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Dynamic Programming and Quantum Mechanical Motion

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Abstract—In this article we show that quantum dynamics is the most natural generalization of classical dynamics from the point of view of optimal control. Employing the techniques of dynamic programming, we derive the Schrödinger equation starting from the Lagrangian defined in terms of Nelson's forward and backward velocities. The generalization to the relativistic case is also analyzed and the Klein Gordon Equation is similarly derived.

1. INTRODUCTION

From the optimal point of view, quantum dynamics is the most natural generalization of classical mechanical laws of motion given rise to by the Hamilton-Jacobi equations. This can be easily extended to a stochastic control system [1]. The usual method in classical and quantum physics is to take the Lagrangian of the deterministic or stochastic system and use a variational method to arrive at the solution [2]. In control theory, a quadratic cost function involving the control variable is formulated and it is minimized over all the control vectors. However, the initialization of dynamic programming by Bellman *et al.* [3–5] brought a sea-change in the methods of solution of control problems. This refers to a multistage decision process analytically more tractable and computationally simpler. The advantage of this formulation is to reduce the dimensions of the process to the proper level, i.e., to the dimensions of the decision policy that confronts one at each stage. Mostly we have an initial value problem situation unlike in the case of the Euler equations, and this method has the mathematical property that monotonicity of convergence is assured and is well suited for applications involving approximations in policy space. The principle of optimality states that whatever the initial state and initial conditions are, the remaining decisions must constitute an optimal policy with regard to the state resulting from the first decision. Hence we arrive at functional equations or iterative discrete equations at each stage. In the next section, we will deal with deterministic motion and the corresponding Hamilton-Jacobi equation.

2. DETERMINISTIC CONTROL

Let a dynamical system move under the control equation

$$\dot{x} = f(t, x, u), \tag{1}$$

where $x \in R^n$ is the position of the system, $u \in \mathcal{U}$ a parameter, and f a sufficiently smooth function. Equation (1) is a well-defined differential equation, and its solution x_u is called the

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trajectory relevant to the control vector $u(t)$. Let the system be connected with a criterion function $J(t_0, x_0, u)$ depending upon a control function u and initial conditions t_0 and x_0 of the trajectory. The control function $u(t)$ is found out such that the boundary conditions are fulfilled and it minimizes $J(t_0, x_0, u)$ and this process is called the deterministic optimal control:

$$-S(x,t) = \min_{u \in \mathcal{U}} J(t,x,u). \tag{2}$$

$u_{t,x}$ denotes the set of all possible $u(t)$, the control functions, such that trajectories $x_u(t)$ equal x at the initial moment t. Let us assume the control function f in equation (1) is u itself, i.e., $\dot{x} = u$, the criterion function is given by

$$J(t,x,u) = \int_t^{t_1} L(t', x(t'), u(t'))\, dt', \tag{3}$$

where L is the Lagrangian. $L(t,x,u) = (1/2)mu^2 - V(t,x)$ so that the dynamic programming principle leads to (assuming $S(;t_1) = 0$)

$$\begin{aligned} S(x,t) &= S(x + u\Delta, t + \Delta) - L(t,x,u)\Delta \\ &= S(x,t) + \frac{\partial S}{\partial t}\Delta + \frac{\partial S}{\partial x}u\Delta - \left(\frac{1}{2}mu^2 - V(t,x)\right)\Delta. \end{aligned} \tag{4}$$

Minimization with respect to u gives

$$\frac{\partial S}{\partial x} - mu = 0. \tag{5a}$$

Hence

$$u = u^* = \frac{1}{m}\frac{\partial S}{\partial x}. \tag{5b}$$

Inserting the minimizing value of $u = (1/m)\frac{\partial S}{\partial x}$ in equation (4), we obtain the Hamilton-Jacobi equation for the deterministic motion:

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 + V(x,t) = 0. \tag{5}$$

Determination of the principal function S solves the entire motion [6]. Equation (5) shows that Lagrangian mechanics of classical motion is a section of deterministic optimal control by dynamic programming method [7].

3. H-J EQUATIONS OF QUANTUM MECHANICS BY DYNAMIC PROGRAMMING TECHNIQUE

We will now investigate the possible connection between quantum mechanics and stochastic control theory. The foundations of quantum probability theory have been initiated and analyzed by various authors. This progress was initiated by Nelson's [8] famous Langevin equations of Brownian motion and deriving the Schrödinger equation, therefore preserving the nondissipative structure of quantum mechanical equations. Using both of these equations, the programming equations have some kind of hyperbolic behaviour with no essential dissipation involved. Along with the continuity equation, these are equivalent to the Schrödinger equation. Variational methods in stochastic mechanics have led to stimulating results [9,10]. As a generalization of the deterministic control equation (1), we have for the stochastic case the following:

$$\dot{x} = f(x,t,u) + \sqrt{\frac{\hbar}{m}}\, dW. \tag{6}$$

The criterion function in the stochastic case is

$$J(t,x,u) = E_{t,x}\int_t^{t_1} L(t',x(t'),u(t'))\,dt', \tag{7}$$

where $E_{t,x}$ represents expectation with initial conditions x at t. Also Nelson's equation for the Brownian motion corresponding to quantum motion is

$$\dot{\mathrm{x}} = b_+(x,t) + \sqrt{\frac{\hbar}{m}}\,dW_+, \tag{8}$$

b_+ is like the drift velocity u in the classical dynamics. Also to preserve time invariance, Nelson added the time reversed equation

$$\dot{\mathrm{x}} = b_-(x,t) + \sqrt{\frac{\hbar}{m}}\,dW_-. \tag{9}$$

The $dW_+ = dW_-$ is the white noise driving force. $L(t,x,v)$ is the canonical one given by

$$L = \frac{1}{2}mv^2 - V(x). \tag{10}$$

But for the stochastic equations defined by equations (8) and (9) used for deriving the Schrödinger equation, we take

$$J = E_{t,x}\int\left[\frac{1}{2}mb_+(t')b_-(t') - V(x,t')\right]dt', \tag{11}$$

where expectation is given by

$$J = \int dx'\int_t^{t_1} dt'\left[\frac{1}{2}mb_+(x',t')b_-(x',t') - V(x',t')\right]\rho(x',t'), \tag{12}$$

and the principal function or the phase function is $S(x,t)$ given by

$$-S(x,t) = \min J(x,t,b_\pm). \tag{13}$$

The Langrangian in equation (11) is a departure from the usual expressions, the kinetic energy is the product of b_+, the forward, and b_-, the backward velocities. This feature introduced by Guerra and Morato [11] is the key factor for deriving the Hamilton-Jacobi equation for quantum motion. For the two stochastic Langevin equations (8) and (9), the Ito differential can be written down [12] easily—D_+ and D_-, the forward and backward total derivatives for any function $F(x,t)$ of the stochastic variable x as

$$D_+F = \frac{\partial F}{\partial t} + b_+\frac{\partial F}{\partial x} + \frac{\hbar^2}{2m}\nabla^2 F, \tag{14}$$

$$D_-F = \frac{\partial F}{\partial t} + b_-\frac{\partial F}{\partial x} - \frac{\hbar^2}{2m}\nabla^2 F. \tag{15}$$

Let us now write the J functional as

$$J = \int_t^{t_1} dt'\int\left[\frac{1}{2}mb_+(x',t')b_-(x',t') - V(x',t')\right]\rho(x',t')\,dx'. \tag{16}$$

Let us ignore the contribution at the upper limit t_1 and rewrite the integral for the term containing b_+ and b_- as

$$\begin{aligned}
J_+ &= \int\int_t^{t_1}\left[\frac{1}{2}mb_+\left(b_+ - \frac{\hbar}{m}\frac{\nabla\rho}{\rho}\right)\right]\rho(x',t')\,dx'\,dt' \\
&= \int dx'\int_t^{t_1} dt'\left[\frac{1}{2}mb_+^2 - \frac{1}{2}\hbar b_+\frac{\nabla\rho}{\rho}\right]\rho \\
&= \int\int_t^{t_1} dt'\left[\frac{1}{2}mb_+^2 dx' + \frac{1}{2}\hbar\partial b_+\right]\rho \qquad \text{by partial integration} \qquad (17)\\
&= \int\int_t^{t_1} dt'\left[\frac{1}{2}mb_-^2 dx' - \frac{1}{2}\hbar\partial b_-\right]\rho, \qquad (18)
\end{aligned}$$

where we have used the expressions for the total drift velocity

$$v = \frac{1}{2}(b_+ + b_-),$$

and the osmotic velocity

$$u = \frac{1}{2}(b_+ - b_-) = \frac{\hbar}{m}\frac{\nabla\rho}{\rho}$$

(from the forward and backward Fokker Plank equations). All the implementations necessary for the dynamic programming method of obtaining equations for S and the principal function are at hand. Since

$$\min_{b_\pm \in B} S(x + b_\pm\Delta, t + \Delta) - \min_{b_\pm \in B}\left[\int L(x', t', b_\pm)\, dx'\rho(x', t')\right]\Delta$$
$$= S(x,t) + \min_{b_\pm \in B} D_\pm S(x,t) - \min_{b_\pm \in B}\int_t^{t+\Delta} L_+(x', b'_\pm, t')\rho(x', t')\, dx'. \quad (19)$$

Since we are putting the initial condition as $x = x(t)$ at t, $\rho(x', t' = t)$ is unity. Hence at the initial instant, the integral is simply $L(x, b_\pm(x', t), t)\Delta$. We have by dynamic programming the following equations:

$$\min_{b_\pm \in B} D_+ S(x,t) - \min_{b_\pm \in B}\frac{1}{2}mb_+^2 - \frac{1}{2}\hbar\frac{\partial b_+}{\partial x} = 0 \quad (20)$$

and

$$\min_{b_\pm \in B} D_- S(x,t) - \min_{b_\pm \in B}\frac{1}{2}mb_-^2 + \frac{1}{2}\hbar\frac{\partial b_-}{\partial x} = 0. \quad (21)$$

We also know that $(1/2)(b_+ + b_-) = v$ and $u = (1/2)(b_+ - b_-)$. Hence $b_+ = u + v$ and $b_- = v - u$, and we have used equations (14), (15), (20), and (21),

$$DS = \frac{1}{2}(D_+ + D_-)S = \frac{\partial S}{\partial t} + v\frac{\partial S}{\partial x} - \frac{1}{2}m(u+v)^2 - \frac{\hbar}{2}\frac{\partial u}{\partial x} - \frac{1}{2}m(v-u)^2. \quad (22)$$

This yields

$$\min_v\left[\frac{\partial S}{\partial t} + v\frac{\partial S}{\partial x} - \frac{1}{2}mv^2 - \frac{1}{2}mu^2 - \frac{\hbar}{2}\frac{\partial u}{\partial x}\right] - V(x) = 0. \quad (23)$$

This minimization yields the first condition

$$\frac{\partial S}{\partial x} - mv = 0, \qquad \text{i.e., } v = \frac{1}{m}\frac{\partial S}{\partial x}. \quad (24)$$

We know that if $\rho(x,t)$, the density, is expressed as e^{2R} and the wave function $\psi = e^R e^{-is/\hbar}$, then

$$v = \frac{1}{m}\frac{\partial S}{\partial x} \quad \text{and} \quad u = \frac{\hbar}{m}\frac{\partial R}{\partial x}. \quad (25)$$

Therefore, substituting equation (25) in equation (23) we obtain the Hamilton-Jacobi equation in Nelson's method

$$\frac{\partial S}{\partial t} + \frac{1}{2m}\left(\frac{\partial S}{\partial x}\right)^2 - \frac{\hbar^2}{2m}\left(\frac{\partial R}{\partial x}\right)^2 - \frac{\hbar}{2m}\frac{\partial^2 R}{\partial x^2} + V(x) = 0. \quad (26)$$

The terms with $\hbar^2$ are Q, the quantum potential or the modification of the classical Hamilton-Jacobi equation due to quantum mechanics [8]. Of course, in the pathwise variational method of Marato, additional terms are introduced to compensate for the variations at the upper end, since even if the end conditions are given at one end, the end conditions at the other end may not get fixed due to the stochasticity entering the problem. This is necessary in variational calculus. We have ignored this in our method. The Ito equations (8) and (9) will lead to the forward and backward Fokker Plank equations which when added will give the continuity equation

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial x}(v\rho). \quad (27)$$

The Hamilton-Jacobi equation (26) and the continuity equation (27) as it is well known are a nonlinearization map of the Schrödinger equation with potential $V(x)$ and a solution of type $\psi = e^R e^{-iS/\hbar}$.

4. RELATIVISTIC GENERALIZATION OF QUANTUM MOTION [13]

To arrive at the relativistic quantum behaviour by extending Nelson's stochastic mechanics [8], we consider a single scalar particle performing diffusion in spacetime. Because of the demand of relativistic covariance, we write the position $x^\mu(\tau)$ in Minkowski spacetime as a function of τ, the proper time (i.e.) in $M^{(4)}$, and $\tau \in R$, $x^\mu = (x^0 = ct, \overline{x})$. The usual definition of Markov property is generalized. Considering the events in $x^\mu(\tau^i)$, we have $E_{\tau'<\tau}; E_\tau; E_{\tau'>\tau}$ and the associated conditional expectations. The Markov property tells us that the future ($\tau' > \tau$) and the past ($\tau' < \tau$) are independent if the present $\tau' = \tau$ is known. However, this is not a correct statement. Let us take a three-dimensional "surface" σ in M^4 and $A_\sigma^\pm$, the regions of M^4 representing the future and past in ordinary time t, with respect to σ. Thus, the probability space of $x^\mu(\tau)$, the σ-algebra $\in_A$ with $X \in A$, and $\tau \in R$ is analyzed. $\in_A$ is controlled by looking at parts of the trajectories in A, i.e., by making physical measurements. Introducing conditional expectations $E_\sigma, E_\sigma^\pm$, the Markov property is

$$E_\sigma^+ E_\sigma^- = E_\sigma^- E_\sigma^+ = E_\sigma, \tag{28}$$

as enunciated by Ruggiero and Guerra [14,15]. In simpler words, $A_\sigma^\pm$ are regions in M^4 in future (+) and the past (−) and Markov disconnection is limited by the light cone. If $x^\mu(\tau)$ is the random process with evolution parameter $\tau \in R$ with invariant density $\rho(x,\tau)$ which has to be accounted for, the displacements Δx along the trajectories are invariantly characterized by the time-like or space-like nature. This later property does not conflict with relativity if creation and annihilation of pairs are admitted. Physical observables are defined in terms of combined expectation values given by equation (29) given below. This brings out the essential nonlocal character of the theory. This approach yields, by means of a stochastic variational principle, a Schrödinger-like equation with proper time dependence. The displacements Δx along the trajectories are characterized by

$$\Delta^\pm x^\mu = \pm[x^\mu(\tau \pm \Delta\tau) - x^\mu(\tau)], \qquad \Delta\tau > 0. \tag{29}$$

Let us use the conditional expectations to define forward and backward velocities $b_\pm(x,\tau)$:

$$E\left[\frac{\Delta^\pm x^\mu}{\Delta\tau} \mid x(\tau) = x,\ (\Delta^\pm x)^2 \geq 0\right] + E\left[\frac{\Delta^\mp x^\mu}{\Delta\tau} \mid x(\tau) = x,\ (\Delta^\mp x)^2 \leq 0\right] \to b_\pm^\mu. \tag{30}$$

The above expression contains both time-like and space-like contributions signifying nonlocal character of relativistic quantum mechanics. b_{+i}^μ and b_{+s}^μ are related to propagation of particle and antiparticle [16,17]. It is well known that the equation of motion in the classical relativistic mechanics for a charge e moving under a field F_ν^μ is

$$m\frac{dx^\mu}{d\tau^2} = \frac{e}{c}F_\nu^\mu \frac{dx^\mu}{d\tau}, \tag{31}$$

and the invariant Lagrangian is given by

$$\mathcal{L} = \frac{1}{2}mg_{\mu\nu}\dot{x}^\mu\dot{x}^\nu - \frac{e}{c}g_{\mu\nu}\dot{x}^\mu\phi^\nu, \tag{32}$$

$g_{\mu\nu}$ is the diagonal metric $(1,-1,-1,-1)$, $\mu,\nu = 0,1,2,3$. $F_{\mu\nu} = \partial_\mu\phi_\nu - \partial\nu\phi\mu$ and $\dot{x}^\mu = \frac{dx^\mu}{d\tau}$. For the random process $x^\mu(\tau)$, the invariant scalar density $\rho(x,\tau)$, $x \in M^4$, is obtained and $x^\mu(\tau)$ is assumed to transform as a vector under Lorentz transformation. Also

$$E\left[\left(\frac{\Delta^\pm x^\mu \Delta^\pm x^\nu}{\Delta\tau} \mid x(\tau) = x,\ (\Delta^\pm x)^2 \geq 0\right) - \left(\frac{\Delta^\mp x^\mu \Delta^\mp x^\nu}{\Delta\tau} \mid x(\tau) = x,\ (\Delta^\mp x)^2 \leq 0\right)\right] \to \frac{\hbar}{m}g^{\mu\nu}. \tag{33}$$

Forgetting the free term in equation (31), let us write the relativistic Lagrangian similar to the earlier expression in Section 2, according to the insight developed by Morato and Guerra [11,18]. Also we define $v^\mu = (1/2)(b_+^\mu + b_-^\mu)$ and the osmotic velocity

$$u^\mu = \frac{1}{2}(b_+^\mu - b_-^\mu) = \frac{\hbar}{2m}\partial_\mu \log \rho. \tag{34}$$

According to Guerra and Ruggiero [14,15], we can define the forward and backward Ito derivatives [12] for the relativistic case as

$$D_\pm F(x,\tau) = \left[\frac{\partial}{\partial\tau} + b_\pm^\mu \partial_\mu \pm \frac{\hbar}{2m}\Box\right] F(x,\tau), \tag{35}$$

F being a function of the random variable x at τ:

$$DF = \frac{1}{2}(D_+ + D_-)F = \left(\frac{\partial}{\partial\tau} + v_\mu \partial^\mu\right) F. \tag{36}$$

The cost function A is obtained from the relativistic Lagrangian [19] for free motion

$$\mathcal{L} = \frac{m}{2} b_+^\mu(x,\tau) b_-^\nu(x,\tau), \tag{37}$$

and the cost function in the relativistic case

$$\begin{aligned} A &= \int_\tau^{\tau_1} E[\mathcal{L}(x(\tau'),\tau')]\, d\tau' \\ &= \int dx' \int_\tau^{\tau_1} d\tau' \mathcal{L}(x'(\tau),\tau')\rho(x',\tau'). \end{aligned} \tag{38}$$

Hence, as we did in the last section, A can be written as

$$A_+ = \iint \mathcal{L}_+(x',\tau')\rho(x',\tau')\, dx'\, d\tau',$$

for initial conditions $x(\tau) = x$ at τ and the condition at the end of τ is ignored:

$$\mathcal{L}_+(x,\tau) = \frac{1}{2}\left(b_{+\mu} b_+^\mu - \frac{\hbar}{m}\partial_\mu b_+^\mu\right), \tag{39}$$

$$\mathcal{L}_-(x,\tau) = \frac{1}{2}\left(b_{-\mu} b_-^\mu + \frac{\hbar}{m}\partial_\mu b_-^\mu\right). \tag{40}$$

By the dynamic programming principle explained in the last section

$$\min_\nu DS = \min_\nu \frac{1}{2}(D_+ + D_-) + \frac{1}{2}(L_+ + L_-) = 0. \tag{41}$$

Since $DS = (\frac{\partial}{\partial\tau} + v_\mu\partial^\mu)S$, we easily obtain the required result as a consequence of minimization that

$$v^\mu = -\frac{1}{m}\partial_\mu S,$$

and hence the Hamilton-Jacobi equation becomes for the relativistic case

$$m^2c^2 + \partial_\mu S \partial^\mu S - \left(\hbar^2 \partial_\mu P \partial^\mu P + \hbar^2 \Box P\right) = 0. \tag{42}$$

Herein, we have introduced the substitution for $S(x,\tau)$ as given by Feynman as [19]

$$S(x,\tau) = S(x) - \frac{1}{2}mc^2\tau. \tag{43}$$

For the case in which a charged particle is moving in an electromagnetic field, the Lagrangian is to be taken as

$$\mathcal{L} = \frac{1}{2} m b_+^\mu(x,\tau) b_-^\mu(x,\tau) - \frac{e}{c} D_s x^\mu \phi^\nu. \tag{44}$$

Instead of the first term as in equation (37), we add a second term $-(e/c)v^\mu\phi^\nu$. In minimizing v^μ, we obtain the minimized value of $\nu^\mu = -(1/m)\partial_\mu(S - (e/c)\phi)$. In other words,

$$v^\mu - \frac{e}{c}\frac{\phi}{m} = -\frac{1}{m}\partial_\mu S. \tag{45}$$

Also we can see that the equation of continuity reads as

$$\frac{\partial \rho}{\partial \tau} + \partial_\mu(\rho v^\mu) = 0. \tag{46}$$

If we take $\psi(x,\tau) = \exp(-(imc^2/2\hbar)\tau)\phi(x)$, we will obtain

$$\Box\phi - \frac{m^2c^2}{\hbar}\phi = 0. \tag{47}$$

We have derived the Hamilton-Jacobi equation for the relativistic Schrödinger evolution equation and consequently the Klein Gordon equation for a given eigenvalue of the mass.

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