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Efficient simulation of quantum state reduction

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The energy-based stochastic extension of the Schrödinger equation is a rather special nonlinear stochastic differential equation on Hilbert space, involving a single free parameter, that has been shown to be very useful for modeling the phenomenon of quantum state reduction. Here we construct a general closed form solution to this equation, for any given initial condition, in terms of a random variable representing the terminal value of the energy and an independent Brownian motion. The solution is essentially algebraic in character, involving no integration, and is thus suitable as a basis for efficient simulation studies of state reduction in complex systems. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1512975]

The standard energy-based stochastic extension of the Schrödinger equation is given by the following stochastic differential equation:

$$\mathrm{d}|\psi_t\rangle = -\mathrm{i}\hat{H}|\psi_t\rangle\mathrm{d}t - \tfrac{1}{8}\sigma^2(\hat{H}-H_t)^2|\psi_t\rangle\mathrm{d}t + \tfrac{1}{2}\sigma(\hat{H}-H_t)|\psi_t\rangle\mathrm{d}W_t\,, \tag{1}$$

with initial condition $|\psi_0\rangle$. Here $|\psi_t\rangle$ is the state vector at time t, $\hat{H}$ is the Hamiltonian operator, W_t denotes a one-dimensional Brownian motion, and

$$H_t = \frac{\langle\psi_t|\hat{H}|\psi_t\rangle}{\langle\psi_t|\psi_t\rangle} \tag{2}$$

is the expectation of $\hat{H}$ in the state $|\psi_t\rangle$. The parameter σ, which has the units $\sigma \sim [\text{energy}]^{-1}[\text{time}]^{-1/2}$, governs the characteristic timescale τ_R associated with the collapse of the wave function induced by (1). This is given by $\tau_R = 1/\sigma^2 V_0$, where V_0 is the initial value of the squared energy uncertainty, which at time t is

$$V_t = \frac{\langle\psi_t|(\hat{H}-H_t)^2|\psi_t\rangle}{\langle\psi_t|\psi_t\rangle}. \tag{3}$$

The stochastic equation (1) is perhaps the simplest known dynamic model for state reduction in quantum mechanics consistent with both the Born probability rules and the principle of energy conservation. Although the mathematical and phenomenological properties of (1) have been studied extensively,[1–4] it has hitherto been necessary to resort to numerical methods to solve dynamical equations of this type,[5] and exact solutions have been unavailable except in very simple cases. The purpose of this article is to present a general analytic solution for the dynamics of $|\psi_t\rangle$.

We begin with a brief overview of the stochastic framework implicit in the extended Schrödinger dynamics given by Eq. (1), following a line of argument developed in Ref. 4. Specifically,

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we introduce the key notions of filtration, conditional expectation, martingale, and supermartingale, and show how these concepts can be used effectively to characterize the reductive properties of (1). We then proceed to establish, by novel use of a *nonlinear filtering* technique, that the energy expectation process (2) can be expressed as the conditional expectation of a random variable representing the terminal value of the energy. As a consequence, we are led to simple analytic expressions for the energy (20) and the state vector (33) in terms of a pair of independent state variables. These results open up the possibility of efficiently simulating the reduction process for a variety of models. Finally, we illustrate the practical advantages of our method by analyzing the timescale associated with the reduction process in the case of a two-state system.

The dynamics of $|\psi_t\rangle$ are defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ with filtration $\{\mathcal{F}_t\}$ $(0 \leqslant t < \infty)$. Here Ω is the sample space over which $\mathcal{F}$ is a σ-field of open sets upon which the probability measure $\mathbb{P}$ is defined.

The filtration determines for each $t \geqslant 0$ the information available at that time. More specifically, the filtration consists of a family $\{\mathcal{F}_t\}$ of σ-subfields of $\mathcal{F}$ such that $s \leqslant t$ implies $\mathcal{F}_s \subset \mathcal{F}_t$. Given a random variable X on $(\Omega, \mathcal{F}, \mathbb{P})$, we write $\mathbb{E}[X|\mathcal{F}_t]$ for the *conditional expectation* of X with respect to the σ-subfield $\mathcal{F}_t \subset \mathcal{F}$. Intuitively, conditioning with respect to $\mathcal{F}_t$ means giving all the information available up to time t. The nesting $\mathcal{F}_s \subset \mathcal{F}_t$ for $s \leqslant t$ thus embodies a notion of causality. For convenience, we use the abbreviation $\mathbb{E}_t[X] = \mathbb{E}[X|\mathcal{F}_t]$, and we note that the conditional expectation satisfies the tower property $\mathbb{E}_s[\mathbb{E}_t[X]] = \mathbb{E}_s[X]$ for $s \leqslant t$. If $\mathbb{E}_t[X] = X$, we say that X is $\mathcal{F}_t$-*measurable*.

The conditional expectation operation allows us to introduce the concept of a martingale, the stochastic analog of a conserved quantity. A process X_t is said to be an $\{\mathcal{F}_t\}$-*martingale* if $\mathbb{E}[|X_t|] < \infty$ and $\mathbb{E}_s[X_t] = X_s$ for all $0 \leqslant s \leqslant t < \infty$. In other words, X_t is an $\{\mathcal{F}_t\}$-martingale if it is integrable and if its conditional expectation, given information up to time s, is the value X_s of the process at that time.

For a concise mathematical representation of the state reduction process, we also require the concept of a supermartingale. A process X_t is an $\{\mathcal{F}_t\}$-*supermartingale* if $\mathbb{E}[|X_t|] < \infty$ and $\mathbb{E}_s[X_t] \leqslant X_s$ for all $0 \leqslant s \leqslant t < \infty$. Intuitively, a supermartingale is on average a nonincreasing process.

The filtration $\{\mathcal{F}_t\}$ with respect to which the state vector $|\psi_t\rangle$ evolves is generated in a standard way by the Wiener process W_t. We signify this by writing $\{\mathcal{F}_t\} = \{\mathcal{F}_t^W\}$. It is straightforward to verify that the energy process H_t is an $\{\mathcal{F}_t^W\}$-martingale, and that the variance process V_t is an $\{\mathcal{F}_t^W\}$-supermartingale. That is to say,

$$\mathbb{E}_s[H_t] = H_s, \tag{4}$$

and

$$\mathbb{E}_s[V_t] \leqslant V_s. \tag{5}$$

These relations can be deduced by applying Ito's lemma to (2) and (3), from which we infer that

$$\mathrm{d}H_t = \sigma V_t \mathrm{d}W_t, \tag{6}$$

and that

$$\mathrm{d}V_t = -\sigma^2 V_t^2 \mathrm{d}t + \sigma \beta_t \mathrm{d}W_t, \tag{7}$$

where

$$\beta_t = \frac{\langle \psi_t | (\hat{H} - H_t)^3 | \psi_t \rangle}{\langle \psi_t | \psi_t \rangle} \tag{8}$$

is the *skewness* of the energy distribution at time t. The fact that (6) has no drift shows that H_t is a martingale, and the fact that the drift in (7) is negative shows that V_t is a supermartingale.

In the case of the ordinary Schrödinger equation with a time-independent Hamiltonian, the energy process (2) is constant. This is usually interpreted as the quantum mechanical expression of an energy conservation law. However, if a system is in an indefinite state of energy, then it is not immediately evident what is meant by energy conservation. The martingale condition $\mathbb{E}_s[H_t]=H_s$ can be interpreted as a *generalized energy conservation law* applicable if a system is in an indefinite state of energy. In particular, it implies that once state reduction has occurred, the probabilistic average of the outcome for the energy must equal the initial expectation.

The supermartingale property satisfied by V_t is the essence of what is meant by a *reduction process*. In fact, it follows from Eq. (7) that the asymptotic behavior of V_t is given by

$$\lim_{t\to\infty}\mathbb{E}[V_t]=0, \tag{9}$$

which signifies the collapse of the wave function. A positive supermartingale with the property that its expectation vanishes in the limit as t goes to infinity is called a *potential* process. Writing H_∞ for the random terminal value of the energy, one can then prove as a consequence of (6) and (7) that

$$H_t=\mathbb{E}_t[H_\infty] \tag{10}$$

and that

$$V_t=\mathbb{E}_t[(H_\infty-H_t)^2]. \tag{11}$$

That is to say, the processes H_t and V_t are respectively the $\mathcal{F}_t^W$-conditional mean and variance of H_∞.

With these facts in hand, we now present a method for solving the stochastic equation (1). Our approach is based on the theory of nonlinear filtering.[6] Filtering techniques have been shown to be useful in quantum optics in connection with the theory of continuous observations, and in some situations phenomenological equations similar to (1) for the *a posteriori* dynamics of a continuously observed system can be derived.[7] We shall, however, regard the dynamics of $|\psi_t\rangle$ as being given, and use the filtering methodology with a different end in view: namely, to construct the *solution* of (1).

The setup is as follows. We denote by E_i $(i=1,2,...)$ the eigenvalues of the Hamiltonian of a given quantum system, and write

$$\pi_i=\frac{|\langle\psi_0|\psi_i\rangle|^2}{\langle\psi_0|\psi_0\rangle\langle\psi_i|\psi_i\rangle} \tag{12}$$

for the transition probability from the given initial state $|\psi_0\rangle$ to the eigenstate $|\psi_i\rangle$ with energy E_i. If the spectrum of $\hat{H}$ is degenerate, then $|\psi_i\rangle$ denotes the Lüders state, i.e., the projection of $|\psi_0\rangle$ onto the linear subspace of states corresponding to the eigenvalue E_i.

Now let the probability space $(\Omega, \mathcal{F}, \mathbb{P})$ be given, and on it specify a random variable H that takes the values E_i with probabilities π_i. We assume that $(\Omega, \mathcal{F}, \mathbb{P})$ comes equipped with a filtration $\{\mathcal{G}_t\}$ with respect to which a standard Brownian motion B_t is specified, and that H and B_t are *independent*. We assign no *a priori* physical significance to H and B_t, which are introduced here simply as an ansatz for obtaining a solution for (1). Next we define the process

$$\xi_t=\sigma Ht+B_t. \tag{13}$$

Intuitively, we can think of ξ_t as giving us a "noisy" representation of the information encoded in the random variable H.

We let $\{\mathcal{F}_t^\xi\}$ denote the filtration generated by the process ξ_t, i.e., the information generated by ξ_t as time progresses, and consider the conditional expectation

$$H_t=\mathbb{E}[H|\mathcal{F}_t^{\xi}]. \tag{14}$$

Clearly, $\mathcal{F}_t^{\xi}\subset\mathcal{G}_t$ since knowledge of H together with the path $\{B_s\}_{0\leqslant s\leqslant t}$ implies knowledge of the path $\{\xi_s\}_{0\leqslant s\leqslant t}$, although the converse is not the case.

It follows from the tower property that H_t is an $\{\mathcal{F}_t^{\xi}\}$-martingale. One can think of H_t as representing an estimate for the value of H given the history of the process ξ_s from time 0 up to time *t*. More precisely, an $\{\mathcal{F}_t^{\xi}\}$-measurable random variable H_t minimizes the expectation of the squared deviation of H from H_t, given the history of ξ_s from time 0 to time *t*, if and only if (14) holds. This can be seen by varying the expression $\mathbb{E}[(H-H_t)^2|\mathcal{F}_t^{\xi}]$ with respect to H_t.

We shall now establish the remarkable fact that the *process H_t defined by (14) is statistically indistinguishable from the energy process (2) associated with the stochastic extension of the Schrödinger equation (1).*

The argument goes as follows. First, because ξ_t is a Markov process satisfying

$$\lim_{t\to\infty} t^{-1}\xi_t=\sigma H, \tag{15}$$

we can replace (14) with the simpler relation $H_t=\mathbb{E}[H|\xi_t]$. In other words, to determine the conditional expectation of H given the path $\{\xi_s\}_{0\leqslant s\leqslant t}$, it suffices to condition on the value ξ_t of the process at the end of the path.

To calculate $\mathbb{E}[H|\xi_t]$, we require a version of the Bayes formula applicable when we consider the probability of a discrete random variable conditioned on the value of a continuous random variable. This is given by

$$\mathbb{P}(H=E_i|\xi_t)=\frac{\pi_i\rho(\xi_t|H=E_i)}{\sum_i\pi_i\rho(\xi_t|H=E_i)}, \tag{16}$$

where

$$\pi_i=\mathbb{P}(H=E_i). \tag{17}$$

Here $\rho(\xi_t|H=E_i)$ denotes the conditional probability density for the continuous random variable ξ_t given that $H=E_i$. Since B_t is a standard Brownian motion, the conditional density for ξ_t is

$$\rho(\xi_t|H=E_i)=\frac{1}{\sqrt{2\pi t}}\exp\left(-\frac{1}{2t}(\xi_t-\sigma E_i t)^2\right). \tag{18}$$

It follows from the Bayes law (16) that the conditional probability for the random variable H is

$$\mathbb{P}(H=E_i|\xi_t)=\frac{\pi_i\exp(\sigma E_i\xi_t-\frac{1}{2}\sigma^2E_i^2t)}{\sum_i\pi_i\exp(\sigma E_i\xi_t-\frac{1}{2}\sigma^2E_i^2t)}. \tag{19}$$

Therefore, multiplying each side of (19) by E_i and summing over *i*, we deduce that the conditional expectation of the random variable H given ξ_t is

$$H_t=\frac{\sum_i\pi_iE_i\exp(\sigma E_i\xi_t-\frac{1}{2}\sigma^2E_i^2t)}{\sum_i\pi_i\exp(\sigma E_i\xi_t-\frac{1}{2}\sigma^2E_i^2t)}. \tag{20}$$

In order to show that H_t is the energy process associated with (1), one further key result is required: namely, that *the process W_t defined by*

$$W_t=\xi_t-\sigma\int_0^t H_s\,\mathrm{d}s \tag{21}$$

is an $\{\mathcal{F}_t^\xi\}$*-Brownian motion*. To verify this, it suffices, by virtue of Lévy's characterization of Brownian motion,[6] to demonstrate (a) that $(\mathrm{d}W_t)^2=\mathrm{d}t$ and (b) that W_t is an $\{\mathcal{F}_t^\xi\}$-martingale. To verify (a) we note that (13) implies

$$\mathrm{d}\xi_t=\sigma H\mathrm{d}t+\mathrm{d}B_t, \tag{22}$$

and thus $(\mathrm{d}\xi_t)^2=\mathrm{d}t$. On the other hand, (21) implies that $\mathrm{d}W_t=\mathrm{d}\xi_t-\sigma H_t\mathrm{d}t$, and hence $(\mathrm{d}W_t)^2=(\mathrm{d}\xi_t)^2$. To establish (b), let (20) define a function $H(\xi,t)$ of two variables such that $H_t=H(\xi_t,t)$:

$$H(\xi,t)=\frac{\Sigma_i\pi_iE_i\exp(\sigma E_i\xi-\frac{1}{2}\sigma^2E_i^2t)}{\Sigma_i\pi_i\exp(\sigma E_i\xi-\frac{1}{2}\sigma^2E_i^2t)}. \tag{23}$$

Then applying Ito's lemma and using the relation $(\mathrm{d}\xi_t)^2=\mathrm{d}t$, we obtain

$$\mathrm{d}H_t=(\partial_tH(\xi_t,t)+\tfrac{1}{2}\partial_\xi^2H(\xi_t,t))\mathrm{d}t+\partial_\xi H(\xi_t,t)\mathrm{d}\xi_t, \tag{24}$$

where $\partial_tH(\xi_t,t)$ denotes $\partial H(\xi,t)/\partial t$ valued at $\xi=\xi_t$, and so on. A calculation making use of (21), (23), and (24) then shows that

$$\mathrm{d}H_t=\sigma V(\xi_t,t)\mathrm{d}W_t, \tag{25}$$

where the function $V(\xi,t)$ is

$$V(\xi,t)=\frac{\Sigma_i\pi_i(E_i-H(\xi,t))^2\exp(\sigma E_i\xi-\frac{1}{2}\sigma^2E_i^2t)}{\Sigma_i\pi_i\exp(\sigma E_i\xi-\frac{1}{2}\sigma^2E_i^2t)}. \tag{26}$$

Because H_t is an $\{\mathcal{F}_t^\xi\}$-martingale, we conclude that W_t is also an $\{\mathcal{F}_t^\xi\}$-martingale, and that establishes (b). We thus deduce that W_t is an $\{\mathcal{F}_t^\xi\}$-Brownian motion, with respect to which ξ_t is a diffusion process satisfying

$$\mathrm{d}\xi_t=\sigma H(\xi_t,t)\mathrm{d}t+\mathrm{d}W_t. \tag{27}$$

Now let $|\psi_0\rangle$ be the initial normalized state vector of the quantum system, and let $\hat{P}_i$ denote for each value of i the projection operator onto the Hilbert subspace corresponding to the energy eigenvalue E_i. We let

$$|\psi_i\rangle=\pi_i^{-1/2}\hat{P}_i|\psi_0\rangle \tag{28}$$

denote the Lüders state corresponding to E_i, and write

$$\Pi_{it}=\mathbb{P}(H=E_i|\xi_t) \tag{29}$$

for the process defined by (19). Then we can establish our main result, that

$$|\psi_t\rangle=\sum_i e^{-\mathrm{i}E_it}\Pi_{it}^{1/2}|\psi_i\rangle \tag{30}$$

satisfies the stochastic extension of the Schrödinger equation (1) with the given initial condition. In particular, by applying Ito's lemma to (19) and using (27) we obtain

$$\mathrm{d}\Pi_{it}=\sigma(E_i-H_t)\Pi_{it}\mathrm{d}W_t. \tag{31}$$

With another application of Ito's lemma we deduce that

$$\mathrm{d}\Pi_{it}^{1/2} = -\tfrac{1}{8}\sigma^2(E_i - H_t)^2\Pi_{it}^{1/2}\mathrm{d}t + \tfrac{1}{2}\sigma(E_i - H_t)\Pi_{it}^{1/2}\mathrm{d}W_t . \tag{32}$$

A short calculation then shows that (30) satisfies the stochastic equation (1), and that the expectation of the operator $\hat{H}$ in the state $|\psi_t\rangle$ is the process (20).

In summary, the stochastic equation (1) can be solved as follows. We let H be a random variable taking the values E_i with the probabilities π_i defined by (12). Letting B_t denote an independent Brownian motion, we define ξ_t as in (13). The solution of (1) is then given by

$$|\psi_t\rangle = \frac{\Sigma_i \sqrt{\pi_i}\,\exp(-\mathrm{i}E_i t + \frac{1}{2}\sigma E_i \xi_t - \frac{1}{4}\sigma^2 E_i^2 t)|\psi_i\rangle}{(\Sigma_i \pi_i \exp(\sigma E_i \xi_t - \frac{1}{2}\sigma^2 E_i^2 t))^{1/2}}, \tag{33}$$

where the $\{\mathcal{F}_t^{\xi}\}$-Brownian motion W_t driving $|\psi_t\rangle$ in (1) is given by (21). Expression (20) for H_t follows at once from (33) since $\langle\psi_i|\hat{H}|\psi_j\rangle = E_i\delta_{ij}$, and for the variance of the energy we deduce that $V_t = V(\xi_t, t)$. To obtain a realization of the process $|\psi_t\rangle$, i.e., to carry out a simulation, we simply choose a value for H in accordance with the given probability law, and then let B_t run its course.

The fact that (20) is indeed a reduction process can be verified directly as follows. Suppose, in a particular realization of the process H_t, the random variable H takes the value E_j for some choice of the index j. Writing $\omega_{ij} = E_i - E_j$ and seting $\xi_t = \sigma E_j t + B_t$, we obtain

$$H_t = \frac{\pi_j E_j + \Sigma_{i(\neq j)} \pi_i E_i \exp(\sigma\omega_{ij} B_t - \frac{1}{2}\sigma^2\omega_{ij}^2 t)}{\pi_j + \Sigma_{i(\neq j)} \pi_i \exp(\sigma\omega_{ij} B_t - \frac{1}{2}\sigma^2\omega_{ij}^2 t)}, \tag{34}$$

for the corresponding realization of H_t. However, the exponential martingale M_{ijt} defined for $i \neq j$ by

$$M_{ijt} = \exp(\sigma\omega_{ij} B_t - \tfrac{1}{2}\sigma^2\omega_{ij}^2 t) \tag{35}$$

that appears in expression (34) has the property

$$\lim_{t\to\infty} \mathbb{P}(M_{ijt} > 0) = 0. \tag{36}$$

Given that

$$H_t = \frac{\pi_j E_j + \Sigma_{i(\neq j)} \pi_i E_i M_{ijt}}{\pi_j + \Sigma_{i(\neq j)} \pi_i M_{ijt}}, \tag{37}$$

we see that H_t converges to the value E_j with probability one. A similar argument shows that if $H = E_j$, then for each value of i we have $\lim_{t\to\infty}\Pi_{it} = 0$ unless $i = j$, which allows us to verify that $|\psi_t\rangle$ converges to the Lüders state corresponding to the energy eigenvalue E_j with probability one.[4]

Therefore, we see that the random variable H can be identified with the terminal value H_∞ of the energy process. The fact that H is not $\mathcal{F}_t^W$-measurable for $t < \infty$ indicates that the "true value" of H is "hidden" until the reduction process is complete. On a related point we note that in stochastic models for state reduction it is sometimes assumed that the driving process W_t is in some way "external" to the quantum system. This assumption, however, is unnecessary: the filtrations associated with W_t, ξ_t, H_t, and $|\psi_t\rangle$ all coincide, and it is thus consistent to regard the innovation process W_t as being endogenous.

The advantage of expressions (20) and (33) from a computational point of view is that H_t and $|\psi_t\rangle$ are expressed *algebraically* in terms of the underlying random variable H and the Brownian motion B_t. These quantities can be thought of as representing independent *state variables* for the reduction dynamics. As a consequence, we are able to investigate properties of the process (1) directly without having to resort to numerical integration. In particular, by use of (33), a numerical simulation of the state reduction of complex systems is feasible, including cases for which the Hamiltonian has a nondiscrete spectrum. It should be emphasized that in our simulation methodology there is no need at any stage for the introduction of a change of probability measure.

In conclusion we present a probabilistic analysis of the timescale associated with the reduction process, in the case of a two-state system with energies E_1 and E_2. The initial state is given by $|\psi_0\rangle$, and the transition probabilities to the energy eigenstates $|E_1\rangle$ and $|E_2\rangle$ are given by π_1 and π_2.

Suppose a measurement of the energy is made, and we condition on the outcome of the measurement being E_1. In that case, according to (37), we have

$$H_t=\frac{\pi_1 E_1+\pi_2 E_2 M_{21t}}{\pi_1+\pi_2 M_{21t}}, \tag{38}$$

where

$$M_{21t}=\exp\left(\sigma\omega_{21}B_t-\tfrac{1}{2}\sigma^2\omega_{21}^2 t\right). \tag{39}$$

Writing $\beta=\frac{1}{4}\sigma^2\omega_{21}^2$ for the parameter that determines the characteristic rate of reduction, we can work out the probability that $M_{21t}<e^{-n}$ for some value of n. Since B_t is normally distributed with zero mean and variance t, we find

$$\mathbb{P}(M_{21t}<e^{-n})=N((\beta t)^{1/2}-\tfrac{1}{2}n(\beta t)^{-1/2}), \tag{40}$$

where $N(x)$ is the standard normal distribution function. Therefore, for example, we see that provided $t>5\tau_R$, we have

$$\mathbb{P}(M_{21t}<e^{-10})>\tfrac{1}{2}, \tag{41}$$

where $\tau_R=1/\beta$. In particular, as H_t draws near E_1 we have the relation

$$H_t-E_1\sim\frac{\pi_2}{\pi_1}(E_2-E_1)M_{21t}. \tag{42}$$

Thus, after only a relatively few multiples of the characteristic reduction timescale, the amount by which H_t differs from E_1 will with high probability be reduced to a tiny fraction of the energy difference E_2-E_1.

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