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Quantum mechanics, control theory and quantum control

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This paper provides a brief review of Rosenbrock's recent work on generating quantum mechanics using dynamic programming, some background knowledge of quantum mechanics and some general issues and problems in developing feedback quantum control.

Key words: control theory; quantum control; quantum mechanics.

1. Introduction

Rosenbrock influenced the entire control research community by his multi-variable frequency domain design method in the early 1980s. We have no intention in this review paper of describing his significant contribution to control theory and control design. Rather, we pay attention to some of his recent works on developing quantum mechanics using control theory, in particular, the dynamic programming and variational principle. Published in this issue includes one of his latest papers on this topic, co-authored by the first author of this paper. We devote this paper to review some of Rosenbrock's works in this area. Rosenbrock used 'Doing quantum mechanics with control theory' for his paper (Rosenbrock, 2000). We may take a few key words out of this title to form 'Quantum control theory', which may not be directly related to Rosenbrock's results in his paper. However, quantum control theory has surely attracted tremendous attention in the control community nowadays. In this paper, we will also touch on some results on this side of the story.

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This paper starts with the introduction of Schrödinger's equation for quantum mechanics in the form shown in any standard textbooks. Then we will briefly review Rosenborck's method of generating quantum mechanics using dynamic programming, and some differences between his quantum mechanics and the standard theory. We then move to discuss general issues of quantum control, starting from measurement, then observability, and further problems in feedback control. In the end, we use dynamic programming again to formulate optimal control for quantum systems with a classical control objective function rather than generating quantum dynamics.

2. Schrödinger's equation

Quantum mechanics is one of the major achievements in physics in the 20th century. The theory started from Planck's observation in 1900 of electromagnetic radiation, and he explained the radiation energy in discrete quanta:

$$E = h\nu \tag{1}$$

where E is the radiation energy, h is a universal constant which is now called Planck's constant, and ν is the radiation frequency. It was then recognized that the radiation sometimes behaves like wave motion, and sometimes like quanta. Discrete energy levels were also observed for electrons in atomic systems. In 1924, de Broglie suggested that matter also has a dual character, and he suggested the following relation between the momentum p and the wavelength h

$$\lambda = \frac{h}{p} \tag{2}$$

His supposition was soon supported by many experimental observations, such as the diffraction of electrons by crystals. This relation between the momentum and wavelength suggests that a wave function may be used to describe localized particles and quanta. As suggested in Schiff (1968), this wave function, $\psi(x, y, z, t)$, which depends in space co-ordinates and time, should have three basic properties, namely, (1) it should be able to interfere with itself; (2) it has a large amplitude where the particle is likely to be; and (3) it should be able to describe the behaviour of single particle such as quanta, rather than its statistical distribution.

Consider the one-dimensional case. We re-write the above two equations as

$$p = \hbar k \tag{3}$$

$$E = \hbar\omega \tag{4}$$

where $k = 2\pi/\lambda$ and $\omega = 2\pi\nu$. A particle with completely undetermined position travelling along x direction with momentum p and energy E is expected to be described by one of the following forms

$$\cos(kx - \omega t),\ \sin(kx - \omega t), e^{i(kx-\omega t)}, e^{-i(kx-\omega t)} \tag{5}$$

A differential equation having one of the above forms as a solution can be easily found. In addition to this, one would require the equation to be linear so that superposition is allowed for wave interference. Another requirement is that the equation should not contain the energy, frequency, or momentum of the particle. For example, if we look at the well-known one-dimensional wave equation

$$\frac{\partial^2 \psi}{\partial t^2} = \gamma \frac{\partial^2 \psi}{\partial x^2} \tag{6}$$

Substituting any of the four forms in Equation (5), it can be obtained that

$$\gamma = \frac{\omega^2}{k^2} = \frac{E^2}{p^2} = \frac{p^2}{2m} \tag{7}$$

This implies that the following equation

$$\frac{\partial^2 \psi}{\partial t^2} = \frac{p^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \tag{8}$$

has all the four forms in (5) as its solutions. However, the above equation contains the momentum p, and therefore it does not satisfy the requirements stated earlier. Noting that

$$E = \frac{p^2}{2m} \tag{9}$$

we have

$$\frac{\omega}{k^2} = \frac{E\hbar}{p^2} = \frac{\hbar}{2m} \tag{10}$$

which only contains the mass of the particle. This suggests that we need a differential equation with a first-order derivative to time and a second-order derivative to x, ie,

$$\frac{\partial \psi}{\partial t} = \gamma \frac{\partial^2 \psi}{\partial x^2} \tag{11}$$

The first and second forms in (5) do not satisfy the above equation. However, the third wave function (ie, $\psi = e^{i(kx-\omega t)}$) does satisfy. Indeed, if $\psi = e^{i(kx-\omega t)}$ is substituted into (11), it can be formulated that

$$\gamma = \frac{i\omega}{k^2} = \frac{iE\hbar}{p^2} = \frac{i\hbar}{2m} \tag{12}$$

which gives the following wave equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \tag{13}$$

This is the one-dimensional Schrödinger's equation for a free particle. Considering a potential energy $V(x, t)$, Schrödinger's equation can then be written as

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi \tag{14}$$

The wave function does not contain the physical parameters such as momentum and energy directly. Thus the standard quantum mechanics has interpretive postulates that each dynamic variable relating to the motion can be represented by a differential operator. For example, the operator for energy is $\hat{E} := i\hbar\partial/\partial t$ and the operator for momentum is $\hat{p} := -i\hbar\partial/\partial x$. If the wave equation is normalized as follows

$$\int \psi^*\psi \, \mathrm{d}x = 1 \tag{15}$$

then it can be interpreted as a probability function. The expected values, denoted by $\langle \cdot \rangle$, can be obtained to give

$$\begin{aligned} \langle E \rangle &= \int \psi^* \hat{E}\psi \, \mathrm{d}x = \int \psi^* \left(i\hbar\frac{\partial}{\partial t}\right)\psi \, \mathrm{d}x = i\hbar \int \psi^* \frac{\partial\psi}{\partial t}\mathrm{d}x \\ \langle p \rangle &= \int \psi^* \hat{p}\psi \, \mathrm{d}x = \int \psi^*(-i, hbar\frac{\partial}{\partial x})\psi \, \mathrm{d}x = -i\hbar \int \psi^* \frac{\partial\psi}{\partial x} \, \mathrm{d}x \end{aligned} \tag{16}$$

The one-dimensional equation can be extended to three-dimensional case with inclusion of forces as

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V(r, t)\psi \tag{17}$$

where r is the position vector, and V denotes the force field.

3. Doing quantum mechanics with control theory

Bellman's dynamic programming is well known to the control community. He has shown how the classic mechanics can be obtained from Hamilton's principle by dynamic programming (Bellman and Dreyfus, 1962). The main theme of Rosenbrock's recent works is to show how quantum mechanics can be obtained using a dynamic program and Hamilton's principle by injecting imaginary noises in the system. Rosenbrock started on this topic of doing quantum mechanics with control theory, or precisely, with the Hamilton principle and Hamilton Jacobian equation, in the 1980s, as shown in his publication in 1985 (Rosenbrock, 1985). Subsequently, he published a number of papers on this topic on various journals (Rosenbrock, 1985, 1986a,b,c, 1995, 1999, 2000). Among them, the best known to the control community is perhaps his paper published in 2000 in *IEEE Transactions on Automatic Control*, which is a mainstream control journal (Rosenbrock, 2000).

For classic mechanics, if $H(x, p, t)$ is the Hamiltonian of a particle with position x and momentum p, the Lagrangian of this particle is given by

$$L(x, p, t) = pv - H(x, p, t) \tag{18}$$

where $v = \mathrm{d}x/\mathrm{d}t$. From the expression $H = pv - L$, we have

$$v = \frac{\partial H}{\partial p} \tag{19}$$

The Hamilton principle can then be stated as

$$\delta_{v,p} \int_t^{t_f} L(x, p, \tau)\,\mathrm{d}\tau = \delta_{v,p} \int_t^{t_f} [pv - H(x, p, \tau)]\,\mathrm{d}\tau = 0 \tag{20}$$

Let $W(x, t)$ denote the optimal value of the integral; we have the Bellman's equation

$$\mathrm{stat}_{v,p}\left[\frac{\mathrm{d}W}{\mathrm{d}t} + pv - H\right] = \mathrm{stat}_{v,p}\left[\frac{\partial W}{\partial t} + v\frac{\partial W}{\partial x} + pv - H\right] = 0 \tag{21}$$

From this equation, immediately we have

$$p = -\frac{\partial W}{\partial x} \tag{22}$$

$$H = \frac{\partial W}{\partial t} \tag{23}$$

Furthermore, from the first equation, we have

$$\frac{\mathrm{d}p}{\mathrm{d}t} = -\left[\frac{\partial^2 W}{\partial x \partial t} + v\frac{\partial^2 W}{\partial x^2}\right] = -\left[\frac{\partial H}{\partial x} - \frac{\partial H}{\partial p}\frac{\partial p}{\partial x}\right] \tag{24}$$

Thus if we regard x and p in $H(x, p, t)$ as independent variables, we have

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \frac{\partial H}{\partial p} \tag{25}$$

$$\frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial H}{\partial x} \tag{26}$$

which are the classic Hamilton's equation.

To inject noise in the system to generate quantum mechanics, the co-ordinate x is replaced by a complex variable $\tilde{x}$, and v in (20) is replaced by $\mathrm{d}\tilde{x} = \tilde{v}\,\mathrm{d}\tau + n\,\mathrm{d}z$, where z is a normalized Wiener process and n is a complex number with $n^2 = -i\hbar h/m$. In this case, Equation (20) is replaced by

$$\delta_{\tilde{v},\tilde{p}} \mathrm{E}\left\{\int_t^{t_f} [\tilde{p}\tilde{v} - \tilde{H}(\tilde{x}, \tilde{p}, \tau)]\,\mathrm{d}\tau\right\} = 0 \tag{27}$$

where E denotes the expectation. Then from dynamic programming, we have

$$
\begin{aligned}
0 &= \mathrm{stat}^{\tilde{v},\tilde{p}}\{\tilde{p}\tilde{v} - \tilde{H} + \mathrm{E}\{\mathrm{d}\tilde{W}\}\} \\
&= \mathrm{stat}_{\tilde{v},\tilde{p}}\left\{\tilde{p}\tilde{v} - \tilde{H} + \frac{\partial \tilde{W}}{\partial t} + \tilde{v}\frac{\partial \tilde{W}}{\partial \tilde{x}} + \frac{n^2}{2}\frac{\partial^2 \tilde{W}}{\partial \tilde{x}^2}\right\}\mathrm{d}t
\end{aligned}
\tag{28}
$$

where $\tilde{W}(\tilde{x}, t)$ denotes the integral value of the stationary solution of (27). To obtain the second equation, we have used $E\mathrm{d}z = 0$, $E\mathrm{d}z^2 = \mathrm{d}t$ and $E(\tilde{v}\,\mathrm{d}t^2 + 2\tilde{v}\mathrm{d}tnh\,\mathrm{d}z + n^2\mathrm{d}z^2) = n^2\,\mathrm{d}t$, with the last property being obtained by taking up to the first order of $\mathrm{d}t$. Similarly to the classic case, we have, from (28),

$$
\frac{\partial \tilde{W}}{\partial \tilde{x}} = -\tilde{p} \tag{29}
$$

$$
\frac{\partial \tilde{W}}{\partial t} = -\frac{n^2}{2}\frac{\partial^2 W}{\partial \tilde{x}^2} + \tilde{H} \tag{30}
$$

Therefore, there is an additional term in the second equation related to the injection of noise. From the second equation, we can obtain Schrödinger's equation. The Hamiltonian for a particle can be written as $H = (p^2/2m) + \mathrm{V}$, where V is the potential energy. Hence we can write

$$
\tilde{H} = \frac{\tilde{p}^2}{2m} + \tilde{V} \tag{31}
$$

Substituting into (30), we have

$$
\frac{\partial \tilde{W}}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \tilde{W}}{\partial \tilde{x}^2} + \frac{\tilde{p}^2}{2m} + \tilde{V} \tag{32}
$$

Let $\tilde{W} = \mathrm{i}\hbar \log \psi$. A direct calculation gives

$$
\frac{\partial \tilde{W}}{\partial t} = i\hbar\psi^{-1}\frac{\partial \psi}{\partial t} \tag{33}
$$

$$
\frac{\partial \tilde{W}}{\partial \tilde{x}} = i\hbar\psi^{-1}\frac{\partial \psi}{\partial \tilde{x}} \tag{34}
$$

and

$$
\begin{aligned}
i\hbar\frac{\partial^2 \tilde{W}}{\partial \tilde{x}^2} &= i\hbar\left[-i\hbar\psi^{-2}\left(\frac{\partial \psi}{\partial \tilde{x}}\right)^2 + i\hbar\psi^{-1}\frac{\partial^2 \psi}{\partial \tilde{x}^2}\right] \\
&= -\left(i\hbar\psi^{-1}\frac{\partial \psi}{\partial \tilde{x}}\right)^2 + \psi^{-1}\left(i\hbar\frac{\partial}{\partial \tilde{x}}\right)^2\psi \\
&= -\tilde{p}^2 - \hbar^2\psi^{-1}\frac{\partial^2 \psi}{\partial \tilde{x}^2}
\end{aligned}
\tag{35}
$$

Substituting the above three equations into Equation (32), we have

$$\psi^{-1} i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \psi^{-1} \frac{\partial^2 \psi}{\partial \tilde{x}^2} + \tilde{V}\psi \tag{36}$$

which gives Schrödinger's equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial \tilde{x}^2} + \tilde{V}\psi \tag{37}$$

Comparing this equation with the one in the standard theory (14), the difference is that the standard theory describes a complex wave equation on a real space, while Equation (37) describes a complex wave equation over a complex domain. The variable $\tilde{x}$ can no longer give the position of the particle. Some postulates are needed to interpret dynamic variables. The postulate proposed in Rosenbrock's paper (Rosenbrock, 2000) is that if the expected value of some property (such as momentum and energy) of the complex image in an ensemble has a real value α on the real axis, then α is the value of the corresponding property of the physical particle. For example, with the operator $\hat{p} = -i\hbar(\partial/\partial \tilde{x})$, we have

$$\tilde{p} = -\frac{\partial \tilde{W}}{\partial x} = \psi^{-1} \hat{p} \psi \tag{38}$$

If we have $\tilde{p} = \alpha$, a real value, then we would say the momentum of the partial is α. In fact, in this case, we have

$$\hat{p}\psi = \alpha\psi \tag{39}$$

which implies that α is an eigenvalue of operator $\tilde{p}$. This is similar to the standard theory that eigenvalue of an operator corresponding to the physical parameter, such as energy eigenvalue in the standard theory in Schiff (1968). There are interpretations of the variables used in the derivation of quantum mechanics, which are detailed in Rosenbrock's recent publications. Other properties such as path integral can also be evaluated using the quantum mechanics derived from the disturbed dynamic programming method. As shown in the paper published in this issue (Rosenbrock and Ding, 2007), the path integral is also independent of the intermediate points, which agrees with the feature established in the standard theory.

Of course, re-establishing the results obtained in the standard quantum mechanics is not the only objective of Rosenbrock's recent work. His aim would be to expect that the alternative way of generating quantum mechanics would give a better description to such features that are not well explained in the standard theory. Just considering the amount of effort devoted in the standard theory of quantum mechanics, Resenbrock realized that it would take a long time to achieve this. It might be worthwhile pursuing this alternative way of generating quantum mechanics.

4. Quantum control

In the previous section, we briefly reviewed how to generate quantum mechanics using classical control theory. Control theory has been successfully applied to macro systems governed by classical mechanics. How do we apply control to micro systems governed by quantum mechanics? In this section, we briefly review and discuss a few issues in control of quantum systems or quantum control.

There has been success in quantum control of a few special cases using control theory, such as optimal control. However, it is very difficult to apply existing control theory to control quantum systems in general, and the difficulty is at least partially due to the quantum measurement, as the quantum measurement has a capacity to disturb the system under estimation. Therefore, the development of quantum control theory requires optimizing over measured strategy, which is not necessary for classical control in general.

With the advance of recent experimental methods, individual quantum systems may be manipulated fast enough on the time scales of the system evolution and it is therefore possible to consider controlling such systems in real time using feedback (Wiseman and Milburn, 1993; Wiseman, 1994). Under feedback control, the dynamics of a system are manipulated using the information of the system obtained through measurement. The objective is usually to maintain a desired state or dynamics in the presence of disturbance. Of course, the main issue of feedback control theory is the development of algorithms to achieve this objective. A fully developed quantum control theory should consider the quantum mechanics of the system and the back action caused by measurement. If we are to apply the concepts and methods of feedback control theory to quantum dynamical systems, we not only need to extend classical control concepts to new regimes but we also need to analyse quantum measurement in a way that is useful for control systems.

A major theoretical challenge of extending feedback control to the quantum mechanical regime is to describe properly the back action of measurement on the evolution of individual quantum systems. With development of the formalism of quantum measurement, in particular the formalism of continuous observation, it is now possible to ask the question of how to deal with the back action caused by the measurement. In fact, the formulation that results from this theory is sufficiently similar to that of classical control theory that the experience gained there provides valuable insights into the problem. The field of quantum-limited feedback was introduced by Wiseman and Milburn (Wiseman and Milburn, 1993; Wiseman, 1994), who considered the instantaneous feedback of some measured photocurrent onto the dynamics of a quantum system. However, there are also important differences that render the quantum problem potentially more complex.

The differences between classical and quantum measurements profoundly affect the design of feedback control algorithms. A classical controller extracts as much information from the system as possible, while in quantum control, irreducible disturbances are inherent to any measurement, and therefore the measurement strategy becomes a significant part of the feedback algorithm. For example, just as the inputs to the system change with time, the measurements too may need to be varied with time so that the best control can be achieved.

4.1 Inherent noise in quantum feedback control

Measurement disturbs a quantum system through the following intrinsic property of quantum mechanics: obtaining accurate knowledge about one observable of a quantum system necessarily limits the information about an observable conjugate to the first. For example, particle position and momentum are conjugate observables, and the uncertainties inherent in the knowledge of both are codified by the famous Heisenberg uncertainty relation. If a chosen feedback control strategy involves measurement, one must take into account the effects of the measurement on the evolution of the quantum system.

A generally applicable model for including those effects is that of a continuous quantum measurement. This model was developed for quantum optics (Carmichael, 1993), a field in which such measurements have been implemented experimentally. Its theoretical footing has also been established in the mathematical physics literature with the help of more abstract reasoning (Barchielli, 1993).

Quantum measurements may introduce unwanted noises in three different ways.

Firstly, one may measure an observable conjugate to the real variable of interest and thereby introduce more uncertainty in the latter variable. More generally, one may attempt to obtain information inconsistent with the state under control. For example, to preserve a state that is the superposition of two position states, position measurements must be avoided because they will destroy the superposition. Thus, in quantum mechanics, the type of measurement chosen must be consistent with the control objectives. This condition is not a problem in classical feedback control.

Secondly, when trying to control the values of observables (Doherty *et al*., 2000), one must consider that the time evolutions of different observables necessarily affect each other over time. Observables whose values are uncertain at one time will cause other observables (perhaps more accurately known) to become uncertain at a later time. For example, a very accurate measurement of the particle position at one time introduces uncertainty into the value of the particle momentum. Because the value of momentum determines the position of the particle at a later time, the momentum uncertainty makes the future position of the particle more uncertain, hence introduces noise into the quantity that is being measured. This mechanism for introducing noise is usually referred to as the back action of a quantum measurement.

Finally, there is randomness of the measurement results. Because the state of the observed system after a measurement depends upon the outcome of the measurement, the more the result fluctuates, the more noise there is in the evolution of the system. For classical measurements, fluctuations in measurement results cannot be any more than the entropy of the system before measurement, ie, the measurement does not introduce any additional noise into the system. In quantum mechanics, however, even if the system state is known precisely, one can still make measurements that change the state in a random way, thereby actually injecting noise into the system. This observation is particularly relevant when the overall state of the system, rather than a specific observable, is being controlled. The situation is further complicated by the fact that, for certain classes of measurements, there is actually a trade-off between the noise injected by the measurement and the information gained by the observer (Doherty *et al*., 2001). As a result, designing measurement strategies is far from being a trivial activity.

4.2 Observability

Observability and controllability are two key concepts in classical control theory, and here we would like to discuss ways in which they may be extended to the quantum domain (Doherty *et al*., 2000). They are useful because they indicate the existence of absolute limits to observation and control in some systems. If it is not possible to completely determine the state of a system given a chosen measurement or to prepare an arbitrary state of the system given the chosen control Hamiltonian, then this will place severe limitations on the feedback control of that system. It is important to note that the definitions of observability and controllability apply classically to noiseless systems (ie, systems with neither process nor measurement noise), although they are relevant for stochastic systems, and it is these systems in which we are naturally interested here.

Consider observability of a system. A system is defined to be observable if the initial state of the system can be decided from the past output, ie, the measurements made on the system from the initial time onwards (Isidori, 1995). It follows that in an observable system, every element in the (classical) state vector affects at least one element in the output vector, so that the relation can be used to obtain the initial state from the outputs. If one considers adding process and measurement noises, then observability is still a useful concept, because it tells us that the outputs, while corrupted by noises, nevertheless provide information about every element in the state vector. Consequently, given imprecise initial knowledge of the state, we can expect our knowledge of all the elements to improve with time. For an unobservable system, there will be at least one state element about which the measurement provides no information. The simplest example of this is a free particle in which the momentum is observed. Since the position never affects the momentum, any initial uncertainty in the position will not be reduced by the measurement. Note that observability is a joint property of a system and the type of measurement that is being made upon it.

It is interesting that there are at least two inequivalent ways in which this concept of observability may be applied to a measured quantum system, and these result from the choice of making an analogy either in terms of the quantum state vector, or a set of quantum observables.

Consider observability defined in terms of a set of observables. The concept of observability applies in this case to whether or not the output contains information about all the physical observables in question. A simple example once again consists of the single particle, in which we can use the position and momentum as the relevant set of observables. If we consider the observation of the position, then the system is observable: the output contains information about both the position and momentum since the momentum continually affects the position. As a result, a large initial uncertainty in both variables is reduced during the observation. Naturally, this is eventually limited by the uncertainty principle. The conditioned state may eventually become pure but there will be a finite limiting variance in the measured quantity since this state must obey the uncertainty relations. In linear systems, the measurement back action noise has a role rather similar to process noise in a classical system, since process noise also leads to non-zero limiting variances of the measured property of the state.

An alternative way to define quantum observability is in terms of the state vector. In this case, the question of observability concerns whether or not the output contains information about all the elements of the quantum state vector. Consider a quantum system in which the observation is the only source of noise. Then, if the system is observable with respect to a particular measurement, as time proceeds one obtains increasingly more information about all the elements of the state vector, and the conditioned state tends to a pure state as $t \to 0$. For an unobservable system, any initial uncertainty in at least one state vector element remains, even in the long time limit. A simple example of a system that is observable in this sense is the measurement of momentum on a free particle (recall that this is unobservable in the previous sense). In this case, it is a simple matter to calculate the time evolution of the purity of the conditioned state to verify that the system is observable. An example of an unobservable system is a set of two non-interacting spins, in which it is an observable of only one of the spins that is measured. In this case, while the state of the measured spin may become pure, clearly the state of the joint system can remain mixed for a suitable choice of an initial state.

A key factor that differs between these examples is that in the observable case the measured quantity (being the momentum) has a non-degenerate eigenspectrum, whereas in the unobservable case the measured quantity (being any observable of the first spin) has degenerate eigenvalues when written as an operator on the full (two-spin) system. It is clear that in the case that the measured observable commutes with the system Hamiltonian the non-degeneracy of the eigenvalues of the observable is a necessary and sufficient condition for observability in this sense. Writing the evolution of the system as multiplication by a series of measurement operators alternating with unitary operators (because of the Hamiltonian evolution), the measurement operators may be combined together since they commute with the unitary operators, and it is readily shown that as $t \to \infty$, one is left with a projection onto the basis of the measured observable. If the eigenvalues of the observable are all different, then the measurement results distinguish the resulting eigenvector, and the result is a pure state. However, if any two of the eigenvectors are degenerate, the measurement results will not distinguish those two states. Consequently, if the system exists initially in a mixture of these two states, it will remain so for all time. Whether this continues to be true in the general case remains an open question.

The controllability of quantum mechanical systems, ie, whether the interaction Hamiltonians available are able to prepare an arbitrary state of a quantum system, can be considered by applying directly the ideas of classical control theory. Interestingly, this has a new interpretation in quantum computation. The gates of the computer must be able to perform an arbitrary unitary operation on the register of qubits; a set of gates with this property is termed universal. Since it may perform arbitrary unitary operations, a universal quantum computer may prepare any desired state of the system from any given initial state. The conditions for controllability of a quantum system were therefore rediscovered as the conditions for universality of a quantum computer.

4.3 Developing control in quantum systems

Open-loop control problems are conceptually straightforward in the quantum context (Habib *et al.*, 2002). One begins with the time evolution operator of the quantum system – the Schrödinger equation for the wave function, the Liouville equation for the density matrix, or more complicated dynamical evolution equations for the density matrix characterizing a system coupled to an environment. A theory for time-dependent variations in the evolution operator is then developed in such a way that the wave function or the density operator at some time is close to some target value. This target value does not have to be unique, nor in fact is the time evolution to that value unique. Although quantum and classical systems are dynamically distinct, the principles for open-loop control are in fact very similar.

The fundamental differences between classical and quantum systems become real issues, however, in the field of closed-loop control. Quantum systems can have two distinct types of feedback control.

4.3.1. Directly coupled quantum feedback: In a system with directly coupled quantum feedback, a quantum variable of the system is coupled to the quantum controller, and a quantum input path from the controller goes directly back to the quantum system. Both the dynamical system and the controller are quantum systems coupled through a unitary interaction. A quantum variable is coupled to the quantum controller, and a quantum input path from the controller goes directly back to the quantum system.

4.3.2. Indirectly coupled quantum feedback: When the quantum feedback is indirect, the quantum dynamical system under control is an observed system. It therefore generates a classical output, also known as the measurement record, which the controller may analyze to provide a best estimate of the original quantum state of the system. The controller then feeds back a classical signal to vary parameters in the quantum evolution operator in accord with the chosen control strategy. A quantum dynamical system can be viewed as having two sets of inputs, one relating to the variation in the classical parameters describing the Hamiltonian and the other representing fully quantum inputs. Similarly, the output channel can be divided into a quantum and a classical channel. The classical channel is, in fact, a piece of the quantum channel that has become classical after observation. The controller analyses the classical record to form an estimate of the dynamical system's state and uses this information to implement the appropriate control.

Hybrid couplings using both direct and indirect quantum feedback channels are easy to envisage. The channel from the system output to the controller input may be directly coupled whereas the channel from the controller output to the system input may be coupled indirectly through a classical path.

In both classical and quantum contexts, the main objective of closed-loop control is to enhance system performance in the presence of noise from both the environment and the uncertainty in the system parameters. To limit the effects of noise, the controller must perform an irreversible operation. Noise generates a large set of undesirable evolutions, and the controller's task is to map this large set to a much smaller one of more desirable evolutions. Mapping from the larger to the smaller set is by definition irreversible. In other words, noise is a source of entropy for the system. To control the system, the controller must extract the entropy from the system under control and put it somewhere else. The controller must therefore have enough degrees of freedom to respond conditionally upon the noise realization. In indirect quantum feedback control, measurement process, coupled with the conditional response of the controller, is the source of entropy reduction. In direct quantum feedback control, the evolution of the system is fully unitary, or quantum mechanical. The quantum controller provides a large Hilbert space of quantum mechanical states. That is precisely where the entropy generated by the noise may be put (or where the history of the effect of the noise on the system may be stored). The quantum controller then reacts conditionally to this quantum record, keeping the entropy of the quantum dynamical system low, while the entropy of the storage location grows continually.

4.4 Quantum optimal control: the quantum Bellman equation

Classically, the optimal control problem can be written in a form that is, at least in principle, amenable to solution via the method of dynamic programming. In the

Section 3, we have shown how to generate quantum mechanics using dynamic programming by injecting noise in the system. Here, we apply dynamic programming to generate an equivalent quantum Bellman equation for optimal quantum control (Doherty *et al.*, 2000).

To define an optimal control problem we must specify a cost function $f(\rho(t), u(t), t)$, which defines how far the system is from the desired state, how much this costs, and how much a given control costs to implement. The problem then involves finding the control that minimizes the value of the cost function integrated over the time during which the control is acting. The important point to note is that the cost function can almost always be written as a function of the conditional density matrix followed by an average over trajectories. This is because the density matrix determines completely the probabilities of all future measurements that can be made on the system, and consequently captures completely the future behaviour of the system as far as future observers are concerned (given that the dynamics are known, of course), which is what one almost always wants to control.

The possible exceptions to this rule come when one is interested in preserving or manipulating unknown information that has been encoded in the system by a previous observer who prepared it in one of a known ensemble of states. Thus as far as the second observer is concerned, the state of the system is found by averaging over these states with the weighting appropriate to the ensemble. However, in this case, it may well be sensible to use a cost function that depends on the ensemble as well as this density matrix. We will restrict ourselves here to what might be referred to as orthodox control objectives, in which it is only the future behaviour of the system that is important, and this is captured by cost functions that depend only on the density matrix (ensemble independent cost functions).

The general statement of our optimal control problem may therefore be written as

$$C = \left\langle \int_0^T f(\rho(t), u(t), t)\,\mathrm{d}t + f_{\mathrm{f}}(\rho_{\mathrm{c}}(T), T) \right\rangle$$

Here C denotes the total average cost for a given control strategy $u(t)$, f is the cost function up until the final time T, f_{f} is the cost function associated with the final state, and $\langle\,\rangle$ denotes the average over all trajectories. The solution is given by minimizing C over $u(t)$, to obtain the minimal cost C_{m}, and resulting optimal strategy $u_{\mathrm{op}}(t)$. Note that the values of u will be different for different trajectories. In this formulation, a cost is specified at each point in time, with the total cost merely the integral over time, and an allowance is explicitly made for extra weighting to be given to the cost of the state at the final time. It is crucial that the cost function takes this local in time form in order that it be rewritten as a Bellman equation.

To derive the quantum Bellman equation, we will consider the problem to be discrete in time, since this provides the clearest treatment. In any case, the continuous limit may be taken at the end of the derivation, if the result is desired. In this case, dividing the interval [0, T] into N steps, the cost function consists of a sum of the costs at times $t_i = t_1, \ldots, t_{N+1}$, with $t_{N+1} = T$ denoting the final time. The idea of dynamic programming (which results from the Bellman equation) is that if the period of control is broken into two steps, then the optimal control during the second step must be the control that would be chosen by optimizing over the later time period alone given the initial state reached after the first step. This allows the optimal control to be calculated from a recursive relation that runs backwards from the final time, or in the continuous-time case from a backwards time differential equation. To derive the Bellman equation, one proceeds as follows.

Trivially, at the final time, given the state $\rho(T)$, the minimal cost is merely the final cost, so $C_{\mathrm{m}}(t_{N+1}) = f_{\mathrm{f}}(\rho(T), T)$. Next, stepping back to the time t_N, the total cost-to-go, given the state $\rho(t_N)$ is

$$C(t_N) = f(\rho_{\mathrm{c}}(t_N), u(t_N), t_N)\Delta t + \int f_{\mathrm{f}}(\rho(T), T) P_{\mathrm{c}}(\rho(T)|\rho_{\mathrm{c}}(t_N), u(t_N))\, \mathrm{d}\rho(T)$$

where P_{c} is the conditional probability density for the state at time T given the state $\rho_{\mathrm{c}}(t_N)$, which is conditioned on any earlier measurement results and controls, and the control $u(t_N)$ at time t_N, so that the integral is simply the conditional expectation value of the cost at the final time. Note that the choice of the control $u(t_N)$ may depend on the measurement result at t_N and that the conditional probability density is conditioned not only on the chosen value of $u(t_N)$ but also on the measurement result at t_N. Since $f_{\mathrm{f}}(\rho(T), T)$ is $C(t_{N+1})$, we have

$$C(t_N) = \min_{u(t_N)}\left[f(\rho_{\mathrm{c}}(t_N), u(t_N), t_N)\Delta t + \int C(t_{N+1}) P_{\mathrm{c}}(\rho(t_{N+1})|\rho_c(t_N), u(t_N))\, \mathrm{d}\rho(t_{N+1})\right]$$

The important step comes when we consider the total cost-to-go at the third-to-last time t_{N-1}. This time there are three terms in the sum. Nevertheless, using the Chapman–Kolmogorov equation for the conditional probability densities, it is straightforward to write the equation for $C(t_{N-1})$ in precisely the same form as that for $C(t_N)$.

From this point, the crucial fact that results in the Bellman equation is this: since the conditional probability densities are positive definite, it follows that the minimum of $C(t_i)$ is only obtained by choosing $C(t_{i+1})$ to be minimum. We can therefore write a backwards-in-time recursive relation for the minimum cost, being

$$C_{\mathrm{m}}(t_i) = \min_{u(t_i)}\left[f(\rho_{\mathrm{c}}(t_i), u(t_i), t_i)\Delta t + \int C_{\mathrm{m}}(t_{i+1}) P_{\mathrm{c}}(\rho(t_{i+1})|\rho_{\mathrm{c}}(t_i), u(t_i))\, d\rho(t_{i+1})\right]$$

which is the discrete time version of the Bellman equation. In other words, this states that an optimal strategy has the property that, whatever any initial states and decisions, all remaining decisions must constitute an optimal strategy with regard to the state that results from the first decision, which is referred to as the optimality principle.

The quantum Bellman equation confirms the intuitive result that any optimal quantum control strategy concerned only with the future behaviour of the system is a function only of the conditional density matrix, and further, that the strategy at time t is only a function of the conditioned density matrix at that time.

The procedure of stepping back through successive time steps from the final time to obtain the optimal strategy is referred to as dynamic programming. This could be used, at least in principle, to solve the problem numerically. In practice, it will be useful to employ some approximate strategy.

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