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# Quantum Representation of Classical Dynamics

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A constructive proof is given to show that there is an exact embedding of a classical system of  $N$  ordinary differential equations (ODEs) within a quantum mechanical system corresponding to a classical phase space of dimension  $2N$ . Doubling the classical phase space allows one to express any set of ODEs through a classical Hamiltonian that is a sum over a set of constraints. The Lagrange multipliers that enforce the constraints are canonically conjugate to the dependent variables of the original ODE and satisfy equations that ensure that the evolution of the system is symplectic. For the quantized system on extended phase space, Heisenberg's uncertainty principle is satisfied by each variable and its canonically conjugate momentum, the Lagrange multiplier. However, there is no uncertainty in a simultaneous measurement for any of the variables of the original ODE. Hence, there is complete fidelity for the quantum representation of the classical system.

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## I. INTRODUCTION

The recent growth in the computing power of quantum coherent devices has spurred great interest in the possibility of using quantum computers to simulate classical dynamics. Ultimately, one dreams of simulating high-dimensional PDEs describing the evolution of fields, fluids, and kinetic probability distribution functions. Using the “method of lines,” PDEs are reduced to large but finite sets of ODEs. Hence, finding a high-fidelity “embedding” of classical dynamics within a quantum mechanical system is of great interest.

There are a number of different strategies one might potentially employ to represent classical dynamics via quantum dynamics. The method that is perhaps most “obvious” to a physicist would be to use any valid quantization of the classical system. The quantum dynamics will track the semi-classical dynamics for arbitrarily long times in the limit that Planck's constant vanishes,  $h \rightarrow 0$ . However, for finite  $h$ , it is well known that there are interesting differences in classical and quantum behavior that begin for sufficiently long observation times. For example, this leads to well-known differences between the manifestation of quantum vs. classical chaos.

An alternate strategy is to directly express the classical Liouville equation as a quantum system with complete fidelity. Assume that one wishes to solve a system of  $N$  classical ODEs with coordinates  $\{z^j\}$  that evolve in time via

$$dz^j/dt = V^j(z, t). \quad (1)$$

The collisionless dynamics of the evolution of the probability distribution function  $f$  is described by the Liouville equation:

$$\partial_t f + \partial_{z^j}(V^j f) = 0. \quad (2)$$

Simply multiplying the Liouville equation by  $i\hbar$  allows one to rewrite this as a Schrödinger-like equation:

$$\hat{\mathcal{H}}f = i\hbar\partial_t f = -i\hbar\partial_{z^j}(V^j f) = \hat{P}_j(V^j f). \quad (3)$$

However, this “Schrödinger equation” is first order in partial derivatives, rather than in the usual second order form. As noted by Chirikov [1], this linear Schrödinger equation precisely tracks the classical evolution.

Performing this “trick” requires doubling the classical phase space from  $\{z^j\}$  to  $\{z^j, P_j\}$ . This is simple to understand from an alternate point of view. Any set of  $N$  classical ODEs can always be generated by using an action principle on a  $2N$  dimensional phase space. The action is

$$S = \int (P_j dz^j - \mathcal{H} dt) \quad (4)$$

with the Hamiltonian

$$\mathcal{H} = P_j V^j(z, t). \quad (5)$$

For this action principle, the Hamiltonian is simply a sum over a set of constraints. Variation with respect to the Lagrange multiplier  $P_j$  generates the classical equation of motion for the  $z^j$  coordinate. Variation with respect to  $z^j$  generates the classical equation of motion for the Lagrange multiplier  $P_j$ :

$$\dot{P}_j = -P_k \partial_{z^j} V^k(z, t). \quad (6)$$

These equations of motion ensure that the transformation of  $\{z^j, P_j\}$  between different points in time always remains symplectic, and, in fact, canonical.

Using this doubly extended phase space implies that the Heisenberg uncertainty principle only applies to the pairs  $\{z^j, P_j\}$ . There is no uncertainty in a simultaneous measurement of any pair of coordinates  $\{z^i, z^j\}$ . Hence, this embedding of the classical system into a quantum system has complete fidelity.

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## II. HAMILTONIAN DYNAMICS

The procedure outlined above works for any system of ODEs, yet Hamiltonian systems of ODEs are of greatest interest from the point of view of fundamental physics.

### A. General Hamiltonian System

A Hamiltonian system of  $N$  equations is defined by its Hamiltonian  $H$  as well as its classical Poisson bracket  $\{A, B\} = J^{jk}(z, t)\partial_{z^j}A\partial_{z^k}B$ . The Poisson bracket must be antisymmetric and must satisfy the Jacobi identity. The classical equations of motion are

$$\dot{z}^j = \{z^j, H\} = J^{jk}\partial_{z^k}H. \quad (7)$$

The corresponding classically constrained Hamiltonian is

$$\mathcal{H} = P_j\{z^j, H\} = P_jJ^{jk}\partial_{z^k}H. \quad (8)$$

This leads to the following dynamics of the Lagrange multipliers:

$$\dot{P}_i = -P_j\partial_{z^i}(J^{jk}\partial_{z^k}H). \quad (9)$$

The ‘‘Schrodinger equation’’ corresponding to the Liouville equation is

$$\hat{\mathcal{H}} = \hat{P}_j\{z^j, H\} = \hat{P}_j(J^{jk}\partial_{z^k}H) \quad (10)$$

$$= -i\hbar(\partial_{z^k}H)J^{jk}\hat{P}_k - i\hbar(\partial_{z^j}J^{jk})(\partial_{z^k}H). \quad (11)$$

Once again, the Heisenberg uncertainty principle only applies to the pairs  $\{z^j, P_{z^j}\}$ .

### B. Canonical Hamiltonian System

For a system of canonical coordinates  $\{q^j, p^j\}$ , the Poisson bracket takes the canonical form  $J^{q^i p^j} = -J^{p^j q^i} = \delta_j^i$ . Hence, the evolution equations are in canonical form

$$\dot{q}^j = \partial_{p_j}H \quad \dot{p}_j = -\partial_{q^j}H. \quad (12)$$

Introducing the Lagrange multipliers  $\{P_j, Q^j\}$  corresponding to  $\{q^j, p^j\}$ , respectively, the constrained Hamiltonian takes the form

$$\mathcal{H} = (P_k\partial_{p_k} - Q^k\partial_{q^k})H. \quad (13)$$

The equations of motion of the Lagrange multipliers are

$$\dot{Q}^j = (P_k\partial_{p_k} - Q^k\partial_{q^k})\partial_{p_j}H \quad (14)$$

$$\dot{P}_j = -(P_k\partial_{p_k} - Q^k\partial_{q^k})\partial_{q^j}H. \quad (15)$$

The quantum Hamiltonian corresponding to the Liouville equation is

$$\hat{\mathcal{H}}f = (\hat{P}_j\partial_{p_j} - \hat{Q}^j\partial_{q^j})Hf \quad (16)$$

$$= -i\hbar(\partial_{p_j}H \cdot \partial_{q^j} - \partial_{q^j}H \cdot \partial_{p_j})f. \quad (17)$$

Once again, the Heisenberg uncertainty principle only applies to the pairs  $\{q^j, P_j\}$  and  $\{p_j, Q^j\}$ , but not to the pairs of  $\{q^j, p_j\}$ .

## III. EXAMPLES

### A. First order Autonomous ODE

The first example is simply an autonomous ODE in a single variable:

$$\dot{z} = V(z) \quad (18)$$

The constrained Hamiltonian is

$$\mathcal{H} = PV(z). \quad (19)$$

The classical dynamics on the extended phase space is

$$\dot{z} = V(z) \quad \dot{P} = -PV'(z). \quad (20)$$

The classical solution to the  $\dot{P}$  equation is simply

$$P = P_0e^{-V(z)}. \quad (21)$$

Since these equations are symplectic, the Jacobian is constant, as can be checked directly from the equations of motion.

For example, the ‘‘velocity’’ for exponential growth is simply  $V = \gamma z$ . The classical solutions on extended phase space are

$$z = z_0e^{\gamma t} \quad P = P_0e^{-\gamma z}. \quad (22)$$

Rewriting the Liouville equation as a ‘‘Schrodinger equation’’ yields

$$\hat{\mathcal{H}}f = \hat{P}Vf = -i\hbar\partial_z(Vf). \quad (23)$$

### B. Harmonic Oscillator

Consider the classical harmonic oscillator in  $\{q, p\}$  coordinates. The classical Hamiltonian of interest is

$$H = \omega_0(q^2 + p^2)/2. \quad (24)$$

The dynamics can be exactly represented by the quantum Hamiltonian

$$\mathcal{H} = \omega_0(pP_q - qQ_p). \quad (25)$$

The additional nontrivial equations of motion for the Lagrange multipliers are

$$\dot{Q}_p = -\omega_0P_q \quad \dot{P}_q = \omega_0Q_p. \quad (26)$$

Hence, the dynamics on the extended phase space consists of two harmonic oscillators which rotate in opposite directions. Rewriting the Liouville equation as a ‘‘Schrodinger equation’’ yields

$$\hat{\mathcal{H}}f = -i\hbar\omega_0(p\partial_q - q\partial_p)f. \quad (27)$$

In action-angle coordinates  $\{J, \theta\}$ , the classical Hamiltonian is

$$H = \omega_0 J. \quad (28)$$

which leads to the constrained Hamiltonian

$$\mathcal{H} = \omega_0 P_\theta \quad (29)$$

which is independent of  $Q^J$ , the Lagrange multiplier corresponding to  $J$ . Rewriting the Liouville equation as a ‘‘Schrodinger equation’’ yields

$$\hat{\mathcal{H}}f = -i\hbar\omega_0\partial_\theta f. \quad (30)$$

Clearly,  $J$ ,  $Q^J$ , and  $P_\theta$  are all conserved on the extended phase space. Hence, there is a difference between

the version in action-angle coordinates and the version in  $\{q, p\}$  space, in that  $dQ^J/dt = 0$ . The dynamics of  $Q^J$  can be modified by adding a function  $E(J)$  to the Hamiltonian above. For example, choosing  $\hat{\mathcal{H}} = \omega_0(P_\theta - J)$  would lead to the same dynamics as in  $\{q, p\}$  space.

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[1] B. V. Chirikov, F. M. Izrailev, D. L. Shepelyansky, *Physica D* 33 (1988) 77.