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FAST TRACK COMMUNICATION

Nonlinearity and constrained quantum motion

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Abstract
The dynamical equation satisfied by the density matrix when a quantum system is subjected to one or more constraints arising from conserved quantities is derived. The resulting nonlinear evolution of the density matrix has the property that it is independent of the specific composition of the pure-state mixture generating the initial state of the system.

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A nonlinear generalization of quantum mechanics was proposed by Mielnik [1, 2], Kibble [3] and Weinberg [4] as an alternative to the linear evolution governed by the Schrödinger equation. The idea of this theory is to replace the linear Hamiltonian operator generating the dynamics of the state vector with a state-dependent operator in such a way that the norm of the state vector remains constant. The properties of such 'nonlinear observables' were subsequently studied in detail by Weinberg [5].

Following Weinberg's analysis, it was argued by Gisin [6, 7] and Polchinski [8] that the existence of dynamical nonlinearities in quantum mechanics might lead to undesirable physical features, such as the possibility of superluminal EPR communication. Indeed, it is often held that the main issue associated with dynamics of the Mielnik–Kibble–Weinberg (MKW) type is that the evolution of a density matrix depends in general on the specific choice of pure-state mixture underlying the initial density matrix. Thus, by observing the dynamics one might be able to infer the particular choice of mixture associated with the initial density matrix (Haag and Bannier [9], Waniewski [10]), which is contrary to the fundamental notion that the initial density matrix is a sufficient characterization of the initial state of the system, and that its composition is irrelevant.

Another potentially problematic aspect of nonlinear quantum mechanics was suggested by Peres [11], who provided an example where the von Neumann entropy decreases with time. Tight experimental bounds on the deviation away from the linear evolution law have been found [12], while criticism of the MKW theory has been strengthened further by Mielnik [13]. As a consequence of these studies, one might conclude that a consensus has emerged to the effect that nonlinear quantum mechanics of the MKW type must be ruled out on physical grounds.

The purpose of the present communication is to report a generalization of the MKW theory that circumvents some of these issues. The nonlinear dynamics that we propose emerges from the consideration of constrained quantum motion. We shall derive the dynamical equation satisfied by a density matrix when unitarity is compromised by the existence of one or more constraints. We demonstrate that although the resulting equations of motion are nonlinear, the associated evolution is autonomous and hence independent of the choice of initial mixture. We conclude that the nonlinearities arising from the type of constraints considered here can be regarded as representing a viable step towards an acceptable generalization of the unitary evolution of quantum mechanics.

Constrained motions appear not infrequently in the general study of dynamical systems [14]. A systematic investigation of constrained motion in classical mechanics from a Hamiltonian point of view was carried out by Dirac [15, 16]. In classical mechanics, the evolution is governed by a symplectic flow on phase space. The idea of Dirac, in essence, is to find the induced symplectic structure on the constraint surface in phase space, and to use this to characterize the dynamics. Dirac's approach has been applied in the quantum context to obtain the constrained dynamical equations satisfied by pure states [17–19] in various examples. In this communication we apply similar techniques to derive constrained equations of motion for mixed states, and to show that in the case of a pure-state density matrix the equations reduce to the results obtained previously. We consider in particular the special case where the constraints are given by the conservation of the expectation values of a family of mutually incompatible observables $\{\hat{\Phi}^k\}$ $(k = 1, \ldots, N)$ satisfying $[\hat{H}, \hat{\Phi}^k] \neq 0$ for all k, where $\hat{H}$ is the Hamiltonian. Given an initial mixed-state density matrix $\hat{\rho}_0$ there are infinitely many different mixtures of pure states that give rise to $\hat{\rho}_0$ [20]. In our scheme, nevertheless, the resulting nonlinear evolution for the density matrix is independent of the specific choice of mixture. We show additionally that the von Neumann entropy is a constant of the motion for one version of the dynamics we consider, and hence that the criticism of Peres does not apply to the constrained dynamics arising in that case.

Let us now present our analysis. As remarked above, the constraints that arise most naturally in the constrained motions of density matrices involve the conservation in expectation of a family of observables $\{\hat{\Phi}^k\}_{k=1,\ldots,N}$ so that

$$\mathrm{tr}(\hat{\rho}\hat{\Phi}^k) = c^k \tag{1}$$

for all k, where $\{c^k\}$ are constants. For the moment we shall assume that N is even. The constraints are taken to be nonredundant in the sense that we require $[\hat{\Phi}^k, \hat{\Phi}^l] \neq 0$ for $k \neq l$ and $[\hat{H}, \hat{\Phi}^k] \neq 0$ for all k. We shall impose (1) by the use of Lagrange multipliers, and write

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = \mathrm{i}[\hat{\rho}, \hat{H}] - \mathrm{i}\sum_{k=1}^{N} \lambda_k[\hat{\rho}, \hat{\Phi}^k] \tag{2}$$

for the proposed dynamics of the density matrix. Here $\{\lambda_k\}$, $k = 1, \ldots, N$, are the Lagrange multipliers conjugate to the constraints $\{c^k\}$. In what follows we employ the usual convention that repeated indices are summed.

The object is to impose the constraints and derive explicit formulae (given by nonlinear functionals of $\hat{\rho}$) for the Lagrange multipliers. To derive the $\{\lambda_k\}$ we observe that equation (1) implies that

$$\mathrm{tr}\left(\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t}\,\hat{\Phi}^k\right) = 0. \tag{3}$$

Substituting (2) in (3) gives

$$\mathrm{tr}([\hat{\rho}, \hat{H}]\hat{\Phi}^k]) - \lambda_j \mathrm{tr}([\hat{\rho}, \hat{\Phi}^j]\hat{\Phi}^k) = 0. \tag{4}$$

By the cyclic property of the trace operation, equation (4) can be rewritten in the form

$$\mathrm{tr}(\hat{\rho}[\hat{H}, \hat{\Phi}^k]) - \lambda_j \mathrm{tr}(\hat{\rho}[\hat{\Phi}^j, \hat{\Phi}^k]) = 0. \tag{5}$$

To proceed we define the antisymmetric matrix w^{jk} by setting

$$w^{jk} = \mathrm{tr}(\hat{\rho}[\hat{\Phi}^j, \hat{\Phi}^k]). \tag{6}$$

Provided that w^{jk} is nonsingular, which we assume holds at least initially, let us write w_{ij} for its inverse so that $w_{ij} w^{jk} = \delta_i^k$. Then the equation reads

$$\mathrm{tr}(\hat{\rho}[\hat{H}, \hat{\Phi}^k]) = \lambda_j w^{jk} \tag{7}$$

and we can solve (5) for the Lagrange multipliers to obtain

$$\lambda_k = w_{jk}\, \mathrm{tr}(\hat{\rho}[\hat{H}, \hat{\Phi}^j]). \tag{8}$$

Substitution of this expression into (2) gives

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = \mathrm{i}[\hat{\rho}, \hat{H}] - \mathrm{i} w_{jk}\, \mathrm{tr}(\hat{\rho}[\hat{H}, \hat{\Phi}^j])[\hat{\rho}, \hat{\Phi}^k]. \tag{9}$$

This is the nonlinear equation of motion satisfied by the density matrix when it is subject to an even number of constraints of the form (1).

Our objective next is to show that in the case of a pure-state density matrix the evolution equation (9) reduces in effect to the nonlinear Schrödinger equation obtained in [18]. In particular, suppose that $\hat{\rho}$ is a time-dependent pure-state density matrix of the form

$$\hat{\rho} = \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle} \tag{10}$$

for some time-dependent state vector $|\psi\rangle$, not necessarily normalized. Then we see that

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = \frac{|\dot{\psi}\rangle\langle\psi|}{\langle\psi|\psi\rangle} + \frac{|\psi\rangle\langle\dot{\psi}|}{\langle\psi|\psi\rangle} - \frac{|\psi\rangle\langle\psi|}{\langle\psi|\psi\rangle^2}(\langle\dot{\psi}|\psi\rangle + \langle\psi|\dot{\psi}\rangle), \tag{11}$$

and hence that

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t}|\psi\rangle = |\dot{\psi}\rangle - \frac{\langle\psi|\dot{\psi}\rangle}{\langle\psi|\psi\rangle}|\psi\rangle. \tag{12}$$

Therefore, for example, if $\hat{\rho}$ is assumed to satisfy the von Neumann equation

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = \mathrm{i}[\hat{\rho}, \hat{H}], \tag{13}$$

we can deduce that $|\psi\rangle$ satisfies the so-called projective Schrödinger equation

$$|\dot{\psi}\rangle - \frac{\langle\psi|\dot{\psi}\rangle}{\langle\psi|\psi\rangle}|\psi\rangle = -\mathrm{i}(\hat{H} - \langle\hat{H}\rangle)|\psi\rangle, \tag{14}$$

where $\langle\hat{H}\rangle$ denotes the expectation of the Hamiltonian:

$$\langle\hat{H}\rangle = \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle}. \tag{15}$$

The projective Schrödinger equation is essentially a slightly 'weakened' form of the full Schrödinger equation

$$|\dot{\psi}\rangle = -\mathrm{i}\hat{H}|\psi\rangle, \tag{16}$$

with the 'unphysical' component of $|\dot{\psi}\rangle$ in the direction of $|\psi\rangle$ removed. Clearly (16) implies (14). It is worth noting, however, that although (16) is linear, the associated projective equation (14), which embodies the physical content of the Schrödinger equation, is nonlinear.

In the case of a constrained quantum system satisfying (2), essentially the same line of argument applies, and a short calculation shows that if $\hat{\rho}$ is a pure-state density matrix then

$$|\dot{\psi}\rangle - \frac{\langle\psi|\dot{\psi}\rangle}{\langle\psi|\psi\rangle}|\psi\rangle = -\mathrm{i}(\hat{H} - \langle\hat{H}\rangle)|\psi\rangle + \mathrm{i}\lambda_k(\hat{\Phi}^k - \langle\hat{\Phi}^k\rangle)|\psi\rangle, \tag{17}$$

where

$$\langle\hat{\Phi}^k\rangle = \frac{\langle\psi|\hat{\Phi}^k|\psi\rangle}{\langle\psi|\psi\rangle}, \tag{18}$$

and where by analogy with (6) and (8) we have defined

$$\lambda_k = w_{jk}\frac{\langle\psi|[\hat{H}, \hat{\Phi}^j]|\psi\rangle}{\langle\psi|\psi\rangle}. \tag{19}$$

Here w_{jk} is the inverse of the matrix w^{ij} defined by

$$w^{ij} = \frac{\langle\psi|[\hat{\Phi}^i, \hat{\Phi}^j]|\psi\rangle}{\langle\psi|\psi\rangle}. \tag{20}$$

This result is consistent with the equation derived in [18], and thus we are able to conclude that the dynamical equation (9) is a natural mixed-state generalization of the constrained equation of motion for pure states.

We remark, as we discuss in more detail below, that the motion generated by the dynamical equation (9) depends only on the initial density matrix, and not on the choice of mixture leading to that matrix. This follows from the fact that the dynamical equation (9) is autonomous in $\hat{\rho}$.

In addition, we can verify, by use of the cyclic property of the trace operation, that the von Neumann entropy, defined by

$$S = -\mathrm{tr}(\hat{\rho}\ln\hat{\rho}), \tag{21}$$

is a constant of motion. The proof is as follows. First we note that if we let $p_n(t)$ denote the components of $\hat{\rho}$ along the diagonal in a Hilbert space basis with respect to which $\hat{\rho}$ is diagonalized, we have

$$\begin{aligned}\frac{\mathrm{d}S}{\mathrm{d}t} &= -\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{tr}(\hat{\rho}\ln\hat{\rho}) \\ &= -\frac{\mathrm{d}}{\mathrm{d}t}\sum_n p_n \ln p_n \\ &= -\sum_n \dot{p}_n \ln p_n \\ &= -\,\mathrm{tr}\left(\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t}\ln\hat{\rho}\right).\end{aligned} \tag{22}$$

Then by use of the dynamical equation (9) for the density matrix we obtain

$$\begin{aligned}\frac{\mathrm{d}S}{\mathrm{d}t} &= -\mathrm{i}\,\mathrm{tr}\left([\hat{H} - \sum_k \lambda_k\hat{\Phi}^k, \hat{\rho}]\ \ln\hat{\rho}\right) \\ &= -\mathrm{i}\,\mathrm{tr}\left([\ln\hat{\rho}, \hat{\rho}]\left(\hat{H} - \sum_k \lambda_k\hat{\Phi}^k\right)\right) \\ &= 0,\end{aligned} \tag{23}$$

by virtue of the cyclic property of the trace, and by use of the fact that $\hat{\rho}$ and $\ln\hat{\rho}$ commute. We can therefore regard (9) as representing a plausible candidate for an acceptable extension of the standard unitary dynamics defined by the von Neumann equation.

We observe that the objections originally raised against nonlinear extensions of quantum mechanics were based implicitly on the essentially mistaken premise that the dynamics of a general mixed-state density matrix can and must be deduced from the dynamics of pure states. More precisely, if the initial density matrix $\hat{\rho}(0)$ happens to admit a decomposition of the form

$$\hat{\rho}(0) = \sum_n p_n \hat{\Pi}_n(0), \tag{24}$$

where $\{\hat{\Pi}_n(0)\}_{n=1,\ldots}$ are normalized projection operators onto a set of pure states $\{|\psi_n\rangle_{t=0}\}_{n=1,\ldots}$, then it was *assumed* that the subsequent dynamics of the density matrix would have to be of the linear form

$$\hat{\rho}(t) = \sum_n p_n \hat{\Pi}_n(t). \tag{25}$$

The point is that in his original analysis Gisin [6, 7] apparently had no way to deduce the dynamics of the density matrix except to regard it as following from the dynamics of pure states. From a modern perspective, however, we can take essentially the opposite view, and regard the density matrix as 'fundamentally' representing the state of the system, from which properties of pure states can be deduced as special cases. Hence, in particular, there is no reason to suppose that the dynamics of $\hat{\rho}$ can or should be deduced, linearly, from the dynamics of a set of hypothetical ensemble constituents. An analogous point of view has been advocated in the work of Czachor [21, 22].

So far we have considered the case for which the number N of conserved observables is even. If N is odd, then the antisymmetric matrix w^{jk} defined in (6) cannot be inverted. Thus, to obtain a system of constrained equations of motion that are applicable to the case for which N is odd we need to modify the foregoing analysis. The idea is to replace the commutator in (2) by a symmetric product of the form

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = \mathrm{i}[\hat{\rho}, \hat{H}] - \lambda_k(\{\hat{\rho}, \hat{\Phi}^k\} - 2\,\mathrm{tr}(\hat{\rho}\hat{\Phi}^k)\hat{\rho}), \tag{26}$$

where $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$ denotes the anticommutator and where the $\{\lambda_k\}$ comprise a set of Lagrange multipliers chosen to ensure the constraints (1), where N need not be even. The plan is to circumvent the problem of the lack of invertibility of w^{jk} arising from the antisymmetric feature of the commutator by replacing it with a symmetric anticommutator $\{\hat{\rho}, \hat{\Phi}^k\}$. The additional trace term on the right-hand side of (26) is to ensure conservation of the total probability so that

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{tr}\hat{\rho} = 0, \tag{27}$$

which follows at once from equation (26).

As before, we determine the Lagrange multipliers by considering the conservation relation (3). Substituting (26) in (3), and using the cyclic property of the trace, we deduce that

$$\mathrm{tr}(\hat{\rho}[\hat{H}, \hat{\Phi}^k]) = -\mathrm{i}\lambda_j(\mathrm{tr}(\hat{\rho}\{\hat{\Phi}^j, \hat{\Phi}^k\}) - 2\,\mathrm{tr}(\hat{\rho}\hat{\Phi}^j)\,\mathrm{tr}(\hat{\rho}\hat{\Phi}^k)). \tag{28}$$

To solve (28) for λ_j we define the symmetric covariance matrix

$$m^{jk} = \mathrm{tr}(\hat{\rho}\{\hat{\Phi}^j, \hat{\Phi}^k\}) - 2\,\mathrm{tr}(\hat{\rho}\hat{\Phi}^j)\,\mathrm{tr}(\hat{\rho}\hat{\Phi}^k). \tag{29}$$

Again, if m^{jk} is nonsingular, we can define its inverse m_{ij} which satisfies $m_{ij}m^{jk} = \delta_i^k$. In this case, we obtain the following expression for the Lagrange multipliers:

$$\lambda_j = \mathrm{i}m_{jk}\,\mathrm{tr}(\hat{\rho}[\hat{H}, \hat{\Phi}^k]). \tag{30}$$

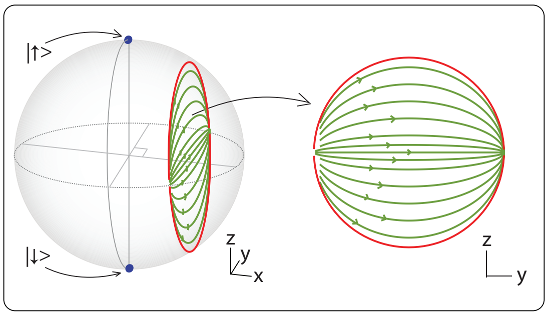

Figure 1. *Constrained dynamics for mixed states in the case of a spin-$\frac{1}{2}$ system*: The state space is a 'Bloch ball' $\mathcal{B}$ of unit radius; pure states form the boundary (surface) of $\mathcal{B}$ and interior points represent mixed states. The Hamiltonian of the system is given by $\hat{H} = \hat{\sigma}_z$. Hence, under unitarity motion the evolution generates a rigid rotation of $\mathcal{B}$ around the z-axis. We constrain the motion by fixing the expectation of $\hat{\sigma}_x$; the resulting constraint surface is a slice of $\mathcal{B}$ perpendicular to the x-axis, as indicated above. Irrespective of the initial condition, the motion converges asymptotically to the pure state for which $\langle\hat{\sigma}_z\rangle = 0$. The integral curves associated with the dynamical equation are shown in the figure.

(This figure is in colour only in the electronic version)

The invertibility of the matrix m^{jk} is ensured by the positive-definiteness of the covariance matrix, which holds if $\hat{\rho}$ is itself nonsingular. Therefore, under this assumption the generalized equation of motion becomes

$$\frac{\mathrm{d}\hat{\rho}}{\mathrm{d}t} = \mathrm{i}[\hat{\rho}, \hat{H}] - \mathrm{i}m_{jk}\,\mathrm{tr}(\hat{\rho}[\hat{H}, \hat{\Phi}^k])(\{\hat{\rho}, \hat{\Phi}^j\} - 2\,\mathrm{tr}(\hat{\rho}\hat{\Phi}^j)\hat{\rho}). \tag{31}$$

We remark, incidentally, that an analogous dynamical equation has been considered in the context of dissipative quantum dynamics [23].

Example. As an illustration let us consider the case of a spin-$\frac{1}{2}$ system for which $\hat{H} = \hat{\sigma}_z$ and the single constraint observable is chosen to be $\hat{\Phi} = \hat{\sigma}_x$. The resulting motion for the density matrix is shown in figure 1. The space of density matrices in this case is a 'Bloch ball' $\mathcal{B}$. The mixed states correspond to the interior points of $\mathcal{B}$ and the pure states form the surface of $\mathcal{B}$. The chosen Hamiltonian would in the unconstrained case generate a rigid rotation around the z-axis. As we constrain the motion of the system by imposing the condition that the expectation of $\hat{\sigma}_x$ must be conserved, the resulting constraint surface corresponds to a cross-section of $\mathcal{B}$ at $x = x_0$, where $\mathrm{tr}(\hat{\rho}\hat{\sigma}_x) = x_0$. From (31) we deduce the equation of motion for the system, and find, as is shown in figure 1, that when the initial state is given by a pure-state density matrix, the state of the system remains pure as it evolves. In this case, the example reduces to the case considered in [24]. The mixed state evolution trajectories are also shown for a choice of initial states in the figure. The equator on the surface of $\mathcal{B}$ corresponds to a set of fixed points. Hence, a state that initially lies at the point to the far left of the cross-section in figure 1 remains fixed, and all other states evolve asymptotically towards the fixed point to the right in the figure.

Returning now to equation (31), we note that in the special case for which $\hat{\rho}$ is a pure-state density matrix of the form (10) we are able to deduce a nonlinear projective Schrödinger equation satisfied by the state vector $|\psi\rangle$ that is applicable to both even and odd number of conserved observables. This is given by

$$|\dot{\psi}\rangle - \frac{\langle\psi|\dot{\psi}\rangle}{\langle\psi|\psi\rangle}|\psi\rangle = -\mathrm{i}(\hat{H} - \langle\hat{H}\rangle)|\psi\rangle - \lambda_k(\hat{\Phi}^k - \langle\hat{\Phi}^k\rangle)|\psi\rangle, \tag{32}$$

which is consistent with the result obtained in [24]. Therefore, (31) constitutes a natural generalization of the result of [24] to the case of general density matrices.

It is interesting to observe that, unlike the motion determined by (9), the motion determined by (31), which is applicable to any number of constraints, does not necessarily preserve the von Neumann entropy. In particular, the entropy production is given by

$$\frac{\mathrm{d}S}{\mathrm{d}t} = -2\lambda_k \operatorname{cov}(\hat{\Phi}^k, \ln\hat{\rho}), \tag{33}$$

where $\operatorname{cov}(\hat{X}, \hat{Y}) = \mathrm{tr}(\hat{\rho}\hat{X}\hat{Y}) - \mathrm{tr}(\hat{\rho}\hat{X})\,\mathrm{tr}(\hat{\rho}\hat{Y})$. The derivative of the entropy vanishes identically for pure states, which is why the pure-state limit (32) is well defined. In general, however, we see that S is not necessarily constant. This is evident in the example shown in figure 1. On the other hand, just as in equation (9), the evolution equation (31) is autonomous and independent of the specific composition of the mixture. Whether the fact that the entropy is variable raises an issue remains an open question.

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