\underbrace{\times \int dy^1..dy^N \; dz^1..dz^N \exp\left[\frac{i}{\hbar}\underbrace{\sum_{j=0}^{N}(y_{j+1}-y_j)p_j^y + (z_{j+1}-z_j)p_j^z}_{\substack{y_\beta p_N^y - y_\alpha p_0^y + z_\beta p_N^z - z_\alpha p_0^z \\ +\sum_{j=1}^N\left[y_j(p_{j-1}^y - p_j^y) + z_j(p_{j-1}^z - p_j^z)\right]}}\right]}_{(2\pi\hbar)^{2N}\cdot\exp\left[\frac{i}{\hbar}\left(y_\beta p_N^y - y_\alpha p_0^y + z_\beta p_N^z - z_\alpha p_0^z\right)\right]\cdot\prod_{j=1}^N \delta(p_{j-1}^y - p_j^y)\delta(p_{j-1}^z - p_j^z)}$$

$$= \int \frac{dp_0^y}{2\pi\hbar}\frac{dp_0^z}{2\pi\hbar} \; \exp\left[\frac{i}{\hbar}\left[p_0^y(y_\beta - y_\alpha) + p_0^z(z_\beta - z_\alpha) - \frac{(p_0^z)^2 t}{2m}\right]\right]$$

$$\underbrace{\times \int dx^1..dx^N \; \frac{dp_0^x}{2\pi\hbar}..\frac{dp_N^x}{2\pi\hbar} \; \exp\left[\frac{i\varepsilon}{\hbar}\sum_{j=0}^{N}\left[\frac{1}{\varepsilon}(x_{j+1}-x_j)p_j^x - \underbrace{\frac{1}{2m}\left[(p_j^x)^2 + (p_0^y - qx_jB)^2\right]}_{\frac{(p_j^x)^2}{2m} + \frac{m}{2}\frac{q^2B^2}{m^2}\left(x_j - \frac{p_0^y}{qB}\right)^2}\right]\right]}_{\substack{\text{transition amplitude for 1-dim. harmonic oscillator} \\ \text{with frequency } \omega_c := \frac{qB}{m}\text{, center } x_0 := \frac{p_0^y}{qB}}}$$

$$= \int \frac{dp_0^y}{2\pi\hbar}\frac{dp_0^z}{2\pi\hbar} \exp\left[\frac{i}{\hbar}\left[p_0^y(y_\beta - y_\alpha) + p_0^z(z_\beta - z_\alpha) - \frac{(p_0^z)^2 t}{2m}\right]\right] \cdot \underbrace{\left\langle x_\beta - \frac{p_0^y}{qB}, t \,\middle|\, x_\alpha - \frac{p_0^y}{qB}, 0\right\rangle_{\omega_c}}_{\substack{\text{transition amplitude for} \\ \text{harmonic oscillator} \\ \text{with frequency } \omega_c}}$$

$$\overset{(A.2)}{=} \underbrace{\sqrt{\frac{m}{i2\pi\hbar t}} \cdot \exp\left[\frac{im}{2\hbar}\frac{(z_\beta - z_\alpha)^2}{t}\right]}_{\substack{\text{transition amplitude for} \\ \text{1-dim. particle along} \\ z\text{-axis, from } z_\alpha \text{ to } z_\beta}} \cdot \left\langle \mathbf{x}_\beta^\perp, t \,\middle|\, \mathbf{x}_\alpha^\perp, 0\right\rangle \quad \Big| \quad (\text{integration of } p_0^z) \tag{4.6}$$

with the *transversal transition amplitude*

$$\left\langle \mathbf{x}_\beta^\perp, t \,\middle|\, \mathbf{x}_\alpha^\perp, 0\right\rangle := \frac{m\omega_c}{2\pi\hbar}\int dx_0 \; \exp\left[\frac{i}{\hbar}m\omega_c x_0(y_\beta - y_\alpha)\right] \cdot \langle x_\beta - x_0, t \,| x_\alpha - x_0, 0\rangle_{\omega_c} \tag{4.7}$$

and *cyclotron frequency* $\omega_c := qB/m$. From section 3 we know that

$$\langle x_\beta - x_0, t\, | x_\alpha - x_0, 0\rangle$$

$$= \sqrt{\frac{m\omega_c}{2\pi\hbar i \sin(\omega_c t)}} \cdot \exp\left\{\frac{im\omega_c}{2\hbar\sin(\omega_c t)}\left[\left((x_\alpha - x_0)^2 + (x_\beta - x_0)^2\right)\cos(\omega_c t) - 2\,(x_\alpha - x_0)\,(x_\beta - x_0)\right]\right\} \quad . \tag{4.8}$$

Inserting into (4.7) and integrating yields

$$\left\langle \mathbf{x}_\beta^\perp, t\, \left| \mathbf{x}_\alpha^\perp, 0\right.\right\rangle = \frac{m\omega_c}{4i\pi\hbar\sin\frac{\omega_c t}{2}} \cdot \exp\left\{\frac{im}{2\hbar}\left[\omega_c(x_\alpha + x_\beta)(y_\beta - y_\alpha) + \frac{\omega_c}{2}\cot\left(\tfrac{\omega_c t}{2}\right)\left[(x_\beta - x_\alpha)^2 + (y_\beta - y_\alpha)^2\right]\right]\right\} \quad . \tag{4.9}$$

Together with (4.6), we finally obtain the transition amplitude

$$\boxed{\langle \mathbf{x}_\beta, t\, | \mathbf{x}_\alpha\rangle = \left[\frac{m}{2\pi\hbar i t}\right]^{\frac{3}{2}} \cdot \frac{\omega_c t}{2\sin\frac{\omega_c t}{2}} \cdot \exp\left[\frac{i}{\hbar}\left[S_{\text{cl}} + S_{\text{bd}}\right]\right]} \tag{4.10}$$

with the classical action

$$\boxed{S_{\text{cl}} = \frac{m}{2}\left[\frac{(z_\beta - z_\alpha)^2}{t} + \omega_c(x_\alpha y_\beta - x_\beta y_\alpha) + \frac{\omega_c}{2}\cot\left(\tfrac{\omega_c t}{2}\right)\left[(x_\beta - x_\alpha)^2 + (y_\beta - y_\alpha)^2\right]\right]} \tag{4.11}$$

and *boundary action*

$$\boxed{S_{\text{bd}} = \frac{m\omega_c}{2}(x_\beta y_\beta - x_\alpha y_\alpha) \quad .} \tag{4.12}$$

The latter actually disappears by choosing the gauge $\widetilde{\mathbf{A}}(\mathbf{x}) := \mathbf{A}(\mathbf{x}) + \nabla f = \frac{1}{2}\mathbf{B} \times \mathbf{x}$ with the gauge function $f(\mathbf{x}) = -\frac{1}{2}\mathbf{x}\mathbf{A}(\mathbf{x})$.[13]. Indeed, in view of section 4.1, this gauge transformation leads to the boundary term $q\left[f(\mathbf{x}_\beta) - f(\mathbf{x}_\alpha)\right] = \frac{qB}{2}\left[x_\alpha y_\alpha - x_\beta y_\beta\right] = -S_{\text{bd}}$ in the new action, yielding the transition amplitude

$$\langle \mathbf{x}_\beta, t\, | \mathbf{x}_\alpha, 0\rangle' = \left[\frac{m}{2\pi\hbar i t}\right]^{\frac{3}{2}} \cdot \frac{\omega_c t}{2\sin\frac{\omega_c t}{2}} \cdot \exp\left[\frac{i}{\hbar}S_{\text{cl}}\right] \quad . \tag{4.13}$$

For further details into the subject see Kleinert[2].

[13]Recall that for any $\varkappa$-homogeneous vector-potential $\mathbf{A}(\mathbf{x})$, inducing the magnetic field $\mathbf{B} := \nabla \times \mathbf{A}$, the gauge $f(\mathbf{x}) := -\frac{\mathbf{x}\mathbf{A}(\mathbf{x})}{\varkappa+1}$ transforms $\mathbf{A}$ into $\mathbf{A}' := \mathbf{A} + \nabla f = \frac{\mathbf{B}\times\mathbf{x}}{\varkappa+1}$.

# A Appendix

This appendix provides with some auxiliary statements, used throughout this article.

## A.1 Gauß-Integrals

For a real, symmetric, positive-definite matrix $\hat{A} \in \mathbb{R}^{n\times n}$ and vector $\mathbf{b} \in \mathbb{R}^n$ one has

$$\int\limits_{\mathbb{R}^n} d^n\mathbf{x}\ \exp\left[-\mathbf{x}^T\hat{A}\mathbf{x} \pm \mathbf{b}^T\mathbf{x}\right] = \sqrt{\frac{\pi^n}{\det \hat{A}}} \cdot \exp\left[\frac{1}{4}\mathbf{b}^T\hat{A}^{-1}\mathbf{b}\right] \tag{A.1}$$

and

$$\int\limits_{\mathbb{R}^n} d^n\mathbf{x}\ \exp\left[-i\mathbf{x}^T\hat{A}\mathbf{x} \pm i\mathbf{b}^T\mathbf{x}\right] = \sqrt{\frac{\pi^n}{i^n \det \hat{A}}} \cdot \exp\left[\frac{i}{4}\mathbf{b}^T\hat{A}^{-1}\mathbf{b}\right] \quad . \tag{A.2}$$

whereas $\sqrt{i} := e^{\frac{i\pi}{4}}$. By complex conjugation, one moreover obtains

$$\int\limits_{\mathbb{R}^n} d^n\mathbf{x}\ \exp\left[i\mathbf{x}^T\hat{A}\mathbf{x} \pm i\mathbf{b}^T\mathbf{x}\right] = \sqrt{\frac{\pi^n i^n}{\det \hat{A}}} \cdot \exp\left[-\frac{i}{4}\mathbf{b}^T\hat{A}^{-1}\mathbf{b}\right] \quad . \tag{A.3}$$

Proofs of these statements can be found in Swanson[1].

## A.2 Determinants

Let $A^{ij} \in \mathbb{C}^{n\times n},\ i,j = 1,..,N$ be diagonal matrices. Then

$$\underbrace{\det\begin{pmatrix} A^{11} & A^{12} & \cdots \\ A^{21} & A^{22} & \\ \vdots & & \ddots \end{pmatrix}}_{\in\mathbb{C}^{nN\times nN}} = \prod_{k=1}^{n} \underbrace{\det\begin{pmatrix} A^{11}_{kk} & A^{12}_{kk} & \cdots \\ A^{21}_{kk} & A^{22}_{kk} & \\ \vdots & & \ddots \end{pmatrix}}_{\in\mathbb{C}^{N\times N}} \tag{A.4}$$

holds.

## A.3 The Zassenhaus formula

Le $X, Y$ be in some Lie algebra $\mathfrak{g}$ of a simply-connected Lie group $G$. Then for $\varepsilon > 0$

$$e^{\varepsilon(X+Y)} = e^{\varepsilon X} e^{\varepsilon Y} e^{-\frac{\varepsilon^2}{2}[X,Y]} e^{\mathcal{O}(\varepsilon^3)} \tag{A.5}$$

holds.

# References


[1] *Path Integrals and Quantum Processes*, M. Swanson
Academic Press Inc., 1992

[2] *Pfadintegrale in Quantenmechanik, Statistik und Polymerphysik*, H. Kleinert
Spektrum Akademischer Verlag, 1993

[3] *Path Integral*, J.Z. Justin
Scholarpedia, 4(2):8674, 2009
http://www.scholarpedia.org/article/Path_integral

[4] *Space-Time Approach to Non-Relativistic Quantum Mechanics*, R.P. Feynman
Reviews of Modern Physics, Vol. 20, No. 2, 1948

[5] *Lecture notes on Path integrals*, A. Wipf
FSU Jena, 2002
http://www.personal.uni-jena.de/∼ p5anwi/lecturenotes.html (May 20, 2010)

[6] *Field Quantization*, W. Greiner, J. Reinhardt
Springer, 1996