Texts and Monographs in Physics

Gert Roepstorff

Path Integral Approach to Quantum Physics

An Introduction

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An Introduction

With 26 Figures

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To Ingrid
who made it all worthwhile

Preface

This book has been written twice. After having written and published it in German in 1990, I started all over again and rewrote the whole story for an English speaking audience. During the first round I received encouraging words and critical remarks from students and colleagues alike which have helped to sustain me the second time around.

In the preface the author usually states that his or her book resulted from a course that he or she gave at some university. I cannot claim that the present book is any exception to the rule. But I expanded and remodelled the original material which circulated as a manuscript so that the printed version would follow a more stringent and coherent architectural plan. In doing so I have concentrated on the conceptual problems inherent in the path integral formalism rather than on certain highly specialized techniques used in applications. Nevertheless, I have also included those methods that are of fundamental interest and have treated specific problems mainly to illustrate them.

The text is designed to introduce graduate students to the functional integration method in contemporary physics as painlessly as possible without their being forced to spend too much time solely in getting oriented in the mathematical intricacies of measure theory. In the development of the method, there is a striking interplay between stochastic processes, statistical physics, and quantum mechanics. This aspect, I felt, should be stressed in a text on path integration. As for the prerequisites, the student is assumed to be familiar with quantum mechanics and, on the mathematical side, with probability theory. Moreover, it is hoped that he or she has grasped the essentials of quantum field theory and elementary particle physics and is open minded.

This expository work is certainly not meant to be a substitute for the conventional operator version of quantum physics: in fact, no attempt has been made to rewrite parts of quantum mechanics or field theory using the rather sophisticated language of path integration. Nor is this work a formal account of all the activities in the field but largely a personal book whose factual details are organized and dominated by my views.

Since I began thinking about path integration, I owe thanks for their guidance to more colleagues than I could possibly name here. My special thanks are due to L. S. Schulman; without him the book could not have come into existence. I owe a great deal to E. H. Lieb who stopped me from making foolish mistakes. I would like to thank R. Haag, J. E. Roberts, and J. Challifour for their sharpening my understanding of quantum field theory. I received advice from W. Thirring, W. Beiglböck, A. Uhlmann, L. Streit, A. Martin, W. Bietenholz, and H. Siedentop. Special thanks go to H. Spohn and M. Demuth for their wisdom and encouragement. I should also like to thank my students C. Beck and M. Ringe for valuable discussions during the preparation of the early draft. I also thank M. Seymour who went carefully through the final draft and pointed out a number of misprints and suggested improvements with regard to style and clarity. Last but not least I am grateful to the Institute for Advanced Study, Princeton, for hospitality.

September 1993 Gert Roepstorff

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1 Brownian Motion

> The main advantages of a discrete approach are pedagogical, inasmuch as one is able to circumvent various conceptual difficulties inherent to the continuous approach. It is also not without a purely scientific interest [...].
>
> *Marc Kac*

> The shortest path between two truths in the real domain passes through the complex domain.
>
> *J. Hadamard*

Physics is often seen as being rooted in, and to the present day deals with, the study of moving bodies. We have every reason to believe that, historically, phenomenological attempts at describing the observed preceded speculations about the underlying dynamical law. This chapter focuses on random motion, first described in 1828 by the British botanist R. Brown, who investigated the pollen of different plants dispersed in water. Years after the discovery scientists began to realize that any kind of inorganic substance, not just "living matter", presents, in principle, the same phenomenon, and thus looked for an explanation. In fact a respectable *theory of Brownian motion* emerged much later (not before 1905) as a result of an interplay between physics and mathematics. At present the prospects for possible applications[1] in the exact sciences seem unlimited: the concepts of Brownian motion are now being used in fields as different as astronomy (stellar dynamics), diffusion, colloid chemistry, polymer physics, quantum mechanics, and elementary-particle physics. The surprise is that the scale of length does not matter at all. Instead what strikes the eye, as a common characteristic, is some kind of universal mathematical structure. Nevertheless, the concept of Brownian motion as a whole together with its highly specialized tools does not seem to fit into the traditional framework of classical mechanics as a deterministic theory that, according to a dictum of A. Sommerfeld, represents the "backbone of mathematical physics".

The apparent irregular motion that we shall describe, nondeterministic as it may be, does not take place without obeying certain rules, and it took the genius of A. Einstein to notice and apply these rules successfully. Through his pioneering work [1.2] the theory of Brownian motion acquired a firm position within the fabric of physics.

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[1] A collection of early significant contributions is presented in [1.1].

1.1 The One-Dimensional Random Walk

The principal features of the problem of the random walk can be elucidated by analyzing the simplest of all cases: the erratic motion of a single point particle in one dimension [1.3]. Imagine the particle suffers displacements along the x-axis in the form of a series of steps of the same length h, each step being taken in either direction within a certain period of time, say of length τ. In essence, one may think of both space and time as being replaced by sequences of equidistant marks: from now on we shall call such models *discrete*.

In addition, supposing that there is no physical factor preferring *right* over *left*, we may postulate that forward and backward steps occur with equal probability $\frac{1}{2}$. Successive steps are assumed to be statistically independent. Hence, the probability is

$$P(ih - jh, \tau) = \begin{cases} \frac{1}{2} & \text{if } |i-j| = 1 \\ 0 & \text{otherwise} \end{cases} \qquad (i, j \in \mathbb{Z}) \tag{1.1.1}$$

for a transition from $x = jh$ to the new position $x = ih$ during the time τ.

In still other words and at a higher level, what we have before us is an example of a stochastic process, more precisely, of a *Markov chain* with a denumerable set of states [1.4]. The process has two obvious properties. It is

homogeneous: the transition probability P is merely a function of the difference $i - j$; and
isotropic: the transition probability does not depend on the direction in space, i.e., P is left unchanged if we replace (i, j) by $(-i, -j)$.

Quite generally, a Markov chain may be characterized by a pair (P, p), where $P = (P_{ij})$ stands for what is called a *transition matrix* and $p = (p_i)$ is the *initial probability distribution*. In simpler terms: p_i is the probability of the event i occurring at starting time $t = 0$. One always has $0 \le p_i \le 1$, $\sum_i p_i = 1$, $0 \le P_{ij} \le 1$, and $\sum_i P_{ij} = 1$. As for our example, the event i is identified with the particle's position $x = ih$ and the matrix P has components

$$P_{ij} = P(ih - jh, \tau). \tag{1.1.2}$$

Caution: this matrix is doubly infinite, $-\infty < i, j < \infty$, and from another point of view it seems more appropriate to call it an *operator*.

After the elapse of time $n\tau$ ($n \in \mathbb{N}$) the accumulated transition probabilities are

$$P(ih - jh, n\tau) = (P^n)_{ij}, \tag{1.1.3}$$

where $P^n = P \cdot P \cdots P$ (n factors) stands for the n-fold matrix product. What about the initial distribution? If, at time $t = 0$ the position of the particle is known with certainty, say $x = 0$, we have $p_i = 0$ for $i \neq 0$ and $p_0 = 1$. After time $n\tau \geq 0$, the system has evolved and produced a new distribution which is $P^n p$. As a matter of convenience, p and $P^n p$ are treated here as vectors. Phrased differently, as a function of n, P^n is the operator of evolution for the system, where we regard n as the relevant time variable. Within this setting, time never assumes negative values.

The operators

$$R = \begin{pmatrix} \ddots & & & & & 0 \\ & 1 & 0 & & & \\ & & \ddots & \ddots & & \\ & & & 1 & 0 & \\ 0 & & & & \ddots & \ddots \end{pmatrix} \qquad L = \begin{pmatrix} \ddots & \ddots & & & & 0 \\ & & 0 & 1 & & \\ & & & \ddots & \ddots & \\ & & & & 0 & 1 \\ 0 & & & & & \ddots \end{pmatrix} \tag{1.1.4}$$

shift the particle's position to the right and left respectively by the amount h. Obviously, $L = R^{-1}$ and thus $RL = LR$. This clarifies the structure of the operator P and its powers: first notice that

$$P = \tfrac{1}{2}(R + L) \tag{1.1.5}$$

and then write

$$P^n = \frac{1}{2^n} \sum_{k=0}^{n} \binom{n}{k} R^k L^{n-k} \tag{1.1.6}$$

to obtain the transition probabilities after n time steps:

$$P(ih - jh, n\tau) = \frac{1}{2^n}\binom{n}{k}, \qquad i - j = k - (n - k). \tag{1.1.7}$$

By appeal to the recursion formula for the binomial coefficients,

$$\binom{n+1}{k} = \binom{n}{k} + \binom{n}{k-1}, \tag{1.1.8}$$

one gets the following remarkable difference equation:

$$P(x, t + \tau) = \tfrac{1}{2}P(x + h, t) + \tfrac{1}{2}P(x - h, t) \tag{1.1.9}$$

with $x = (i - j)h$ and $t = n\tau$. Equation (1.1.9) may be rewritten as

$$\frac{P(x, t + \tau) - P(x, t)}{\tau} = \frac{h^2}{2\tau} \frac{P(x + h, t) - 2P(x, t) + P(x - h, t)}{h^2}. \tag{1.1.10}$$

The point is, the difference equation has got pretty close to some differential equation. Now, think of h and τ as *microscopic* quantities and pass to a macroscopic (large scale) description of a random walk by a limiting process $h \to 0$, $\tau \to 0$ with

$$D = \frac{h^2}{2\tau}\,, \tag{1.1.11}$$

the *diffusion constant*, held fixed. This process turns x und t into continuous variables: $x \in \mathbb{R}$, $t \in \mathbb{R}_+$ which conforms much better with our normal view of space and time. As a highly satisfactory result, we obtain from (1.1.10) the one-dimensional diffusion equation[2]:

$$\frac{\partial}{\partial t}P(x,t) = D\frac{\partial^2}{\partial x^2}P(x,t). \tag{1.1.12}$$

The results of a computer simulation of the one-dimensional diffusive motion using two different diffusion constants are shown in Fig.1.1.

Equation (1.1.12) and its multidimensional variants form the basis of Einstein's theory of Brownian motion. As a result of the limiting procedure, no meaning can be attributed to the velocity of the Brownian particle. This is clearly indicated by $h/\tau \to \infty$. Phrased in more mathematical terms: though continuous, a typical Brownian path is nowhere differentiable as a function of time.

Einstein reasoned that the diffusion constant should be of the form $D = k_B T/f$, where k_B, T, and f are Boltzmann's constant, the temperature, and the friction constant respectively. For f he used Stokes's law $f = 6\pi a\eta$ for a single, rigid, spherical particle of radius a inserted into a fluid of viscosity η. The radius of the Brownian particle is to be taken large compared to both the radius of the bombarding solvent molecules and their mean free path. Next, Einstein suggested using the mean square displacement for a Brownian particle starting at the origin, $\langle x^2 \rangle = 2Dt$, to determine the diffusion constant D, which, when we know a and η, ultimately yields a value for Avogadro's constant N since $k_B = R/N$. Consistency with other ways of obtaining N showed once more the validity of the molecular kinetic theory and thus the reality of atoms.

Einstein's relation between D and f represents the first instance of the fluctuation–dissipation connection of statistical physics: a fluctuation (the mean square displacement per unit time) is connected with a dissipative quantity (the friction constant).

The diffusion equation and the heat equation formally look the same. However, there is a distinction in the interpretation of the function $P(x,t)$ and the constant D. The reader familiar with the theory of heat conduction knows that the solution of the initial value problem $P_0(x,0) = \delta(x)$ is the Gauss function

$$P_0(x,t) = \frac{1}{2\sqrt{\pi D t}} \exp\left\{-\frac{x^2}{4Dt}\right\} \qquad (t > 0). \tag{1.1.13}$$

In terms of Brownian motion this choice of initial data means that the particle starts at the origin. By the classical theorem of Laplace and De Moivre, i.e., convergence of the binomial distribution towards the normal distribution, the transition probability for the discrete random walk, P,

[2] Notice: it is $h^{-1}P_{ij}$ that approaches $P(x,t)$. The extra factor h^{-1} takes care of the fact that the normalization $\sum_i P_{ij} = 1$ changes to $\int dx\, P(x,t) = 1$.