Abstract

We outline a new approach to the steering problem for quantum systems relying on \textit{Nelson’s stochastic mechanics} and on the \textit{theory of Schrödinger bridges}. The method is illustrated by working out a simple Gaussian example.

1 Introduction

The problem of steering a quantum system from a given state \( \psi_0 \) at time \( t_0 \) to another given state \( \psi_1 \) at time \( t_1 \) applying an external potential function lies at the heart of the field of control for quantum systems. The applications are manifold, including control of molecular dynamics, quantum computing, nuclear magnetic resonance, quantum communications, etc., see [1]-[12], and references therein. In its entirety, the problem consists in finding a control potential function \( V_c(x,t) \) in a suitable class such that, if \( V_i(x,t) \) is the ambient potential function, the solution \( \psi(x,t) \) of the controlled Schrödinger equation

\[
\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m} \Delta \psi - \frac{i}{\hbar} [V_i(x) + V_c(x,t)] \psi, \quad (1)
\]

\[
\psi(x,t_0) = \psi_0(x), \quad (2)
\]

satisfies \( \psi(x,t_1) = \psi_1(x) \). Of course, the first natural question to pose is the controllability question for the Schrödinger equation. Since this is a distributed-parameter bilinear system, the problem is highly nontrivial, and only very limited results are so far available [1]. The problem can be effectively studied for N-level systems that approximate in a suitable way the infinite-dimensional system [4].

2 Elements of stochastic mechanics and Schrödinger bridges

In this paper, we outline a completely new approach to the steering problem for the Schrödinger equation relying on \textit{Nelson’s stochastic mechanics} [13]-[21] and on the \textit{theory of Schrödinger bridges}, cf. [23, 22] and references therein. We remark, in passing, that this method has nothing to do with the results of [24]-[26], where the theory of Schrödinger bridges and reciprocal processes was employed to construct different versions of stochastic mechanics.

Nelson’s stochastic mechanics is a quantization procedure for classical dynamical systems based on diffusion processes. Given a quantum evolution \( \left\{ \psi(x,t); t_0 \leq t \leq t_1 \right\} \), where \( x \in \mathbb{R}^n \), a \( n \)-dimensional Markov diffusion process \( \left\{ x(t); t_0 \leq t \leq t_1 \right\} \), called \textit{Nelson’s process}, is associated to it as follows. The (forward) Ito differential of \( x(t) \) is given by

\[
dx(t) = \left[ \frac{\hbar}{m} \nabla (\Re \log \psi(x(t),t) + \Im \log \psi(x(t),t)) \right] dt + \sqrt{\frac{\hbar}{m}} dw(t), \quad (3)
\]

where \( w \) is a standard, \( n \)-dimensional Wiener process. Moreover, the probability density \( \rho(x,t) \) of \( x(t) \) satisfies

\[
\rho(x,t) = |\psi(x,t)|^2, \quad \forall t \in [t_0,t_1]. \quad (4)
\]

The construction of the Nelson process corresponding to \( \psi(x,t) \) in the case where \( \psi(x,t) \) vanishes requires considerable care. It will always be assumed that \( \psi \) is of class \( C^{2,1} \) with

\[
||\nabla \psi||_2^2 \in L^1_{\text{loc}}([t_0, +\infty)). \quad (5)
\]
This is Carlen’s finite action condition. Under these hypotheses, the Nelson measure may be constructed, [15, 17, Chapter IV], and references therein. Let us now outline the theory of the Schrödinger bridges. The Kullback-Leibler pseudo-distance between two probability densities \( p(\cdot) \) and \( q(\cdot) \) is defined by

\[
H(p, q) := \int_{\mathbb{R}^n} \log \frac{p(x)}{q(x)} \, p(x) \, dx.
\]

This concept can be considerably generalized. Let \( \Omega := C([t_0, t_1], \mathbb{R}^n) \), let \( W_x \) denote Wiener measure on \( \Omega \) starting at \( x \), and let

\[
W := \int W_x \, dx
\]

be stationary Wiener measure. Let \( \mathbb{D} \) be the family of distributions on \( \Omega \) that are equivalent to \( W \). For \( Q, P \in \mathbb{D} \), we define the relative entropy \( H(Q, P) \) of \( Q \) with respect to \( P \) as

\[
H(Q, P) = E_Q [\log \frac{dQ}{dP}].
\]

It then follows from Girsanov’s theorem that [22]

\[
H(Q, P) = H(q(t_0), p(t_0)) + E_Q \left[ \int_{t_0}^{t_1} \frac{1}{2} [\beta^Q(t) - \beta^P(t)] \cdot [\beta^Q(t) - \beta^P(t)] \, dt \right]
\]

\[
= H(q(t_1), p(t_1)) + E_Q \left[ \int_{t_0}^{t_1} \frac{1}{2} [\gamma^Q(t) - \gamma^P(t)] \cdot [\gamma^Q(t) - \gamma^P(t)] \, dt \right].
\]

Here \( q(t_0) \) is the marginal density of \( Q \) at \( t_0 \), \( \beta^Q \) and \( \gamma^Q \) are the forward and the backward drifts of \( Q \), respectively. Now let \( \rho_0 \) and \( \rho_1 \) be two everywhere positive probability densities. Let \( \mathbb{D}(\rho_0, \rho_1) \) denote the set of distributions in \( \mathbb{D} \) having the prescribed marginal densities at \( t_0 \) and \( t_1 \). Given \( P \in \mathbb{D} \), we consider the following problem:

Minimize \( H(Q, P) \) over \( \mathbb{D}(\rho_0, \rho_1) \).

This problem is connected through Sanov’s theorem to a problem of large deviations of the empirical distribution, according to Schrödinger original motivation [23, 22]. If there is at least one \( Q \) in \( \mathbb{D}(\rho_0, \rho_1) \) such that \( H(Q, P) < \infty \), it may be shown that there exists a unique minimizer \( Q^* \) in \( \mathbb{D}(\rho_0, \rho_1) \) called the Schrödinger bridge from \( \rho_0 \) to \( \rho_1 \) over \( P \). If (the coordinate process under) \( P \) is Markovian with forward drift field \( b^P_+(x, t) \) and transition density \( p(\sigma, x, \tau, y) \), then \( Q^* \) is also Markovian with forward drift field

\[
b^Q_+(x, t) = b^P_+(x, t) + \nabla \log \phi(x, t),
\]

where the function \( \phi \) solves together with another function \( \phi \) the system

\[
\phi(t, x) = \int p(t, x, t_1, y) \phi(t_1, y) \, dy,
\]

\[
\dot{\phi}(t, x) = \int p(t, y, t, x) \phi(t, y) \, dy
\]

with the boundary conditions

\[
\phi(x, t_0) \phi(x, t_0) = \rho_0(x), \quad \phi(x, t_1) \phi(x, t_1) = \rho_1(x).
\]

Moreover, we have \( \rho(x, t) = \phi(x, t) \phi(x, t), \forall t \in [t_0, t_1] \).

### 3 Steering for quantum systems

We now show that the theory of Schrödinger bridges can be employed, jointly with stochastic mechanics, to attack the steering problem for quantum systems. First of all, observe that everything we said about Schrödinger bridges continues to hold if we consider finite-energy diffusions with diffusion coefficient equal to \( \frac{\hbar}{m} \) rather than \( 1 \). Let \( \psi_0 \) and \( \psi_1 \) be the given initial and final quantum states. Consider a reference quantum evolution \( \{\psi(x, t); t_0 \leq t \leq t_1\} \) solving the Schrödinger equation

\[
\partial \psi \over \partial t = \frac{i}{\hbar} \left[ H \psi \right] \frac{\hbar}{m} \nabla S(x, t) + \frac{\hbar}{m} \nabla \log \phi(x, t),
\]

and satisfying Carlen’s finite action condition (5). Let \( P \in \mathbb{D} \) be the Markovian measure of the Nelson process associated to \( \{\psi(x, t)\} \) as in (3)-(4). Hence, in particular, the probability density satisfies \( \rho(x, t) = |\psi(x, t)|^2 \). Thus, if we write

\[
\psi(x, t) = \exp[R(x, t) + \frac{i}{\hbar} S(x, t)],
\]

the forward drift of the Nelson process is then given by

\[
b^P_+(x, t) = \frac{1}{m} \nabla S(x, t) + \frac{\hbar}{m} \nabla R(x, t).
\]

We then have the following result.

**Theorem 1** Let \( Q^* \) be the Schrödinger bridge from \( |\psi_0|^2 \) to \( |\psi_1|^2 \) over \( P \) (see previous section). Then, \( Q^* \) has forward drift field

\[
b^Q_+(x, t) = \frac{1}{m} \nabla S(x, t) + \frac{\hbar}{m} \nabla R(x, t) + \frac{\hbar}{2m} \Delta \phi(x, t),
\]

where the function \( \phi \) solves together with another function \( \phi \) the system

\[
\frac{\partial \phi}{\partial t} + \left( \frac{1}{m} \nabla S + \frac{\hbar}{m} \nabla R \right) \cdot \nabla \phi + \frac{\hbar}{2m} \Delta \phi = 0, \quad (6)
\]

\[
\frac{\partial \phi}{\partial t} + \nabla \left( \frac{1}{m} \nabla S + \frac{\hbar}{m} \nabla R \right) \phi - \frac{\hbar}{2m} \Delta \phi = 0, \quad (7)
\]

with the boundary conditions

\[
\phi(x, t_0) \phi(x, t_0) = |\psi_0|^2(x), \quad \phi(x, t_1) \phi(x, t_1) = |\psi_1|^2(x).
\]

The one-time probability density of \( Q^* \) satisfies

\[
\tilde{\rho}(x, t) = \phi(x, t) \phi(x, t).
\]

Define, for \( t \in [t_0, t_1] \),

\[
\tilde{S}(x, t) = S(x, t) + \hbar R(x, t) + \frac{\hbar}{2} \log \frac{\phi(x, t)}{\phi(x, t)},
\]

\[
\tilde{R}(x, t) = \frac{1}{2} \log \tilde{\rho}(x, t).
\]
Let \( \{ \tilde{\psi}(x,t); t_0 \leq t \leq t_1 \} \) be defined by
\[
\tilde{\psi}(x,t) = \exp[\tilde{R}(x,t) + \frac{i}{\hbar}\tilde{S}(x,t)].
\]

Then, \( \{ \tilde{\psi}(x,t) \} \) solves the Schrödinger equation (1) with controlling potential function \( V_\epsilon(x,t) \) given by
\[
V_\epsilon(x,t) = V(x) - V_0(x) + \frac{\hbar^2}{m} \left[ \frac{\Delta \sqrt{\rho(x,t)}}{\sqrt{\rho(x,t)}} - \frac{\Delta \sqrt{\rho(x,t)}}{\sqrt{\rho(x,t)}} \right],
\]
and we have
\[
|\tilde{\psi}(x,t_0)| = |\psi_0(x)|, \quad |\tilde{\psi}(x,t_1)| = |\psi_1(x)|.
\]

Moreover, the Schrödinger bridge \( Q^* \) is indeed the Nelson process associated to the new quantum evolution \( \{ \tilde{\psi}(x,t); t_0 \leq t \leq t_1 \} \).

Proof: As is well known [13], \( R \) and \( S \) satisfy the system of nonlinear p.d.e.’s:
\[
\frac{\partial R}{\partial t} + \frac{1}{m} \nabla R \cdot \nabla S + \frac{1}{2m} \Delta S = 0, \tag{11}
\]
\[
\frac{\partial S}{\partial t} + \frac{1}{2m} \nabla S \cdot \nabla S + V - \frac{\hbar}{2m} [\nabla R \cdot \nabla R + \Delta R] = 0. \tag{12}
\]
A long calculation employing definitions (8)-(9), and equations (6), (7), (11) and (12) establishes (10). The last assertion follows at once observing that (8)-(9) imply
\[
b_\epsilon^Q(x,t) = \frac{1}{m} \nabla \tilde{S}(x,t) + \frac{\hbar}{m} \nabla \tilde{R}(x,t).
\]

Remark 1 Notice that when \( V(x) = V_\epsilon(x) \), namely the reference quantum evolution takes place in the ambient potential \( V_\epsilon \), the controlling potential reduces to
\[
V_\epsilon(x,t) = \frac{\hbar^2}{m} \left[ \frac{\Delta \sqrt{\rho(x,t)}}{\sqrt{\rho(x,t)}} - \frac{\Delta \sqrt{\rho(x,t)}}{\sqrt{\rho(x,t)}} \right].
\]

Instead, when the ambient potential is zero, we get the following remarkable invariance property:
\[
V_\epsilon(x,t) - \frac{\hbar^2}{m} \frac{\Delta \sqrt{\rho(x,t)}}{\sqrt{\rho(x,t)}} = V(x) - \frac{\hbar^2}{m} \frac{\Delta \sqrt{\rho(x,t)}}{\sqrt{\rho(x,t)}}.
\]

The quantity
\[
- \frac{\hbar^2}{2m} \frac{\Delta \sqrt{\rho(x,t)}}{\sqrt{\rho(x,t)}}
\]
is called quantum potential in quantum mechanics [14, 27] because it appears in the Hamilton-Jacobi like equation (12).

Remark 2 The quantum evolution \( \{ \tilde{\psi}(x,t); t_0 \leq t \leq t_1 \} \) has, by construction, the desired absolute values at times \( t_0 \) and \( t_1 \). Notice that any choice of the “reference process” \( P \) produces a quantum evolution with these properties, and a corresponding control potential function. Thus, we can try to choose \( P \) (our “free parameter”) so that the phase function \( \tilde{S}(x,t) \) has the prescribed initial and final values, thereby achieving the desired steering, see the example in the following section.

4 Example

The aim is that of shifting the mean of a Gaussian wave packet, that is, passing from the initial quantum state
\[
\psi_0(x) = \left( \frac{\omega}{\pi} \right)^{1/4} \exp(-\omega x^2/2)
\]
\[
= \exp(R_0(x) + iS_0(x)) \tag{13}
\]
at \( t = 0 \) to the final quantum state
\[
\psi_1(x) = \left( \frac{\omega}{\pi} \right)^{1/4} \exp(-\omega(x-1)^2/2)
\]
\[
= \exp(R_1(x) + iS_1(x)) \tag{14}
\]
at \( t = 1 \). As we shall show elsewhere [28], to solve this simple problem a direct approach is actually feasible. We choose here to solve the problem via the theory of Schrödinger bridges, in order to illustrate the method of the previous section. For notational convenience, let us assume that we are in a reference system where \( m = \hbar = 1 \) and that \( \omega = \pi \). We will often omit in the sequel the function arguments \( t \) and \( x \). Let us take as reference evolution
\[
\psi(x,t) = \exp(R(x,t) + iS(x,t)), \tag{15}
\]
where
\[
R(x,t) = -\frac{\omega}{2}(x - m(t))^2 \tag{16}
\]
\[
S(x,t) = cx + d(t), \tag{17}
\]
with
\[
m(t) = m_1 + m_2 \tag{18}
\]
\[
c = m(t) = m_2 \tag{19}
\]
and \( d \) is to be specified. The Schrödinger system (6)-(7) is given by the following two equations for \( \phi \) and \( \dot{\phi} \):
\[
\frac{\partial \phi}{\partial t} + \left( \frac{\partial S}{\partial x} + \frac{\partial R}{\partial x} \right) \frac{\partial \phi}{\partial x} + \frac{1}{2} \frac{\partial^2 \phi}{\partial x^2} = 0 \tag{20}
\]
\[
\frac{\partial \phi}{\partial t} + \frac{\partial}{\partial x} \left( \frac{\partial S}{\partial x} + \frac{\partial R}{\partial x} \right) \phi - \frac{1}{2} \frac{\partial^2 \phi}{\partial x^2} = 0 \tag{21}
\]
with boundary conditions
\[
\phi(x,0) \phi(x,0) = \rho_0(x) = \exp(-\omega x^2) \tag{22}
\]
\[
\phi(x,1) \phi(x,1) = \rho_1(x) = \exp(-\omega(x-1)^2) \tag{23}
\]
Assuming that

\[ \phi(x, t) = \exp(\alpha(t)x^2 + \beta(t)x + \gamma(t)) \]

we find the following sets of equations for \( \alpha, \dot{\alpha}, \beta, \dot{\beta}, \) and \( \gamma, \dot{\gamma} \):

\[
\begin{cases}
  \dot{\alpha} - 2\alpha\omega + 2\alpha^2 &= 0 \\
  \beta + 2\alpha\omega + \omega\beta + 2\alpha\beta &= 0 \\
  \dot{\gamma} + \gamma + \omega\beta + \frac{1}{2}\beta^2 + \alpha &= 0
\end{cases}
\]

and

\[
\begin{cases}
  \dot{\dot{\alpha}} - 2\dot{\alpha}\omega - 2\dot{\alpha}^2 &= 0 \\
  \ddot{\beta} + 2\alpha\dot{\omega} + \omega\dot{\beta} - 2\dot{\alpha}\dot{\beta} &= 0 \\
  \ddot{\gamma} - \omega + c\beta + \omega\beta + \frac{1}{2}\beta^2 - \dot{\alpha} &= 0
\end{cases}
\]

The boundary conditions (22)-(23) yield the constraints on the values of \( \alpha, \dot{\alpha}, \beta, \dot{\beta}, \) and \( \gamma, \dot{\gamma} \) at \( t = 0, 1 \):

\[
\begin{cases}
  \alpha_0 + \dot{\alpha}_0 &= -\omega \\
  \beta_0 + \dot{\beta}_0 &= 0 \\
  \gamma_0 + \dot{\gamma}_0 &= 0
\end{cases}
\]

and

\[
\begin{cases}
  \alpha_1 + \dot{\alpha}_1 &= -\omega \\
  \beta_1 + \dot{\beta}_1 &= 2\omega \\
  \gamma_1 + \dot{\gamma}_1 &= -\omega
\end{cases}
\]

It is easy to see that

\[
\begin{align*}
\dot{\beta}(t) &= 2\omega\dot{m}(t) - e^{-\omega t}(\beta_0 + 2\omega m_1) . \\
\beta_0 &= 2\omega \frac{1 + m_1 e^{-\omega t} - (m_1 + m_2)}{e^{\omega t} - e^{-\omega t}} .
\end{align*}
\]

Given \( \beta \) and \( \dot{\beta} \), it is possible to obtain \( \gamma \) and \( \dot{\gamma} \) (by integration), where \( \gamma_0 \) is so far to be specified. Thus, we get

\[
\begin{align*}
\gamma(t) &= \gamma_0 + \frac{\beta_0^2}{4\omega}(1 - e^{-2\omega t}) + \dot{\beta}_0(m_1 - e^{-\omega t}m(t)) \\
\gamma(t) &= -\gamma_0 + \frac{1}{4\omega}[\beta_0^2(1 - e^{-2\omega t}) \\
&+ 4\dot{\beta}_0\omega e^{-2\omega t}(e^{\omega t}m(t) - m_1) \\
&+ 4\omega^2 e^{-2\omega t}(e^{\omega t}m(t) - m_1)^2]
\end{align*}
\]

It can be checked that the constraint \( \gamma_1 + \dot{\gamma}_1 = -\omega \) is always satisfied, whatever the value of \( \gamma_0 \). Matching the phase at \( t = 0, 1 \) requires that

\[
\begin{align*}
S(x, 0) + R(x, 0) + \ln \phi(x, 0) &= S_0(x) + \frac{1}{2} \ln \rho_0(x) \\
S(x, 1) + R(x, 1) + \ln \phi(x, 1) &= S_1(x) + \frac{1}{2} \ln \rho_1(x),
\end{align*}
\]

or equivalently that

\[
\begin{align*}
m_2 + \omega m_1 + \beta_0 &= 0 \\
\gamma_0 - \frac{\omega}{2} m_1^2 + d_0 &= 0 \\
m_2 + \omega(m_1 + m_2) + \beta_1 - \omega &= 0 \\
\frac{\omega^2}{2}(m_1 + m_2)^2 + \gamma_1 + \frac{\omega}{2} + d_1 &= 0 ,
\end{align*}
\]

where \( d_0 \) and \( d_1 \) are the values of \( d(t) \) at \( t = 0, 1 \). Some computations show that eqns. (34) and (37)-(40) are satisfied by the following values

\[
\begin{align*}
m_1 &= -\frac{e^{\omega t} - 1}{2 - 2e^{\omega t} + \omega + \omega e^{\omega t}} \\
m_2 &= \frac{\omega e^{\omega t} + 1}{2 - 2e^{\omega t} + \omega + \omega e^{\omega t}} \\
\beta_0 &= -\frac{\omega}{2 - 2e^{\omega t} + \omega + \omega e^{\omega t}} \\
\gamma_0 &= \frac{\omega}{2 (2 - 2e^{\omega t} + \omega + \omega e^{\omega t})} \\
d_0 &= 0 \\
d_1 &= -\frac{\omega(1 + e^{\omega t})(1 - e^{\omega t} + \omega + \omega e^{\omega t})}{(2 - 2e^{\omega t} + \omega + \omega e^{\omega t})^2}.
\end{align*}
\]

A possible choice for \( d(t) \) is then

\[ d(t) = d_1 t . \]

By choosing \( m, d, \alpha, \dot{\alpha}, \beta, \dot{\beta}, \) and \( \gamma, \dot{\gamma} \) according to equations (30)-(33), (35)-(36), (41)-(47), both the reference evolution (15) and the solution \( \phi, \dot{\phi} \) of the Schrödinger system (20)-(23) are completely specified. The expressions of the controlled quantum evolution \( \tilde{\psi}(x, t) \) and of the controlling potential function \( V_c(x, t) \) can then be derived as in Theorem 1.

References


