

Quantum dynamics of two coupled qubits

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We investigate the difference between classical and quantum dynamics of coupled magnetic dipoles. We prove that in general the dynamics of the classical interaction Hamiltonian differs from the corresponding quantum model, regardless of the initial state. The difference appears as nonpositive-definite diffusion terms in the quantum evolution equation of an appropriate positive phase-space probability density. Thus, it is not possible to express the dynamics in terms of a convolution of a positive transition probability function and the initial condition as can be done in the classical case. It is this feature that enables the quantum system to evolve to an entangled state. We conclude that the dynamics are a quantum element of nuclear magnetic resonance quantum-information processing. There are two limits where our quantum evolution coincides with the classical one: the short-time limit before spin-spin interaction sets in and the long-time limit when phase diffusion is incorporated.

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I. INTRODUCTION

Recent work in quantum-information theory has suggested that quantum computers are more powerful than their classical counterparts [1–6]. In quantum communication, there already exist algorithms which have been proved to outperform their classical counterparts [7,8]. The situation in computation is not as clear: we know of problems which have quantum algorithms that are exponentially faster but only when compared to the known classical ones [1,3,5,6,9] (not the optimum ones). The special power of quantum computers is only a conjecture as we have no proof that we cannot simulate efficiently quantum systems using classical computers. Although most physicists would believe this efficient simulation to be impossible, this is at the foundation of the distinction between classical and quantum computation.

If quantum computers are indeed more powerful than classical ones, could we pinpoint the origin of this power to one or a few elements in the quantum-mechanical theory? In the “folklore,” the power of quantum computation has been attributed to entanglement. In quantum computers where the initial states are pure it has been claimed [10,11] that the presence of entanglement distinguishes quantum and classical algorithms. Indeed the evolution of a quantum system starting in a pure state and evolving unitarily without entanglement (which could occur if there were no interactions between the components) can be efficiently simulated by a classical system; on the other hand, a classical simulation of generic quantum evolution for a pure state has no known efficient algorithm. At the basis of this argument is the ability to efficiently simulate a system by a classical computer.

The argument employed in Ref. [11], which uses the existence of an efficient classical simulation in the absence of entanglement, does not carry through when the initial state is mixed (i.e., not a pure state). That is, for some highly mixed state [12] such as the state of nuclear spins present in liquid-

state nuclear magnetic resonance (NMR), we do not know how to efficiently simulate the evolution of the system on a classical computer. For these states, the density matrix can be represented as a sum of separable states with positive coefficient (to be interpreted classically as probabilities to be in the respective states). However, under generic unitary evolutions, the choice of separable states must change. No efficient algorithms exist to relate the initial separable states to the final ones for an increasing number of spins.

We do not yet have a generic quantitative measure for entanglement, although we do have a measure for absence of entanglement. Pure states are defined as being separable, or nonentangled, if they can be expressed as products of subsystem (such as qubit) wave functions. For mixed states, this notion is generalized to the existence of at least one expansion of the state in terms of separable pure states with positive coefficients. Thus an equal mixture of the maximally entangled state of two spins (Bell states) does not contain any entanglement because this density matrix can be re-expressed in terms of separable states (for example, the computational states with equal probability). The separable states of spin-half systems could be described at a given time as a probability distribution of a set of classical tops.

The notion of entanglement for mixed states has been developed in the context of quantum communication. One definition corresponds to the number of maximally entangled states that can be an extracted ensemble of these states [13]. But a computation is inherently a dynamical process, and we do not know in general how to describe the evolution of one mixed separable state to another using an efficient classical description, in contradistinction to the pure state case. The quantum device can thus provide some information more efficiently than a classical device could.

If mixed states are used as initial states of a quantum computer, entanglement does not seem to play the essential role in distinguishing quantum and classical algorithms as it might if we used pure states. A particular example of a quan-

tum algorithm without a known efficient classical counterpart is the one given in Ref. [14]. The algorithm gives the distribution of eigenvalues of a quantum Hamiltonian. It uses as an input state an extremely mixed state, one with a single qubit in a pure state (a pseudopure state [15] would also do) and all other qubits are maximally mixed. This algorithm uses extremely mixed states but can still outperform known classical algorithms. For a small number of qubits there will definitely be no entanglement if a pseudopure state of the first bit is used; as we increase the number of bits there may or may not be entanglement. But even if it happens at the n th qubit, the algorithm will not go through any phase transition; thus, it would be meaningless to refer to the algorithm as classical before the presence of entanglement and as quantum afterwards. What distinguishes this algorithm from the classical analog is that the rules for transforming the density matrix are the quantum rules, and we do not know how to efficiently simulate them by the classical rules.

The algorithm in Ref. [14] is especially relevant in the context of recent discussions of experiments in quantum-information processing using liquid-state NMR technology [10,16]. The algorithm in Ref. [14] could be implemented in liquid-state NMR. The authors of [10] commented: “The results in this letter suggest that current NMR experiments are not true quantum computations, since no entanglement appears in the physical states at any stage.” This statement makes the assumption that entanglement is the necessary element of quantum computation following the suggestion in [11]. In the same paper [10] however, it was recognized that it may not be so easy to separate quantum dynamics and entanglement when trying to pinpoint the power of quantum computation; “The results in this letter suggest that current NMR experiments are not true quantum computations, since no entanglement appears in the physical states at any stage. We stress, however, that we have not proved this suggestion, since we would need to analyze the power of general unitary operations in their action on separable states. To reach a firm conclusion, much more needs to be understood about what it means for a computation to be a ‘quantum’ computation.” However, the claim that the evolution of unentangled pure states can be efficiently simulated by a classical computer [11] does not carry through to mixed states. The power of quantum computation can come from properties of the dynamics, not the state. This was also recognized by Schack and Caves [16]. Indeed, the real origin of the criteria in [11] is the dynamical evolution of the system not the state itself. If we apply the type of unitary transformation used in [11] to a highly mixed state (so that entanglement might not appear) it is as hard to simulate on a classical computer as when the state is initially pure. This point was not considered in Ref. [10].

Recognizing this fact, Schack and Caves attempted to explain some liquid-state NMR experiments using classical dynamics, without success [17]. They did not derive an equation of motion for the behavior of the spins but rather provided a model which described the effect of “gates” on the states. Their model did predict an exponential decay of the signal as a function of the number of gates going as $(1 + 2^{2n-1})^{-g}$ for n the number of qubits in the experiment and

g the number of gates [18]. Even in the three-qubit experiments they commented upon, the gates defined by Schack and Caves are not the physical gates implemented in the experiment as this would have ruled out their model. In the seven-qubit experiment of Ref. [19], the model predicted a decrease in the signal-to-noise ratio of $\sim 10^{40}$ smaller than observed, a number which unquestionably rules out the model. Discrepancies of their theory with older NMR experiments, although not called quantum computing at the time, are plentiful in the NMR literature, and the readers can review experiments performed twenty years ago [20,21].

What does make the quantum dynamics so hard to simulate? Could there be other classical models which explain NMR experiments? Can we understand the origin of the discrepancy between classical and quantum evolution? In this paper we compare the evolution of two coupled spin-half particles under quantum and classical evolution. The work of the last fifty years in NMR shows the consistency of experimental results with quantum mechanics and the failure to find a classical description; “The dynamics of isolated spins can be understood in terms of the motion of classical magnetization vectors. To describe coupled spins, however, it is necessary to have recourse to a quantum-mechanical formalism where the state of the system is expressed by a state function or, more generally, by a density operator [22].” Here, we will give the explicit origin for this difference for the simplest choice of a classical model; the one with the same Hamiltonian as the quantum model. In the next section we derive the evolution equation for classical and quantum interacting spin-half particles, explicitly demonstrating that the classical theory (with the same Hamiltonian) cannot reproduce the quantum equations. We then discuss implications of these equations and draw conclusions.

II. CLASSICAL AND QUANTUM DYNAMICS OF COUPLED SPIN-HALF PARTICLES

We investigate the equations of motion of classical and quantum spin-half particles and show that the quantum behavior is fundamentally different from the classical one. We show that even in the cases where the density is highly mixed (nonentangled) the evolution leads to different observable quantities. There is some ambiguity in exactly what is meant by the classical dynamics of such a system. We must agree on some ground rules to make a meaningful comparison. Semiclassical dynamics has a long history and some rules have been established [23]. We will assign a classical analogue for a quantum problem by demanding that the same functional form of the Hamiltonian be used but with the corresponding classical phase-space variables substituted for the quantum canonical operators.

In the case of a spin-half system this would appear to present some problems, but the situation is clearer if we always work in the irreducible representations of the total angular momentum of the system. There are two subspaces corresponding to total angular momentum; quantum numbers $s=1$ and $s=0$. The dynamics of a single spin-half system will conserve angular momentum. However, for two spin-half systems, with arbitrary one- and two-qubit interactions,

angular momentum need not be conserved and these subspaces will become coherently mixed. It will suffice, however, to consider one particular two qubit gate that does conserve angular momentum, which is an important two qubit gate for quantum computing and for which the classical and quantum dynamics are completely different except on a short-time scale. Furthermore, this is precisely the two qubit gate accessible in NMR quantum computing.

In order to produce entangled states of single spin-half systems, a variety of possible interactions could be used; however, in NMR the natural interaction is of the form

$$H_2 = \frac{J}{4} \hat{\sigma}_z^{(1)} \hat{\sigma}_z^{(2)} \quad (2.1)$$

with $\hbar = 1$ and the subscript 2 indicating that the interaction is between two qubits. The dynamics of two spin states that follows from this Hamiltonian is given by a unitary operator $U_2(t)$ where

$$U_2(t) = \exp\left[-i \frac{J}{4} t \hat{\sigma}_z^{(1)} \hat{\sigma}_z^{(2)}\right]. \quad (2.2)$$

In addition to this two-spin unitary operator or ‘‘gate,’’ generic quantum computation needs single spin dynamics. This is easily generated by the scalar coupling of a spin-half magnetic dipole with an applied magnetic field. The Hamiltonian for these single spin rotations for the spin labeled i is

$$H_1 = \vec{B}(t) \cdot \vec{\sigma}^{(i)}, \quad (2.3)$$

where the subscript 1 indicates that the Hamiltonian applies to a single qubit, and the corresponding unitary operator is

$$U_1(t) = \exp[-i \vec{B} \cdot \vec{\sigma}^{(i)}]. \quad (2.4)$$

We can now use U_1 and U_2 to generate an entangled state. For example, the Bell state

$$|\phi^+\rangle = \frac{|\downarrow\rangle_1 \otimes |\downarrow\rangle_2 + |\uparrow\rangle_1 \otimes |\uparrow\rangle_2}{\sqrt{2}} \quad (2.5)$$

is generated from the product state $|\downarrow\rangle_1 \otimes |\downarrow\rangle_2$ by

$$|\phi^+\rangle = e^{-i\pi/4} e^{i(\pi/4)\sigma_x^{(2)}} e^{i(\pi/4)\sigma_z^{(1)}} e^{-i(\pi/4)\sigma_y^{(2)}} e^{-i(\pi/4)\sigma_z^{(1)}\sigma_z^{(2)}} \\ \times e^{i(\pi/4)\sigma_y^{(2)}} e^{-i(\pi/4)\sigma_y^{(1)}} |\downarrow\rangle_1 \otimes |\downarrow\rangle_2. \quad (2.6)$$

In liquid-state NMR we do not begin with initial pure states, but we begin with a mixed state-density operator

$$\rho_\epsilon = \mathcal{Z}^{-1} e^{-\beta H} \quad (2.7)$$

with H the system (individual nuclear spins on a single molecule) Hamiltonian, $\beta = (k_B T^{-1})$ and $\mathcal{Z} = \text{tr} \rho_\epsilon$ [22]. At high temperature, as is the case for present-day liquid-state NMR quantum computation [15,24], the state is very close to the identity so

$$\rho_\epsilon \sim \frac{(1-\epsilon)}{2^N} \mathbb{1} + \epsilon \rho_1, \quad (2.8)$$

where $d = 2^N$ is the dimension of the Hilbert space for N qubits, $\mathbb{1}$ is the identity operator in this tensor product space, and ρ_1 is an arbitrary density operator. For example, in the case of a molecule with two spins and scalar coupling we have,

$$H = \hbar \omega_1 \hat{\sigma}_z^{(1)} + \hbar \omega_2 \hat{\sigma}_z^{(2)} + J \sigma_z^{(1)} \sigma_z^{(1)} \quad (2.9)$$

with $J \ll \omega_1, \omega_2$, and thus

$$\rho_\epsilon \approx \frac{\mathbb{1}}{4} + \frac{\epsilon}{4} (\hat{\sigma}_z^{(1)} + \mu \hat{\sigma}_z^{(2)}), \quad (2.10)$$

where μ is the ratio of the Larmor frequencies of spin 2 and 1. By a carefully tailored sequence of rf pulses, any two-spin unitary transformation of this state can be achieved. Furthermore, using a spatially nonuniform magnetic-field pulse (a gradient pulse) and averaging the varying phases over the sample, we can effect particular nonunitary transformations [25]. With these two techniques it is possible to prepare the system in a so-called *pseudopure state* of the form

$$\rho_\epsilon \approx \frac{(1-\epsilon)}{2^N} \mathbb{1} + \epsilon |\Psi\rangle\langle\Psi| \quad (2.11)$$

for $|\Psi\rangle\langle\Psi|$ a pure, and possibly entangled, state for N spins. It is possible to place bounds on the value of ϵ for which the total state in Eq. (2.10) is entangled [10], that is, a state which cannot be written as a convex combination of factorizable density operators. In typical experiments $\epsilon \approx 10^{-5}$, a value which is too small for these states to be entangled. The pseudopure states produced in two qubit NMR quantum-information processing experiments are not entangled and thus the spin-spin correlations at a fixed time have a purely classical interpretation.

Even though entangled states have not yet been produced in NMR quantum-information processing experiments, this does not mean that the system is not quantum mechanical. The important question is whether there is a classical description of the dynamics of these experiments. This is a question that can and must be answered in a way that does not depend on the initial and final states of the system. It is a question concerning the propagator, or Green’s function, for the dynamics, not the initial and final states. It is possible that the initial and final states may exhibit no quantum correlations and have a perfectly valid classical description, yet not be connected by a classical dynamical model, be it deterministic or stochastic. In the case of stochastic dynamics the answer to this question will involve a specification of transition probabilities. As we show below, via a particular but well-motivated classical model, it is possible that the initial and final states are described by separable states (and thus could be interpreted as a perfectly valid classical probability distribution) yet no positive transition probability exists to connect them either globally or infinitesimally.

The quantum dynamics of a single spin-half system, described by the Hamiltonian Eq. (2.3), is equivalent to the classical dynamics of the corresponding magnetic dipole in an applied field [16,22]. In both cases we find a linear precession of the average magnetic dipole about the direction of the applied field. Of course the states involved in the classical and quantum case are quite different. In the quantum case we can express the time-dependent state of the spin as

$$\rho(t) = \frac{1}{2} [1 + \vec{n}(t) \cdot \vec{\sigma}] \quad (2.12)$$

with $\vec{n}(t)$ a unit vector and $\vec{\sigma} = \vec{e}_x \hat{\sigma}_x + \vec{e}_y \hat{\sigma}_y + \vec{e}_z \hat{\sigma}_z$. If the quantum Hamiltonian is $\hat{H} = \vec{B} \cdot \vec{\sigma}$ the quantum dynamics are given by the solution to the Bloch equations:

$$\frac{d\vec{n}}{dt} = -\vec{B} \times \vec{n}. \quad (2.13)$$

This is the same equation of motion as a classical (unit) magnetic dipole, \vec{n} , in a magnetic field \vec{B} . The equation describes the linear precession of a point, \vec{n} , on the unit sphere around the direction of \vec{B} at a rate $|\vec{B}|$.

Instead of a single classical dipole, suppose we had a distribution of dipoles described by some initial probability distribution function on the sphere, $Q_0(\vec{n})$. As the precession on the sphere is linear, each vector will precess at the same rate $|\vec{B}|$ around the direction of \vec{B} . The distribution at time is then simply $Q_0(\vec{n}(t))$. In other words the solution of Eq. (2.13) is the characteristic equations for the equation of motion of the distribution function. The distribution simply rotates without distortion at a constant rate around \vec{B} .

However, the classical and quantum dynamics that result for two magnetic dipoles interacting via the spin-spin interaction Eq. (2.1), an entangling interaction, are very different as we show below. Thus we conclude that, while at present liquid-state NMR may not have access to entangled quantum states, it does allow us to realize quantum dynamics for those states that will not be realized classically. It is the dynamics that are quantum in liquid-state NMR not the states. Liquid-state NMR allows us to experimentally study the quantum dynamics of many coupled qubits and at present probably the most interesting element is to understand the amount of control we have on these dynamics. The corresponding classical system, with the same Hamiltonian, could never achieve this.

To explain this we first note an equivalence between the spin-spin interaction of Eq. (2.1) and a nonlinear top model. Consider the collective angular momentum operator \hat{S}_z defined by

$$\hat{S}_z = \frac{1}{2} (\hat{\sigma}_z^{(1)} + \hat{\sigma}_z^{(2)}). \quad (2.14)$$

It is then easy to see that

$$\hat{S}_z^2 = \frac{1}{2} (1 + \hat{\sigma}_z^{(1)} \hat{\sigma}_z^{(2)}). \quad (2.15)$$

Thus, up to an irrelevant additive constant, we obtain

$$H_2 \equiv \frac{J}{2} \hat{S}_z^2. \quad (2.16)$$

The question of the dynamics is reduced to studying the quantum and classical dynamics of this nonlinear top. Note that this Hamiltonian commutes with \hat{S}^2 the total angular momentum operator. Thus the system cannot evolve out of the subspaces corresponding to the irreducible representations of a two-spin system. There are two such subspaces, the triplet with $s=1$ and the singlet with $s=0$. If we begin with the state in which both spins are down, we cannot leave the triplet subspace with this Hamiltonian. Of course combinations of the two-spin and single-spin unitary operators will mix the two irreducible subspaces. However, the quantum and classical dynamics that result from the nonlinear top interaction (with the same Hamiltonian form), equivalently the two-spin interaction, are different regardless of the initial states, as we now show. To be specific we will consider the dynamics restricted to the triplet ($s=1$) subspace.

We will follow closely the presentation of Sanders [26] concerning the classical and quantum dynamics of nonlinear tops. We will assume that the physical interaction between two spins is fixed as the scalar coupling of two magnetic dipoles. The corresponding Hamiltonian is then fixed and we can compare the dynamics of observable quantities that results when the interaction is treated either quantum mechanically or classically. It is conceivable that the exact quantum dynamics could be simulated exactly by a different classical Hamiltonian. After all we could always simulate the quantum system on a classical computer, which is indeed a classical system with a very complex time-dependent Hamiltonian. However, we believe it is unlikely that any classical Hamiltonian, no matter how complex, could simulate the quantum dynamics over a fixed time interval. We will return to this point in the discussion section below.

The classical dynamics of a nonlinear top is defined by the Hamiltonian

$$H = \omega S_z + \frac{J}{2s} S_z^2, \quad (2.17)$$

where we have included a linear precession term with ω the linear precession frequency. In this case the quantity S_z is the z component of the classical angular momentum of the top. The first term describes the linear precession of the angular momentum vector about the z axis at the constant rate ω . The second term describes a nonlinear precession about the z axis at a frequency that depends on the z component of angular momentum. The classical mechanics is described by the motion of a point in a spherical phase space embedded in the three-dimensional Euclidean space with coordinates S_x, S_y, S_z with $S_x^2 + S_y^2 + S_z^2 = s^2$ [27]. The classical states are probability distributions which describes an ensemble of tops with a distribution of angular momentum directions (every top in the ensemble has the same magnitude of total angular momentum). The points on the sphere of radius s are conveniently parametrized in polar coordinates as

$$\mathbf{S}/s = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta). \quad (2.18)$$

However, we will use the stereo-graphic projection of the sphere onto the complex plane defined by the map

$$z = e^{i\phi} \tan \theta/2. \quad (2.19)$$

The north pole ($S_z = s$) is mapped to the origin ($z = 0$) and the south pole is mapped to infinity. The equator is mapped to the unit circle. In this conformal mapping, distributions with circular contours are mapped to distributions with circular contours in the complex plane. The dynamics of a distribution of points is easily described. A linear precession about the z axis simply causes a distribution of a point to rotate about the origin in the complex plane without changing its shape. However, the nonlinear precession causes the distribution to shear as different parts of the distribution with different values for S_z may have different precession rates. In the long-time limit the distribution will tend to become smeared around the origin in the complex plane (see Sanders [26] for a pictorial representation). As we will see this is very different from what happens in the quantum case where the shearing ceases after some time and revivals and fractional revivals of the initial state occur.

In order to make a comparison with the quantum dynamics we need to consider the dynamics of a distribution of points on the sphere. This is because a quantum state cannot be perfectly localized at a point on the sphere. The classical state of the system is described by a probability distribution $Q(z)$ of the vector \mathbf{S} corresponding to z . The expectation values for the components of angular momentum are given by

$$\mathcal{E}(S_z) = \int d\mu(z) Q(z) \frac{s(1 - |z|^2)}{1 + |z|^2}, \quad (2.20)$$

$$\mathcal{E}(S_x - iS_y) = \int d\mu(z) Q(z) \frac{2sz^*}{1 + |z|^2}, \quad (2.21)$$

where the integration measure in the stereographic plane is

$$d\mu(z) = \frac{2s+1}{\pi} (1 + |z|^2)^{-2}. \quad (2.22)$$

We have chosen the prefactor $2s+1$ as a scaling of the classical probability distribution, which makes the comparison with the quantum case more convenient.

The classical dynamics are described by a Liouville equation

$$\frac{\partial Q}{\partial t} = \{H, Q\}, \quad (2.23)$$

where the Poisson bracket $\{, \}$ may be determined using $\{S_i, S_j\} = \sum_k \epsilon_{ijk} S_k$. The Liouville equation is a first-order partial differential equation of the form

$$\frac{\partial Q(z, t)}{\partial t} = -\dot{z} \frac{\partial}{\partial z} Q(z, t) + \text{c.c.}, \quad (2.24)$$

where the equations of motion are

$$\dot{z} = i \left(\omega + J \frac{1 - |z|^2}{1 + |z|^2} \right) z. \quad (2.25)$$

The solution to this is easily found after noting that $|z|^2$ is a constant of motion. Thus

$$z(t) = \exp \left[-it \left(\omega + J \frac{1 - |z|^2}{1 + |z|^2} \right) \right] z(0), \quad (2.26)$$

which in polar coordinates becomes

$$\theta(t) = \theta_0, \quad (2.27)$$

$$\phi(t) = \phi_0 - \omega t - Jt \cos \theta_0, \quad (2.28)$$

where ϕ_0, θ_0 are the initial values. In this form it is particularly easy to see that the dynamics are a rotational shear of the sphere around the z axis.

The solution for the probability density is

$$Q(z, t) = \int d^2z' \mathcal{T}(z, z'; t) Q(z', 0), \quad (2.29)$$

where the propagator is defined by

$$\mathcal{T}(z, z'; t) = \delta^2(z'(t) - z), \quad (2.30)$$

where $z'(t)$ is the solution to the equation of motion for time t starting with the initial point z' . When $J=0$ we recover the previous result for a classical magnetic dipole; the distribution simply rotates, without distortion, at a constant rate ω about the z axis. The effect of the nonlinear term proportional to J causes a rotational shearing of the distribution around the z axis.

We may include additional stochastic dynamics on top of the Hamiltonian dynamics. However, it is important to note that if $Q(z, t)$ is a probability distribution then the propagators \mathcal{T} must be positive and may be interpreted as transition probabilities. The Hamiltonian Liouville evolution is a special case. As the propagator is simply the Green's function for the evolution equation the positivity requirement for the propagator restricts the allowed form of evolution equations. It is well known that the allowed forms correspond to Fokker-Planck equations and can contain at most second-order derivatives with positive definite diffusion matrices [28]. In other words, if the propagators are to be positive the evolution equation is necessarily restricted regardless of the initial or final conditions. We may thus define allowed classical dynamics either in terms of positive transition probabilities or in terms of the differential operator for the dynamics.

To compare the quantum and classical dynamics we now need to define a relevant quantum distribution. It is argued in Refs. [26,29] that the appropriate object is the matrix element of the quantum density operator in a coherent state basis. In the case of the harmonic oscillator, these are the coherent states of the Heisenberg-Weyl group, and the resulting distribution is a true (i.e., positive) probability distribution for simultaneous measurement of position and momentum [30]. In the case of angular momentum we can use the $SU(2)$ coherent states [31] defined by

$$|z\rangle = R(z)|s,s\rangle_z \quad (2.31)$$

$$= (1+|z|^2)^{-s} \sum_{m=0}^{2s} \binom{2s}{m}^{1/2} \times z^m |s,s-m\rangle_z, \quad (2.32)$$

where $|s,m\rangle$ are the $2s+1$ eigenstates of \hat{S}_z , and the rotation operator is

$$\hat{R}(z) = \exp[-i\theta \mathbf{n} \cdot \hat{S}] \quad (2.33)$$

with the unit vector $\mathbf{n} = (\sin\phi, \cos\phi, 0)$. The states $|z\rangle$ are product states in terms of the qubits, which are rotated from the state $|0\rangle_1|0\rangle_2$ by the angle ϕ and θ on the Bloch sphere:

$$|z\rangle = \frac{1}{(1+|z|^2)} (|0\rangle_1 + z|1\rangle_1) \otimes (|0\rangle_2 + z|1\rangle_2).$$

The function

$$Q(z,t) = \text{Tr}(\rho(t)|z\rangle\langle z|) \quad (2.34)$$

is a true (that is positive) probability distribution for measurements defined by the projection operator valued measure $|z\rangle\langle z|d^2z/2\pi$. Note that all allowed distributions are necessarily positive (and bounded) from the construction of $Q(z,t)$ as a trace of the product of a positive operator and a projection operator. For example, the Q function for a particular atomic coherent state $|z_0\rangle$ is

$$Q(z) = \left[\frac{(1+z_0^*z)(1+z_0z^*)}{(1+z_0z_0^*)(1+zz^*)} \right]^{2s}. \quad (2.35)$$

The first moments are given by integrals over the Q function as

$$\langle \hat{S}_x - i\hat{S}_y \rangle = \int d\mu(z) Q(z) \frac{2(s+1)z^*}{1+|z|^2}, \quad (2.36)$$

$$\langle \hat{S}_z \rangle = \int d\mu(z) Q(z) \left(\frac{(s+1)(1-|z|^2)}{1+|z|^2} \right). \quad (2.37)$$

The important point to notice is that the averages of \hat{S}_\pm are given by the same functional form as the classical case, apart from an additional term that becomes negligible in the semiclassical limit as $s \rightarrow \infty$. The second-order moments are given by

$$\langle \hat{S}_-^2 \rangle = \int d\mu(z) Q(z) \left(\frac{2(2s+3)(s+1)z^*{}^2}{(1+|z|^2)^2} \right), \quad (2.38)$$

$$\begin{aligned} \langle \hat{S}_z^2 \rangle &= \int d\mu(z) Q(z) \\ &\times \left(\frac{(s+1)^2 - 2s(s+2)|z|^2 + (s^2 + 4s + 5)|z|^4}{(1+|z|^2)^2} \right). \end{aligned} \quad (2.39)$$

Thus, even though the Q function is a true probability distribution, its marginals do not give the quantum expectation values; an additional rule is needed to connect averages over the Q function to the quantum averages. This is analogous to the case for the harmonic-oscillator coherent states [29]. In the case of a spherical phase space, however, the difference appears already at the level of the first-order moments.

Taking matrix elements of the quantum Liouville equation

$$\frac{d\rho}{dt} = -i[H, \rho], \quad (2.40)$$

we obtain the evolution equation

$$\frac{\partial}{\partial t} Q(z,t) = -i \left(\omega + J \frac{1-|z|^2}{1+|z|^2} - \frac{J}{2s} z \frac{\partial}{\partial z} \right) z \frac{\partial}{\partial z} Q(z,t) + \text{c.c.} \quad (2.41)$$

This equation is linear in Q ; thus, ρ_1 in Eq. (2.8) will obey exactly the same equation. In the limit of $s \rightarrow \infty$, with ω, λ held constant, the equation reduces to the first-order differential equation of classical dynamics. The difference between quantum and classical dynamics is due to the second-order differential operators. Note that while these terms are second order, they are certainly not of the kind expected for a diffusion equation, as the corresponding diffusion matrix would not be positive definite. This is a familiar feature of the difference between classical and quantum dynamics as reflected in the dynamics of a quasiprobability distribution and was first noted in the context of quantum optics [32].

In Ref. [26] it was shown how extreme this difference could be. For example, at times $t = \pi s/J$, an initial coherent state (or coherent pseudopure state) $|z_0\rangle$ would evolve in the rotating frame ($\omega=0$) into the pure state

$$2^{-1/2} [e^{-i\pi/4}|z_0\rangle + (-1)^s e^{i\pi/4}|-z_0\rangle] \quad (2.42)$$

for which the resulting Q function is double peaked. The state is entangled in terms of the pure state representation. No state such as this could ever be obtained from the classical dynamics given in Eq. (2.29) starting from the initial state Eq. (2.35).

III. DISCUSSION

We noted above that the difference between the quantum and classical dynamics appears through the second-order derivatives in Eq. (2.41). How does this difference become manifest in the propagator for the equation? It is far from clear that we can find a positive propagator corresponding to the differential operator on the right-hand side of Eq. (2.41), especially as this equation is not of Fokker-Planck form (the diffusion matrix is not positive definite). Nonetheless all initial and final Q functions must be positive by construction. We now show that the quantum evolution of the Q function cannot be written in terms of transition probability propagators. Despite this it can be obtained uniquely from the initial condition, $Q(z,t=0)$

To begin we define the Q -function amplitude for a pure state $|\psi(t)\rangle$

$$Q(z,t) = \langle z | \psi(t) \rangle. \quad (3.1)$$

The Q function is given by the modulus squared of the Q -function amplitude, $Q(z,t) = |Q(z,t)|^2$. The linearity of the Schrödinger equation now requires that the dynamics of the Q amplitude can be written in terms of a linear propagator

$$Q(z,t) = \int d^2z' \mathcal{L}(z,z';t) Q(z',0), \quad (3.2)$$

where $Q(z,0)$ is the Q -function amplitude for the initial state, and the propagator (for $s=1$) is constructed from the unitary time evolution operator $U(t)$ as

$$\begin{aligned} \mathcal{L}(z,z_1;t) &= \langle z | U(t) | z_1 \rangle \\ &= \frac{1}{(1+|z|^2)(1+|z_1|^2)} \\ &\quad \times \left(\exp \left[-i \left(\omega + \frac{J}{2s} \right) t \right] \right. \\ &\quad \left. + 2z^* z_1 + z^{*2} z_1^2 \exp \left[-i \left(-\omega + \frac{J}{2s} \right) t \right] \right). \end{aligned} \quad (3.4)$$

Thus the Q -function dynamics can be written in integral form as

$$\begin{aligned} Q(z,t) &= \int d^2z_1 d^2z_2 \mathcal{L}(z,z_1;t) \mathcal{L}^*(z,z_2;t) \\ &\quad \times Q(z_1,0)^* Q(z_2,0). \end{aligned} \quad (3.5)$$

In the case of a general initial state $\rho(0)$ the equation becomes

$$Q(z,t) = \int d^2z_1 d^2z_2 \mathcal{L}(z,z_1;t) \mathcal{L}^*(z,z_2;t) \langle z_1 | \rho(0) | z_2 \rangle. \quad (3.6)$$

This last expression seems to suggest we need to know more than just the initial condition $Q(z,0)$, but this is not the case. The matrix elements of ρ in the coherent-state basis suffice to uniquely determine the state and thus uniquely determine the off-diagonal matrix elements [31] by analytic continuation. A similar statement may be made about the propagator in Eq. (3.6). We only need to know the diagonal matrix element of $U^\dagger |z\rangle \langle z | U$ in order to determine the total propagator in Eq. (3.6). Thus knowledge of the initial Q function $Q(z,0)$ and a positive linear propagator $\mathcal{K}(z,z_1;t) = \langle z_1 | U(t)^\dagger | z \rangle \langle z | U(t) | z_1 \rangle$ uniquely determines the solution to the quantum evolution equation for the Q function. This is of course also true for the classical evolution equation, through a simple convolution of the initial state and the propagator. However, the propagation integral in the quantum case, Eq. (3.6), is not a positive (or even real) function and can have no interpretation as a transition probability.

It is generally accepted that uncontrolled interactions with an environment enable the quantum and classical dynamics to be reconciled when states of the environment are averaged over [33]. In the case of two coupled spins, there are a variety of possible environmental interactions. In order to illustrate the principle of decoherence, we take the simplest possible case in which both spins are coupled equally to the same environment with a Hamiltonian that conserves the total z component of angular momentum \hat{S}_z . While this collective dephasing model is not very realistic for NMR experiments, it will illustrate how decoherence can cause the quantum propagator in Eq. (3.6) to become diagonal.

The collective dephasing master equation is given by [26]

$$\dot{\rho} = \mathcal{D}\rho = -i[H, \rho] - \frac{\gamma}{2s} [\hat{S}_z, [\hat{S}_z, \rho]]. \quad (3.7)$$

The general solution for the Q function may then be written as

$$Q(z,t) = \int d^2z_1 \int d^2z_2 \mathcal{P}(z; z_1, z_2, t) \langle z_1 | \rho(0) | z_2 \rangle, \quad (3.8)$$

where the propagator is given in terms of the coherent-state matrix elements of the dynamically propagated off-diagonal projector

$$\mathcal{P}(z; z_1, z_2, t) = \langle z | e^{\mathcal{D}t} (|z_1\rangle \langle z_2|) | z \rangle. \quad (3.9)$$

For short times we can expand this to linear order in t . The dominant non-Hamiltonian terms in total spin s are given by

$$\begin{aligned} \mathcal{P}(z; z_1, z_2, t) &= \left[1 - \frac{\gamma s t}{2} \left(\frac{|z_1|^2 - |z_2|^2}{(1+|z_1|^2)(1+|z_2|^2)} \right)^2 \right] \\ &\quad \times \mathcal{P}(z; z_1, z_2, 0) + \dots \end{aligned} \quad (3.10)$$

The cofactor of $\gamma s t / 2$ is less than unity. For two spin-half systems with $s=1$, the coherence decay rate is then set entirely by γ , which could be small compared to the time scale set by the coherent interaction J^{-1} . When the initial state is concentrated on $|z_1| = |z_2|$ the decoherence is also small. The coherence decay rate for large semiclassical systems for which $s \gg 1$ can be large. Of course the resulting propagator is not the same as the classical Hamiltonian result [Eq. (2.29)] in the absence of dephasing as the coupling to the environment would add some level of phase diffusion to the classical dynamics as well, broadening the δ function in Eq. (2.29). In the case of $s=1$ considered here one would need to consider all the terms in the short-time expansion for $\mathcal{P}(z; z_1, z_2, t)$, but it remains the case that terms with large values of $|z_1| - |z_2|$ are rapidly suppressed.

Other two-qubit interactions might be considered, for example, the exchange interaction [34],

$$H_{\text{ex}} = \frac{J}{4} \vec{\sigma}^{(1)} \cdot \vec{\sigma}^{(2)} = \frac{J}{2} \left(\vec{S} \cdot \vec{S} - \frac{3}{2} \right), \quad (3.11)$$

where the total spin operator is $\vec{S} = (\vec{\sigma}^{(1)} + \vec{\sigma}^{(2)})/2$. This is the Hamiltonian for a rigid body with an isotropic moment of inertia with no external torques and with moment of inertia J^{-1} . The classical phase space is a cylinder with canonical coordinates S on the axis of the cylinder and θ around the circumference. The classical equations are the same as those of a free mass with periodic boundary conditions in position at $\pm\pi$: $\dot{\theta} = Js$ and $\dot{S} = 0$. The first of these again indicates a rotational shearing of a localized distribution on the phase space. When the shearing causes different parts of the state to overlap on the classical phase space, we expect the corresponding quantum system to exhibit interference fringes. Thus the quantum and classical dynamics of two interacting magnetic dipoles with such an interaction must differ. (Clearly such an interaction would need a different mechanism in classical systems as exchange interactions are quantum mechanical.)

As we have seen, the nonlinear top can generate the superposition state $(e^{-i\pi/4}|s,s\rangle_z + e^{-i\pi/4}|s,-s\rangle_z)$. A similar state can be generated by a sequence of CNOT gates on $N = \log_2(2j+1)$ qubits. A product state of N qubits can be written in terms of a binary string $|X\rangle = \prod_i |x_i\rangle$, where x_i is the i th term of the string X . Alternatively X could encode an integer k in binary form. The maximally entangled state of N qubits, $|000\dots 0\rangle + |111\dots 1\rangle$ would then take the form $|0\rangle + |M\rangle$, where $M = 2^N$. Such a state is easily generated in a quantum computer by a single Hadamard gate on the first qubit followed by a cascaded sequence of controlled-NOT gates. If we change the notation for angular momentum states so that $|s, m-s\rangle_z = |m\rangle$, where $m = 0, 1, \dots, 2s$, then the angular momentum superposition state generated by the nonlinear top is equivalent to the maximally entangled state. This equivalence suggests that a nonlinear top may itself be made to act as a quantum computer in the $2s+1$ dimensional Hilbert space. Indeed numerical evidence exists [35] that a time-dependent Hamiltonian of the form $H(t) = \vec{B}(t) \cdot \vec{S} + J(t)S_z^2$ can generate any state in the Hilbert space by a suitable choice of the time-dependent coefficients. We

conjecture that a sequence of pulses $U(\theta_n, \phi_n, \chi_n) = \exp(-i\theta_n \vec{n}_n \cdot \vec{S}) \exp(-i\chi_n S_z^2)$, where $\vec{n} = (\cos\phi, \sin\phi, 0)$ will suffice to perform quantum algorithms in the Hilbert space of the nonlinear top. Further work remains to be done to determine whether there are interesting efficient algorithms in terms of the number of pulses and (say) $\log(s)$.

IV. CONCLUSION

We have investigated classical and quantum Hamiltonians of the nonlinear top and show that they produce different observables even in the presence of highly mixed states. This shows that even if a state is separable, its classical and quantum evolution can differ. Thus this fortifies the claim that the evolution is one of the quantum elements of liquid-state NMR quantum information processing. However it does not prove that bulk ensemble NMR quantum computation is uniquely quantum. We have used a particular classical model, that is one motivated by the physics of two interacting magnetic dipoles, to compare the quantum and classical dynamics. It may well be the case that for states that are close to the maximally mixed state there is another classical model (in effect a hidden variable model) that correctly describes the dynamics as far as is required to model the observed results in NMR experiments [16].

Even if the transformation of the state is not classical, our present paper does not show that using these mixed state qubits is as powerful as a pure state quantum computer. If we use the pseudopure state as has been done in present experiments, the signal-to-noise ratio decreases exponentially, thus rendering the algorithms inefficient. In this case liquid-state NMR does not provide any advantage (with respect to speed) over classical computers. In the absence of noise, Schulman and Vazirani [36] have shown how to efficiently transform the initial mixed state into a pure state. Some simulations of quantum systems evolving under unitary transform and the algorithm suggested in [37] could also be implemented efficiently as long as noise is negligible. Thus liquid-state NMR

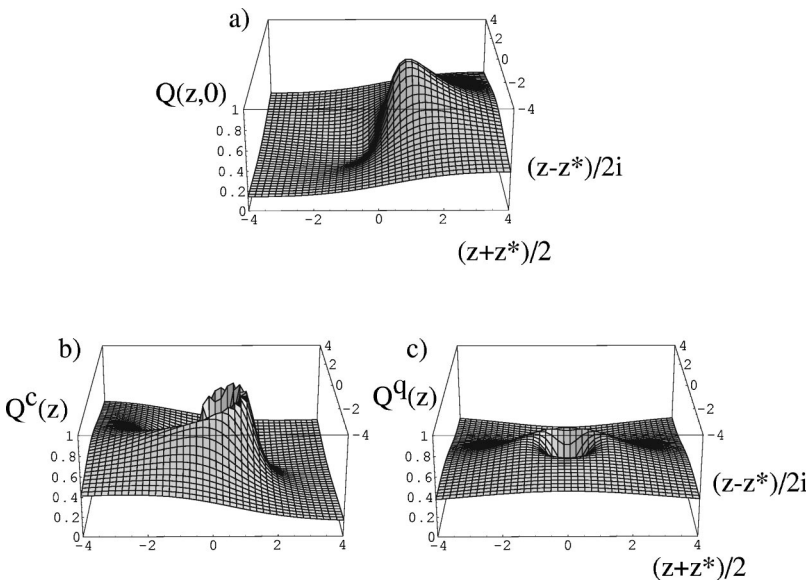


FIG. 1. Comparison between the classical and quantum evolution of the $Q(z)$ function. The initial state is given by (a). It corresponds to the distribution for the quantum state $|z=1\rangle$. (b) and (c) depict the classical and quantum distribution at time $t = 2\pi/J$ (for $\omega=0$). The classical evolution follows the equation of motion Eq. (2.24) and the quantum one Eq. (2.41). The discrepancy between the classical evolution and the quantum one is evident.

(in the absence of noise, i.e., on time scales smaller than T_2) offers a testing ground for QIP. The dynamics are correct. Moreover it has the right error model to provide a test bed for small quantum computations (up to roughly 10 qubits). The difference between liquid-state NMR and other proposals for quantum computation is that, in the former case we do not have, even in principle, a method to make the quantum evolution robust. In practice this does not distinguish NMR from other present devices as none have approached the accuracy needed for scalability.

In the present paper we have neglected the possibility of hidden variables. The reason is that there is a trivial hidden variable model that would explain all the present experiments in QIP (including not only NMR but also other technologies) as long as observations are not made on spacelike surfaces. The model can be thought of as a classical computer that simulates the quantum evolution and tells the bits of the physical system how to behave so they mimic quantum mechanics. Although this model can describe all the experiments in QIP today, the amount of resources it uses compared to its quantum counterpart always seem to be exponential in the size of the problem (the model of Schack and Caves is such a model). It is important that the resources account for not only the signal-to-noise but all resources as it is usually easy to trade one resource for another. We would like to conjecture that what distinguishes classical and quantum computation is the amount of algorithmic information

required to produce the answer of some problem starting from a fiducial state. Classical devices require an exponential amount of algorithmic information compared to a quantum computer to answer certain problems. Simulating liquid-state NMR experiments is one such problem compared to known classical algorithms.

So where did the power of quantum computation come from? In this paper we have argued that the power comes from the dynamics of the system. A similar argument has been made by others [10,16]. We have criticized the view that entanglement is the source of power of quantum computation by giving algorithms and dynamical evolution, which do not depend on entanglement. There may be a variety of elements which make these devices more powerful, and for another unusual method to quantum compute see [38]. However, as long as we lack a proof that we cannot simulate quantum systems efficiently, it is hard to attribute the source of the power of quantumness, and we await more powerful arguments.

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