

Feynman path integral

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(Dated: October 25, 2018)

From the viewpoints of Schrödinger and Heisenberg, we have been studying quantum mechanics. We shall now venture into the third viewpoint based on the *path integral*, invented by R. F. Feynman, to look at the quantum systems. This viewpoint is particularly suitable to see the topological aspect of the systems. Here we shall learn the Feynman path integral method for treating simplest case, namely, a free particle.

I. BASIC IDEA [1]

It is said [1] that Feynman's path integral method is inspired by the mysterious remark in Dirac's book (page 128) [2], which states that

$$\exp \left[\frac{i}{\hbar} \int_{t_i}^{t_f} dt L(q, \dot{q}) \right] \text{ corresponds to } \langle q_f, t_f | q_i, t_i \rangle, \quad (1)$$

where $L(q, \dot{q})$ is the classical Lagrangian of a particle of mass m in a 1-dimensional potential $V(q)$,

$$L(q, \dot{q}) = \frac{1}{2} m \dot{q}^2 - V(q), \quad (2)$$

and $\langle q_f, t_f | q_i, t_i \rangle$ is the quantum probability amplitude for the particle to go from a space-time point (q_i, t_i) to (q_f, t_f) .

The exact correspondence, in the end Feynman found, can indeed be written by the space-time integral

$$\begin{aligned} \langle q_f, t_f | q_i, t_i \rangle &= \int_{q_i}^{q_f} Dq \exp \left[\frac{i}{\hbar} \int_{t_i}^{t_f} dt L(q, \dot{q}) \right] \\ &= \int_{q_i}^{q_f} Dq \exp \left[\frac{i}{\hbar} S[q] \right], \end{aligned} \quad (3)$$

where

$$\int_{q_i}^{q_f} Dq = \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \hbar \Delta t} \right)^{\frac{N}{2}} \int_{-\infty}^{\infty} dq_{N-1} \int_{-\infty}^{\infty} dq_{N-2} \cdots \int_{-\infty}^{\infty} dq_1. \quad (4)$$

is a infinite-dimensional path integral with $\{q_f, q_{N-1}, q_{N-2}, \dots, q_1, q_i\}$ representing a single path (trajectory) of the particle in a coordinate space and $S[q]$ is the action. Let us see how this *Feynman path integral*, Eq. (3), is emerged.

II. INTEGRAL OVER PATHS THROUGH PHASE SPACE [3]

The quantum probability amplitude for the particle $\langle q_f, t_f | q_i, t_i \rangle$ in Eq. (3) was written in the Heisenberg picture. This can be rewritten in the Schrödinger picture as

$$\langle q_f, t_f | q_i, t_i \rangle = \langle q_f | \exp \left[-\frac{i}{\hbar} H(t_f - t_i) \right] | q_i \rangle, \quad (5)$$

where

$$H = \frac{1}{2m} p^2 + V(q) \quad (6)$$

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is the Hamiltonian with p being the momentum conjugate of q . Chopping the time interval $t \equiv t_f - t_i$ into $N \gg 1$ steps lead to

$$e^{-\frac{i}{\hbar}Ht} = \left[e^{-\frac{i}{\hbar}H\Delta t} \right]^N, \quad (7)$$

where $\Delta t = \frac{t}{N}$. Now supposing that Δt is very short time interval (compared to the dominant time scale of the Hamiltonian dynamics) so that we can factorize $e^{-\frac{i}{\hbar}H\Delta t}$ in Eq. (7) into an easily diagonalized form, that is,

$$\begin{aligned} e^{-\frac{i}{\hbar}H\Delta t} &\cong \left(1 - i\frac{H}{\hbar}\Delta t \right) + \mathcal{O}(\Delta t^2) \\ &= \left(1 - \frac{i}{\hbar}\frac{p^2}{2m}\Delta t \right) \left(1 - \frac{i}{\hbar}V(q)\Delta t \right) + \mathcal{O}(\Delta t^2) \\ &\cong e^{-\frac{i}{\hbar}\frac{p^2}{2m}\Delta t} e^{-\frac{i}{\hbar}V(q)\Delta t} + \mathcal{O}(\Delta t^2). \end{aligned} \quad (8)$$

We thus have

$$\langle q_f, t_f | q_i, t_i \rangle = \langle q_f | \underbrace{e^{-\frac{i}{\hbar}\frac{p^2}{2m}\Delta t} e^{-\frac{i}{\hbar}V(q)\Delta t}}_1 \underbrace{e^{-\frac{i}{\hbar}\frac{p^2}{2m}\Delta t} e^{-\frac{i}{\hbar}V(q)\Delta t}}_2 \dots \underbrace{e^{-\frac{i}{\hbar}\frac{p^2}{2m}\Delta t} e^{-\frac{i}{\hbar}V(q)\Delta t}}_N | q_i \rangle. \quad (9)$$

Here we introduce the *resolution of identity*,

$$1 = \int dq_k |q_k\rangle \langle q_k| \int dp_k |p_k\rangle \langle p_k|, \quad (10)$$

and insert N of them into Eq. (9) leading to

$$\begin{aligned} \langle q_f, t_f | q_i, t_i \rangle &= \langle q_f | \underbrace{\int dq_N |q_N\rangle \langle q_N|}_1 \int dp_N |p_N\rangle \langle p_N| \underbrace{e^{-\frac{i}{\hbar}\frac{p^2}{2m}\Delta t} e^{-\frac{i}{\hbar}V(q)\Delta t}}_1 \int dq_{N-1} |q_{N-1}\rangle \langle q_{N-1}| \\ &\quad \int dp_{N-1} |p_{N-1}\rangle \langle p_{N-1}| \underbrace{e^{-\frac{i}{\hbar}\frac{p^2}{2m}\Delta t} e^{-\frac{i}{\hbar}V(q)\Delta t}}_2 \int dq_{N-2} |q_{N-2}\rangle \langle q_{N-2}| \\ &\quad \dots \int dp_1 |p_1\rangle \langle p_1| \underbrace{e^{-\frac{i}{\hbar}\frac{p^2}{2m}\Delta t} e^{-\frac{i}{\hbar}V(q)\Delta t}}_N | q_i \rangle. \end{aligned} \quad (11)$$

We can simplify Eq. (11) as

$$\begin{aligned} \langle q_f, t_f | q_i, t_i \rangle &= \int \prod_{k=1}^{N-1} dq_k \int \prod_{k=1}^N dp_k \langle q_f | p_N \rangle e^{-\frac{i}{\hbar}\frac{p_N^2}{2m}\Delta t} e^{-\frac{i}{\hbar}V(q_{N-1})\Delta t} \langle p_N | q_{N-1} \rangle \\ &\quad \langle q_{N-1} | p_{N-1} \rangle e^{-\frac{i}{\hbar}\frac{p_{N-1}^2}{2m}\Delta t} e^{-\frac{i}{\hbar}V(q_{N-2})\Delta t} \langle p_{N-1} | q_{N-2} \rangle \\ &\quad \dots \langle q_1 | p_1 \rangle e^{-\frac{i}{\hbar}\frac{p_1^2}{2m}\Delta t} e^{-\frac{i}{\hbar}V(q_i)\Delta t} \langle p_1 | q_i \rangle. \end{aligned} \quad (12)$$

Remembering that within the position representation

$$\langle q | p \rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{qp}{\hbar}}, \quad (13)$$

Eq. (12) can be further simplified and given as a $(2N-1)$ -dimensional integral

$$\begin{aligned} \langle q_f, t_f | q_i, t_i \rangle &= \int \prod_{k=1}^{N-1} dq_k \int \prod_{k=1}^N \frac{dp_k}{2\pi\hbar} e^{-\frac{i}{\hbar}\left(\frac{p_N^2}{2m} + V(q_{N-1}) - p_N \frac{q_f - q_{N-1}}{\Delta t}\right)\Delta t} \\ &\quad e^{-\frac{i}{\hbar}\left(\frac{p_{N-1}^2}{2m} + V(q_{N-2}) - p_{N-1} \frac{q_{N-1} - q_{N-2}}{\Delta t}\right)\Delta t} \dots e^{-\frac{i}{\hbar}\left(\frac{p_1^2}{2m} - V(q_i) - p_1 \frac{q_1 - q_i}{\Delta t}\right)\Delta t} \\ &= \int \prod_{k=1}^{N-1} dq_k \int \prod_{k=1}^N \frac{dp_k}{2\pi\hbar} \exp \left[-\frac{i}{\hbar}\Delta t \sum_{k=0}^{N-1} \left(\frac{p_{k+1}^2}{2m} + V(q_k) - p_{k+1} \frac{q_{k+1} - q_k}{\Delta t} \right) \right], \end{aligned} \quad (14)$$

where we set $q_0 = q_i$. Note that the third term in the exponent takes care of the *connection* between the chunks of the time interval. For the case of path integral of spin that term corresponds to the *topological term* [3].

Now by taking the continuum limit, that is, $N \rightarrow \infty$ while keeping $t = N\Delta t$ constant, we have

$$\begin{aligned} \langle q_f, t_f | q_i, t_i \rangle &= \int \underbrace{\prod_{k=1}^{N-1} dq_k}_{\int Dq} \int \underbrace{\prod_{k=1}^N \frac{dp_k}{2\pi\hbar}}_{\int Dp} \exp \left[-\frac{i}{\hbar} \int_0^t dt' \left(\frac{p(t')^2}{2m} + V(q(t')) - p(t')\dot{q}(t') \right) \right] \\ &= \int Dq \int Dp \exp \left[\frac{i}{\hbar} \int_0^t dt' (p(t')\dot{q}(t') - H(q(t'), p(t'))) \right], \end{aligned} \quad (15)$$

where we used

$$\Delta t \sum_{k=0}^{N-1} \Rightarrow \int_0^t dt' \quad (16)$$

$$\frac{q_{k+1} - q_k}{\Delta t} \Rightarrow \dot{q}(t')|_{t'=k\Delta t}, \quad (17)$$

with \Rightarrow indicating the continuum limit. Equation (15) is the *Hamiltonian formulation of the path integral*.

III. INTEGRAL OVER PATHS THROUGH COORDINATE SPACE [3]

The Hamiltonian formulation of the path integral, Eq. (15) represents Feynman's idea that the quantum probability amplitude $\langle q_f, t_f | q_i, t_i \rangle$ can be obtained by *summing over all possible paths in the phase space*. There is an analogous formula based on Lagrangian and the philosophy is to get $\langle q_f, t_f | q_i, t_i \rangle$ by *summing over all possible paths in the configuration space*. To this end, we just need to carry out the integration over Dp in Eq. (15). This can be done by the following procedure. First, rewrite the path integral as

$$\langle q_f, t_f | q_i, t_i \rangle = \int Dq \exp \left[-\frac{i}{\hbar} \int_0^t dt' V(q) \right] \int Dp \exp \left[-\frac{i}{\hbar} \int_0^t dt' \left(\frac{p^2}{2m} - p\dot{q} \right) \right], \quad (18)$$

and recognize that the second integrand is quadratic in p . Second, to execute the integration over p with *Gaussian integration* (see Appendix) go back to the finite-dimensional integral form,

$$\begin{aligned} \int Dp \exp \left[-\frac{i}{\hbar} \int_0^t dt' \left(\frac{p^2}{2m} - p\dot{q} \right) \right] &\Rightarrow \int \prod_{k=1}^N \frac{dp_k}{2\pi\hbar} \exp \left[-\frac{i}{\hbar} \Delta t \sum_{k=1}^N \left(\frac{p_k^2}{2m} - p_k \dot{q}_k \right) \right] \\ &= \left(\frac{1}{2\pi\hbar} \right)^N \int d\mathbf{p} \exp \left[-\frac{1}{2} (\mathbf{p}^T \mathbf{A} \mathbf{p}) + \mathbf{j}^T \mathbf{p} \right], \end{aligned} \quad (19)$$

where

$$\mathbf{p} = \begin{bmatrix} p_1 \\ p_2 \\ p_3 \\ \vdots \\ p_N \end{bmatrix}; \quad (20)$$

$$\mathbf{A} = \begin{bmatrix} \frac{i}{m\hbar}\Delta t & 0 & 0 & \cdots & 0 \\ 0 & \frac{i}{m\hbar}\Delta t & 0 & \cdots & 0 \\ 0 & 0 & \frac{i}{m\hbar}\Delta t & & \\ \vdots & \vdots & & \ddots & \\ 0 & 0 & & & \frac{i}{m\hbar}\Delta t \end{bmatrix}; \quad (21)$$

$$\mathbf{j} = \begin{bmatrix} \frac{i}{\hbar}q_1\Delta t \\ \frac{i}{\hbar}q_2\Delta t \\ \frac{i}{\hbar}q_3\Delta t \\ \vdots \\ \frac{i}{\hbar}q_N\Delta t \end{bmatrix}. \quad (22)$$

Third, perform the Gaussian integration (see Eq. (A4)):

$$\left(\frac{1}{2\pi\hbar}\right)^N \int d\mathbf{p} \exp\left[-\frac{1}{2}(\mathbf{p}^T \mathbf{A} \mathbf{p}) + \mathbf{j}^T \mathbf{p}\right] = \left(\frac{m}{2\pi i \hbar \Delta t}\right)^{\frac{N}{2}} \exp\left[-\frac{i}{\hbar}\Delta t \sum_{k=1}^N \left(-\frac{1}{2}mq_k^2\right)\right]. \quad (23)$$

Here we used the following trick (inverse of *Hubbard-Stratonovich transformation*). First, by shifting the integration vector according to

$$\mathbf{p} \rightarrow \mathbf{p} + \mathbf{A}^{-1}\mathbf{j}, \quad (24)$$

the left-hand-side of Eq. (23) becomes

$$\begin{aligned} & \int d\mathbf{p} \exp\left[-\frac{1}{2}(\mathbf{p} + \mathbf{A}^{-1}\mathbf{j})^T \mathbf{A} (\mathbf{p} + \mathbf{A}^{-1}\mathbf{j}) + \mathbf{j}^T (\mathbf{p} + \mathbf{A}^{-1}\mathbf{j})\right] \\ &= \left(\int d\mathbf{p} \exp\left[-\frac{1}{2}\mathbf{p}^T \mathbf{A} \mathbf{p}\right]\right) \exp\left[\frac{1}{2}\mathbf{j}^T \mathbf{A}^{-1}\mathbf{j}\right]. \end{aligned} \quad (25)$$

Next, by the further variable transformation

$$\mathbf{p} \rightarrow \mathbf{O}\mathbf{p}, \quad (26)$$

the above equation becomes

$$\begin{aligned} & \int d\mathbf{p} \exp\left[-\frac{1}{2}\mathbf{p}^T \underbrace{\mathbf{O}^T \mathbf{A} \mathbf{O}}_{\mathbf{D}: \text{diagonal matrix}} \mathbf{p}\right] \exp\left[\frac{1}{2}\mathbf{j}^T \mathbf{A}^{-1}\mathbf{j}\right] \\ &= \int \prod_i dp_i \exp\left[-\frac{1}{2}d_i p_i^2\right] \exp\left[\frac{1}{2}\mathbf{j}^T \mathbf{A}^{-1}\mathbf{j}\right] \\ &= \prod_i \sqrt{\frac{2\pi}{d_i}} \exp\left[\frac{1}{2}\mathbf{j}^T \mathbf{A}^{-1}\mathbf{j}\right], \end{aligned} \quad (27)$$

which is equivalent to the right-hand-side of Eq. (23). Finally, by taking the continuum limit again we can complete the integration over Dp as

$$\int Dp \exp \left[-\frac{i}{\hbar} \int_0^t dt' \left(\frac{p^2}{2m} - p\dot{q} \right) \right] = \lim_{N \rightarrow \infty} \left(\frac{m}{2\pi i \hbar \Delta t} \right)^{\frac{N}{2}} \exp \left[-\frac{i}{\hbar} \int_0^t dt' \left(-\frac{1}{2} m \dot{q}_k^2 \right) \right]. \quad (28)$$

By plugging Eq. (28) into Eq. (18) we reach the same conclusion as Feynman, i.e., Eq. (3)!

A. Example: free particle

Having get the beautiful formula Eq. (3), this formula per se is little use. Consider the the simplest example, free particle with mass m . In this case the Hamiltonian is

$$H = \frac{p^2}{2m}. \quad (29)$$

We shall now see that even in this simplest case the calculation of $G_{\text{free}}(q_f, q_i; t) \equiv \langle q_f, t_f | q_i, t_i \rangle$ with the Feynman path integral method is rather clumsy and cumbersome. We shall see the true power of the Feynman path integral method later on.

To avoid the divergence problem inherent in the path integral in the continuum limit [3], the starting point to get the formula of $G_{\text{free}}(q_f, q_i; t)$ is again the discretized finite-dimensional integral, Eq (14) with $V(q_k) = 0$:

$$\int \prod_{k=1}^{N-1} dq_k \int \prod_{k=1}^N \frac{dp_k}{2\pi\hbar} \exp \left[\frac{i}{\hbar} \sum_{k=1}^N \left(p_k (q_k - q_{k-1}) - \frac{p_k^2}{2m} \Delta t \right) \right]. \quad (30)$$

Here we notice that the integrations over $\{q_1, q_2, \dots, q_{N-1}\}$ are separately performed and

$$\int dq_k \exp \left[\frac{i}{\hbar} q_k (p_k - p_{k+1}) \right] = 2\pi\hbar \delta_{p_k p_{k+1}} \quad (31)$$

for $k = 1, 2, \dots, N-1$. Thus Eq. (30) becomes

$$(2\pi\hbar)^{N-1} \int \frac{dp_N}{2\pi\hbar} \int \prod_{k=1}^{N-1} \frac{dp_k}{2\pi\hbar} \delta_{p_k p_{k+1}} \exp \left[\frac{i}{\hbar} \left(\underbrace{(p_N q_N - p_1 q_0)}_{\text{leftover}} + \sum_{k=1}^N \left(-\frac{p_k^2}{2m} \Delta t \right) \right) \right]. \quad (32)$$

Performing the integration over p_N we have

$$(2\pi\hbar)^{N-2} \int \frac{dp_{N-1}}{2\pi\hbar} \int \prod_{k=1}^{N-2} \frac{dp_k}{2\pi\hbar} \delta_{p_k p_{k+1}} \exp \left[\frac{i}{\hbar} \left((p_{N-1} q_N - p_1 q_0) + \sum_{k=1}^{N-1} \left(-\frac{p_k^2}{2m} \Delta t \right) - \frac{p_{N-1}^2}{2m} \Delta t \right) \right]. \quad (33)$$

Then performing the integration over p_{N-1} we have

$$(2\pi\hbar)^{N-3} \int \frac{dp_{N-2}}{2\pi\hbar} \int \prod_{k=1}^{N-3} \frac{dp_k}{2\pi\hbar} \delta_{p_k p_{k+1}} \exp \left[\frac{i}{\hbar} \left((p_{N-2} q_N - p_1 q_0) + \sum_{k=1}^{N-2} \left(-\frac{p_k^2}{2m} \Delta t \right) - \frac{p_{N-2}^2}{2m} 2\Delta t \right) \right]. \quad (34)$$

Iterating this integration over p_k up to $k = 2$ leads to

$$\begin{aligned} G_{\text{free}}(q_f, q_i; t) &= \lim_{N \rightarrow \infty} \int \frac{dp_1}{2\pi\hbar} \exp \left[\frac{i}{\hbar} \left((p_1 q_N - p_1 q_0) + \left(-\frac{p_1^2}{2m} \Delta t \right) - \frac{p_1^2}{2m} (N-1) \Delta t \right) \right] \\ &= \lim_{N \rightarrow \infty} \int \frac{dp_1}{2\pi\hbar} \exp \left[\frac{i}{\hbar} \left((q_N - q_0) p_1 - \frac{t}{2m} p_1^2 \right) \right] \\ &= \int \frac{dp_1}{2\pi\hbar} \exp \left[\frac{i}{\hbar} \left((q_f - q_i) p_1 - \frac{t}{2m} p_1^2 \right) \right], \end{aligned} \quad (35)$$

where $q_0 = q_i$ and $q_N = q_f$. This is the Gaussian-form integral with respect to p_1 . Performing the Gaussian integration over p_1 (see Eq. (A2)) we have

$$G_{\text{free}}(q_f, q_i; t) = \sqrt{\frac{1}{4\pi \left(\frac{i\hbar}{2m} \right) t}} \exp \left[-\frac{(q_f - q_i)^2}{4 \left(\frac{i\hbar}{2m} \right) t} \right] \Theta(t), \quad (36)$$

where the step function, $\Theta(t)$, is introduced to account for the causality. Note that this is like a solution of a classical diffusion equation with the diffusion constant $D = \frac{i\hbar}{2m}$.

B. Example: free particle in momentum representation

Consider again the path integral of a free particle with mass m with $H = \frac{p^2}{2m}$. This time, however, we are interested in a form in the momentum representation, that is, $\langle p', t | p, 0 \rangle$, which can be given by

$$\begin{aligned} \langle p', t | p, 0 \rangle &= \langle p', t | \underbrace{\int dq' |q', t\rangle}_{1} \underbrace{\langle q', t | \int dq |q, 0\rangle}_{1} \langle q, 0 | p, 0 \rangle \\ &= \int dq \int dq' \langle q', t | q, 0 \rangle \left(\frac{1}{2\pi\hbar} \exp \left[\frac{i}{\hbar} (pq - p'q') \right] \right). \end{aligned} \quad (37)$$

Plugging Eq. (35) into Eq. (37) we have

$$\begin{aligned} \langle p', t | p, 0 \rangle &= \int dq \int dq' \left(\int \frac{dp_1}{2\pi\hbar} \exp \left[\frac{i}{\hbar} \left((q - q') p_1 - \frac{t}{2m} p_1^2 \right) \right] \right) \left(\frac{1}{2\pi\hbar} \exp \left[\frac{i}{\hbar} (pq - p'q') \right] \right) \\ &= \frac{1}{(2\pi\hbar)^2} \int dp_1 \exp \left[-\frac{i}{\hbar} \left(\frac{t}{2m} p_1^2 \right) \right] \underbrace{\int dq \exp \left[\frac{i}{\hbar} q (p + p_1) \right]}_{2\pi\hbar\delta(p+p_1)} \underbrace{\int dq' \exp \left[-\frac{i}{\hbar} q' (p' + p_1) \right]}_{2\pi\hbar\delta(p'+p_1)} \\ &= \delta(p' - p) \exp \left[-\frac{i}{\hbar} \left(\frac{p^2}{2m} \right) t \right] \\ &= \delta(p' - p) \exp \left[-\frac{i}{\hbar} Ht \right]. \end{aligned} \quad (38)$$

This is indeed the sensible result: under the free particle hamiltonian $H = \frac{p^2}{2m}$ the linear momentum is conserved and the time evolution of the eigenstate $|p, 0\rangle$ acquires the dynamical phase factor $e^{-\frac{i}{\hbar} Ht}$ during time t .

Appendix A: Gaussian integration

First, some mathematics. The most fundamental Gaussian integration is

$$\int_{-\infty}^{\infty} dx e^{-\frac{1}{2}ax^2} = \sqrt{\frac{2\pi}{a}}. \quad (A1)$$

An interesting and useful Gaussian integration is

$$\int_{-\infty}^{\infty} dx e^{-\frac{1}{2}ax^2 + bx} = \sqrt{\frac{2\pi}{a}} e^{\frac{b^2}{2a}}. \quad (A2)$$

The Multi-dimensional expansion of Eq. (A1) is

$$\int_{-\infty}^{\infty} d\mathbf{v} e^{-\frac{1}{2}\mathbf{v}^T \mathbf{A} \mathbf{v}} = (2\pi)^{\frac{N}{2}} \frac{1}{\sqrt{\det[\mathbf{A}]}} \quad (A3)$$

and that of Eq. (A2) is

$$\int_{-\infty}^{\infty} d\mathbf{v} e^{-\frac{1}{2}\mathbf{v}^T \mathbf{A} \mathbf{v} + \mathbf{j} \cdot \mathbf{v}} = (2\pi)^{\frac{N}{2}} \frac{1}{\sqrt{\det[\mathbf{A}]}} e^{\frac{1}{2}\mathbf{j}^T \mathbf{A}^{-1} \mathbf{j}}, \quad (A4)$$

[1] J. J. Sakurai, *Modern Quantum Mechanics*, revised ed. (Addison-Wesley, Reading, MA, 1994).

[2] P. A. M. Dirac, *Quantum Mechanics*, 4th ed. (Oxford University Press, London, 1958).

[3] A. Altland and B. D. Simons, *Condensed Matter Field Theory*, 2nd ed. (Cambridge University Press, Cambridge, 2010).