(90

13. Pfadintegralformulierung der QM

Litt: R. P. Feynman, A. R. Hibbs
"QM and Path Integrals
(McGraw Hill, New York (1965))
H. Kleinert
"Path Int. in QM, Statistics, ..."
(World Scientific, Singapore (2004))

– Aus meinen QFT I/II
Vorlesungen

Chapter 8

Path integral formulation of QFT

So far, we have studied QFT in the canonical formalism with operator-valued fields, in the Heisenberg representation. Richard Feynman has formulated another representation of both QM and QFT, which is very intuitive and does not use operators. Its mathematical status, however, is still in development. This method is particularly powerful if one wants to quantize gauge theories - this is why it is necessary to discuss it - and it also allows one to derive the Feynman rules very easily, and to discuss problems beyond perturbation theory, although we will not go into the latter here.

13.1

8.1 Path integrals in QM

The path integral formulation of QM centers around the transition amplitude for a QM particle from a position $x(t)$ at a time t to a position $x'(t')$ at time t'. It starts from the Heisenberg picture, where the time dependent operators $\mathbf{X}(t)$ and $\mathbf{P}(t)$ have their respective eigenvectors $|x(t)\rangle$ and $|p(t)\rangle$, with time developments

$$\mathbf{X}(t) = e^{i\mathbf{H}(t-t_0)/\hbar}\mathbf{X}(t_0)e^{-i\mathbf{H}(t-t_0)/\hbar} \tag{8.1}$$

$$|x(t)\rangle = e^{i\mathbf{H}(t-t_0)/\hbar}|x(t_0)\rangle \tag{8.2}$$

and similarly for $\mathbf{P}$ and p. The factors of $\hbar$ have been reinserted here for clarity. Note that the sign in eq. (8.2) is opposite to that of the Schrödinger equation. Note also that this equation describes a transition in time, while the position does not change. Finally, in eq. (8.1), $\mathbf{X}(t_0) = \mathbf{X}_S$; in the Schrödinger picture, t_0 is usually taken to be 0.

Let us start at the end of our discussion of the path integral formulation, 91

with the result:

$$\boxed{\langle x'(t')|x(t)\rangle = \int \mathcal{D}x\mathcal{D}p \exp\left[i\int_t^{t'} d\tau \left\{p(\tau)\frac{dx}{d\tau} - \mathbf{H}(p,x)\right\}/\hbar\right]} \tag{8.3}$$

Here, $\int \mathcal{D}x$ is a *path integral*, in mathematical circles known as *functional integral*, an integral over all possible paths $x(\tau)$ connecting x and x', with $x(t) = x$ and $x(t') = x'$.

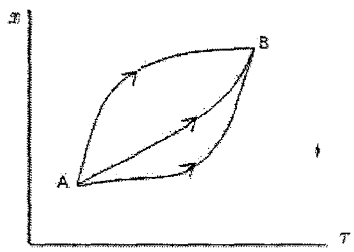


Figure 8.1: Integrate over all possible paths

$\int \mathcal{D}p$ does not have boundary conditions, since the problem asks for the transition amplitude between positions, but not between momenta. (As a small aside: note that the exponent is just the classical action times $i/\hbar$.)

After discretization of the time integral, it becomes a product of integrals at $\tau_1, \tau_2, \ldots$ over $x(\tau_1), x(\tau_2), \ldots$:

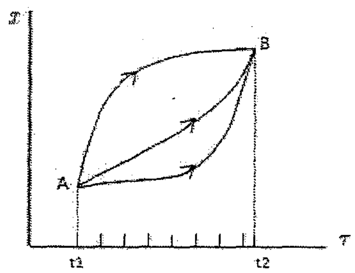


Figure 8.2: Discretization of the time integral

$$\int \mathcal{D}x \exp\left(\int d\tau \ldots\right) \to \prod_i \int_{-\infty}^{\infty} dx(\tau_i)$$

Defining $\delta\tau := \tau_i - \tau_{i-1}$, one eventually has to take the limit $\delta\tau \to 0$, which is mathematically demanding. Obviously, the integral over $\mathcal{D}x$ does not need to be evaluated at the endpoints, since these are fixed.

92

Now, let us derive this result. From the canonical formalism, we have the following formula:

$$\langle x'(t')|x(t)\rangle = \langle x'|\, e^{-i\mathbf{H}(t'-t)/\hbar}\,|x\rangle \tag{8.4}$$

where $|x\rangle$ is a Schrödinger state. Decomposing the interval into N bits, $t'-t = N\epsilon$, gives

$$\langle x_N|\, e^{-i\mathbf{H}\epsilon/\hbar}\,|x_{N-1}\rangle\, \langle x_{N-1}|\, e^{-i\mathbf{H}\epsilon/\hbar}\,|x_{N-2}\rangle\, \langle x_{N-2}|\cdots$$
$$\cdots|x_1\rangle\, \langle x_1|\, e^{-i\mathbf{H}\epsilon/\hbar}\,|x_0\rangle$$

where $x_N = x'$ and $x_0 = x$, and $\mathbf{H} = \frac{\mathbf{P}^2}{2m} + V(\mathbf{X})$. Consider one of these matrix elements, to order ϵ:

$$\begin{aligned}
&\langle x_{k+1}|\, e^{-i\mathbf{H}\epsilon/\hbar}\,|x_k\rangle = \langle x_{k+1}|\, 1 - \frac{i\mathbf{H}}{\hbar}\epsilon + \ldots |x_k\rangle = \\
&\quad \langle x_{k+1}|x_k\rangle - i\epsilon \int \frac{dp_k}{2\pi\hbar} \left\{ V\left(\frac{x_{k+1}+x_k}{2}\right) \langle x_{k+1}|p_k\rangle\, \langle p_k|x_k\rangle + \right. \\
&\qquad \left. \langle x_{k+1}|p_k\rangle \left\langle p_k \left| \frac{\mathbf{P}^2}{2m} \right| x_k \right\rangle \right\} + \cdots = \\
&\int \frac{dp_k}{2\pi\hbar} \left[1 - \frac{i\epsilon}{\hbar}\left(\frac{p_k^2}{2m} + V\left(\frac{x_{k+1}+x_k}{2}\right)\right)\right] \exp\left(\frac{ip_k}{\hbar}(x_{k+1}-x_k)\right) + \ldots
\end{aligned} \tag{8.5}$$

Note: for more complicated $\mathbf{X}/\mathbf{P}$-mixed operators one needs *Weyl ordering*, a symmetrization of the operator sequence in $\mathbf{X}/\mathbf{P}$; see Peskin & Schröder, p. 281 for more on this topic. Note that the argument in $V(\frac{x_{n+1}+x_n}{2})$ is written like this for cosmetic reasons; we could just as well have written x_n, since in the end, the limit $N \to \infty$ will be taken. Continuing our derivation, let us define

$$\theta(\epsilon) = \int \frac{dp_k}{2\pi\hbar} \exp\left(-\frac{i\epsilon}{\hbar}\left(\frac{p_k^2}{2m} + V\left(\frac{x_k+x_{k+1}}{2}\right) - p_k\frac{x_{k+1}-x_k}{\epsilon}\right)\right) \tag{8.6}$$

which is the right hand side of eq. (8.5) to order $\mathcal{O}(\epsilon)$. Multiplying all θ's and taking the limit $\epsilon \to 0$, we have

$$\langle x'(t')|x(t)\rangle = \int \mathcal{D}x\mathcal{D}p\, \exp\left[i\int_t^{t'} dt \left(\frac{p\dot{x} - H(p,q)}{\hbar}\right)\right] \tag{8.7}$$

with $x(t) = x$ and $x(t') = x'$. This limit * is of course accompanied by some higher-level mathematics. The naïve expression, however, has to be based on the discretized version we started from. Concretely, for physicists, this means that in QFT, numerical lattice calculations are an adequate way to approach this integral. Note that the continuous and differentiable functions are a dense set of measure zero in the functional integral.

* "Trotter formula"

(93

The dp_k-integration in eq. (8.6) can be performed: it is just a Gaussian integral, here restricted to one dimension for simplicity. It is solved by completing the square:

$$
\begin{aligned}
&-\frac{p_k^2\epsilon}{2m} + p_k(x_k - x_{k+1}) = \\
&-\frac{1}{2}\left[\frac{p_k^2}{m}\epsilon - 2p_k(x_k - x_{k+1}) + \frac{(x_k - x_{k+1})^2}{\epsilon}m\right] + \frac{1}{2}m\frac{(x_k - x_{k+1})^2}{\epsilon} = \\
&-\frac{p_k'^2}{2}\frac{\epsilon}{m} + \frac{1}{2}m\frac{(x_k - x_{k+1})^2}{\epsilon}
\end{aligned}
$$

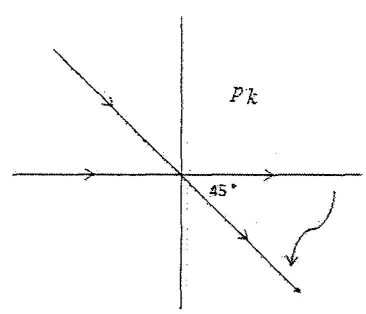
with $p_k' := \frac{p_k}{\cancel{m}} - \frac{x_k - x_{k+1}}{\epsilon}m$. Using the standard Gaussian integral,

$$\int_{-\infty}^{\infty} dx e^{-\alpha x^2} = \left(\frac{\pi}{\alpha}\right)^{1/2} \tag{8.8}$$

(*) we can perform the p_k'-integral. The first part becomes

"Fresnel integral" $$\int_{-\infty}^{\infty} \frac{dp_k'}{2\pi\hbar}\exp\left(-\frac{1}{2}\frac{i\epsilon}{\hbar m}p_k'^2\right) = \frac{\sqrt{\hbar m/i\epsilon}}{2\pi\hbar}\int_{-\infty}^{\infty} dy e^{-y^2/2} = \frac{1}{2\pi\hbar}\sqrt{\frac{2\pi\hbar m}{i\epsilon}}$$

where $y = p_k'\sqrt{i\epsilon/\hbar m}$. Note that due to the presence of $\sqrt{i}$ in the conversion from p_k' to y, this substitution constitutes a 45-degree rotation of the integration path:



So, the final result, the product of all the separate integrals, is

$$\prod_{j=1}^{N-1}\int dx_j \left(\sqrt{\frac{m}{i\epsilon\hbar 2\pi}}\right)^N \exp\left(i\sum_{i=1}^{N}\epsilon\left\{\frac{m}{2}\frac{(x_i - x_{i-1})^2}{\epsilon^2} - V(x_i)\right\}/\hbar\right)$$

which, after taking ϵ to zero and N to infinity, becomes:

$$\boxed{\langle x(t)|x'(t')\rangle = \int \mathcal{D}x \exp\left(i\int_t^{t'} d\tau \mathcal{L}(x,\dot{x})/\hbar\right)} \tag{8.9}$$

(*) $$\int_{-\infty}^{+\infty} dx \exp\left(-\frac{i}{2}\alpha x^2\right) = e^{-i\pi/4}\left(\frac{2\pi}{\alpha}\right)^{1/2}$$

Gauss $$\int_{-\infty}^{+\infty} dx \exp(-\alpha x^2) = \left(\frac{2\pi}{\alpha}\right)^{1/2}$$

(94

with singular integration measure ($\sim \epsilon^{-N/2}$) and Lagrangian density $\mathcal{L} = \frac{m\dot{x}^2}{2} - V(x)$.

The x-space path integral is less general (namely only for H quadratic in p) than the first version, but for our purpose, we can settle for this one.

Remarks

- For $\langle x'(t')|\,\mathrm{T}(\mathrm{O}_1(t_1)\mathrm{O}_2(t_2)\dots)\,|x(t)\rangle$, the operators $\mathrm{O}_1, \mathrm{O}_2, \dots$ act in the time slices around $t_1, t_2, \dots$. Then, $\langle x(t_1)|\,\mathrm{O}_1(t_1)\,|x(t_1')\rangle = O_1(x(t_1))\delta(t_1 - t_1')$ where O_1 is a function. Thus, we obtain time-ordering in the path integral, which is decomposed into time slices. This remark is also important if the potential has the shape of a matrix in more complicated settings.
- The oscillating behaviour of the Feynman exponential, which makes the convergence of the integral a more subtle affair, can be avoided if we go to imaginary, or Euclidean, time ($t = x^0 = -ix^4 = -it_{\mathrm{E}}$). This so-called *Wick rotation* helps us to define certain expressions properly. Of course, one has to rotate back at the end of the calculation .

8.1.1 Vacuum expectation values

When going to QFT, we will be interested in vacuum expectation values (cf. correlation functions in statistical physics). Let us briefly investigate them here:

$$\langle 0|\,\mathrm{T}(\mathbf{x}(t_1)\dots\mathbf{x}(t_n))\,|0\rangle = ?$$

Let us start from

$$\langle x_T(T)|\,\mathrm{T}(\mathbf{x}(t_1)\dots\mathbf{x}(t_n))\,|x_{-T}(-T)\rangle = \int_{x_{-T}}^{x_T} \mathcal{D}x\, x(t_1)\dots x(t_n)\times \exp\left(-\int d\tau_e\left(\frac{m\dot{x}^2}{2} + V(x)\right)\right) \tag{8.10}$$

where τ_e stands for Euclidean (Wick-rotated) time. Now,

$$|x_{-T}(-T)\rangle = e^{(-T)H}\,|x_{-T}(0)\rangle = \sum_n |n\rangle\,\langle n|x_{-T}\rangle\, e^{-E_nT}$$

where $|x_{-T}(0)\rangle$ is also written $|x_{-T}\rangle$, and is a Schrödinger vector, which at $t=0$ coincides with the corresponding Heisenberg vector. When T is large, only the ground state contributes. Then, eq. (8.10) becomes

$$= \langle x_T(0)|0\rangle\,\langle 0|\,\mathrm{T}(\mathbf{x}(t_1)\dots\mathbf{x}(t_n))\,|0\rangle\,\langle 0|x_{-T}(0)\rangle\, e^{-2E_0T}$$

Dividing by $\langle x_T(T)|x_{-T}(-T)\rangle$, like in the Gell-Mann-Low formula, removes the outer parts, leaving

$$\langle 0|\,\mathrm{T}(\mathbf{x}(t_1)\dots\mathbf{x}(t_n))\,|0\rangle = \lim_{T\to\infty} Z_T \int_{x_{-T}}^{x_T} \mathcal{D}x\, x(t_1)\dots x(t_n)e^{-S} \tag{8.11}$$

13.2 Der "Propagator" $G(x',t',x,t) = \langle x'(t')|x(t)\rangle$

mit $t' \geq t$ ist im Schrödinger-Bild

$$G(x',t',x,t) = \langle x'| \underbrace{\theta(t'-t)\, \underbrace{e^{-i/\hbar \int_t^{t'} dt\, H(\cancel{t})}}_{\text{später } T(\ldots) \text{ zeitgeordnet}}}_{G^+(t',t) \quad \text{"retardierte Green-f."}} |x\rangle$$

mit $(i\hbar\partial_t - H)\, G^+ = \delta(t'-t)$

$\boxed{\text{F.T.}}$ $$\tilde{G}^+(\omega + i\epsilon) = \int_{-\infty}^{+\infty} dt\, e^{i/\hbar\,(\omega - H + i\epsilon)t} = \frac{1}{\omega - H + i\epsilon}$$

$$\tilde{G}(x',x,\omega) = \sum_n \underbrace{\langle x'|E_n\rangle}_{\psi_n(x')} \underbrace{\langle E_n| \ldots |E_n\rangle}_{\text{diagonal}} \overset{\psi_n^*(x)}{\langle E_n|x\rangle}$$

$$= \sum_n \frac{\psi_n(x')\,\psi_n^*(x)}{\omega - E_n + i\epsilon}$$

$\to e^{-i/\hbar\, E_n(t'-t)}$ ohne F.T.

→ S. 101

so gilt $$\boxed{\psi(x',t') = \int dx\, G(x',t',x,t)\,\psi(x,t)}$$

mit $\psi(x,t) = \langle x|\psi(t)\rangle \ldots$

und $|\psi(t')\rangle = G^+(t',t)\,|\psi(t)\rangle$

$(\to \langle x'|\psi(t')\rangle = \langle x'|G^+(t',t)|x\rangle\langle x|\psi(t)\rangle)$

Summe!

$\psi(x,t)$ erfüllt die Schrödinger-Gleichung, wie wir sofort aus der obigen unitären Zeitentwicklung sehen, aber auch aus dem Pfadintegral über infinitesimale Zeiten:

(1 Schritt)

$$\psi(x',t+\Delta t) = \sqrt{\frac{m}{i\Delta t\, 2\pi\hbar}} \int dx\, e^{i\Delta t\left(\frac{m}{2\hbar}\left(\frac{x'-x}{\Delta t}\right)^2 - V\left(\frac{x+x'}{2}\right)/\hbar\right)} \psi(x)$$

x-Werte mit $\left|\frac{x'-x}{\Delta t}\right|^2 \frac{m}{\hbar} \gg 1$ werden wegoszilliert (Fresnelsches Int.)

(bzw. nach Rotation ins "Euklidische" weggedämpft)

$\Rightarrow$ Entwickle $\psi(x)$ bei x'

$$\psi(x,t) = \psi(x',t) + \partial_x\psi \times (x'-x) + \frac{1}{2!}\partial_x^2\psi \times (x'-x)^2 + \ldots$$

$$\sqrt{\ldots}\int_{-\infty}^{+\infty} dx\, e^{i\, m/2\hbar\, \frac{(x'-x)^2}{\Delta t}} = 1$$

$$\sqrt{\ldots}\int_{-\infty}^{+\infty} dx\, (x'-x)\, e^{\ldots} = 0$$

(zur Einfachheit 1D)

$$\underbrace{\sqrt{\ldots}\int_{-\infty}^{+\infty} dx}_{!}\ \frac{(x'-x)^2}{2!} e^{\ldots} = i\frac{\Delta t\, \hbar}{2m}$$

$$\rightsquigarrow \psi(x',t+\Delta t) = \psi(x',t) + i\frac{\Delta t\, \hbar}{2m}\partial_x^2\psi(x',t) - i\frac{\Delta t}{\hbar} V(x')$$

wobei wir $e^{-i\Delta t/\hbar\, V\left(\frac{x+x'}{2}\right)}$ zur ersten Ordnung in Δt entwickelt haben. Dies ist für $\Delta t \to 0$ die Schrödinger Gl.

$$i\hbar\dot\psi(x) = \left(-\frac{\hbar^2}{2m}\partial_x^2 + V(x)\right)\psi(x) \quad (x' \to x)$$

In den bekannten Fällen "freie Theorie", harmonischer Oszillator, Wasserstoffatom ist die Pfadintegralmethode zwar durchführbar, aber wesentlich aufwändiger als die Lösung der Schrödingergleichung. Wichtig wird das Pfadintegral bei der Lösung von QM-Problemen jenseits der Störungstheorie, bei denen man also nicht nach einer bekannten Lösung entwickeln kann, in der Quantenfeldtheorie bei der Ableitung der "Feynman Regeln", insbesondere bei den nichtabelschen Eichtheorien des Standard-Modells, bei der Diskussion von "Solitonen", "Instantonen" $\longrightarrow$ d.h. nicht zuletzt bei Tunnel-problemen!

Hier einige simple Hinweise:

13.3 freie Theorie: (i) Man kann den Propagator direkt im diskretisierten Pfadintegral im Limes $\Delta t \to 0$ ausrechnen (Übung?)

$$H = \frac{p^2}{2m}$$

$$\langle x_b(t_b) \mid x_a(t_a) \rangle = \frac{1}{(2\pi i \hbar (t_b - t_a)/m)^{1/2}} \exp\left(\frac{i}{\hbar} \frac{m}{2} \frac{(x_b - x_a)^2}{t_b - t_a} \right)$$

(*)

Notation ändern!

(ii) Man kann auch das "Sattelpunktverfahren" benutzen: suche ein Extremum des Exponenten $iS/\hbar$: dies ist gerade eine klassische Lösung (der Mechanik)

$$x_{cl}(t) = x_a + \frac{x_b - x_a}{t_b - t_a}(t - t_a) \quad \text{mit} \quad x_{cl}(t_a) = x_a, \quad x_{cl}(t_b) = x_b$$