Dynamic programming and path integrals

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Abstract – **Dynamic programming gives a new method for computing the wave function in quantum mechanics. The paper compares this method with Feynman's path integral method.**

1 Introduction

As in earlier publications [1-5], Schrödinger's equation can be obtained from the variational principle

$$\underset{\tilde{v},\tilde{p}}{\delta}\,\mathcal{E}\int_t^{t_f}\left[\tilde{p}\tilde{v}-\tilde{H}(q,\tilde{p},\tau)\right]d\tau=0,\ dq=\tilde{v}dt+ndz \tag{1}$$

This is given here for a single particle in one dimension and the notation is defined in the Appendix. Bellman's equation [6] is

$$\underset{\tilde{v},\tilde{p}}{\text{stat}}\left\{\frac{\partial\tilde{W}}{\partial t}+\tilde{v}\frac{\partial\tilde{W}}{\partial q}-\frac{i\hbar}{2m}\frac{\partial^2\tilde{W}}{\partial q^2}+\tilde{p}\tilde{v}-\tilde{H}\right\}=0 \tag{2}$$

where the 'cost' $\tilde{W}(q,t)$ is the stationary expected value of the integral in (1); $\tilde{W}$ here has the opposite sign to the one that would be expected because t is at the lower limit of integration in (1). Because n in (1) is complex, the variables $\tilde{p}$, $\tilde{v}$, etc. become complex, which is indicated where necessary by the tilde. From (2) we obtain

$$\tilde{p}=-\frac{\partial\tilde{W}}{\partial q},\quad \tilde{v}=\frac{\partial\tilde{H}}{\partial\tilde{p}},\quad \frac{\partial\tilde{W}}{\partial t}=\frac{i\hbar}{2m}\frac{\partial^2\tilde{W}}{\partial q^2}+\tilde{H} \tag{3}$$

and with $\tilde{W}=i\hbar\log\psi$, $\tilde{\mathcal{H}}=\partial\tilde{W}/\partial t$,

$$\tilde{\mathcal{H}}\psi=i\hbar\frac{\partial\psi}{\partial t}=\left[\frac{\hat{p}^2}{2m}+\tilde{V}\right]\psi=\hat{H}\psi \tag{4}$$

which is Schrödinger's equation extended by analytical continuation from real x to complex q.

We have therefore embedded the orthodox theory, of complex functions on a real space, in a theory of complex functions on a complex space. The variable q can no longer give the position of the particle, and we say that it defines the position of a 'complex image'. To revert to the orthodox theory we make the following postulate:
If the expected value of some property (such as momentum $\tilde{p}$ or energy $\tilde{\mathcal{H}}$) of the complex images in an ensemble has the real value α on the real axis, then α is the value of the corresponding property of the physical particles.

Thus if α is a real constant and we have $\tilde{\mathcal{H}}=\psi^{-1}\hat{H}\psi=\alpha$, then $\hat{H}\psi=\alpha\psi$ which can be satisfied only if α is an eigenvalue of the operator $\hat{H}$ and ψ is a corresponding eigenvector. Similarly for the momentum, $\tilde{p}=\psi^{-1}\hat{p}\psi=\alpha$ gives $\hat{p}\psi=\alpha\psi$, and we can follow the same procedure for x if we introduce an operator $\hat{x}$ by $x=\psi^{-1}\hat{x}\psi=\alpha$, giving $\hat{x}\psi=\alpha\psi$, for which the eigenfunctions are $\psi=\delta(x-\alpha)$.

2 Discrete-time formulation

Bellman's functional equation, which gives rise to (2), is

$$\tilde{W}(q,t)=\underset{\tilde{v}}{\text{stat}}\,\mathcal{E}\left\{\tilde{L}(q,\tilde{v},t)dt+\tilde{W}(q+dq,t+dt)\right\} \tag{5}$$

where we have used $\tilde{p}\tilde{v}-\tilde{H}=\tilde{L}$, and from (5) we can obtain a discrete-time approximation to the solution of (4). The natural boundary condition at t_f is a function $\tilde{W}(q_f,t_f)$, which could be given numerically or algebraically. As a special case, we can choose a penalty function at t_f which forces all trajectories to end in the vicinity of some point Q at t_f. More simply, as below, only trajectories ending at Q may be included in the calculation. This is done for comparison with path integrals: it introduces a difficulty, which is well-known in control theory, because $\tilde{v}$ then tends to infinity at t_f.

As an example, consider a free particle moving from x at t to x_f at t_f. The classical action W has $\partial^2W/\partial x^2$ independent of x, whence as in §4 below it follows that the optimal trajectory for the particle lies on the real axis. Numbering time intervals backwards from $t_f=t_0$ to $t=t_N$ as in Figure 1 we consider trajectories that terminate at (x_0,t_0). At t_2 we choose x_2, and then v_2 as a candidate for the optimal velocity at (x_2,t_2). We consider the time intervals t_0-t_1, t_1-t_2, both of these being short enough to allow their squares to be neglected. The Lagrangian for the free particle is $\tilde{L}=m\tilde{v}^2/2$, and we write $\xi=x_2+v_2(t_1-t_2)$ so that choice of ξ is equivalent to choice of (real) v_2, and then approximate to $\tilde{W}_2$ at (x_2,t_2) by

$$\tilde{W}_2=\underset{\xi}{\text{stat}}\,\mathcal{E}\left\{\frac{m(\xi-x_2)^2}{2(t_1-t_2)}+\frac{m(x_0-\xi-nz)^2}{2(t_0-t_1)}\right\} \tag{6}$$

$$=\underset{\xi}{\text{stat}}\int_{-\infty}^{\infty}\left\{\frac{m(\xi-x_2)^2}{2(t_1-t_2)}+\frac{m(x_0-\xi)^2}{2(t_0-t_1)}-\frac{i\hbar z^2}{2}\left[\frac{1}{t_0-t_1}\right]\right\}P(z)dz$$

The probability density is $P(z)=\left[2\pi(t_1-t_2)\right]^{-1/2}\exp\left[-z^2/2(t_1-t_2)\right]$, giving $\mathcal{E}z^2=(t_1-t_2)$, and differentiating with respect to ξ for optimality we have

$$\frac{\xi - x_2}{t_1 - t_2} = \frac{x_0 - \xi}{t_0 - t_1} \tag{7}$$

so that the optimal v on the two intervals is the same, and is equal to $(x_0 - x_2)/(t_0 - t_2)$, giving

$$\tilde{W}_2 = \frac{m(x_0 - x_2)^2}{2(t_0 - t_2)} - \frac{i\hbar}{2}\left[\frac{t_1 - t_2}{t_0 - t_1}\right] \tag{8}$$

In the same way, extending $\tilde{W}_2$ by analytic continuation to complex q,

$$\tilde{W}_3 = \underset{\xi}{\text{stat}}\, \mathcal{E}\left\{\frac{m(\xi - x_3)^2}{2(t_2 - t_3)} + \tilde{W}_2(\xi + nz, t_2)\right\}$$
$$= \frac{m(x_0 - x_3)^2}{2(t_0 - t_3)} - \frac{i\hbar}{2}\left[\frac{t_1 - t_2}{t_0 - t_1} + \frac{t_2 - t_3}{t_0 - t_2}\right] \tag{9}$$

and by induction

$$\tilde{W}_N = \frac{m(x_0 - x_N)^2}{2(t_0 - t_N)} - \frac{i\hbar}{2}\left[\sum_{j=1}^{N-1}\frac{t_j - t_{j+1}}{t_0 - t_j}\right] \tag{10}$$

which approximates to

$$\tilde{W}(x, t; x_f, t_f) = \frac{m(x_f - x)^2}{2(t_f - t)} - \frac{i\hbar}{2}\int_t^{t_f}\frac{d\tau}{t_f - \tau} \tag{11}$$

where both limits of integration are now shown in $\tilde{W}$.

Neglecting the upper limit of integration in (11), which is justified in §4 below, we then have for the kernel (propagator, Green's function) $K = \exp(\tilde{W}/i\hbar)$

$$K(x, t; x_f, t_f) = \alpha(t_f - t)^{-1/2} \exp\left[\frac{m(x_f - x)^2}{2i\hbar(t_f - t)}\right] \tag{12}$$

where α is a normalising constant. This expression can be extended to the complex plane by analytical continuation. It will be seen from (12) that $|K|$, which determines the particle density, arises from the complex trajectories which accompany the real optimal trajectory.

3 Path integration

By path integration here we mean the computational procedure suggested originally by Feynman [7], not the later development described, for example, by Schulman [8]. The basis of the procedure is to consider the passage of a particle from a fixed point x_2 at t_2 to a second fixed point x_0 at t_0. At x_2, since the position is known, the velocity is undetermined. Then at an intermediate time t_1, the particle will be found with equal probability at any point x_1 on the real axis. Assigning the contribution $\exp(W/i\hbar)$ to K along any path, where W is the classical action for the path, the contributions are summed over all possible paths. This calculation can be iterated backwards in time, as in §2, to give a comparison with dynamic programming. In place of (6) we then have for the free particle, on summing over all possible (real) paths from x_2 to x_0,

$$K_2 = \exp(\tilde{W}/i\hbar) = \int_{-\infty}^{\infty}\exp\left[\frac{m(\xi - x_2)^2}{2i\hbar(t_1 - t_2)} + \frac{m(x_0 - \xi)^2}{2i\hbar(t_0 - t_1)}\right]d\xi \tag{13}$$

subject to a correction given below. The result is

$$K_2 = \alpha\left[\frac{t_0 - t_2}{(t_0 - t_1)(t_1 - t_2)}\right]^{-1/2} \exp\left[\frac{m(x_0 - x_2)^2}{2i\hbar(t_0 - t_2)}\right] \tag{14}$$

where α is a constant. This calculation gives $K_3, K_4, \ldots K_N$ as in §2.

The result in (14) is clearly incorrect: t_1 has not been eliminated, and if all the time intervals are made equal to ε, K_N has a multiplier ε^N. To correct (14), it is only necessary to associate multipliers $(t_0 - t_1)^{-1/2}$ and $(t_1 - t_2)^{-1/2}$ with paths from t_1 to t_0 and t_2 to t_1 respectively. These multipliers do not arise directly from the path integral formulation, but have to be supplied by other means: "This seems to be characteristic of various methods for doing path integrals; a great deal can be worked out by some general methods, but often a multiplying factor is not fully determined" [7, pp.60-61].

4 Real optimal trajectory

In the path integral procedure there is a tacit assumption that on the real axis the velocity, and therefore also the momentum, is real. Then on putting $\tilde{W} = S + i\hbar R$, with S and R real when q is real, we have

$$\tilde{p} = -\frac{\partial}{\partial x}(S + i\hbar R), \qquad \frac{\partial R}{\partial x} = 0, \tag{15}$$

Taking real and imaginary parts in (3)

$$\frac{\partial S}{\partial t} = \frac{1}{2m}\left(-\frac{\partial S}{\partial x}\right)^2 + V \tag{16}$$

$$\frac{\partial R}{\partial t} = \frac{1}{2m}\frac{\partial^2 S}{\partial x^2} \tag{17}$$

Equation (16) is the equation obtained for the classical action W on putting $n = 0$ in (1). If the boundary conditions are the same (and are necessarily real) we can therefore identify S with W. Also, from (15), R is a function only of t, and so also is the function on the right-hand side of (17), and

$$R = \frac{1}{2m}\int\frac{\partial^2 W(x, t)}{\partial x^2}dt + \beta \tag{18}$$

where β is a constant. We therefore obtain for the quantum mechanical system

$$\tilde{W} = S + i\hbar R = W + \frac{i\hbar}{2m}\int\frac{\partial^2 W(x, t; x_f, t_f)}{\partial x^2}dt + i\hbar\beta \tag{19}$$

so that if $\tilde{v}(q, t)$ is real for real q, $\tilde{W}$ is given by (19). When the boundary conditions x and x_f on the integral in

(1) are real, to say that $\tilde{v}(q,t)$ is real for real q is the same as saying that the optimal trajectory $q(t)$ is real.

Conversely, if some classical system makes the integrand in (18) independent of x, there exists a quantum mechanical system satisfying (1) with the same boundary conditions and with $\tilde{v}(q,t)$ real for real q, and for this system $\tilde{W}$ is given by (19). For on substituting this $\tilde{W}$ in (3) we have

$$\frac{\partial \tilde{W}}{\partial t} - \frac{i\hbar}{2m}\frac{\partial^2 \tilde{W}}{\partial x^2} - \tilde{H}$$
$$= \frac{\partial W}{\partial t} + \frac{i\hbar}{2m}\frac{\partial^2 W}{\partial x^2} - \frac{i\hbar}{2}\frac{\partial^2 W}{\partial x^2} - H = 0 \qquad (20)$$

since in $\tilde{H}$, $\tilde{p}$ is equal to p.

There may, however, be other quantum mechanical systems corresponding to the classical system just considered. For example the classical oscillator has

$$W = \frac{m\omega}{2\sin\omega(t_f - t)}\left[\left(x_f^2 + x^2\right)\cos\omega(t_f - t) - 2x_f x\right] \qquad (21)$$

with

$$\frac{1}{m}\frac{\partial^2 W}{\partial x^2} = \omega\cot\omega(t_f - t) \qquad (22)$$

independent of x. It therefore has an associated quantum mechanical system with

$$\tilde{W} = W + \frac{i\hbar}{2}\int \omega\cot\omega(t_f - t)\,dt$$
$$= W - \frac{i\hbar}{2}\log\sin\omega(t_f - t) + i\hbar\beta \qquad (23)$$

giving

$$K = \exp\left(\tilde{W}/i\hbar\right) = \alpha\left[\sin\omega(t_f - t)\right]^{-1/2}\exp\left(W/i\hbar\right) \qquad (24)$$

where α is a normalising constant. This system has $\tilde{v}$ real on the real axis, but there is in addition an infinite set of solutions of (1) having energy $\omega\hbar/2, 3\omega\hbar/2, \ldots$, and with $\tilde{v}$ pure imaginary on the real axis.

5 Complex optimal trajectory

The quantum oscillator in the ground state has

$$\tilde{L} = m\tilde{v}^2/2 - m\omega^2 q^2/2, \psi = \exp\left(-m\omega q^2/2\hbar - i\omega t/2\right)$$
$$\tilde{W} = i\hbar\log\psi = -im\omega q^2/2 + \hbar\omega t/2$$
$$\tilde{v} = -\left(\partial\tilde{W}/\partial q\right)/m = i\omega q \qquad (25)$$

so that the optimal velocity is not in general real and the optimal trajectories are $q(t) = r\exp(i\omega t)$ with r constant. There is now no fixed terminal point for the trajectories, and the end condition at t_f is supplied by a given $\tilde{W}(q_f, t_f)$.

Using the notation of Figure 1 we put $\tilde{W}_0 = -im\omega q_0^2/2 + \hbar\omega t_0/2$ as in (25), and following the procedure in §2 we have

$$\tilde{W}_1 = \operatorname*{stat}_{\zeta}\mathcal{E}\left\{\frac{m(\zeta - q_1)^2}{2(t_0 - t_1)} - \frac{m\omega^2 q_1^2(t_0 - t_1)}{2} + \tilde{W}_0(\zeta + nz, t_0)\right\}$$
$$= \operatorname*{stat}_{\zeta}\left\{\frac{m(\zeta - q_1)^2}{2(t_0 - t_1)} - \frac{im\omega}{2}\left[\zeta^2 + n^2(t_0 - t_1)\right]\right\}$$
$$- \frac{m\omega^2 q_1^2(t_0 - t_1)}{2} + \frac{\hbar\omega t_0}{2} \qquad (26)$$

and for the stationary value

$$\frac{\partial\tilde{W}_1}{\partial\zeta} = \frac{m(\zeta - q_1)}{t_0 - t_1} - im\omega\zeta = 0$$

$$\zeta = q_0 = \frac{q_1}{1 - i\omega(t_0 - t_1)} \approx q_1\left[1 + i\omega(t_0 - t_1)\right] \qquad (27)$$

to first order. Then substituting this last expression for the optimal ζ in (26) and simplifying we have, again to first order,

$$\tilde{W}_1 \approx -i\omega q_1^2/2 + \hbar\omega t_1/2 \qquad (28)$$

Equation (28) agrees with (25), and (27) gives

$$\tilde{v}_1 = (q_0 - q_1)/(t_0 - t_1) \approx i\omega q_1 \qquad (29)$$

also as in (25). Iteration of the stagewise calculation will therefore generate an approximation to the solution of (1) along an optimal trajectory with the given end condition. This is to be expected, because the procedure in §2 is (with appropriate modifications for complex variable) a standard method for approximating to the solution of (1).

The above calculation verifies the procedure in §2 for the example (25), but since $\tilde{W}_0$ was given algebraically no new information is obtained. If on the other hand $\tilde{W}_0$ were given as a numerical function of q at t_0, the calculation would no longer be empty, and it would generate the function $\tilde{W}$ at earlier times.

The path integral method proceeds differently [7, p.57] by first computing K and then using the formula

$$\psi(x,t) = \int_{-\infty}^{\infty} K(x,t;x_0,t_0)\psi(x_0,t_0)\,dx_0 \qquad (30)$$

This is not easy to evaluate directly, but can be solved by indirect methods [7, pp.200-201]. Whereas (26) leads to the evaluation of $\tilde{W}$, and hence ψ, along an optimal trajectory, (30) describes the evolution of ψ on the real axis.

6 Comparison of the methods

When the optimal trajectory is real, as in §2 and §3, There is a close resemblance between certain aspects of the dynamic programming and the path integral procedures, though in some other respects they differ strongly. When the optimal trajectory is complex, on the other hand, as in §5, the two methods have nothing in common. Both methods, in principle, have the same scope in providing a solution of Schrödinger's equation. Path integration, in its later form [8], is extensively developed and widely employed. Dynamic programming, at least in its real-variable form, has long been used in control theory as a way of obtaining solutions of stochastic variational problems such as (1). We therefore seem to have two valid methods of solution with no apparent way of relating one to the other.

The two methods depend in fact on two different consequences of the variational principle (1). Path integration relies upon the linearity of Schrödinger's equation. Dynamic programming relies upon the direction of causal influence in time, which ensures that an optimal (future) cost can be defined at a given q and t, regardless of how this state was reached. The two different procedures that result can lead to the same conclusion in two apparently irreconcilable forms.

For example, the result in (19) gives

$$K = \alpha\left\{\exp\frac{1}{2m}\int\frac{\partial^2 W\left(x,t;x_f,t_f\right)}{\partial x^2}dt\right\}\exp(W/i\hbar) \qquad (31)$$

which can be compared with the van Vleck formula [8], valid under the same conditions,

$$K = \alpha\left[-\frac{\partial^2 W\left(x,t;x_f t_f\right)}{\partial x\,\partial x_f}\right]^{1/2}\exp(W/i\hbar) \qquad (32)$$

where α in each equation is available for normalisation. The two formulae are entirely different in form, and one cannot be derived from the other. Yet when applied to K satisfying the appropriate conditions both give the same result, as can be seen from (12) and (24). The conclusion to which one is led is that there is some deeper mathematical structure underlying these results.

7 Discussion

The development given above has been limited to a single particle in one dimension. This was done so that important features should not be obscured by details, but there is no serious difficulty in generalising to any number of particles in three dimensions [3,4]. The Hamiltonian is assumed to have the form

$$H(x,p,t) = \frac{1}{2}\sum_{j,k=1}^{3n} h_{j,k}(x,t)p_j p_k + \sum_{j=1}^{3n} h_j(x,t)p_j + h_0(x,t) \qquad (33)$$

and the development from (1) to (4) follows straightforwardly [cf. 2,3].

The use of dynamic programming could result in new methods of calculation, though the chief development so far is to illuminate the connection between quantum and classical mechanics and to show how phenomena such as interference can be explained [4].

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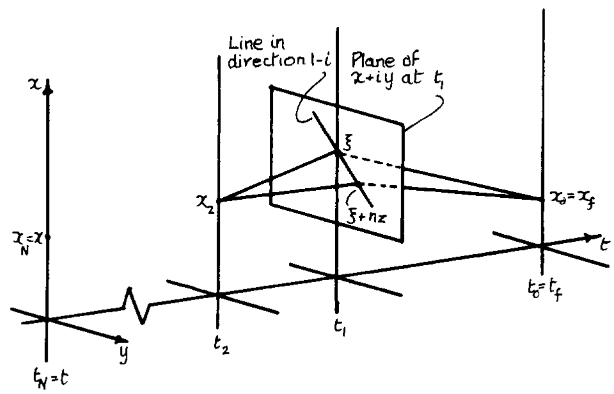

Figure 1 Optimal trajectory for a free particle
From x_2 at t_2 a tentative choice of velocity v_2 gives $\xi = x_2 + v_2(t_1 - t_2)$. This tentative trajectory is perturbed by noise to give points such as $\xi + nz$, where z has probability density $P(z) = \left[2\pi(t_1 - t_2)\right]^{-1/2}\exp\left[-z^2/2(t_1 - t_2)\right]$. Integrating the contribution to $\tilde{W}$ from the two intervals for all z we obtain the value of $\tilde{W}$ at (x_2,t_2) on the assumption that the velocity at (x_2,t_2) is $(\xi - x_2)/(t_1 - t_2)$. Then we seek a stationary value of $\tilde{W}_2$ with respect to ξ. This is the required $\tilde{W}_2$, and the optimal v_2 is obtained at the same time. Once $\tilde{W}_2$ has been obtained for a suitable set of points x_2 (or has been obtained as an explicit function of x_2 and t_2) the procedure can be iterated to give $\tilde{W}_3, \tilde{W}_4$, etc.

Appendix Notation

The symbols and definitions given here are those that apply in the theory derived from (1). Those accompanied by * do not appear in the standard treatment of quantum mechanics. Those which do appear in the standard treatment (for example $\hat{p}$) are shown as functions of q arising from (1), though in the standard theory they appear as functions of the real variable x.

$\mathcal{E}$:– expectation taken over an ensemble

$\hbar = h/2\pi$:– where h is Planck's constant

$H(x,p,t) = \partial W/\partial t$:– classical Hamiltonian expression for the energy, in which p and x are independent variables; but when derived from W on an optimal trajectory p becomes a function of x and t

* $\widetilde{H}(q,\widetilde{p},t)$:– obtained by substituting $q, \widetilde{p}$ for x, p in $H(x,p,t)$; not equal to the energy

* $\mathfrak{H}(q,\widetilde{p},t) = \partial\widetilde{W}/\partial t$:– q.m. energy

$\hat{H}(q,\hat{p},t)$:– q.m. energy operator, obtained by substituting $q, \hat{p}$ for x, p in $H(x,p,t)$

$L(x,v,t) = pv - H$:– classical Lagrangian

* $\widetilde{L}(q,\widetilde{v},t) = \widetilde{p}\widetilde{v} - \widetilde{H}$:– q.m. Lagrangian

m :– mass

$n^2 = -i\hbar/m$:– n is coefficient of noise process

$p = -\partial W/\partial x$:– classical momentum

* $\widetilde{p} = -\partial\widetilde{W}/\partial q$:– q.m. momentum

$\hat{p} = -i\hbar\partial/\partial q$:– q.m. momentum operator

$v = \partial H/\partial p$:– classical velocity

* $\widetilde{v} = \partial\widetilde{H}/\partial\widetilde{p}$:– q.m. velocity

$V(x,t)$:– classical potential energy

* $\widetilde{V}(q,t)$:– obtained by substituting q for x in $V(x,t)$

* $\widetilde{W}$:– q.m. action integral as in (1)

z :– Gaussian noise process

$\psi = \exp(\widetilde{W}/i\hbar)$:– wave function satisfying Schrödinger's equation

* $\underset{\widetilde{v},\widetilde{p}}{\text{stat}}$:– stationary value obtained by varying the functions $\widetilde{v}$, $\widetilde{p}$

* $\underset{\widetilde{v},\widetilde{p}}{\delta}$:– variation of the succeeding expression with respect to $\widetilde{v}$, $\widetilde{p}$