SIX

Doing the Integral: Free Particle and Quadratic Lagrangians

The prescription for evaluating a path integral suggests that the task is formidable, but in some instances the calculation can be done in full.

For a free particle, $V=0$, and $\mathbf{A}=0$. The three-dimensional propagator is simply the product of three one-dimensional propagators, so there is no point in cluttering our equations with vectors. We wish to evaluate

$$\begin{aligned} G(x,t;y) &= \int_{y0}^{xt} dx(\tau)\exp\left[\frac{i}{\hbar}\int_0^t \frac{m}{2}\left(\frac{dx}{d\tau}\right)^2 d\tau\right] \\ &= \lim_{N\to\infty}\left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{(N+1)/2}\int dx_1\cdots dx_N \exp\left[\frac{im}{2\hbar\varepsilon}\sum_{j=0}^{N}(x_{j+1}-x_j)^2\right] \end{aligned} \tag{6.1}$$

(where $x_{N+1}=x$, $x_0=y$ and $\varepsilon=t/(N+1)$). This integral turns out to be easy to do because of the following identity

$$\int_{-\infty}^{\infty} du\sqrt{\frac{a}{\pi}}\, e^{-a(x-u)^2}\sqrt{\frac{b}{\pi}}\, e^{-b(u-y)^2}=\sqrt{\frac{ab}{\pi(a+b)}}\,\exp\left[-\frac{ab}{a+b}(x-y)^2\right] \tag{6.2}$$

This formula is proved by completing the square in the exponential. The fact that the expression can depend only on $(x-y)$ is obvious by a change of variables. Using (6.2) consider the integral on x_1 in (6.1).

Including two of the $(m/2\pi i\hbar\varepsilon)^{1/2}$ factors this is

$$\left(\frac{m}{2\pi i\hbar\varepsilon}\right)\int dx_1 \exp\left[\frac{im}{2\hbar\varepsilon}(x_1-x_0)^2+\frac{im}{2\hbar\varepsilon}(x_2-x_1)^2\right] \tag{6.3}$$

which equals

$$\sqrt{\frac{m}{2\pi i\hbar(2\varepsilon)}}\ \exp\left[\frac{im}{2\hbar(2\varepsilon)}(x_2-x_0)^2\right] \tag{6.4}$$

The effect of the x_1 integration is to change ε to 2ε (both in the square root and in the exponential) and to replace $(x_2-x_1)^2+(x_1-x_0)^2$ by $(x_2-x_0)^2$. The integral over x_2 changes 2ε to 3ε (both in the square root and in the exponential) and yields the term $(x_3-x_0)^2$ in the exponential.

This is continued for all N integrals. The ε becomes $(N+1)\varepsilon$, which is just t, and the distance squared appearing in the exponential becomes $(x_{N+1}-x_0)^2$, which is $(x-y)^2$. There is no longer any N dependence so the limit operation is trivial and we obtain the result

$$G(x,t;y)=\sqrt{\frac{m}{2\pi i\hbar t}}\ \exp\left[\frac{im}{2\hbar t}(x-y)^2\right] \tag{6.5}$$

For a free particle the classical path from $(y,0)$ to (x,t) is

$$x(\tau)=y+\frac{\tau}{t}(x-y) \tag{6.6}$$

The classical action is

$$S=\int_0^t \frac{m}{2}\left(\frac{x-y}{t}\right)^2 d\tau=\frac{m}{2}\frac{(x-y)^2}{t} \tag{6.7}$$

Evidently the phase in (6.5) is just the classical action (divided by $\hbar$), and we find that the classical path gives the exact propagator for a free particle.

The second example to be studied is a quadratic Lagrangian, which includes as special cases the simple harmonic oscillator and the uniform force field. The Lagrangian is

$$L=\tfrac{1}{2}m\dot{x}^2+b(t)x\dot{x}-\tfrac{1}{2}c(t)x^2-e(t)x \tag{6.8}$$

and we wish to evaluate

$$G(x_b,t_b;x_a,t_a)=\int_{x_a t_a}^{x_b t_b} dx(\tau)\exp\left(\frac{i}{\hbar}\int_{t_a}^{t_b} L\,d\tau\right) \tag{6.9}$$

The change of variables that we now perform demands a certain amount of belief in the formal object in (6.9), but since the answer we get in the end can be checked by applying Schrödinger's equation there is no harm done if we proceed optimistically. Let $\bar{x}(t)$ be the solution of the Euler-Lagrange equation

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}}\right)-\frac{\partial L}{\partial x}=0 \tag{6.10}$$

or

$$m\ddot{x}+(c+\dot{b})x+e=0 \tag{6.11}$$

with boundary conditions $x(t_a)=x_a$, $x(t_b)=x_b$. Let

$$y(\tau)=x(\tau)-\bar{x}(\tau) \tag{6.12}$$

be the new "integration variable" in (6.9). The "Jacobian" of this change of variables is 1. What this means is that if (6.9) were written out as a limit, each x_j, would be replaced by $y_j=x_j-\bar{x}(t_j)$, which is just a translation. The action term in (6.9) behaves simply. This is most easily seen by working formally

$$\int L\,dt=S(x(\tau))=S(y(\tau)+\bar{x}(\tau))$$

$$=S(\bar{x}(\tau))+\left.\frac{\delta S}{\delta x}\right|_{\bar{x}}y(\tau)+\frac{1}{2}\left.\frac{\delta^2 S}{\delta x^2}\right|_{\bar{x}}y(\tau)^2 \tag{6.13}$$

The Taylor expansion of S terminates after its second derivative, since S is a quadratic functional. Furthermore, the first derivative term is zero since this is just the definition of $\bar{x}$—the classical path is that for which the first variation of S vanishes. Finally, again because S is quadratic, $\frac{1}{2}\delta^2 S/\delta x^2$ is the same quadratic form as S except that the term that was linear in x does not appear. It follows that

$$S(\bar{x}+y)=S(\bar{x})+\tfrac{1}{2}\delta^2 S y^2 \tag{6.14}$$

$S(\bar{x})$ can be factored out of the path integral over $dy(\tau)$. Taking into account the fact that the boundary conditions for each $y(\tau)$ are

$$y(t_a)=0$$
$$y(t_b)=0 \tag{6.15}$$

[by (6.12)], we obtain

$$G(x_b, t_b; x_a, t_a) = \exp\left[\frac{iS(x_b, t_b; x_a, t_a)}{\hbar}\right]\tilde{G}(0, t_b; 0, t_a) \tag{6.16}$$

where $S(x_b, t_b; x_a, t_a)$ is the action along the classical path $\bar{x}$ from (x_a, t_a) to (x_b, t_b) and $\tilde{G}$ is the Green's function for the Lagrangian $L = \frac{1}{2}m\dot{x}^2 + bx\dot{x} - \frac{1}{2}cx^2$.

Evaluation of the factor $\tilde{G}(0, t_b; 0, t_a)$, a function of time only, gives us the opportunity to do the first respectable integral of the book. Taking the usual definitions we have

$$\tilde{G}(0, t_b; 0, t_a) = \lim_{N\to\infty} \int dy_1 \cdots dy_N \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{(N+1)/2}$$
$$\times \exp\left\{\frac{i}{\hbar}\sum_{j=0}^{N}\left[\frac{m}{2\varepsilon}(y_{j+1} - y_j)^2 - \tfrac{1}{2}\varepsilon c_j y_j^2\right]\right\} \tag{6.17}$$

where $c_j = c(t_j)$, $t_j = t_a + (j/N)(t_b - t_a)$ and where we have dropped the term $bx\dot{x}$ because of its irrelevance in the one-dimensional problem. (In three dimensions an $\mathbf{x}\cdot\dot{\mathbf{x}}$ term has physical consequences and we leave as an exercise the development of the analogue of the results we shall obtain in one dimension.)

To deal with the multitude of integrals in (6.17) we define an N vector η

$$\eta = \begin{bmatrix} y_1 \\ \vdots \\ y_N \end{bmatrix} \tag{6.18}$$

and note that the argument of the exponent in (6.17) can be written

$$-\eta^T \sigma \eta \tag{6.19}$$

where T signifies transpose and σ is the matrix

$$\sigma = \frac{m}{2\varepsilon\hbar i}\begin{bmatrix} 2 & -1 & & & & \\ -1 & 2 & -1 & & & \bigcirc \\ & -1 & 2 & \ddots & & \\ & & & \ddots & & \\ & \bigcirc & & \ddots & 2 & -1 \\ & & & & -1 & 2 \end{bmatrix} + \frac{i\varepsilon}{2\hbar}\begin{bmatrix} c_1 & & \bigcirc \\ & \ddots & \\ \bigcirc & & c_N \end{bmatrix} \tag{6.20}$$

Equation 6.17 can now be concisely written

$$\tilde{G} = \lim_{N\to\infty} \left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{(N+1)/2} \int d^N\eta \exp(-\eta^T\sigma\eta) \tag{6.21}$$

There is a variety of ways to evaluate the integral in (6.21). We use a straightforward approach. Consider

$$\int d^N\eta e^{-\eta^T\sigma\eta} \tag{6.22}$$

where σ is of the form $i\tilde{\sigma}$ with $\tilde{\sigma}$ real and Hermitian. Then σ can be diagonalized by a unitary matrix:

$$\sigma = U^\dagger \sigma_D U \tag{6.23}$$

where σ_D is the diagonal matrix of eigenvalues of σ (call these σ_α) and U is unitary. For real eigenvectors U is also real; let $\zeta = U\eta$. The vector ζ is real and $\{\zeta\}$ is an N dimensional vector space. Note that because $|\det U| = 1$ the Jacobian for going from $d^N\eta$ to $d^N\zeta$ is 1. Therefore

$$\int d^N\eta e^{-\eta^T\sigma\eta} = \int d^N\zeta e^{-\zeta^T\sigma_D\zeta} = \prod_{\alpha=1}^{N} \sqrt{\frac{\pi}{\sigma_\alpha}} = \frac{\pi^{N/2}}{\sqrt{\det\sigma}} \tag{6.24}$$

provided there are no zero eigenvalues. If there are any zero eigenvalues the integral simply does not exist.

The evaluation of $\det\sigma$ proceeds by a well-known technique. Our interest is in

$$\tilde{G}(0,t_b;0,t_a) = \lim_{N\to\infty} \left[\left(\frac{m}{2\pi i\hbar\varepsilon}\right)^{N+1} \frac{\pi^N}{\det\sigma}\right]^{1/2}$$

$$= \lim_{N\to\infty} \left[\frac{m}{2\pi i\hbar} \cdot \frac{1}{\varepsilon} \cdot \frac{1}{\left(\frac{2i\hbar\varepsilon}{m}\right)^N \det\sigma}\right]^{1/2} \tag{6.25}$$

Define f as

$$f(t_b,t_a) = \lim_{N\to\infty} \left[\varepsilon\left(\frac{2i\hbar\varepsilon}{m}\right)^N \det\sigma\right] \tag{6.26}$$

From (6.20) it follows that

$$\left(\frac{2i\hbar\varepsilon}{m}\right)^N \det\sigma = \det\left\{\begin{bmatrix} 2 & -1 & & & \bigcirc \\ -1 & 2 & & & \\ & & \ddots & \ddots & \\ & & \ddots & \ddots & -1 \\ \bigcirc & & & -1 & 2 \end{bmatrix} - \frac{\varepsilon^2}{m}\begin{bmatrix} c_1 & & \bigcirc \\ & \ddots & \\ \bigcirc & & c_N \end{bmatrix}\right\} \equiv \det\sigma'_N \equiv p_N \tag{6.27}$$

where σ'_N is defined to be the matrix in the brackets. We first define truncated $j\times j$ matrices σ'_j—but ε remains $(t_b-t_a)/(N+1)$—that consist of the first j rows and columns of σ'_N and whose determinants are p_j. By expanding σ'_{j+1} in minors, the following recursion formula for the p_j is easy to show:

$$p_{j+1} = \left(2 - \frac{\varepsilon^2}{m}c_{j+1}\right)p_j - p_{j-1}, \qquad j=1,\ldots,N \tag{6.28}$$

where $p_1 = 2 - \varepsilon^2 c_1/m$ and p_0 is defined to be $+1$. When (6.28) is rewritten in the form

$$\frac{p_{j+1}-2p_j+p_{j-1}}{\varepsilon^2} = -\frac{c_{j+1}p_j}{m} \tag{6.29}$$

it becomes evident that p_N will be obtained by solving a differential equation. If we now let

$$\varphi(t) = \varepsilon p_j \tag{6.30}$$

for $t = t_a + j\varepsilon$ we observe that (6.29) implies that in the limit $\varepsilon\to 0$, $\varphi(t)$ satisfies the equation

$$\frac{d^2\varphi}{dt^2} = -\frac{c(t)}{m}\varphi \tag{6.31}$$

The initial values for φ follow from

$$\varphi(0)=\varepsilon p_0 \to 0$$

$$\frac{d\varphi(0)}{dt}=\varepsilon\left(\frac{p_1-p_0}{\varepsilon}\right)=2-\frac{\varepsilon^2}{m}c_1-1\to 1, \qquad \text{as } N\to\infty \tag{6.32}$$

Consequently $f(t_b, t_a)=\varphi(t_b)$ is obtained by solving the differential equation

$$m\frac{\partial^2 f(t,t_a)}{\partial t^2}+c(t)f(t,t_a)=0 \tag{6.33}$$

with the initial conditions

$$f(t_a,t_a)=0, \qquad \frac{\partial f}{\partial t}(t,t_a)\bigg|_{t=t_a}=1 \tag{6.34}$$

We have thus arrived at the following form for the Green's function for the quadratic Lagrangian given in (6.8):

$$G(x_b,t_b;x_a,t_a)=\sqrt{\frac{m}{2\pi i\hbar f(t_b,t_a)}}\,\exp\left[\frac{i}{\hbar}S_c(x_b,t_b;x_a,t_a)\right] \tag{6.35}$$

where S_c is the action along the classical path and f is given by (6.33) and (6.34).

Exercise: Under what circumstance can there be more than one classical path connecting the given end points?

Exercise: Show that (6.5) (the free particle) is a special case of (6.35).

We next specialize the foregoing results to the simple harmonic oscillator. For this system $e(t)\equiv 0$ and $c(t)\equiv m\omega^2=\text{const}$. Equations 6.33 and 6.34 are easily solved to yield

$$f(t_b,t_a)=\frac{\sin\omega T}{\omega} \tag{6.36}$$

where $T=t_b-t_a$. The more tedious job of evaluating $S(x_b, t_b; x_a, t_a)$ along the classical path is left as an exercise.

Exercise: Show that the action along the classical path from (x_a, t_a) to (x_b, t_b), $T=t_b-t_a$, is

$$S(x_b, t_b; x_a, t_a)=\frac{m\omega}{2\sin\omega T}\left[(x_b^2+x_a^2)\cos\omega T-2x_a x_b\right] \tag{6.37}$$

The exact Green's function is therefore

$$G(x_b, t_b; x_a, t_a)=\sqrt{\frac{m\omega}{2\pi i\hbar\sin\omega T}} \times\exp\left\{\frac{im\omega}{2\hbar\sin\omega T}\left[(x_b^2+x_a^2)\cos\omega T-2x_a x_b\right]\right\}. \tag{6.38}$$

The particle in a uniform field is even simpler. The Lagrangian is

$$L=\tfrac{1}{2}m\dot{x}^2-ex \tag{6.39}$$

[so that $e(t)\equiv e=\text{const.}$] and you can easily show that*

$$G(x_b, t_b; x_a, t_a) =\sqrt{\frac{m}{2\pi i\hbar T}}\exp\left\{\frac{i}{\hbar}\left[\frac{m(x_b-x_a)^2}{2T}-\tfrac{1}{2}eT(x_b+x_a)-\frac{e^2T^3}{24m}\right]\right\} \tag{6.40}$$

Finally we quote the result for

$$L=\tfrac{1}{2}m\dot{x}^2-\frac{m\omega^2}{2}x^2-e(t)x \tag{6.41}$$

The function $f(T)$ is the same as that given in (6.36), since the function $e(t)$ has no effect on f, while the classical action is

$$\begin{aligned}S(x_b, t_b; x_a, t_a)=\frac{m\omega}{2\sin\omega T}\Bigg[&(x_b^2+x_a^2)\cos\omega T-2x_a x_b\\ &-\frac{2x_b}{m\omega}\int_{t_a}^{t_b}e(t)\sin\omega(t-t_a)\,dt\\ &-\frac{2x_a}{m\omega}\int_{t_a}^{t_b}e(t)\sin\omega(t_b-t)\,dt\\ &-\frac{2}{m^2\omega^2}\int_{t_a}^{t_b}\int_{t_a}^{t}e(t)e(s)\sin\omega(t_b-t)\sin\omega(s-t_a)\,ds\,dt\Bigg].\end{aligned} \tag{6.42}$$

*Beware of misprints in Feynman and Hibbs, Equation 3-62.

Exercise: Obtain a closed form expression for the (time dependent) Green's function for a charged particle in three dimensions under the following circumstances:

(a) Uniform electric field.

(b) Uniform magnetic field.

NOTES

Methods for handling the quadratic Lagrangian are legion and have been well developed since the earliest work on path integrals. Oddly enough papers on the subject continue to appear and may give some historian of science material for a case history on the nondiffusion of knowledge. Our treatment of the quadratic Lagrangian is similar to those of

I. M. Gelfand and A. M. Yaglom, *J. Math. Phys.* **1**, 48 (1960)

E. W. Montroll, *Commun. Pure and Appl. Math.* **5**, 415 (1952)

There is no shortage of other methods, and any document purporting to be an introduction to path integration will have some derivation of the results.

APPENDIX: EXACTNESS OF THE SUM OVER CLASSICAL PATHS

For all path integrals evaluated above, the result was expressible entirely in terms of the classical path. It turns out that every propagator that anyone has ever been able to evaluate exactly and in closed form is a sum over "classical paths" only. There has even appeared in the literature the claim that *all* propagators are given exactly as a sum over classical paths. Recall that we are discussing the time dependent propagator, so that quantum mechanical tunneling, which is a phenomenon at fixed energy, does not constitute an immediate contradiction to the foregoing claim. Nevertheless, we shall see (Sections 15 and 16) that the propagator near a caustic does not vanish and shall even get an expression for its value in the shadow region—that is, in the region where no classical paths penetrate. This absence of classical paths is not due to a fixing of the energy but is rather a consequence of the focusing effect of the potential responsible for the caustic. Other counterexamples have also been suggested.*

*E. Nelson gave the following counterexample. Let the potential V be zero except in a small region where it is smooth and small. For sufficiently small times and for two points near each other but far from the support of V there is no classical path between these points that "feels" V. Nevertheless, we know that for arbitrarily small times the propagator is influenced by V.

As seen in this section Lagrangians (or Hamiltonians) for which the sum over classical paths is exact include those that are at most quadratic in the coordinate and its derivative. This will also be evident in our development of the WKB method where a quadratic Lagrangian has the special property that the third variation of the action, $\delta^3 S$, and all higher variations, are automatically zero.

Another situation leading to the exact sum over classical paths is where the particle is confined in a simple geometry by perfectly reflecting walls. A trivial example of this is the free particle confined to the positive x axis (ignore y and z) by a potential $V(x) = +\infty$ for $x<0$. The propagator is

$$G(b,T;a,0) = \sqrt{\frac{1}{2\pi i T}}\left[e^{i(b-a)^2/2T} - e^{i(b+a)^2/2T}\right] \tag{6.43}$$

where we have taken $\hbar = m = 1$ for convenience. See the discussion following (9.38) for a proof of this assertion. Now the two terms in (6.43) can be associated with the two classical paths from a to b in time T: one direct path with action $(b-a)^2/2T$ and one reflected path with action $(b+a)^2/2T$. The only difficulty from the path integral point of view is the minus sign for the reflected path. If a turning point were involved, a relative phase of $\pi/2$ might appear, but there is no way for a phase of π to occur in one dimension. There is an *ad hoc* way to put in the sign, a way that has been employed in the more difficult problem of an obstacle in two or three dimensions. One pastes another copy of the positive real axis onto the existing one, calculates the classical path to the image of the final point in the new space ignoring what transpires where they are attached (in higher dimensions there is a creep wave), and adds the propagators associated with the two images of the final point. The relative sign with which they are taken is determined by the boundary condition at the obstacle. For vanishing wave function the two contributions must be subtracted. If one desired vanishing derivative of the wave function, the terms would be added.

This rule, while correct, is an embarrassment to the purist so long as it has not been derived in a purely path integral context. In the sum over paths the only change that has occurred is that integrals of the form

$$\int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_N$$

have had the range of integration restricted to $x_i > 0$, $i = 1, \ldots, N$. It is not clear if this is enough to recover the correct form easily, since for any given mesh in time there may be ranges in x for which one needs both direct and reflected paths even for the "infinitesimal" propagator.

Despite the foregoing "embarrassment" the propagator does involve classical paths only. It is thus likely that the propagator is given exactly by such a sum in those geometries for which the "method of images" works in electrodynamics. In both cases one uses special properties of the geometry to satisfy the boundary conditions.

There is another, more subtle, situation where the sum over classical paths is exact. This is for Green's functions for free motion on the group manifolds of Lie groups. This was first found to be true for $SU(2)$ and at the time conjectured to hold for the larger class. Subsequently, Dowker proved the result for a large class of group manifolds. However, the exactness of the sum is not generally true for homogeneous spaces such as $S^2 = SU(2)/U(1)$. Further discussion of curved space path integrals is given in Section 24. Here we only wish to remark that while other examples of exact sums may seem in a sense trivial, the curved space path integral with its plethora of $g_{\mu\nu}$'s and curvature terms looks anything but. Of course that may only mean that one simply needs the right coordinates to make the group manifold path integral look trivial too. It may also be possible to define harmonic oscillator like potentials on group manifolds and obtain closed form Green's functions for them.

Finally we refer the reader to Section 31 for remarks on systems with solition modes and global invariants and on the possibility that such systems might yield exact semiclassical "approximations."

Notes

An expression for the propagator in terms of classical paths only appears in

M. Clutton-Brock, *Proc. Camb. Phil. Soc.* **61**, 201 (1965)

The Green's function in the presence of a reflecting obstacle has been calculated by

V. S. Buslaev, in *Topics in Mathematical Physics*, Sh. Birman, Ed., Consultants Bureau, New York, 1967, p. 67

Exactness of the sum over classical paths for $SU(2)$ is shown in

L. S. Schulman, *Phys. Rev.* **176**, 1558 (1968)

and for Lie group manifolds by

J. S. Dowker, *J. Phys. A* **3**, 451 (1970)

J. S. Dowker, *Ann. Phys.* **62**, 561 (1971)