TECHNIQUES AND APPLICATIONS OF PATH INTEGRATION

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Techniques and Applications of Path Integration

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Preface

This book originated in a course given at the Technion some 10 years ago during my first stay, as a visitor, in Israel. Things were different then. Path integrals were not in the mainstream of anything, and I think those who studied this topic did so more from an aesthetic turn of mind than for practical reasons. Either that, or they still carried forth the ideas of the 1950s when path integration had its great, early successes. My own interest in the subject is accidental—while reading an article in Schwinger's reprint collection on quantum electrodynamics the pages slipped and the book fell open to Feynman's *Reviews of Modern Physics* paper. This I read, and resolved, as a thesis topic, to try to produce a path integral for spin.

Path integration has come a long way in the 1970s. In statistical physics it was the basic framework for the first formulation of the renormalization group transformation. It is used extensively in studying systems with random impurities. In particle physics it is basic to the instanton industry and finds application in studies of gauge field theory (even though some of the methods used had been developed for other problems in the 1960s). In chemical, atomic, and nuclear physics path integrals have been applied to semiclassical approximation schemes for scattering theory. And in rigorous studies of quantum field theory and statistical mechanics the functional integral is used again and again.

This is a book of techniques and applications. My aim is to say what the path integral is and then by example to show how it can and has been used. The approach is that of a physicist with a weakness for but not an addiction to mathematics. The level is such that anyone with a reasonable first course in quantum mechanics should not find difficulty although some of the applications presuppose specialized knowledge; even then, on topics of special interest to me I have supplied background material unrelated to path integrals.

The implications of path integrals for a general understanding of quantum mechanics have been beautifully expounded in Feynman's original *Reviews of Modern Physics* paper and in his book on path integrals with Hibbs. For this reason I have touched only lightly on these matters. The Feynman-Hibbs book also includes many applications of path integration, some of which have been given brief treatment here. The emphasis in that volume is on applications developed by Feynman himself, and while they form a considerable body of knowledge there is still enough left over for the present book.

The first part of the book develops the techniques of path integration. Our basic derivation of the path integral presents it as a mathematically justified consequence of the usual quantum mechanics formalism (via the Trotter product formula). Of course we also talk of summing the quantity $\exp(iS/\hbar)$ over all paths, despite the lack of rigorous justification for such terminology. In fact some of our work makes extensive use of this view. Nevertheless, while I have been willing to work without the full blessings of theorems at every step, I have tried to avoid some of the pitfalls that path integrals offer to the unwary. In particular there is a good deal of discussion of the relation $(\Delta\,\text{distance})^2 \sim (\Delta\,\text{time})$, a central property of paths entering the Feynman sum over histories. Some of the usual quantum formalism is recovered from the path integral but no great emphasis is placed on this goal. The explicitly solvable path integrals—the harmonic oscillator and variations thereof—are written out, and it is thus shown that the awesome task of summing over paths can in fact occasionally be done. At this early stage we also introduce the Wiener integral, formal first cousin of the path integral and legitimate integral over paths. Here we are able to indulge in an occasional rigorous proof and present a calculation of a first passage time, illustrating the profound connection provided by the Wiener integral between probability and potential theory.

The choice of applications that appear in this book requires a special apology. For a topic to be treated here, I had to first know about it, next understand it (or think I did), then find it amusing, exciting, fundamental, or possessing some similar quality, and finally have the time to present it. There are undoubtedly works that satisfy the third of my criteria but miss out on some other count. Section 32, being a brief treatment of some omissions, reflects the fact that the book had to be finished some time although many beautiful applications would not appear.

As to the applications that do appear.... A lot of space is devoted to the semiclassical approximation. Although the mathematical justification for the stationary phase approximation to the functional integral is not strong, this is an important application, at least in terms of consumer interest. Also, one of the features of Feynman's formulation of quantum mechanics that first impressed me was that the correspondence limit ($\hbar \to 0$) was a wave of the hand away (via the stationary phase approximation). Of course converting the hand waving arguments to mathematics is still an uncompleted job, but that does not detract from the beauty of the ideas. I must also confess that I am drawn to the semiclassical approximation not so much by consumer interest but rather by the way in which so many different strands of nineteenth and twentieth century mathematics are brought together. Between Sections 11 and 18 the following topics—all relevant to the matter at hand—are taken up: (1) variational principles of classical mechanics and *minimum* (rather than merely extremum) properties of paths—the Jacobi equation; (2) the Morse index theorem; (3) asymptotic analysis, order relations, and so on; (4) Sturm-Liouville theory; (5) Thom's catastrophe theory; (6) *uniform* asymptotic analysis.

Starting from semiclassical results it is not difficult to derive both approximations for scattering theory (Section 19) and a path integral theory of optics (Section 20). The optics calls for some unnatural definitions but I think the reward is worth the temporary inelegance: semiclassical results for path integrals lead at once to geometrical (and even physical) optics with a possibility of getting Keller's "geometrical diffraction" theory too (that possibility is suggested but not carried out in this book).

Probably the most famous early application of path integration is to the polaron and we treat that here too. What makes the polaron special from the standpoint of selling path integrals is that it is one of the few places where the path integral not only helps you discover an answer, but also remains the best way to calculate the answer even after you know it. I like the polaron because it is a tractable field theory; the benefits obtained from using the path integral are entirely analogous to those gotten in quantum electrodynamics, but for the latter all steps are more difficult because of the infinities, the vector character of the field, and gauge problems. Results of the path integral treatment of Q.E.D. are mentioned briefly in Section 32.

Three sections are devoted to the problem of formulating a path integral for spin. Not surprisingly I place the most emphasis on the approach I myself have worked on. To be honest, if I had to solve the problem of a hydrogen atom in a magnetic field I would not use this formalism. Nevertheless, the method shows there is *some* way to treat spin by path integrals. It would also appear that some of the connections to homotopy theory developed in the course of working out a path integral for spin are turning out to be important in gauge theories. Unfortunately, path integral treatments of gauge theories get only the briefest mention in this book; this is one of the gaps I especially regret.

The section on relativistic propagators is both central to the book and an incidental side topic. It is central, because if you wish to think of path integrals as telling you something fundamental about quantum mechanics then you had better have a relativistic formulation, since that's the way the world is. On the other hand, the most dramatic part of Section 25 deals with particles in the strong gravitational fields near black holes. This application certainly demonstrates the versatility of path integration. For this section some background in general relativity is needed.

Statistical mechanical applications of path integration could easily take up a book on their own. The partition function, the basic object of statistical physics, is most conveniently written as a functional integral for many physical systems. In Sections 26 to 30 both general developments and specific applications are treated. Systems with random impurities are studied although our greatest expositional efforts are not concentrated on the currently most popular developments. The references however cover some of the missing material. The instantons of the 1970s and all their aliases first appeared as critical droplets in path integral studies of metastability in first order phase transitions. Our own treatment takes a neutral view of the physics and presents the method as a way of doing an analytical continuation. The renormalization group and scale transformations have been an important recent application of functional integration and Section 30 deals with this.

The section on coherent states finds itself in the statistical mechanics department almost by accident: one of the applications of this form of the path integral is to the statistical mechanics of boson field theories. Rightfully this could have been put with the section on the phase space path integral with which it has strong ties. As to the section on the phase space path integral, I have included it somewhat reluctantly. Although the reader will soon find that I am not overly fussy about dotting all my mathematical i's, I think that phase space path integrals have more troubles than merely missing details. On this basis they should have been left out of the book; however, I often have conversations with people who use this form of the path integral and they want to know what all the fuss is about. Section 31 aims to answer that question.

The final section gives various applications that I just *couldn't* leave out, and of course, so as to finally finish the book (gestating lo these five years), some topics were left out.

Each section of the book has its own set of references and notes, since I felt that this gave the best opportunity to present background and ancillary material. For convenience however these references are included by author in the index.

There is some previously unpublished work in the book. Much of this occurs in the sections on the semiclassical approximation. The material on caustics was reported in a 1973 conference and was never fully written up, pending its appearance here.

It is a pleasure to thank the many students and colleagues who helped me in the completion of this book. I would like to mention especially Steve Coyne, Gianfausto Dell'Antonio, Mark Kac, Don Lichtenberg, Ady Mann, David McLaughlin, Rebecca McCraw, Charles Newman, Michael Revzen, Roman Shtokhamer, Barry Simon, David Wallace, Arthur Wightman, and Joshua Zak. Although many skilled hands have gone into the typing of the manuscript I am particularly grateful to Judy Huffaker Hammond and Gila Ezion for their help.

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PART II SELECTED APPLICATIONS OF THE PATH INTEGRAL

PART ONE

Introduction

ONE

Introducing and Defining the Path Integral

The best place to find out about path integrals is in Feynman's paper.* Our approach is not to use path integrals as a way of arriving at quantum mechanics, although Feynman has used this point of view in his book with Hibbs. Rather we assume knowledge of quantum mechanics and deduce the path integral formalism from it. This gets us into the subject quickly.

The wave function of a nonrelativistic spinless particle in one dimension evolves according to Schrödinger's equation

$$H\psi = i\hbar \frac{\partial \psi}{\partial t} \tag{1.1}$$

$$H = T + V = \frac{1}{2m}p^2 + V = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V \tag{1.2}$$

Our interest is in the propagator or Green's function G which satisfies the equation

$$\left(H - i\hbar\frac{\partial}{\partial t}\right)G(t, t_0) = -i\hbar 1\delta(t - t_0) \tag{1.3}$$

in operator notation. In coordinate space this is written

$$\left(H_x - i\hbar\frac{\partial}{\partial t}\right)G(x, t; y, t_0) = -i\hbar\delta(x - y)\delta(t - t_0) \tag{1.4}$$

The G's are related by

$$G(x, t; y, t_0) = \langle x|G(t, t_0)|y\rangle \tag{1.5}$$

*For references see notes at the end of the section.

Knowing G means having a solution to the time dependent Schrödinger equation in the sense that if $\psi(t_0)$ is the state of the system at t_0, $\psi(t)$, given by

$$\psi(t)=G(t,t_0)\psi(t_0) \tag{1.6}$$

is the state at t. For time independent H an operator solution of (1.3) can immediately be written down:

$$G(t,t_0)=\theta(t-t_0)\exp\left[-\frac{iH(t-t_0)}{\hbar}\right] \tag{1.7}$$

where θ is the step function. Since H is assumed to be time independent we can, without loss of generality, take $t_0=0$. Then for $t>0$ we have

$$G(x,t;y)=\langle x|e^{-iHt/\hbar}|y\rangle \tag{1.8}$$

where the argument 0 has been deleted.

The path integral arises from the fact that

$$e^A=(e^{A/N})^N \tag{1.9}$$

Letting $\lambda=it/\hbar$ yields

$$G(x,t;y)=\langle x|e^{-\lambda(T+V)/N}e^{-\lambda(T+V)/N}\cdots e^{-\lambda(T+V)/N}|y\rangle \tag{1.10}$$

with the product in the brackets taken N times. Now we make use of a fundamental fact about the exponential of two operators, namely

$$e^{-\lambda(T+V)/N}=e^{-\lambda T/N}e^{-\lambda V/N}+O\left(\frac{\lambda^2}{N^2}\right) \tag{1.11}$$

This is proved easily enough,* and in a power series expansion the coefficient of the λ^2/N^2 term is

$$A=\tfrac{1}{2}[V,T]$$

In subsequent manipulations we assume that the $O(1/N^2)$ term is well behaved, that it stays bounded when applied to states, and so on. For reasonable potentials this assumption is justified; more is said on this topic in the appendix.

*An expansion is conveniently generated by looking at derivatives of $\exp(\lambda T/N)\exp(-\lambda(T+V)/N)\exp(\lambda V/N)$.

What we are now aiming for is to replace the term

$$\left[e^{-\lambda(T+V)/N}\right]^N=\left[e^{-\lambda T/N}e^{-\lambda V/N}+O(1/N^2)\right]^N \tag{1.12}$$

by the term

$$\left[e^{-\lambda T/N}e^{-\lambda V/N}\right]^N \tag{1.13}$$

For real numbers (rather than operators) this replacement is a reflection of a fundamental fact about the exponential. The expression

$$\left(1+\frac{x+y_n}{n}\right)^n$$

converges to e^x despite the presence of y_n so long as $y_n \to 0$ as $n\to\infty$. (A proof of this assertion can be had by taking large enough n that $|y_n|<\delta$ and by using the bound

$$\left(1+\frac{x-\delta}{n}\right)^n<\left(1+\frac{x+y_n}{n}\right)^n<\left(1+\frac{x+\delta}{n}\right)^n$$

and assuming n large enough that $|(x-\delta)/n|<1$.)

For operators a bit of care is required, and the trick is to express the difference of (1.12) and (1.13) in a peculiar way:

$$\begin{aligned}
&(e^{-\lambda T/N}e^{-\lambda V/N})^N-(e^{-\lambda(T+V)/N})^N\\
&\quad=\left[e^{-\lambda T/N}e^{-\lambda V/N}-e^{-\lambda(T+V)/N}\right](e^{-\lambda(T+V)/N})^{N-1}\\
&\qquad+e^{-\lambda T/N}e^{-\lambda V/N}\left[e^{-\lambda T/N}e^{-\lambda V/N}-e^{-\lambda(T+V)/N}\right]e^{-\lambda(T+V)(N-2)/N}\\
&\qquad+\cdots+(e^{-\lambda T/N}e^{-\lambda V/N})^{N-1}\left[e^{-\lambda T/N}e^{-\lambda V/N}-e^{-\lambda(T+V)/N}\right]
\end{aligned} \tag{1.14}$$

Equation 1.14 is an identity. It contains N terms, each of which has the factor $\exp(-\lambda T/N)\exp(-\lambda V/N)-\exp(-\lambda(T+V)/N)$, which by (1.11) is of order $1/N^2$. Hence in the limit the difference is zero. (In an appendix mention is made of various finer points in the estimate.)

We have therefore justified the replacement of (1.10) by

$$G(x,t;y)=\lim_{N\to\infty}\langle x|(e^{-\lambda T/N}e^{-\lambda V/N})^N|y\rangle \tag{1.15}$$

In effect we have given a heuristic proof of the Trotter product formula. From here, getting the path integral is just a few easy steps. The identity operator, in the form

$$\int dx_j |x_j\rangle\langle x_j|, \qquad j=1,\ldots,N-1 \tag{1.16}$$

is inserted between each term in the product in (1.15), yielding

$$G(x,t;y)=\lim_{N\to\infty}\int dx_1\cdots dx_{N-1}\prod_{j=0}^{N-1}\langle x_{j+1}|e^{-\lambda T/N}e^{-\lambda V/N}|x_j\rangle \tag{1.17}$$

(for convenience we have taken $y=x_0$, $x=x_N$). The multiplication operator V is diagonal in coordinate space so that

$$\exp\left(-\frac{\lambda V}{N}\right)|x_j\rangle=|x_j\rangle\exp\left(-\frac{\lambda V(x_j)}{N}\right) \tag{1.18}$$

Next we require coordinate space matrix elements of $\exp(-\lambda T/N)$ (between states $\langle\eta|$ and $|\xi\rangle$, say), and to obtain these we insert a complete set of momentum states

$$1=\int dp|p\rangle\langle p| \qquad \text{with} \qquad \langle p|\xi\rangle=(2\pi\hbar)^{-1/2}\exp\left(-\frac{ip\xi}{\hbar}\right) \tag{1.19}$$

This gives

$$\begin{aligned}\langle\eta|e^{-\lambda T/N}|\xi\rangle&=\int dp\langle\eta|e^{-\lambda T/N}|p\rangle\langle p|\xi\rangle\\&=\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}dp\, e^{-\lambda p^2/2mN}e^{ip(\eta-\xi)/\hbar}\end{aligned} \tag{1.20}$$

This is our first Gaussian integral of the book, but far from the last. The general formula is

$$\int_{-\infty}^{\infty}e^{-ay^2+by}\,dy=\sqrt{\frac{\pi}{a}}\;e^{b^2/4a} \tag{1.21}$$

Using (1.21), (1.20) becomes

$$\langle\eta|e^{-\lambda T/N}|\xi\rangle=\sqrt{\frac{mN}{2\pi\lambda\hbar^2}}\;e^{-mN(\eta-\xi)^2/2\lambda\hbar^2} \tag{1.22}$$