FRONTIERS OF PATH INTEGRATION

L. S. Schulman

Physics Department, Clarkson University
Potsdam, NY 18999-5880 USA

Introduction

The last session of the 1993 Bangkok path integral conference bore the title of this article and represented an invitation to the present writer and ultimately to other conference participants to identify and comment upon important open questions in the field. It was not a conference summary. I did not take my mandate entirely literally and instead spoke of (and present below) various topics that I consider interesting or important; however, I would not try to defend them as the most important. About halfway into the session I opened the floor to other participants for their views, and will give a condensed version below of some of their comments. It is inevitable that my rendition will have unintended omissions and distortions.

For the reader who would like a further view of “frontiers” of path integration, besides that implicit in the present volume, I can recommend the book, Lectures on Path Integration: Trieste 1991, that arose out of a workshop and conference at ICTP.

Although, as indicated, I passed up the opportunity to define the future of the field, I did feel that the grandiose title offered license to pontificate just a bit. This is embodied in the following paragraph.

Pure thought

I wish to offer advice of general value in theoretical physics and which is especially relevant to the path integral community. The advice is to stay close to things, to material objects, to data, to physics. There is significant risk of total irrelevance for those who indulge in pure thought. This advice is sensationalized in Fig. 1, an improvement over the crude drawing of Rodin’s famous statue that I used at the conference. Of course this is an exaggeration and surely I am myself guilty of the sin I now condemn. Nevertheless, the most lasting and significant contributions of the path integral have been those with direct physical impact. You could argue that Feynman’s original paper on the path integral was at that stage without such impact, but bear in mind that few of us, in our finest moments, come near to Feynman’s level and recall that even he “stooped” to the polaron system to give the path integral one of its most important accomplishments.

Elimination of background oscillator degrees of freedom

Indeed, even today some of the “frontiers” involve the very principle developed by Feynman for the polaron (actually, originally for electrodynamics). That principle is the elimination of an interacting field—whose internal dynamics must be at least approximately harmonic—through explicit functional integration and its replacement by an effective interaction. The most recent large industry based on that technique deal with quantum/dissipation effects in Josephson junctions. At this conference we heard a new application dealing with protons in Niobium as well as extensions of older techniques, for example the treatment of polarons in magnetic fields.

Chemical applications

Now we all know that path integrals have had significant impact on polymer physics (and this too was reviewed here in Bangkok) but it is worth mentioning that there is a big frontier out there that seldom makes it to our conferences. Perhaps the problem is one of scientific sociology or perhaps it’s the sheer mass of the Journal of Chemical Physics, but there is a great deal of path integral activity among chemists that does not reach our ears. Apropos of polymers, I mention work of Berne in which one writes the classical partition function

\[ Z = \int dx_1 \ldots dx_N \exp \left( -\beta K \sum (x_{j+1} - x_j)^2 + \ldots \right) \]  

(1)

As for the polymer case, one is truly interested in the terms of the sum without the limit, in which each term contributes infinitesimally (although taking the limit may at times be expedient). Using Eq. (1), the classical problem becomes a quantum one for beads on a string. I will not go into particular applications here, but refer to a few articles from the chemical literature.

Quantum chaos

Another topic, jointly and enthusiastically explored by both physicists and chemists is quantum chaos. The expansion of Gutzwiller will be known to readers,
but I wish to mention recent work on the time dependent propagator in which the semiclassical approximation turns out to be amazingly accurate. This is a paper of Heller and Tomsovic on the quantum mechanics of the stadium billiard. The boundary value problem fixes phase space regions (essentially coherent states) and, for longish times, tens of thousands of classical paths satisfy the conditions. Despite this, and especially despite the potential mischief arising from caustics, the propagator turns out to be well approximated semiclassically. As indicated in a more detailed analysis of this work, it is not entirely clear that for dynamical systems more realistic than the billiard this correspondence is maintained; nevertheless, this is a surprising and compelling result.

Relativistic propagators and the path decomposition expansion

For several years I have been trumpeting a result named by its authors the "path decomposition expansion," or "PDX." This is a method for (sort of) breaking coordinate space into regions. Instead of the familiar, single time, all coordinate space relation,

$$ G(x, t; y) = \int dz G(x, t - s; z)G(z, s; y) \ , \tag{2} $$

there is a relation involving restricted propagators calculated in only part of coordinate space and summing also over times (that the system last or first entered or left the region of interest). I give only the simplest form: $x, c, y \in \mathcal{R}, y < c < x$

$$ G(x, t; y) = \int_0^t ds G(x, t - s; c) \frac{i\hbar}{2m} \frac{\partial}{\partial z} G^*(z, s; y) \bigg|_{s = c} \tag{3} $$

where $G^*(z, s; y)$ is the propagator for a particle restricted to the region $y < c$. There is now an interesting use of this formula, a use that is in itself the clarification of an old problem. This is a paper of Halliwell and Ortiz. They were puzzled because the composition law for relativistic propagators is more complicated than what appears above in Eq. (2). In particular, it involves derivatives. What they found was that these derivatives arise because the relativistic formula can be phrased as applications of the path decomposition formula. (N.B., the derivative in Eq. (3).) One starts with a path integral with a fifth parameter (a la Feynman) in which particle paths can go forward and backward with respect to physical time. Then one uses (the multidimensional generalization of) Eq. (3) with the intervening surface (generalizing the point "c" above) a spacelike surface separating initial and final events.

A rigorous path integral?

Another frontier of path integration has been recognized as such since the subject came into existence. This is the mathematical problem of defining the path integral. Considerable thought has been put into this and for all I know a successful proposal already been offered. However, if one designs success as the use of the method by someone other than the proposer or the students of the proposer, then this requirement has not yet been met. At this conference a new direction has been suggested by Nakamura using nonstandard analysis. Aspects of this model relate to work of Gaveau, et al. and in that article it was mentioned that because the "imaginary Poisson measure" did not suffer the same problems as the corresponding Feynman/Wiener object, the nonrelativistic limit of Feynman's checkerboard path integral might help in discovering a rigorous form of the path integral. In fact I did not hold out too much hope for this since I knew what the limiting object looked like (the usual nonrelativistic path integral). Perhaps though with nonstandard analysis a more subtle limit can be made. I look forward to hearing more about this.

An exercise

My next topic is not so grandiose as a "frontier," but is an exercise that should be easy, but which I haven't solved. The following question was posed by Ted Jacobson: show the unitarity of the time evolution operator directly from global path summation. From

$$ U(t) = e^{-iHt/\hbar} \ , \ G(x, t; y) = \langle x | U | y \rangle \ , \text{ and } U(t)\dag U(t) = 1 \ , \tag{4} $$

we know that

$$ \int dz G(x, -t; z)G(z, t; y) = \delta(x - y) \tag{5} $$

and

$$ \int dz G^*(z, t; x)G(z, t; y) = \delta(x - y) \tag{6} $$

Therefore the integral of the path integrals must also give a delta function. That is,
\[ \int dz \sum_{\Gamma_1, \Gamma_2} \exp \left( \frac{i}{\hbar} \left[ -S(x_1(\cdot)) + S(x_2(\cdot)) \right] \right) = \delta(z - y) \],

where \( x_1 \in \Gamma_1, x_2 \in \Gamma_2, \) and

\[ \Gamma_1 = \{ \text{paths with } x(0) = x, x(t) = x \} \]
\[ \Gamma_2 = \{ \text{paths with } x(0) = y, x(t) = x \} \]

The exercise is to prove Eq. (7) using global path summation arguments. What I mean to exclude by the word “global” is the writing of both path integrals (in Eq. (7)) in discrete time form. Then the integral over \( z \) would yield a \( \delta \)-function in the infinitesimally near spatial arguments and Eq. (7) would be established by going back to \( \varepsilon \) (= \( t/N \)) at a time.

Relativistic path integral for spin

Finally I wish to recall what I still consider to be a fundamental open question of path integration. This is the providing of a clean, intellectually satisfying relativistic path integral for particles with spin. This may be a foolish and presumptuous question. Foolish because it violates the precept embodied in Fig. 1, and presumptuous because of its implicit rejection of the many ideas that have been offered in this regard (which include by the way some of my own). It may also be true that the project is simply impossible. Part of what I mean by “intellectually satisfying” is a path integral with continuous paths. There are well-known relativistic limitations on the concept of position operator, and the pristine extension of Feynman’s ideas, summing over curves in an ordinary manifold, may implicitly require an unavailable concept of position.

Discussion

In the open discussion that followed the above presentation, Fig. 1 was repeatedly attacked. I took the position that my intent had been provocative and that in that I had clearly been successful.

On a substantive level, Klauder and Kleinert mentioned examples of relativistic path integrals, for example those involving not merely paths but more complicated objects, such as “ribbons.” Others, for example Melek, spoke in favor of the Grassmann approach for the relativistic path integral.

Other discussion, by Adachi, concerned the problems of caustics in the path integral. In the coherent state path integral one is naturally led to a complex classical mechanics in which there are caustics associated with “noncontributing paths” and the associated Stokes phenomena are more difficult to handle than other caustic-related problems I had taken up (and which go away with averaging). It is not clear (to me, at least) whether these difficulties are an artifact of the coherent state representation, or whether even in the usual classical mechanics—where they do not seem to occur—there is some way in which the problem is manifested. An example of how this could occur would be as a result of Fourier transforming, where complex \((t)\) singularities in the classical action might show up. Another issue raised by Adachi was the uniformity of the asymptotic expression that I used in my expansion for caustics. In fact, it is uniform in the sense that (for example) the Airy function is a single analytic object containing two different (lower order) asymptotic objects. However, one can use further coordinate transformations to extend its validity to a larger region. This was done by Levit and Smilansky at about the same time (1970s) that I developed my expression. This, by the way, is an example of the message of Fig. 1. I had done my work in violation of the sentiments I associate with that figure. Under the circumstances, the most you can get is credit for asking a good question. Levit and Smilansky did their work in order to fit experimental data and as a result came out with a greater range of validity. The difference is quantitative rather than qualitative; nevertheless, it’s what it takes to fit the data.

The issue of caustics and quantum chaos also led to the question (asked by this writer) of the caustic structure for the kicked rotator.

Kleinert made a strong case for fluctuating surfaces being a frontier of path integration. Not only is the class of geometric objects richer, but the dominant dynamical term may be different. For example, in studying surfaces connected with red blood cells, the leading term is \( z^2 \), leading to violent fluctuations of biological significance for efficient absorption of Oxygen. The oil-water interface in oil wells was also mentioned for its economic significance with Kleinert alluding to a potential for immediate personal economic significance—with the physicist in the role of consultant.

The subject of surfaces is discussed by the way in an article by Bruinsma in the book of lectures that I mentioned earlier as a general source for “frontier” material.

Papadopolous discussed other boundary specifications for the classical action, in particular he gave the advantages of fixing the spatial end points and varying the time.

Klauder mentioned current activity on quaternionic quantum mechanics and
pointed to associated path integral questions.

The session and the meeting were closed by V. Sa-yakanit.

Acknowledgment

This work was supported in part by NSF grant PHY 90 15558.

References

1. H. Cerdeira, S. Lundqvist, D. Mugnai, A. Ranfagni, V. Sa-yakanit and L.
   S. Schulman, Lectures on Path Integration: Trieste 1991, World Scientific,

2. D. F. Coker and B. J. Berne, Quantum calculations on excess electrons in
disordered media, in Excess Electrons in Dielectric Media, J.-P. Jay-Gerlin
Z. H. Lin, B. J. Berne and G. Martyna, Density Dependence of Excess Elec-
Tuckerman, B. J. Berne and G. J. Martyna, Reversible Multiple Time Scale
Molecular Dynamics, preprint, 1992. W. H. Miller, Semidclassical Methods in
H. Miller, Time Correlation Function and Path Integral Analysis of Quantum
Rate Constants, J. Phys. Chem. 93, 7009 (1989). N. Maki and W. H. Miller,
Exponential power series expansion for the quantum time evolution operator,

3. S. Tomsovic and E. J. Heller, Semiclassical Dynamics of Chaotic Motion:

4. L. S. Schulman, Caustics and the semiclassical propagator for chaotic systems,
in Path Integrals from meV to MeV: Tuzing 1992, H. Grabert, A. Inomata, L.

5. A. Auerbach and S. Kivelson, The Path Decomposition Expansion and Mul-
Tunneling and the Path Decomposition Expansion, in Lectures on Path Inte-
gration: Trieste 1991, H. A. Cerdeira et al., eds., World Scientific, Singapore
(1993).

6. J. J. Halliwell and M. E. Ortiz, Sum-Over-Histories Origin of the Composition

7. T. Nakamura, A nonstandard representation of Feynman's path integrals, J.

8. B. Gaveau, T. Jacobson, M. Kac and L. S. Schulman, Relativistic Extension of
the Analogy between Quantum Mechanics and Brownian Motion, Phys. Rev.

9. S. Levit and U. Smilansky, The Hamiltonian Path Integrals and the Uniform
Fig. 1. Variation on Rodin’s Thinker.