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The Path Integral Formulation of Quantum Mechanics

We turn now to a topic that is important already for ordinary quantum mechanics and essential in quantum field theory: the so-called path integral. In the setting of ordinary quantum mechanics (of the sort we have been considering in this book), the integrals in question are over spaces of "paths," that is, maps of some interval $[a, b]$ into $\mathbb{R}^n$. In the setting of quantum field theory, the integrals are integrals over spaces of "fields," that is, maps of some region inside $\mathbb{R}^d$ into $\mathbb{R}^n$. Formal integrals of this sort abound in the physics literature, and it is typically difficult to make rigorous mathematical sense of them—although much effort has been expended in the attempt! In this chapter, we will develop a rigorous integral over spaces of paths by using the *Wiener measure*, resulting in the Feynman–Kac formula.

We begin with the Trotter product formula, which will be our main tool in deriving the path integral formulas. From there we turn to the (heuristic) path integral formula of Feynman, and then to the rigorous version of Feynman's result obtained by M. Kac, the so-called Feynman–Kac formula. Although it is not feasible to give complete proofs of all results presented here, we give enough proofs to get a flavor of the mathematics involved. We will prove a version of the Trotter product formula and, assuming the existence of the Wiener measure, a version of the Feynman–Kac formula.

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20.1 Trotter Product Formula

The Lie product formula (Point 7 of Theorem 16.15) says that for all X and Y in $M_n(\mathbb{C})$, we have

$$e^{X+Y} = \lim_{m\to\infty} (e^{X/m} e^{Y/m})^m.$$

The Trotter product formula asserts that a similar result holds for certain classes of *unbounded* operators on Hilbert spaces.

Theorem 20.1 (Trotter Product Formula) *Suppose that A and B are self-adjoint operators on $\mathbf{H}$ and that $A+B$ is densely defined and essentially self-adjoint on $\mathrm{Dom}(A) \cap \mathrm{Dom}(B)$. Then the following results hold.*

1. *For all $\psi \in \mathbf{H}$, we have*

$$\lim_{N\to\infty} \left\| e^{it(A+B)}\psi - (e^{itA/N} e^{itB/N})^N \psi \right\|. \tag{20.1}$$

2. *If A and B are bounded below, then for all $\psi \in \mathbf{H}$, we have*

$$\lim_{N\to\infty} \left\| e^{-t(A+B)}\psi - (e^{-tA/N} e^{-tB/N})^N \psi \right\|. \tag{20.2}$$

In both results, the expression $A + B$ refers to the unique self-adjoint extension of the operator defined on $\mathrm{Dom}(A) \cap \mathrm{Dom}(B)$.

In the usual terminology of functional analysis, (20.1) asserts that the operators $(e^{itA/N} e^{itB/N})^N$ converge to $e^{it(A+B)}$ in the "strong operator topology," and similarly with (20.2).

We will give a proof of this result in the special case in which $A + B$ is densely defined and self-adjoint on $\mathrm{Dom}(A) \cap \mathrm{Dom}(B)$. This condition holds, for example, whenever the Kato–Rellich theorem (Theorem 9.37) applies. See Sect. A.5 of [14] for a proof of the version stated above.

Proof. Since all the operators in Point 1 of the theorem are unitary, it is easy to see that if the result holds on some dense subspace W of $\mathbf{H}$, it holds on all of $\mathbf{H}$. In Point 2 of the theorem, we first make a simple reduction to the case where A and B are non-negative, and then have the same conclusion, since all operators involved will then be contractions.

We will prove Point 1 of the theorem, with the proof of Point 2 being similar. Let us introduce the notation $S_s := e^{is(A+B)}$ and $T_s := e^{isA} e^{isB}$. What we want to prove is that for each $\psi \in \mathbf{H}$, the quantity $\left\|(S_t - (T_{t/N})^N)\psi\right\|$ tends to zero as N tends to infinity. Now, a simple calculation shows that

$$\left\|(S_t - (T_{t/N})^N)\psi\right\| = \left\| \sum_{j=0}^{N-1} (T_{t/N})^j (S_{t/N} - T_{t/N}) (S_{t/N})^{N-j-1} \psi \right\|. \tag{20.3}$$

Since $S_\cdot$ is a one-parameter unitary group, $(S_{t/N})^{N-j-1}\psi = S_s\psi$, where $s = (N-j-1)t/N$. Thus, if we let $\psi_s = S_s\psi$, we have

$$\left\|(S_t - (T_{t/N})^N)\psi\right\| \leq N \sup_{0\leq s\leq t} \left\|(S_{t/N} - T_{t/N})\psi_s\right\|. \tag{20.4}$$

Now, for any ψ in $\mathrm{Dom}(A+B)$, we have

$$\lim_{N\to\infty} N(S_{t/N}\psi - \psi) = it(A+B)\psi,$$

by Stone's theorem. Meanwhile, according to Exercise 2, we have

$$\lim_{s\to 0} \frac{1}{s}(T_s - I)\psi = iA\psi + iB\psi, \tag{20.5}$$

for all $\psi \in \mathrm{Dom}(A) \cap \mathrm{Dom}(B)$. (This result is clear at the heuristic level.) Thus,

$$\begin{aligned}\lim_{N\to\infty} N(S_{t/N} - T_{t/N})\psi &= \lim_{N\to\infty} N(S_{t/N} - I)\psi - \lim_{N\to\infty} N(T_{t/N} - I)\psi \\ &= it(A+B)\psi - it(A+B)\psi = 0 \end{aligned} \tag{20.6}$$

for every $\psi \in \mathrm{Dom}(A) \cap \mathrm{Dom}(B)$.

Let $W = \mathrm{Dom}(A) \cap \mathrm{Dom}(B)$, which is, by assumption, dense in $\mathbf{H}$, equipped with the norm $\|\cdot\|_1$ given by

$$\|\psi\|_1 = \|\psi\| + \|(A+B)\psi\|.$$

Since we are assuming $A+B$ is self-adjoint, and thus also closed, on W, we see that W is a Banach space with respect $\|\cdot\|_1$ (Exercise 6 in Chap. 9). Now, the operators $N(S_{t/N} - T_{t/N})$ are certainly bounded from W to $\mathbf{H}$, for each N. Furthermore, (20.6) shows that for each $\psi \in W$, we have

$$\sup_N \left\|N(S_{t/N} - T_{t/N})\psi\right\| < \infty.$$

Thus, by the principle of uniform boundedness (Theorem A.40), there is a constant C such that

$$\left\|N(S_{t/N} - T_{t/N})\psi\right\| \leq C\,\|\psi\|_1$$

for all $\psi \in W$. It then follows (Exercise 3) that $\left\|N(S_{t/N} - T_{t/N})\psi\right\|$ tends to zero *uniformly* on every compact subset of W.

Suppose, now, that for each $\psi \in W$, the $s \mapsto \psi_s$ is continuous in W. If so, the image of the compact interval $[0,t]$ under $s \mapsto \psi_s$ will be compact in W, and so $\left\|N(S_{t/N} - T_{t/N})\psi_s\right\|$ will tend to zero uniformly in s. Thus, by (20.4), we will have Point 1 of the theorem. To establish the desired continuity, we first note that by Lemma 10.17, the operators $S_s = e^{is(A+B)}$

preserve $\mathrm{Dom}(A+B)$, which is equal to W, by assumption. Then for any $s, r \in [0,t]$ and $\psi \in W$, we have

$$\begin{aligned}
&\left\| e^{is(A+B)}\psi - e^{ir(A+B)}\psi \right\|_1 \\
&= \left\| e^{is(A+B)}\psi - e^{ir(A+B)}\psi \right\| + \left\| (A+B)(e^{is(A+B)}\psi - e^{ir(A+B)}\psi) \right\| \\
&= \left\| (e^{is(A+B)} - e^{ir(A+B)})\psi \right\| + \left\| (e^{is(A+B)} - e^{ir(A+B)})(A+B)\psi \right\|, \quad (20.7)
\end{aligned}$$

where we have used Lemma 10.17 again in the second equality. The strong continuity of $e^{is(A+B)}$ (Proposition 10.14) then ensures that the right-hand side of (20.7) tends to zero as s approaches r. ■

20.2 Formal Derivation of the Feynman Path Integral

In this section, we apply Point 1 of the Trotter product formula to the operator

$$-\frac{1}{\hbar}\hat{H} = \frac{\hbar}{2m}\Delta - \frac{1}{\hbar}V(X). \tag{20.8}$$

Let us call the operators on the right-hand side of (20.8) A and B, respectively, and let us assume V is sufficiently nice that $\hat{H}$ is essentially self-adjoint on $\mathrm{Dom}(A) \cap \mathrm{Dom}(B)$. Any bounded potential certainly has this property, as do many unbounded potentials. (See, e.g., Theorem 9.38.)

Point 1 of Theorem 20.1 then tells us that

$$e^{-it\hat{H}/\hbar}\psi = \lim_{N\to\infty}\left(\exp\left\{\frac{it\hbar\Delta}{2mN}\right\}\exp\left\{-\frac{itV(X)}{N\hbar}\right\}\right)^N \psi.$$

Under mild assumptions on ψ, Theorem 4.5 (extended to n dimensions) tells us that $\exp(it\hbar\Delta/(2mN))$ may be computed as

$$e^{it\hbar\Delta/(2mN)}\psi(\mathbf{x}_0) = \left(\frac{mN}{it\hbar}\right)^{n/2}\int_{\mathbb{R}^n}\exp\left\{i\frac{mN}{2t\hbar}\left|\mathbf{x}_1 - \mathbf{x}_0\right|^2\right\}\psi(\mathbf{x}_1)\, d\mathbf{x}_1.$$

Meanwhile, $\exp(-itV(X)/(N\hbar))$ is simply a multiplication operator.

Thus, assuming that Theorem 4.5 applies at each stage, we have

$$\begin{aligned}
&\left[\left(\exp\left\{\frac{it\hbar\Delta}{2mN}\right\}\exp\left\{-\frac{itV(X)}{N\hbar}\right\}\right)^N\psi\right](\mathbf{x}_0)\\
&= C\int_{\mathbb{R}^n}\exp\left\{i\frac{mN}{2t\hbar}\left|\mathbf{x}_1-\mathbf{x}_0\right|^2\right\}\exp\left\{-\frac{itV(\mathbf{x}_1)}{N\hbar}\right\}\\
&\times\int_{\mathbb{R}^n}\exp\left\{i\frac{mN}{2t\hbar}\left|\mathbf{x}_{N-1}-\mathbf{x}_{N-2}\right|^2\right\}\exp\left\{-\frac{itV(\mathbf{x}_{N-1})}{N\hbar}\right\}\\
&\times\cdots\times\int_{\mathbb{R}^n}\exp\left\{i\frac{mN}{2t\hbar}\left|\mathbf{x}_N-\mathbf{x}_{N-1}\right|^2\right\}\exp\left\{-\frac{itV(\mathbf{x}_N)}{N\hbar}\right\}\\
&\times\psi(\mathbf{x}_N)\,d\mathbf{x}_N\,d\mathbf{x}_{N-1}\cdots\,d\mathbf{x}_1,
\end{aligned}$$

where $C=(mN/(it\hbar))^{nN/2}$. Letting $\varepsilon=t/N$ and assuming we can freely rearrange the order of integration, we obtain

$$\begin{aligned}
&(e^{-it\hat{H}/\hbar}\psi)(\mathbf{x}_0)\\
&=\lim_{N\to\infty}C\int_{(\mathbb{R}^n)^N}\exp\left\{\frac{i}{\hbar}\sum_{j=1}^N\varepsilon\left[\frac{m}{2}\left|\frac{\mathbf{x}_j-\mathbf{x}_{j-1}}{\varepsilon}\right|^2-V(\mathbf{x}_{j-1})\right]\right\}\\
&\times\psi(\mathbf{x}_N)\,d\mathbf{x}_1\,d\mathbf{x}_2\cdots d\mathbf{x}_N.
\end{aligned}\tag{20.9}$$

So far, the argument is mostly rigorous, coming from the Trotter product formula and Theorem 4.5. The nonrigorous part comes in attempting to evaluate the limit on the right-hand side of (20.9). Let us think of the values $\mathbf{x}_j$, $j=0,\ldots,N$ as constituting the values of a path $\mathbf{x}(s)$ at the points $s_j:=j\varepsilon=jt/N$:

$$\mathbf{x}_j=\mathbf{x}(jt/N).$$

Since the distance between s_{j-1} and s_j is ε, the quantity $|\mathbf{x}_j-\mathbf{x}_{j-1}|/\varepsilon$ is an approximation to the derivative of $x(s)$ with respect to s. Meanwhile, the sum over j in the right-hand side of (20.9) is an approximation to an integral. Thus, if we then take the limit of the right-hand of (20.9) in a totally nonrigorous fashion, we obtain

$$\begin{aligned}
&(e^{-it\hat{H}/\hbar}\psi)(\mathbf{x}_0)\\
&=C\int_{\substack{\text{paths with}\\ \mathbf{x}(0)=\mathbf{x}_0}}\exp\left\{\frac{i}{\hbar}\int_0^t\left[\frac{m}{2}\left|\frac{d\mathbf{x}}{ds}\right|^2-V(\mathbf{x}(s))\right]\,ds\right\}\psi(\mathbf{x}(t))\,\mathcal{D}\mathbf{x}.
\end{aligned}\tag{20.10}$$

Here, C is a normalization constant and $\mathcal{D}\mathbf{x}$ is something like "Lebesgue measure" on the space of all paths $\mathbf{x}(\cdot)$ mapping $[0,t]$ into $\mathbb{R}^n$. (The quantity $\mathbf{x}$ in the expression $\mathcal{D}\mathbf{x}$ is a *path*, not a point in $\mathbb{R}^n$.)

The reader who is familiar with the Lagrangian approach to mechanics will recognize the expression in square brackets in the exponent on the right-hand side of (20.10) as the *Lagrangian* of the particle, $L = T - V$, where $T = (1/2)m\,|v|^2$ is the kinetic energy and V is the potential energy. The integral of the Lagrangian over some time interval is called the *action functional*, denoted by the letter $\mathcal{S}$. That is to say, given a path $\mathbf{x}(\cdot)$, we define the action functional of $\mathbf{x}(\cdot)$ over a time-interval $[a, b]$ as follows:

$$\mathcal{S}(\mathbf{x}(\cdot), a, b) := \int_a^b \left[\frac{m}{2} \left| \frac{d\mathbf{x}}{ds} \right|^2 - V(\mathbf{x}(s)) \right] ds. \tag{20.11}$$

In Lagrangian mechanics, one shows that the solutions to Newton's law are precisely the *stationary points* of the action functional. Using the notation in (20.11), we may rewrite (20.10) as

$$(e^{-it\hat{H}/\hbar}\psi)(\mathbf{x}_0) = C \int_{\substack{\text{paths with} \\ \mathbf{x}(0)=\mathbf{x}_0}} \exp\left\{ \frac{i}{\hbar} \mathcal{S}(\mathbf{x}(\cdot), 0, t) \right\} \psi(\mathbf{x}(t))\ \mathcal{D}\mathbf{x}. \tag{20.12}$$

This formula is the *Feynman path integral formula*.

Now, knowledge of Lagrangian mechanics is not directly relevant to the derivation of the Feynman path integral formula. Nevertheless, it is intriguing that the an important quantity from *classical* mechanics should appear in the Feynman path integral formula in *quantum* mechanics. Indeed, this appearance raises the possibility that one can use the path integral formula to make connections between quantum mechanics and classical mechanics. Indeed, the "method of stationary phase" (when applied, formally, in an infinite-dimensional setting) asserts that for small values of $\hbar$, the main contribution to the right-hand side of (20.12) comes from regions near the stationary points of the action functional, namely the classical trajectories. Using this method, Gutzwiller was able to derive his famous trace formula, which provides predictions of typical eigenvalue spacings for Schrödinger operators based on the behavior of the underlying classical system. More information about this fascinating subject can be found in books on "quantum chaos," including [19] by Gutzwiller himself.

It is notoriously difficult to attach a rigorous meaning to the right-hand side of the Feynman path integral formula. Note that the formal expression "$\mathcal{D}\mathbf{x}$" is the limit as N tends to infinity of the integral over $(\mathbb{R}^n)^N$ in (20.9) with respect to the Lebesgue measure (i.e., the measure given by $d\mathbf{x}_1\, d\mathbf{x}_2 \cdots d\mathbf{x}_N$). Thus, "$\mathcal{D}\mathbf{x}$" should be something like Lebesgue measure on the space of all paths (maps from $[0, t]$ into $\mathbb{R}^n$). However, it is known that an infinite-dimensional vector space (say, a Banach space) does not have any "reasonable" (say, σ-finite) translation-invariant measure that could play the role of Lebesgue measure. Furthermore, the absolute value of the constant C is easily seen to be infinite. Thus, we certainly cannot take the right-hand side of (20.12) literally.

A better approach is to avoid looking at the component parts of the Feynman path integral and instead to look at the whole expression against which the function $\psi(\mathbf{x}(t))$ is being integrated. If we could attach a rigorous meaning to the expression

$$C \exp\left\{\frac{i}{\hbar}\mathcal{S}(\mathbf{x}(\cdot), 0, t)\right\} \mathcal{D}\mathbf{x}, \tag{20.13}$$

as, say, a complex-valued measure on the space of continuous paths, then this could serve to give a meaning to the path integral. It is known, however, that there is no complex measure on the space of paths that makes the Feynman path integral formula true. The oscillatory behavior produced by the i in the exponent in (20.13) makes it difficult to give a rigorous meaning to the Feynman path integral in its original form.

20.3 The Imaginary-Time Calculation

In trying to give a rigorous meaning to the path integral formula of Feynman, Kac proceeded by considering the "imaginary time" time-evolution operator $\exp(-t\hat{H}/\hbar)$, which is just the usual time-evolution operator $\exp(-it\hat{H}/\hbar)$ evaluated with t replaced by $-it$. The idea is that if one can use path integrals to understand the operators $\exp(-t\hat{H}/\hbar)$, one can go back to the "real time" operator $\exp(-it\hat{H}/\hbar)$ by analytic continuation with respect to t.

The counterpart of Theorem 4.5 for $\exp(-t\hbar\Delta/(2m))$ (proved in the same way) is

$$(e^{-t\hbar\Delta/(2m)}\psi)(\mathbf{x}_0) = \left(\frac{m}{2\pi t\hbar}\right)^{n/2} \int_{\mathbb{R}^n} \exp\left\{-\frac{m}{2t\hbar}\left|\mathbf{x}_1 - \mathbf{x}_0\right|^2\right\} \psi(\mathbf{x}_1)\, d\mathbf{x}_1.$$

Unlike Theorem 4.5, however, the above expression holds for all $\psi \in L^2(\mathbb{R}^n)$, with absolute convergence of the integral for every $\mathbf{x}_0 \in \mathbb{R}^n$. Applying the Trotter product formula and rearranging the integral as before gives

$$\begin{aligned}
&(e^{-t\hat{H}/\hbar}\psi)(\mathbf{x}_0) \\
&= \lim_{N\to\infty} C \int_{(\mathbb{R}^n)^N} \exp\left\{-\frac{1}{\hbar}\sum_{j=1}^{N} \varepsilon \left[\frac{m}{2}\left|\frac{\mathbf{x}_j - \mathbf{x}_{j-1}}{\varepsilon}\right|^2 + V(\mathbf{x}_{j-1})\right]\right\} \\
&\times \psi(\mathbf{x}_N)\, d\mathbf{x}_1\, d\mathbf{x}_2 \cdots d\mathbf{x}_N.
\end{aligned} \tag{20.14}$$

If V is, say, bounded below, then there is no difficulty in changing the order of integration, because of the rapid decay of the integrand. Note that there is a relative sign change between the two terms in square brackets,

compared to (20.9). Taking a formal limit as before gives

$$(e^{-t\hat{H}/\hbar}\psi)(\mathbf{x}) = C \int_{\substack{\text{paths with} \\ \mathbf{x}(0)=\mathbf{x}_0}} \exp\left\{-\frac{1}{\hbar}\int_0^t \left[\frac{m}{2}\left|\frac{d\mathbf{x}}{ds}\right|^2 + V(\mathbf{x}(s))\right] ds\right\} \psi(\mathbf{x}(t))\, \mathcal{D}\mathbf{x}. \tag{20.15}$$

Note that the integral in the exponent on the right-hand side is *not* the classical action in (20.11), because the potential term has the wrong sign.

Kac's idea was to separate out the quadratic part of the exponent on the right-hand side of (20.15) and attempt to interpret the expression

$$C \exp\left\{-\frac{1}{\hbar}\int_0^t \frac{m}{2}\left|\frac{d\mathbf{x}}{ds}\right|^2 ds\right\} \mathcal{D}\mathbf{x} \tag{20.16}$$

as a measure on the space of paths. Specifically, this is a *Gaussian* measure, one with a (formal) density with respect to the Lebesgue measure that is the exponential of a quadratic expression. There is a well-developed theory of Gaussian measures on infinite-dimensional spaces. Although there is no Lebesgue measure in the infinite-dimensional case, one can construct Gaussian measures as limits of Gaussian measures on spaces of large finite dimension.

20.4 The Wiener Measure

Kac identified the formal expression in (20.16) as the *Wiener measure*. To be precise, for each fixed $\mathbf{x}_0 \in \mathbb{R}$, there is a Wiener measure $\mu_{\mathbf{x}_0}$, where $\mu_{\mathbf{x}_0}$ is supported on the set of paths $\mathbf{x} : [0,t] \to \mathbb{R}$ with $\mathbf{x}(0) = \mathbf{x}_0$. The Wiener measure was developed by Norbert Wiener as a rigorous embodiment of Albert Einstein's mathematical model of Brownian motion. Einstein, in one of his 1905 papers, had proposed that the random motion of a very small particle in water was due to collisions between the particle and the water molecules. Einstein postulated that the *increments* of a Brownian path $\mathbf{x}$ [quantities of the form $\mathbf{x}(t) - \mathbf{x}(s)$] should be independent for disjoint time intervals and should be normal random variables with mean zero and variance proportional to $t - s$. The following theorem shows that there is a unique measure on the space of continuous paths satisfying Einstein's criteria. Let $\mathcal{C}_{\mathbf{x}_0}([0,t];\mathbb{R}^n)$ denote the space of continuous maps $\mathbf{x}(\cdot)$ of $[0,t]$ into $\mathbb{R}^n$ satisfying $\mathbf{x}(0) = \mathbf{x}_0$, equipped with the supremum norm.

Theorem 20.2 (Wiener) *For each vector $\mathbf{x}_0 \in \mathbb{R}^n$ and each pair of positive numbers σ and t, there exists a unique measure $\mu^\sigma_{\mathbf{x}_0}$ on the Borel σ-algebra in $\mathcal{C}_{\mathbf{x}_0}([0,t];\mathbb{R}^n)$ such that the following condition holds. For each*

sequence $0 = t_0 < t_1 < \cdots < t_N \leq t$ *of real numbers and each non-negative measurable function* f *on* $(\mathbb{R}^n)^N$, *we have*

$$\int_{C_{\mathbf{x}_0}([0,t];\mathbb{R}^n)} f(\mathbf{x}(t_1), \mathbf{x}(t_2), \ldots, \mathbf{x}(t_N))\ d\mu^{\sigma}_{\mathbf{x}_0}(\mathbf{x})$$
$$= C \int_{\mathbb{R}^N} \exp\left\{ -\frac{1}{2\sigma} \sum_{j=1}^{N} \frac{|\mathbf{x}_j - \mathbf{x}_{j-1}|^2}{t_j - t_{j-1}} \right\} f(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N)\ d\mathbf{x}_1 \cdots\ d\mathbf{x}_N, \tag{20.17}$$

where

$$C = \prod_{j=1}^{N} \frac{1}{\sqrt{2\pi\sigma(t_j - t_{j-1})}}.$$

Note that the right-hand side of (20.17) is extremely similar to the right-hand side of (20.14), except that there are no terms involving the potential V in the exponent in (20.17). Thus, it is reasonable to think that the Wiener measure is a rigorous version of the formal expression in (20.16). It should be noted, however, that the heuristic expression (20.16) is misleading in one important respect. That expression suggests that the measure is supported on paths $\mathbf{x}(\cdot)$ for which $d\mathbf{x}/dt$ belongs to $L^2([0,t];\mathbb{R}^n)$, since the exponential factor would seemingly "damp out" any paths for which this is not the case. This conclusion is, however, incorrect. [One should, in general, be extremely cautious in drawing conclusions based on purely formal expressions such as the one in (20.16).] Actually, the "typical" path with respect to the Wiener measure is nowhere differentiable; that is, the set of paths $\mathbf{x}(t)$ that are differentiable for even one value of t form a set of measure zero.

This discrepancy is actually a general feature of Gaussian measures on infinite-dimensional spaces: They are always supported on a larger space than the formal expression would suggest. In the case of the Wiener measure, the space on which the measure actually lives (the space of continuous functions) is nice enough that no difficulties arise in the formulation of our main result, the Feynman–Kac formula. In the setting of quantum field theory, however, issues concerning the support of a Gaussian measure become serious difficulties. See Sect. 20.6 for more information.

20.5 The Feynman–Kac Formula

The Wiener measure gives a rigorous interpretation to the expression in (20.16). Thus, the Wiener measure encapsulates everything in (20.15) except for the term involving V in the exponent and the factor of $\psi(\mathbf{x}(t))$. This reasoning accounts for the form of the following result.

Theorem 20.3 (Feynman–Kac Formula) *Suppose $V : \mathbb{R}^3 \to \mathbb{R}$ can be expressed as the sum of a function in $L^2(\mathbb{R}^3)$ and a bounded function. Then for all $\mathbf{x}_0 \in \mathbb{R}^3$, we have*

$$\begin{aligned}&(e^{-t\hat{H}/\hbar}\psi)(\mathbf{x}_0)\\&= \int_{\mathcal{C}_{\mathbf{x}_0}([0,t];\mathbb{R}^3)} \exp\left\{-\frac{1}{\hbar}\int_0^t V(\mathbf{x}(s))\ ds\right\}\psi\left(\mathbf{x}(t)\right)\ d\mu^\sigma_{\mathbf{x}_0}(\mathbf{x}),\end{aligned}$$

where $\mu^\sigma_{\mathbf{x}_0}$ is the Wiener measure on $\mathcal{C}_{\mathbf{x}_0}([0,t];\mathbb{R}^3)$ and where $\sigma = \hbar/m$.

Of course, similar results hold in other dimensions, under suitable assumptions on the potential. We refer the interested reader to [37] or [14] for details on different versions of the Feynman–Kac formula. Theorem 20.3 cannot be obtained directly from the Trotter product formula, because the limit in (20.14) is an L^2 limit rather than a pointwise limit. We will content ourselves with proving an "integrated" version of the Feynman–Kac formula for nice potentials; Theorem 20.3 is Theorem 6.5 of [37].

Definition 20.4 *Let $\mathcal{C}([0,t];\mathbb{R}^n)$ denote the space of all continuous paths on $[0,t]$ with values in $\mathbb{R}^n$. For all $\sigma > 0$, let μ^σ be the measure on $\mathcal{C}([0,t];\mathbb{R}^n)$ given by*

$$\mu(E) = \int_{\mathbb{R}^n} \mu^\sigma_{\mathbf{x}_0}(E)\ d\mathbf{x}_0.$$

Proposition 20.5 *Suppose $V : \mathbb{R}^n \to \mathbb{R}$ is bounded and continuous. Then for all $\phi, \psi \in L^2(\mathbb{R}^n)$, we have*

$$\begin{aligned}&\langle \phi, e^{-t\hat{H}/\hbar}\psi\rangle\\&= \int_{\mathcal{C}([0,t];\mathbb{R}^n)} \overline{\phi(\mathbf{x}(0))}\exp\left\{-\frac{1}{\hbar}\int_0^t V(\mathbf{x}(s))\ ds\right\}\psi\left(\mathbf{x}(t)\right)\ d\mu^\sigma(\mathbf{x}),\end{aligned}$$

where μ^σ is as in Definition 20.4 and where $\sigma = \hbar/m$.

Proof. We begin with (20.14) and apply Theorem 20.2 with parameters chosen as follows. We take $\sigma = \hbar/m$, we take the sequence $\langle t_j\rangle$ to be given by $t_j = jt/N$, and we take f to be the function given by

$$f(\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N) = \psi(\mathbf{x}_N).$$

Theorem 20.2 then allows us to express the right-hand side of (20.14) as an integral against the Wiener measure, giving

$$\begin{aligned}&(e^{-t\hat{H}/\hbar}\psi)(\mathbf{x}_0)\\&= \lim_{N\to\infty}\int_{\mathcal{C}_{\mathbf{x}_0}([0,t];\mathbb{R}^n)} \exp\left\{-\frac{1}{\hbar}\sum_{j=1}^N \frac{t}{N}V\left(\mathbf{x}\left(\frac{jt}{N}\right)\right)\right\}\psi(\mathbf{x}(t))\ d\mu^\sigma_{\mathbf{x}_0}(\mathbf{x}).\end{aligned}$$

Since the limit in the above equation is an L^2 limit, we may move the inner product with ϕ inside the limit on the right-hand side. The integral with respect to $\mu^\sigma_{\mathbf{x}_0}$ and the integral with respect to $d\mathbf{x}_0$ may then be combined into a single integral with respect to μ^σ, giving

$$\langle \phi, e^{-t\hat{H}/\hbar}\psi\rangle = \lim_{N\to\infty} \int_{\mathcal{C}([0,t];\mathbb{R}^n)} \overline{\phi(\mathbf{x}(0))} \times \exp\left\{-\frac{1}{\hbar}\sum_{j=1}^{N} \frac{t}{N} V\left(\mathbf{x}\left(\frac{jt}{N}\right)\right)\right\} \psi\left(\mathbf{x}(t)\right)\ d\mu^\sigma(\mathbf{x}). \tag{20.18}$$

Now, since V is continuous,

$$\lim_{N\to\infty} \sum_{j=1}^{N} \frac{t}{N} V\left(\mathbf{x}\left(\frac{jt}{N}\right)\right) = \int_0^t V(\mathbf{x}(s))\ ds,$$

for every continuous path $\mathbf{x}$. Furthermore, it is easily seen that the "distribution" of the quantity $\mathbf{x}(s)$ with respect to the measure μ^σ is the Lebesgue measure on $\mathbb{R}^n$, for any $s \in [0,t]$. Thus, the function $\mathbf{x} \mapsto \phi(\mathbf{x}(0))$ is square-integrable with respect to μ^σ, with L^2 norm equal to the L^2 norm of ϕ over $\mathbb{R}^n$, and similarly for $\mathbf{x} \mapsto \psi(\mathbf{x}(t))$. It follows that the quantity $\overline{\phi(\mathbf{x}(0))}\psi\left(\mathbf{x}(t)\right)$ is an L^1 function on $\mathcal{C}([0,t];\mathbb{R}^n)$. Since V is bounded, we may apply dominated convergence to move the limit inside the integral, at which point we obtain the desired result. ■

20.6 Path Integrals in Quantum Field Theory

In this section, we briefly discuss the path integral approach to quantum field theory. We consider quantum field theory in a space–time of dimension d, so that space has dimension $d-1$. The configuration space for the classical version of the theory is the collection of "spatial" fields, that is, maps $\phi(\mathbf{x})$ of $\mathbb{R}^{d-1}$ into some finite-dimensional vector space V. A *path* in the space of fields is then a map $\phi(\mathbf{x},t)$ of $\mathbb{R}^{d-1}\times\mathbb{R} \cong \mathbb{R}^d$ into V. In the path integral approach to quantum field theory (which is the most commonly used approach to the subject), one considers integrals over the space of such paths.

Let us consider, as a simple example, what is called ϕ^4 theory. In this theory, the fields ϕ map into $\mathbb{R}$ and we consider a path integral of the form

$$C\int_{\mathcal{F}_d} \exp\left\{-\frac{1}{\hbar}\int_{\mathbb{R}^d}\left[c_1\left\|\nabla\phi(\mathbf{x})\right\|^2 + c_2\phi(\mathbf{x})^2 + c_3\phi(\mathbf{x})^4\right]\ d\mathbf{x}\right\} \times F(\phi)\ \mathcal{D}\phi, \tag{20.19}$$

for some functional $F(\phi)$ on the space of fields. [The expression in (20.19) is, more precisely, a "Euclidean" or "imaginary time" path integral. Such

an integral is the counterpart in quantum field theory of the integral occurring in the Feynman–Kac formula in quantum mechanics.] In (20.19), $\mathcal{F}_d$ represents the space of all "fields" (i.e., functions) mapping our space–time $\mathbb{R}^d$ into $\mathbb{R}$. In an attempt to make sense of this heuristic expression, we may follow the strategy we used in deriving the Feynman–Kac formula by separating out the quadratic part of the exponent. We look, then, for a measure μ on $\mathcal{F}_d$ given by the heuristic expression

$$d\mu(\phi) \text{ “=” } C \exp\left\{-\frac{1}{\hbar}\int_{\mathbb{R}^d}\left[c_1 \left\|\nabla\phi(\mathbf{x})\right\|^2 + c_2\phi(\mathbf{x})^2\right] d\mathbf{x}\right\} \mathcal{D}\phi. \quad (20.20)$$

Using the theory of Gaussian measures, one can construct a rigorously defined measure corresponding to the heuristic expression in (20.20). There is, however, a serious difficulty with this approach: The measure μ is supported on very "rough" fields, much rougher than the heuristic expression suggests. In fact, we have the following result.

Proposition 20.6 *For all $d \geq 1$, there exists a Gaussian measure on the space $\mathcal{F}_d$ of fields on $\mathbb{R}^d$ corresponding to the heuristic expression (20.20). For $d \geq 2$, however, this measure is not supported on any space of ordinary functions, but rather on a space of distributions.*

We will not prove this result here; see Sect. 8.5 of [14] for more information. Here, then, is the problem with the path integral approach to quantum field theory on space–times of dimension $d \geq 2$: The functional $\int_{\mathbb{R}^d} \phi(x)^4\, dx$ does not make sense for a "typical" field with respect to the measure μ in (20.20). As a result, we cannot make sense of (20.19) simply by absorbing all the Gaussian part into the definition of the measure μ, since what is left over is not a μ-almost everywhere defined functional of ϕ. Indeed, even a local integral, of the form $\int_U \phi(x)^4\, dx$ for some bounded region U in $\mathbb{R}^d$, fails to be almost-everywhere defined with respect to μ. After all, if $\int_U \phi(x)^4\, dx$ made sense, then ϕ would be a locally L^4 function, rather than a distribution.

It should be emphasized that the difficulty described in the previous paragraph is not just a technicality that can be swept away by some simple trick. Furthermore, this difficulty is not specific to ϕ^4 theory, but is present in all "nontrivial" field theories. In all interesting field theories, the fields defined by the Gaussian part of the path integral are fundamentally "too rough" to allow us to make sense of the non-Gaussian part of the integral. This phenomenon is *the* fundamental mathematical difficulty in the path integral approach to quantum field theory.

To have a chance to make rigorous sense of path integrals in quantum field theory, one has to employ a complicated regularization process known as renormalization. This process has, so far, been carried out in a rigorous fashion only for a very small number of field theories. One of the Clay Millennium Prize problems is to make rigorous sense out of the Yang–Mills

field theory in four space–time dimensions. See [14] for a detailed survey of the mathematical issues connected with the path integral approach to quantum field theory. See also [13] for a treatment of quantum field theory and renormalization with a greater eye toward the physical content.

Since the roughness of the fields is a major problem in trying to give a rigorous meaning to path integrals, let us think for moment why it arises. Suppose we wish to construct a Gaussian measure from a certain heuristic expression of the form $\mu = Ce^{-Q(x)}\mathcal{D}x$, where Q is a positive-definite quadratic functional of x. A reasonable approach is to consider the (real) Hilbert space $\mathbf{H}$ for which $\|x\|_H^2 = Q(x)$. [In the case of (20.20), $\mathbf{H}$ would be the "Sobolev space" of fields having one derivative in L^2.] The heuristic expression for the Gaussian measure then takes the form

$$d\mu(x) = Ce^{-\|x\|_{\mathbf{H}}^2}\,\mathcal{D}x. \tag{20.21}$$

One might now try to approximate μ by Gaussian measures μ_N on Hilbert spaces $\mathbf{H}_N$ of dimension $N < \infty$. If $\dim \mathbf{H} < \infty$, then the expression (20.21) is perfectly rigorous, where the constant C may be taken to normalize μ to be a probability measure. A simple calculation (Exercise 4), however, shows that for any R, we have

$$\lim_{N\to\infty} \mu_N(B_{R,N}) = 0,$$

where $B_{R,N}$ denotes the ball of radius R in $\mathbf{H}_N$. This means that in the $N \to \infty$ limit, all of the "mass" of the measure is outside the ball of radius R, for *every* R. Thus, in the limit, the measure is supported entirely on points x where $\|x\|_H = \infty$, that is, on points that are not actually in $\mathbf{H}$. The measures μ_N *do* converge to a measure μ as N tends to infinity, but μ *does not* live on $\mathbf{H}$, but on some larger space $B \supset \mathbf{H}$. The original space $\mathbf{H}$ is a set of μ-measure zero inside B. See [16] for more information. In the case of the measure μ corresponding to the heuristic expression in (20.20), μ does not—as the expression suggests—live on the Sobolev space of fields with one derivative in L^2, but on a larger space, which turns out to be a space of distributions.

20.7 Exercises

1. Verify the identity (20.3) in the proof of the Trotter product formula.
2. Verify (20.5) in the proof of the Trotter product formula, using Stone's theorem and the following identity:

$$\frac{1}{s}(e^{isA}e^{isB} - I)\psi = e^{isA}(iB\psi) + e^{isA}\left(\frac{1}{s}(e^{isB} - I)\psi - iB\psi\right) + \frac{1}{s}(e^{isA} - I)\psi.$$

3. Suppose $\{A_N\}$ is a family of bounded operators mapping a Banach space W_1 to a Banach space W_2. Suppose that for some constant C, we have $\|A_N\| \leq C$ for all N. Finally, suppose that $\|A_N\psi\| \to 0$ as $N \to \infty$, for every $\psi \in W$.

   (a) Show that for each $\psi \in W$ and each $\varepsilon > 0$, there exists a neighborhood U of ψ and an integer M such that

   $$\|A_N\phi\| < \varepsilon$$

   for all $\phi \in U$ and $N \geq M$.

   (b) If K is a compact subset of W, show that $\|A_N\psi\|$ tends to zero *uniformly* for $\psi \in K$.

4. (a) Let $\mathbf{H}_N$ be an N-dimensional Hilbert space. Show that the measure

   $$d\mu_N(x) := \pi^{-N/2}e^{-\|x\|^2}dx$$

   is a probability measure. Here dx is the Lebesgue measure on $\mathbf{H}_N$, normalized to that the unit cube has volume 1.

   Hint: Use Proposition A.22.

   (b) Let $B_{R,N}$ denote the ball of radius R in $\mathbf{H}_N$. Show that for each $R < \infty$, there exists number $a_R < 1$ such that

   $$\mu_N(B_{R,N}) < (a_R)^N.$$

   Thus, $\lim_{N\to\infty} \mu_N(B_{R,N}) = 0$.

   Hint: The ball $B_{R,N}$ is contained in a cube centered at the origin with side length $2R$.