Classical model for bulk-ensemble NMR quantum computation

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Abstract

We present a classical model for bulk-ensemble NMR quantum computation: the quantum state of the NMR sample is described by a probability distribution over the orientations of classical tops, and quantum gates are described by classical transition probabilities. All NMR quantum computing experiments performed so far with three quantum bits can be accounted for in this classical model. After a few entangling gates, the classical model suffers an exponential decrease of the measured signal, whereas there is no corresponding decrease in the quantum description. We suggest that for small numbers of quantum bits, the quantum nature of NMR quantum computation lies in the ability to avoid an exponential signal decrease.

I. INTRODUCTION

The original proposals [1,2] for quantum computing using high-temperature, liquid-state nuclear magnetic resonance (NMR) sparked an explosion of interest. The resulting work on NMR quantum-information processing has attracted a great deal of attention. In addition to a long list of publications [1–20], there have been numerous news reports, especially on the recent NMR experiments on quantum error correction [5] and quantum teleportation [4].

The fundamental information-processing elements in NMR are two-level nuclear spins, called quantum bits, or *qubits* for short, which are bound together in a single molecule. A liquid NMR sample contains a macroscopic number of molecules, each of which functions as an independent information-processing system. The molecules are initially in thermal equilibrium at high temperature; the nuclear spins are only weakly polarized along the direction of a strong applied magnetic field. NMR techniques cannot control the quantum states of

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individual molecules; instead, all the molecules in the sample are manipulated in parallel. Moreover, NMR readout techniques are sensitive to the average magnetization of the entire sample. For these reasons the use of high-temperature, liquid-state NMR techniques for quantum-information processing is called *bulk-ensemble quantum computation*. Clever techniques have been devised to map the coherent quantum-mechanical manipulations required for quantum computation to this situation in which one neither controls nor makes measurements on individual molecules [1,2,8,11,13].

This paper deals exclusively with bulk-ensemble quantum-information processing, not with proposals (see, for example, Ref. [21]) for using nuclear spins in situations, as in solid-state systems, where they can be highly polarized. Although the paper is phrased in terms of and aimed at NMR quantum computation, the analysis is not specific to NMR and could be applied to any realization of (low-polarization) bulk-ensemble quantum computation.

Bulk-ensemble NMR quantum computation is in principle scalable to many qubits [20], but it is unclear whether it will ever lead to useful quantum computations involving more than a few dozen qubits [1,3]. Nevertheless, the experiments performed so far, which use only a few qubits, are cited as important demonstrations of the principles of quantum-information processing and quantum computation. There has, however, been persistent skepticism about whether these experiments demonstrate genuine quantum-information processing. Recently these doubts have been brought into sharper focus [22] with the realization that all quantum states used in present NMR experiments are *separable* [23], i.e., unentangled. Entanglement is generally thought to be an essential feature of quantum computation [24,25], although there have been suggestions that the power of quantum computation cannot be so simply characterized [26–28].

In this paper we explore the "quantumness" of bulk-ensemble quantum computation. There being no general definition of what it means to be doing genuine quantum-information processing, we begin by proposing three different criteria, which are investigated in the remainder of the paper.

- According to the first criterion, an N-qubit NMR experiment does not demonstrate genuine quantum-information processing if all quantum states that occur during the experiment are *separable* (unentangled), i.e., are equivalent to classical ensembles of spinning tops. The motivation for this criterion is that for separable states, the statistics of any measurement performed on the NMR sample can be described in the language of classical probabilities for spin orientations. With respect to this criterion, NMR experiments for up to about 15 qubits do not demonstrate genuine quantum-information processing [23]. There is, however, an immediate objection to this criterion: even if all states involved in the experiment are classical, the transformations between the states might be essentially quantum mechanical, not having any description in classical language.

- Our second criterion addresses this objection by stating that an N-qubit NMR experiment does not demonstrate genuine quantum-information processing if we can construct an *overall classical model* for the experiment, by which we mean that in addition to the experiment's satisfying the first criterion, the transformation T that maps the initial quantum state to the final quantum state can be described by classical transition probabilities. The transition probabilities are required to be fully specified by T; in particular, they must be independent of the initial and final states. We formulate an overall classical model below, which shows that, with respect to this second criterion, NMR experiments for up to about 6 qubits do not demonstrate genuine quantum-information processing. An objection to this second criterion is that an overall classical model does not constitute a valid model for a quantum computation, because the complexity of the overall transition probabilities might increase exponentially with problem size; according to this objection, computational complexity is at the heart of the question of whether a given computation is quantum mechanical.

- Our third criterion incorporates this objection as follows. It states that an N-qubit NMR experiment does not demonstrate genuine quantum information processing if we can construct a *gate-by-gate classical model*, by which we mean that in addition to the first criterion being satisfied, any elementary gate U implemented in the experiment can be described by classical transition probabilities, which, as before, are fully specified by U and which, apart from trivial contributions for the qubits not involved in the gate, are independent of the total number of qubits [29]. We devise a gate-by-gate classical model below. It shows that all 3-qubit quantum computing experiments performed so far [4–8] do not demonstrate genuine quantum-information processing according to this third criterion.

We emphasize that the point of constructing gate-by-gate classical models is to answer the following question: Can the *information processing* that occurs in bulk-ensemble quantum computation be accounted for in classical language? The purpose is not to provide a detailed physical model of all aspects of a particular realization of a bulk-ensemble quantum computer. Thus we consider a model successful if it provides transition probabilities for the elementary quantum gates that are used to perform the information processing. In an NMR experiment, an elementary 2-qubit gate, such as a controlled-NOT gate, is built up from many smaller building blocks and requires a complex sequence of radio-frequency pulses, but in constructing classical models, we adopt the view that this underlying sequence of pulses is not important for assessing whether an NMR experiment is doing genuine quantum-information processing.

In the NMR literature, transformations are often represented by diagrams that depict spins as arrows evolving on spheres; see, e.g., Ref. [30] or the "effective fields picture" in Ref. [14], where a diagram representing a controlled-NOT gate is given. This diagram illustrates what is new in our approach. The diagram assumes that the sample is split into two subpopulations, according to whether the control qubit is up or down. Thus it provides a classical description of the gate for initial conditions corresponding to spin-up–spin-down (computational-basis) states of the control qubit, but not for arbitrary, possibly entangled initial states. Consequently, it does not give a classical model of the controlled-NOT gate in the sense of our third criterion.

We emphasize that our gate-by-gate classical model is not the same as a simulation of a quantum algorithm on a classical computer. First, in our classical *model*, measurement statistics are determined by probabilities for classical spin orientations; this means that our classical model provides a *local* hidden-variable description of the experiment. In contrast, in a classical *simulation*, where one calculates the quantum amplitudes in, say, the computational basis, one can regard the entire state vector, a nonlocal object, as a hidden variable

[29]. Second, the computational complexity of a classical simulation increases exponentially with the number of gates [24], whereas the complexity of our transition probabilities for an entangling gate increases only linearly with the number of qubits.

Equally important is a difference between our gate-by-gate classical model and the quantum description of an NMR experiment. In our classical model, the strength of the magnetization signal decreases exponentially with the number of entangling gates. Though this decrease can be staved off for a few entangling steps, it cannot be put off indefinitely. Such a decrease is absent from the quantum description. Thus it is straightforward to design experiments that cannot be described by our classical model. Two-qubit experiments that fall into this class are Ref. [9] and probably also Ref. [10], although in the latter case this is not clear from the published data. In order to prove conclusively, however, that a bulk-ensemble NMR experiment demonstrates genuine quantum-information processing in the sense of the third criterion given above, one must rule out *all* gate-by-gate classical models, not just the particular model given in this paper. We stress that quantum mechanics accounts for all aspects of very sophisticated NMR experiments. Classical models are not meant to provide an alternative physical description of these experiments, but rather to contribute to understanding whether there is anything genuinely quantum mechanical about the *information processing* in the experiments.

The paper is organized as follows. In Sec. II, we give a brief description of bulk-ensemble NMR quantum computation, and in Sec. III, we summarize the proof given in Ref. [23] that the states used in high-temperature NMR experiments are classical up to about 15 qubits in the sense of the first criterion above. In Sec. IV, we define the transition probabilities that are used in our overall and gate-by-gate classical models. Used directly in a gate-by-gate classical model, these transition probabilities give rise to a signal decrease by a constant factor at each entangling multi-qubit operation. Section V shows how to modify the gate-by-gate model so as to avoid this signal decrease for a small number of entangling steps. In Sec. VI we consider the implications of our results for bulk-ensemble NMR quantum-information processing.

II. NMR QUANTUM-INFORMATION PROCESSING

All NMR quantum computing experiments performed so far [4–16] work according to the following principles. The state of the sample is described by a density operator ρ for the N spins (qubits) in each molecule. The molecules are prepared in an initial state

$$\rho = (1-\epsilon)M + \epsilon\rho_1 \ , \tag{2.1}$$

where $M = I/2^N$ is the maximally mixed density operator for N qubits (I is the unit operator) and ρ_1 is a density operator, usually chosen to be the projector onto the computational-basis state $|0\dots0\rangle$. The parameter ϵ scales like

$$\epsilon = \frac{\alpha N}{2^N} \ . \tag{2.2}$$

Here $\alpha = h\bar{\nu}/2kT$, where $\bar{\nu}$ is the average resonant frequency of the active spins in the strong magnetic field, determines the polarization of the sample. If ρ_1 is a pure state, ρ is called a pseudopure state [1]. Procedures for synthesizing a pseudopure state from an initial thermal density operator are described in Refs. [2,8,11,13].

For typical molecules in present magnetic-field strengths, the average resonant frequency is roughly $\bar{\nu} \sim 300\,\mathrm{MHz}$, which at room temperature, gives $\alpha \sim 2 \times 10^{-5}$. It is difficult to know the actual value of α and ϵ in the experiments, because the polarization is not calibrated absolutely. In evaluating the experiments, we adopt the scaling of Eq. (2.2), with a conservative value of $\alpha = 2 \times 10^{-6}$, which is meant to take into account inefficiencies in the experiments, especially loss of polarization involved in the synthesis of a pseudopure state. The results of this paper do not depend significantly on the exact value for α chosen.

One interpretation of ϵ is that it specifies the fraction of molecules in the sample that occupy the desired initial state ρ_1. This interpretation is not unique, and it is not mandated or even preferred by quantum mechanics. It is sometimes promoted to the level of a physical fact by advocates of NMR quantum computation, yet it becomes a physical fact only if one actually prepares a fraction of the molecules in a particular state [31], a situation that does not apply to a high-temperature NMR experiment. The freedom to interpret ρ in terms of other ensembles underlies the conclusions of this paper.

After synthesis of the desired initial state, a sequence of radio-frequency pulses, alternating with continuous evolution, is applied to the sample. We first consider the case where the evolution is described by a unitary transformation U. Applying the unitary operator U to ρ results in the state

$$\rho^{\mathrm{out}} \equiv U\rho U^\dagger = (1-\epsilon)M + \epsilon U\rho_1 U^\dagger \equiv (1-\epsilon)M + \epsilon\rho_1^{\mathrm{out}} \,. \tag{2.3}$$

The totally mixed part of the state is unaffected by the unitary transformation. The output state retains the form (2.1) with the same value of ϵ, but—and this is the essence of the bulk-ensemble paradigm for quantum computation—ρ_1 undergoes the desired unitary transformation.

The same conclusions hold for transformations implemented using gradient pulses together with diffusion in the sample [8]; these are equivalent to mixtures of unitary transformations, as in

$$\rho^{\mathrm{out}} \equiv \sum_l p_l U_l \rho U_l^\dagger = (1-\epsilon)M + \epsilon \sum_l p_l U_l \rho_1 U_l^\dagger \equiv (1-\epsilon)M + \epsilon\rho_1^{\mathrm{out}} \,, \tag{2.4}$$

where the $p_l \geq 0$ are probabilities. We assume that decoherence also preserves the form of the density operator, leaving ϵ unchanged. This assumption is certainly justified when decoherence is simulated by unitary transformations, as in the gradient pulses used to simulate decoherence in Ref. [5]. It is also true for naturally occurring decoherence for times short compared to the characteristic time for relaxation to thermal equilibrium. These are the times of interest for quantum-information processing.

The last step in any NMR experiment is the readout. By applying radio-frequency pulses and then measuring the transverse magnetization of the sample, one can determine all expectation values of the form

$$\mathrm{tr}\Big(\rho^{\mathrm{out}}\sigma_{\beta_1} \otimes \cdots \otimes \sigma_{\beta_N}\Big) = \epsilon\, \mathrm{tr}\Big(\rho_1^{\mathrm{out}}\sigma_{\beta_1} \otimes \cdots \otimes \sigma_{\beta_N}\Big) \,. \tag{2.5}$$

The tensor product in this expression includes one operator for each spin; σ_{β_k} denotes the unit operator I for the kth spin if $\beta_k = 0$, and it denotes a Pauli matrix if $\beta_k = 1, 2,$ or 3.

In writing Eq. (2.5) and all such expectation values in this paper, it is assumed that there is at least one Pauli matrix in the tensor product (not all the β's are zero). The maximally mixed part of the density operator does not contribute to the measured expectation values, which are determined by the state ρ_1^{out} that undergoes the desired evolution. The parameter ϵ appears naturally as a measure of the strength of the magnetization signal (or of the signal-to-noise ratio).

Throughout this paper we use the phrase "bulk-ensemble quantum computation" to refer to any scheme that uses an ensemble of information-processing elements, each consisting of N qubits, in the manner described in this section. The processing elements, prepared initially in a highly mixed state of the form (2.1), are manipulated in parallel as in Eq. (2.3), and the readout, involving the entire ensemble, yields expectation values of the form (2.5). Our results apply to any such bulk-ensemble scheme.

III. SEPARABILITY OF STATES USED IN NMR

Our conclusions rest on the freedom to write states of the form (2.1) in terms of probability distributions over spin orientations for N classical tops. We review one such representation [23], the foundation for our work, which provides a classical description for all states of the form (2.1) provided that

$$\epsilon \le \eta \equiv \frac{1}{1+2^{2N-1}} \, . \tag{3.1}$$

If we assume that $\alpha = 2 \times 10^{-6}$ in Eq. (2.2), this inequality holds for $N < 16$ qubits.

The argument is straightforward [23]. The most general pure product state of N qubits has the form

$$P_1(\tilde{n}) \equiv P_1(\vec{n}_1, \ldots, \vec{n}_N) = \frac{1}{2^N}(I + \vec{n}_1 \cdot \vec{\sigma}) \otimes \cdots \otimes (I + \vec{n}_N \cdot \vec{\sigma}) \, , \tag{3.2}$$

This state can be interpreted as N classical tops pointing in the directions given by the unit vectors $\vec{n}_1, \ldots, \vec{n}_N$, denoted collectively by $\tilde{n}$. Since the operators $P_1(\tilde{n})$ form an overcomplete basis in the space of linear operators acting on N qubits, any N-qubit density operator ρ can be expanded as

$$\rho = \int d\Omega_{\tilde{n}}\, w^{\rho}(\tilde{n}) P_1(\tilde{n}) \, , \tag{3.3}$$

where $d\Omega_{\tilde{n}} \equiv d\Omega_{\vec{n}_1} \cdots d\Omega_{\vec{n}_N}$. The overcompleteness means that the expansion coefficients are not unique. One choice is

$$w^{\rho}(\tilde{n}) \equiv \mathrm{tr}\Big(\rho Q_1(\tilde{n})\Big) \, , \tag{3.4}$$

where the operators $Q_1(\tilde{n})$ are defined by

$$Q_1(\tilde{n}) \equiv \frac{1}{(4\pi)^N}(I + 3\vec{n}_1 \cdot \vec{\sigma}) \otimes \cdots \otimes (I + 3\vec{n}_N \cdot \vec{\sigma}) \, . \tag{3.5}$$

The representation (3.4), which is analogous to the P representation for a harmonic oscillator, was introduced by Arecchi *et al.* [32] and studied in detail by Scully and Wódkiewicz [33]. The expansion coefficients $w^\rho(\tilde{n})$ can be positive or negative, but they obey the bound

$$w^\rho(\tilde{n}) \geq \begin{pmatrix} \text{smallest} \\ \text{eigenvalue} \\ \text{of } Q_1(\tilde{n}) \end{pmatrix} = -\frac{2^{2N-1}}{(4\pi)^N} \ . \tag{3.6}$$

When $w^\rho(\tilde{n})$ is everywhere nonnegative, it can be interpreted as a classical probability distribution for the N spins to point in the directions $\vec{n}_1, \ldots, \vec{n}_N$. Since the maximally mixed density operator M has probability density $w^M(\tilde{n}) = 1/(4\pi)^N$, it follows that for a density operator ρ of the form (2.1) with $\epsilon \leq \eta$,

$$w^\rho(\tilde{n}) = \frac{1-\epsilon}{(4\pi)^N} + \epsilon w^{\rho_1}(\tilde{n}) \geq \frac{1-\epsilon/\eta}{(4\pi)^N} \geq 0 \ . \tag{3.7}$$

A density operator for a joint system is *separable* if it can be written as a nonnegative linear combination of product density operators. When $w^\rho(\tilde{n})$ is everywhere nonnegative, the expansion (3.3) provides a separable representation for ρ. Related work on the separability of states near the maximally mixed state can be found in Refs. [31] and [34]. Separable states have no quantum entanglement [35]. The importance of separability in this paper is that a separable state of N qubits can be interpreted in terms of an ensemble of classical tops, because the expectation values (2.5) measured in NMR experiments have the standard form for an ensemble with probability distribution $w^\rho(\tilde{n})$:

$$\mathrm{tr}\Big(\rho\,\sigma_{\beta_1} \otimes \cdots \otimes \sigma_{\beta_N}\Big) = \int d\Omega_{\tilde{n}}\, w^\rho(\tilde{n})\, \underbrace{\mathrm{tr}\Big(P_1(\tilde{n})\sigma_{\beta_1} \otimes \cdots \otimes \sigma_{\beta_N}\Big)}_{=\,(n_1)_{\beta_1}\cdots(n_N)_{\beta_N}} \ . \tag{3.8}$$

In this expression, $(n_j)_{\beta_j} = 1$ if $\beta_j = 0$, and $(n_j)_{\beta_j}$ is a Cartesian component of the vector $\vec{n}_j$ if $\beta_j = 1, 2$, or 3.

Although a classical interpretation of the expectation values (2.5) is all we need for understanding the measurements in bulk-ensemble quantum computation, we can demonstrate a much stronger result: for separable states of N qubits, all measurements, including nonfactorizable measurements, can be interpreted in terms of an ensemble of classical top orientations. To see this, consider an arbitrary measurement on the N qubits, its statistics described by a positive-operator-valued measure (POVM) with POVM elements E_α [36]. The probability to obtain result α is

$$\mathrm{tr}(\rho E_\alpha) = \int d\Omega_{\tilde{n}}\, w^\rho(\tilde{n})\mathrm{tr}\Big(P_1(\tilde{n})E_\alpha\Big) \ . \tag{3.9}$$

Here the quantity $\mathrm{tr}\Big(P_1(\tilde{n})E_\alpha\Big) \geq 0$ can be interpreted as the conditional probability to obtain result α, given that the spins point in the directions specified by $\tilde{n}$. Thus, as long as $w^\rho(\tilde{n}) \geq 0$, the measurement statistics can be interpreted in terms of an ensemble of classical tops [37].

If one adopts our first criterion, none of the NMR experiments performed to date has done any genuine quantum-information processing, since they all use 2 or 3 qubits. Yet the fact that all states—initial, intermediate, and final—that occur in a given NMR experiment are equivalent to ensembles of classical tops does not mean, by itself, that there is a classical model for the entire experiment. To see this, consider the following naïve attempt to describe a unitary transformation U by classical transition probabilities:

$$w^{U\rho U^\dagger}(\tilde{n}) = \mathrm{tr}\Big(U\rho U^\dagger Q_1(\tilde{n})\Big) = \int d\Omega_{\tilde{m}}\, w^\rho(\tilde{m})\, \underbrace{\mathrm{tr}\Big(UP_1(\tilde{m})U^\dagger Q_1(\tilde{n})\Big)}_{\equiv\, t_U(\tilde{n}|\tilde{m})} \; . \tag{3.10}$$

The transition function $t_U(\tilde{n}|\tilde{m})$ is not a transition probability because it assumes negative values; for example, for the trivial case of the identity transformation, $U = I$, we have

$$t_I(\tilde{n}|\tilde{m}) = \mathrm{tr}\Big(P_1(\tilde{m})Q_1(\tilde{n})\Big) = \frac{1}{(4\pi)^N}\prod_{j=1}^{N}(1 + 3\vec{m}_j\cdot\vec{n}_j) \; . \tag{3.11}$$

The expansion coefficients $w^{P_1(\tilde{m})}(\tilde{n}) = \mathrm{tr}\Big(P_1(\tilde{m})Q_1(\tilde{n})\Big)$ in Eq. (3.11) are the coefficients for the pure product state $P_1(\tilde{m})$. That these coefficients can be negative might seem to be a drawback of our representation, but in fact it is an essential feature of a program to construct a classical model. To see this, suppose that we could use a representation w^ρ, linear in ρ, to construct a classical model for all unitary operators acting on density operators sufficiently close to the maximally mixed state. This means that there is a nonnegative transition probability $w_U(\tilde{n}|\tilde{m}) \ge 0$ such that

$$w^{U\rho U^\dagger}(\tilde{n}) = \int d\Omega_{\tilde{m}}\, w_U(\tilde{n}|\tilde{m}) w^\rho(\tilde{m}) \tag{3.12}$$

for all unitary operators U and for all density operators ρ of the form (2.1), provided ϵ is sufficiently small. Applying Eq. (3.12) to the case where ρ_1 is a pure state P and using the linearity of w^ρ, we get immediately that

$$w^{UPU^\dagger}(\tilde{n}) = \int d\Omega_{\tilde{m}}\, w_U(\tilde{n}|\tilde{m}) w^P(\tilde{m}) \; . \tag{3.13}$$

If $w^P(\tilde{m})$ is everywhere nonnegative, we get a nonnegative representation for $UPU^\dagger$ and, hence, conclude that $UPU^\dagger$ is separable. This can't be true, however, because we can always choose U to map P to an entangled state. The conclusion is that w^P must go negative for all pure states P. This tells us something useful only for pure product states, because all other pure states are entangled and necessarily have a representation that goes negative. The representation we are using, embodied in Eq. (3.4), does go negative for all pure product states.

Returning now to the first criterion, we note that even though it is not the whole story, it is the right criterion for judging claims of having produced entangled states using bulk-ensemble NMR. For example, as pointed out in Ref. [23], the claim of Laflamme *et al.* [6] to have created a 3-qubit Greenberger-Horne-Zeilinger (GHZ) entangled state is incorrect. Despite the authors' assertion, "We describe the creation of a Greenberger-Horne-Zeilinger state of the form $(|000\rangle + |111\rangle)/\sqrt{2}$ (three maximally entangled quantum bits) using nuclear magnetic resonance. ... We have thus extended the space of entangled quantum states explored systematically to three quantum bits ... ," no entanglement was created in that experiment; the statistics of any measurement performed on the purported GHZ state could have been explained in terms of classical correlations contained in $w^\rho(\tilde{n})$. Similar conclusions apply to the experiments in which Chuang *et al.* [11] and Cory *et al.* [8] claim to have created 2-qubit Einstein-Podolsky-Rosen (EPR) entangled states. The states created in these experiment were unentangled, though Chuang *et al.* write, "As an application of the controlled-NOT gate, we used it in a simple quantum circuit to create entangled states from the thermal mixture. ... We have experimentally confirmed this (nonclassical) behavior, and the signature of the entanglement—a purely *non-classical* effect—is the strong reverse diagonal measured in the density matrix," and Cory *et al.* refer to applying the "spin-coherence XOR gate to a one-spin superposition to create an entangled state."

Indeed, the first criterion can be applied to any NMR experiment that claims to have manipulated quantum *states* in a particular way. For example, in describing the NMR version of quantum teleportation [4], a 3-qubit experiment, the authors assert, "Quantum-mechanical systems have information processing capabilities that are not possible with classical devices. One example is quantum teleportation, in which the quantum state of a system is transported from one location to another without moving through the intervening space. ... Here we report an experimental implementation of full quantum teleportation over inter-atomic distances using liquid-state nuclear magnetic resonance." This claim cannot be supported, because the quantum state at all stages of the experiment could be interpreted in terms of classical correlations among spin directions. What the experiment achieved was a reshuffling of these classical correlations. Nonetheless, as noted above, this conclusion does not imply that there is a classical model for the entire experiment.

IV. TRANSITION PROBABILITIES FOR QUANTUM GATES

The essence of a classical model lies in the construction of nonnegative transition probabilities to describe unitary transformations. We first consider product unitaries, i.e., unitary transformations of the form $V = V_1 \otimes \cdots \otimes V_N$, and then tackle the tougher task of entangling unitaries, i.e., unitary transformations that are not product unitaries.

The expansion coefficients for the output state are given by

$$w^{V\rho V^\dagger}(\tilde{n}) = \mathrm{tr}\Big(V\rho V^\dagger Q_1(\tilde{n})\Big) = \mathrm{tr}\Big(\rho V^\dagger Q_1(\tilde{n}) V\Big) \ . \tag{4.1}$$

For a product unitary V, the unitary transform of $Q_1(\tilde{n})$ factors into a product of transformations for each qubit. If we introduce the 3-dimensional rotation operator R_k (an orthogonal transformation) corresponding to the unitary operator V_k, i.e., $V_k^\dagger \vec{\sigma} V_k = R_k \vec{\sigma}$, and use the fact that $\vec{n}_k \cdot R_k \vec{\sigma} = R_k^{-1} \vec{n}_k \cdot \vec{\sigma}$, then the unitary transform of $Q_1(\tilde{n})$ assumes the form

$$V^\dagger Q_1(\tilde{n}) V = Q_1(R_1^{-1}\vec{n}_1, \ldots, R_N^{-1}\vec{n}_N) = Q_1(\tilde{R}^{-1}\tilde{n}) \ . \tag{4.2}$$

Here $\tilde{R}$ stands for the rotations on all the qubits. Now the output expansion coefficients assume the form

$$w^{V\rho V^\dagger}(\tilde{n}) = w^\rho(\tilde{R}^{-1}\tilde{n}) = w^\rho(R_1^{-1}\vec{n}_1, \ldots, R_N^{-1}\vec{n}_N) \ . \tag{4.3}$$

Not surprisingly, the action of the product unitary V is equivalent to rotating each of the classical tops. The corresponding nonnegative transition probabilities are $w(\tilde{n}|\tilde{m}) =$

$\delta(\tilde{R}^{-1}\tilde{n}-\tilde{m})$. This result shows that, for product unitaries, our transition probabilities are equivalent to the simple classical diagrams often used in the NMR literature [30].

Before proceeding to entangling unitaries, we describe how decoherence is incorporated into our classical models. In some experiments decoherence is simulated as a mixture of product unitary transformations; an example is the use of gradient pulses in Ref. [5]. In current experiments, naturally occurring decoherence processes can be regarded as acting independently on the various qubits; on time scales short compared to the thermal relaxation time, they preserve the maximally mixed density operator. Any decoherence process that satisfies these two properties can be described as a mixture of product unitaries [38]. Thus decoherence can be handled in our classical models as a mixture of rotations of the qubits.

To describe general, entangling unitaries, we need to introduce some additional notation. For an arbitrary density operator ρ and for $0<\theta\le 1$, we define

$$\rho_\theta \equiv (1-\theta)M+\theta\rho\,. \tag{4.4}$$

Furthermore, we define the states

$$P_\theta(\tilde{n}) \equiv (1-\theta)M+\theta P_1(\tilde{n}) \tag{4.5}$$

and associated operators

$$Q_\theta(\tilde{n}) \equiv \frac{1-\theta^{-1}}{(4\pi)^N}\,I+\theta^{-1}Q_1(\tilde{n})\,. \tag{4.6}$$

For a general unitary operator U, we define the transition probabilities

$$w_U(\tilde{n}|\tilde{m}) \equiv \mathrm{tr}\Big(UP_\eta(\tilde{m})U^\dagger Q_1(\tilde{n})\Big)=\frac{1-\eta}{(4\pi)^N}+\eta t_U(\tilde{n}|\tilde{m})\ge 0\,, \tag{4.7}$$

where $t_U(\tilde{n}|\tilde{m})$ is defined in Eq. (3.10). The nonnegativity of these transition probabilities follows from the argument leading to Eq. (3.7), since $UP_\eta(\tilde{m})U^\dagger$ is a state of the form (2.1) with $\epsilon=\eta$.

It is straightforward to write down the transition probabilities for elementary entangling gates. As an illustration, we compute them for the controlled-phase gate,

$$\begin{aligned} U=C_{ij} &= |0\rangle\langle 0|\otimes 1+|1\rangle\langle 1|\otimes\sigma_3 \\ &= \frac{1}{2}(1+\sigma_3)\otimes 1+\frac{1}{2}(1-\sigma_3)\otimes\sigma_3\,, \end{aligned} \tag{4.8}$$

acting on qubits i and j. We obtain

$$\begin{aligned} w_{C_{ij}}(\tilde{n}|\tilde{m}) &= \mathrm{tr}\Big(C_{ij}P_\eta(\tilde{m})C_{ij}Q_1(\tilde{n})\Big) \\ &= \frac{1}{(4\pi)^N}\Bigg(1-\eta+\eta\prod_{l\ne i,j}(1+3\vec{m}_l\cdot\vec{n}_l) \\ &\qquad\times\Big([1+3(m_i)_3(n_i)_3][1+3(m_j)_3(n_j)_3]+9(\vec{m}_i\times\vec{n}_i)_3(\vec{m}_j\times\vec{n}_j)_3 \\ &\qquad\quad+3[(m_i)_3+3(n_i)_3](\vec{m}_{j\perp}\cdot\vec{n}_{j\perp})+3[(m_j)_3+3(n_j)_3](\vec{m}_{i\perp}\cdot\vec{n}_{i\perp})\Big)\Bigg)\,, \end{aligned} \tag{4.9}$$

where $\vec{m}_\perp$ is the projection of $\vec{m}$ into the 1-2 plane, obtained by setting m_3 to zero. As in this example, the qubits not involved in an entangling gate do appear in the transition probabilities, but in a simple, universal way.

Applying the transition probabilities (4.7) to an input ensemble $w_{\rm in} \equiv w^\rho(\tilde{n})$, we obtain a classical output ensemble

$$
\begin{aligned}
w_{\rm out}(\tilde{n}) &\equiv \int d\Omega_{\tilde{m}}\, w_U(\tilde{n}|\tilde{m}) w_{\rm in}(\tilde{m}) \\
&= \mathrm{tr}\Bigg(U \underbrace{\left[\int d\Omega_{\tilde{m}}\, w^\rho(\tilde{m}) P_\eta(\tilde{m}) \right]}_{=\,\rho_\eta} U^\dagger Q_1(\tilde{n}) \Bigg) \\
&= w^{U\rho_\eta U^\dagger}(\tilde{n}) \\
&= \frac{1-\eta}{(4\pi)^N} + \eta w^{U\rho U^\dagger}(\tilde{n}) \;.
\end{aligned} \tag{4.10}
$$

Unlike the quantum output ensemble $w^{U\rho U^\dagger}(\tilde{n})$, the classical output ensemble suffers an increase in the fraction of molecules that are maximally mixed. This means that the magnetization signal produced by the classical output ensemble is a factor of η smaller than in the quantum description:

$$
\begin{aligned}
\int d\Omega_{\tilde{n}}\, w_{\rm out}(\tilde{n}) (n_1)_{\beta_1} \cdots (n_N)_{\beta_N} &= \mathrm{tr}\Big(U\rho_\eta U^\dagger \sigma_{\beta_1} \otimes \cdots \otimes \sigma_{\beta_N} \Big) \\
&= \eta\, \mathrm{tr}\Big(U\rho U^\dagger \sigma_{\beta_1} \otimes \cdots \otimes \sigma_{\beta_N} \Big) \;.
\end{aligned} \tag{4.11}
$$

If we use the transition probabilities (4.7) to describe transitions of the spin directions in a gate-by-gate classical model of an NMR quantum computation, the magnetization signal of the model loses a factor of η at each entangling gate. Though such a model gives a satisfactory account of an NMR experiment in which one ignores the strength of the signal, we can formulate a better model that avoids the decay for a few entangling gates.

V. GATE-BY-GATE CLASSICAL MODEL

The key idea in constructing an improved model is to introduce auxiliary, "hidden" spins $\vec{a}_1, \ldots, \vec{a}_N \equiv \tilde{a}$, one for each qubit. We also need a "counter index" k, which increments by 1 at each entangling gate. In the improved model, we can avoid the decay of the signal for K entangling gates, where K is the largest integer such that

$$
\epsilon \le \eta^{K+1} \;. \tag{5.1}
$$

We assume that $\epsilon \le \eta^2$ to ensure that $K \ge 1$. It is useful to introduce the function

$$
\eta_k \equiv \begin{cases} \eta^{K-k} \,, & 0 \le k < K, \\ 1 \,, & k \ge K. \end{cases} \tag{5.2}
$$

Between the kth and $(k+1)$th entangling gates ($k \ge 0$), we represent a density operator ρ by the expansion coefficients

$$w_k^\rho(\tilde{a}) \equiv \mathrm{tr}\Big(\rho Q_{\eta_k}(\tilde{a})\Big) \; . \tag{5.3}$$

It is easy to show that these expansion coefficients are related to the original coefficients (3.4) by

$$w_k^\rho(\tilde{a}) = \frac{1-\eta_k^{-1}}{(4\pi)^N} + \eta_k^{-1} w^\rho(\tilde{a}) \tag{5.4}$$

and that ρ can be expanded as

$$\rho = \int d\Omega_{\tilde{a}}\, w_k^\rho(\tilde{a}) P_{\eta_k}(\tilde{a}) \; . \tag{5.5}$$

For density operators of the form (2.1), Eqs. (5.4) and (3.7) imply that

$$w_k^\rho(\tilde{a}) \geq \frac{1-\epsilon/\eta^{K+1}}{(4\pi)^N} \geq 0 \tag{5.6}$$

for all $k \geq 0$. Throughout the experiment, the expansion coefficients $w_k^\rho(\tilde{a})$ can be interpreted as probability distributions.

In our improved classical model, the gate operations manipulate the hidden spins; the effect of a gate shows up in the observable spins $\tilde{n}$ through the correlations of $\tilde{n}$ with $\tilde{a}$. Between the kth and $(k+1)$th entangling gates, this correlation is described by the joint distribution

$$w_k^\rho(\tilde{n}, \tilde{a}) \equiv q_k(\tilde{n}|\tilde{a}) w_k^\rho(\tilde{a}) \; , \tag{5.7}$$

where

$$q_k(\tilde{n}|\tilde{a}) \equiv \frac{1-\eta_k}{(4\pi)^N} + \eta_k \delta(\tilde{n}-\tilde{a}) \tag{5.8}$$

is a conditional probability distribution. The marginal distribution for the observable spin variables,

$$\int d\Omega_{\tilde{a}}\, w_k^\rho(\tilde{n}, \tilde{a}) = \frac{1-\eta_k}{(4\pi)^N} + \eta_k w_k^\rho(\tilde{n}) = w^\rho(\tilde{n}) \; , \tag{5.9}$$

is just the right mixture of $w_k^\rho(\tilde{n})$ with the uniform distribution to produce the distribution $w^\rho(\tilde{n})$ that gives the measured expectation values.

We now define transition probabilities for quantum gates, distinguishing as before between product unitaries and entangling unitaries. For a product unitary V, we find, by an argument analogous to the previous one, that

$$w_k^{V\rho V^\dagger}(\tilde{n}, \tilde{a}) = w_k^\rho(\tilde{n}, \tilde{R}^{-1}\tilde{a}) \; . \tag{5.10}$$

The effect of V is to rotate the hidden spins. Decoherence is handled, as previously, by mixtures of product unitaries.

To deal with an entangling unitary transformation U, we first note that the transition probabilities $w_U(\tilde{a}|\tilde{b})$ defined in Eq. (4.7) can be expressed as

$$w_U(\tilde{a}|\tilde{b}) = \mathrm{tr}\Big(UP_{\eta\theta}(\tilde{b})U^\dagger Q_\theta(\tilde{a})\Big) \geq 0\ . \tag{5.11}$$

Using this result, together with Eq. (5.5), we find

$$\begin{aligned}
\int d\Omega_{\tilde{b}}\, w_U(\tilde{a}|\tilde{b}) w_k^\rho(\tilde{b}) &= \mathrm{tr}\Bigg(U \underbrace{\Big[\int d\Omega_{\tilde{b}}\, P_{\eta\eta_{k+1}}(\tilde{b}) w_k^\rho(\tilde{b})\Big]}_{=\begin{cases}\rho\ , & 0\le k<K\\ \rho_\eta\ , & k\ge K\end{cases}} U^\dagger Q_{\eta_{k+1}}(\tilde{a})\Bigg) \\
&= \begin{cases} w_{k+1}^{U\rho U^\dagger}(\tilde{a})\ , & 0 \le k < K,\\ w_{k+1}^{U\rho_\eta U^\dagger}(\tilde{a})\ , & k \ge K. \end{cases}
\end{aligned} \tag{5.12}$$

To describe the effect of the $(k+1)$th entangling gate, we use transition probabilities

$$w_{k+1}^U(\tilde{n},\tilde{a}|\tilde{m},\tilde{b}) \equiv q_{k+1}(\tilde{n}|\tilde{a}) w_U(\tilde{a}|\tilde{b})\ , \tag{5.13}$$

which take the input ensemble $w_{\mathrm{in}} \equiv w_k^\rho(\tilde{n},\tilde{a})$ to an output ensemble

$$\begin{aligned}
w_{\mathrm{out}}(\tilde{n},\tilde{a}) &= \int d\Omega_{\tilde{m}}\, d\Omega_{\tilde{b}}\, w_{k+1}^U(\tilde{n},\tilde{a}|\tilde{m},\tilde{b}) w_{\mathrm{in}}(\tilde{m},\tilde{b}) \\
&= q_{k+1}(\tilde{n}|\tilde{a}) \int d\Omega_{\tilde{b}}\, w_U(\tilde{a}|\tilde{b}) w_k^\rho(\tilde{b}) \\
&= \begin{cases} w_{k+1}^{U\rho U^\dagger}(\tilde{n},\tilde{a})\ , & 0 \le k < K,\\ w_{k+1}^{U\rho_\eta U^\dagger}(\tilde{n},\tilde{a})\ , & k \ge K. \end{cases}
\end{aligned} \tag{5.14}$$

We have now constructed a gate-by-gate classical model in which there is no loss of magnetization signal for the first K entangling gates. How this works can be summarized as follows. The initial distribution $w_0^\rho(\tilde{a})$ of the hidden spin variables is chosen to have as little contribution from the uniform distribution as is consistent with nonnegativity. At each entangling gate, the ensemble of hidden spins suffers an increase in the proportion of molecules that are maximally mixed, but the observable spins retain the statistics of the quantum description by becoming more tightly correlated with the hidden spins. After K entangling gates, the observable and hidden spins become δ-correlated; thus from the $(K+1)$th entangling gate on, the signal decreases by a factor of η at each entangling gate.

VI. DISCUSSION

Consider a bulk-ensemble NMR experiment whose parameter ϵ satisfies the condition $\epsilon \leq \eta^2$ that underlies the argument in Sec. V. If we assume $\alpha = 2\times 10^{-6}$ in Eq. (2.2), this condition is fulfilled for $N \leq 6$ qubits. The model constructed in Sec. V provides an overall classical model in the sense of our second criterion: the unitary transformation U that maps the initial state to the final state is described in the model, with no loss of magnetization signal, by the transition probabilities $w_1^U(\tilde{n},\tilde{a}|\tilde{m},\tilde{b})$; mixtures of such transition probabilities are used to incorporate decoherence. The predictions of the model for the signal derived from the output state are identical to the quantum predictions. Since all NMR experiments to date involve 2 or 3 qubits, this overall classical model applies to all such experiments.

We turn now to the implications of the gate-by-gate classical model constructed in Sec. V. If we assume again that $\alpha = 2 \times 10^{-6}$, in a 2-qubit experiment the model proceeds through $K = 5$ entangling gates with no signal loss, and in a 3-qubit experiment, through $K = 3$ entangling gates. We illustrate the implications by considering a particular 3-qubit experiment, the NMR version of quantum teleportation [4]. After preparation of a pseudopure state by the gradient-pulse technique [8], the teleportation experiment consisted of four operations: (i) an entangling 2-qubit gate, (ii) a 2-qubit mapping of the Bell basis to the computational basis, (iii) decoherence of two qubits in the computational basis, and (iv) a conditional 3-qubit unitary. Our model incorporates the decoherence step as a mixture of classical rotations of the hidden spins. Since the model can account for $K = 3$ entangling gates without loss of signal, it provides a gate-by-gate classical model whose predictions are identical to the quantum predictions. This experiment therefore does not demonstrate genuine quantum-information processing in the sense of our third criterion. For a larger value of α, when $K = 2$, our model predicts a drop in signal by a factor of $\eta = 1/33$ at the third entangling step. Nevertheless, even when $K = 2$, the classical model can still account for the teleportation experiment if the first two 2-qubit gates are "compiled" into a single 3-qubit gate.

Similar conclusions apply to the other 3-qubit experiments performed to date [5–8] and to most of the 2-qubit experiments [8,11–16]. The 2-qubit experiment described in Ref. [9] ran through 15 entangling gates with an approximately exponential signal-to-noise decrease that is, however, much slower than the factor of $\eta = 1/9$ per entangling gate predicted by our model after the first $K = 5$ steps. The 2-qubit experiment reported in Ref. [10] implemented up to 14 entangling gates, but the absence of signal-to-noise data makes comparison with our model difficult.

This paper, together with Ref. [23], begins the task of establishing standards for assessing the quantumness of bulk-ensemble NMR quantum computation [39,40]. Our gate-by-gate classical model erects a hurdle in the way of NMR quantum-information processing. "Testing" our classical model is not the point, for no one would contend that it describes the physics that underlies an NMR experiment. The point is that experiments that fail to clear the hurdle can be explained in classical language and thus do no genuine quantum-information processing according to our third criterion.

It will be easy for NMR experimenters to clear our hurdle, by measuring the signal-to-noise ratio in experiments involving many entangling gates, like the experiment reported in Ref. [9]. Yet jumping over our hurdle is probably not sufficient to provide a warranty of genuine quantum-information processing, for that would require showing that a given experiment is inconsistent with *all* gate-by-gate classical models, not just the model formulated in this paper. There are reasons for believing that our classical model is not optimal, the most cogent of which is that the model's transition probabilities for an entangling gate transform qubits that are unaffected by the gate. Avenues for improving the model include the following: (i) investigating more efficient representations both for quantum states near the maximally mixed density operator and for the transition probabilities between states, (ii) seeking gate representations that are more efficient when fewer qubits are involved in the gate, and (iii) addressing the extent to which one is allowed to "compile" successive entangling unitaries into a single operation (compiling is routine in NMR experiments as a method for reducing the length of a computation).

We conjecture, however, that no matter how efficient the gate representations are made, an ultimate signal decrease is an unavoidable consequence of any attempt to describe entangling unitaries classically, even when the unitaries act only on separable states. Indeed, more interesting than our results would be a demonstration of this conjecture. Should the conjecture prove to be correct, one could conclude that the quantumness of NMR quantum computation, for small numbers of qubits, lies in the ability to avoid any signal decrease. More broadly, we speculate that the power of quantum-information processing comes not from entanglement itself [26–28], but rather from the information-processing capabilities of entangling unitaries.

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[26] Knill and Laflamme [19] analyze the "Power of one qubit of quantum information" by considering a model for ensemble computation using input states in which one qubit is in a pure state and all the other qubits are in a maximally mixed state. They note that although the apparent power of quantum computers "is frequently attributed to 'quantum parallelism,' interference phenomena derived from the superposition principle,

and the ability to prepare and control pure states according to the Schrödinger equation," their results suggest that "the usual reasons given for why quantum computation appears to be so powerful may have to be revised."
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[29] It is likely that there are Bohm-type "nonlocal" hidden-variable models for N qubits. Such a model would look like the Bohmian description of translational degrees of freedom [for an introduction to Bohmian mechanics, see the articles in *Bohmian Mechanics and Quantum Theory: An Appraisal*, edited by J. T. Cushing, A. Fine, and S. Goldstein (Kluwer, Dordrecht, 1996)] and would reproduce all the predictions of quantum mechanics by incorporating the state vector directly into the model. It would, however, violate the assumptions of our third criterion, in that the transition probabilities for a gate would depend on the initial state or would include qubits not involved in a gate in a nontrivial way.
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[37] Consider the case of two qubits ($N = 2$), initially in a computational-basis state ρ, which undergo a nonfactorizable unitary transformation U that takes computational-basis states to (entangled) Bell states. After the unitary dynamics, the two qubits are measured in the computational basis; let F_α denote the POVM elements of this measurement. The measurement statistics can be regarded as coming from a measurement of factorizable POVM F_α on the entangled state $U\rho U^\dagger$ or as a measurement of a nonfactorizable POVM $E_\alpha = U^\dagger F_\alpha U$ on the separable state ρ. According to the discussion surrounding Eq. (3.9), the latter can be given a classical interpretation, whereas the former cannot. The discrepancy is resolved in the following way: introduce a tensor-product decomposition of the four-dimensional Hilbert space in which the computational-basis states and the Bell states switch roles, the original computational-basis states becoming Bell states and the original Bell states becoming product states (this new decomposition corresponds to a different way of dividing the two-qubit system into two subsystems); analyzed in this new tensor-product decomposition, the measurement of E_α on ρ becomes identical to the measurement of F_α on $U\rho U^\dagger$ and cannot be given a classical interpretation. These considerations are relevant to states of the form (2.1), with $\epsilon \leq \eta$, for

these states are separable relative to *all* decompositions of the 2^N-dimensional Hilbert space into a tensor product of N two-dimensional spaces. This *super-separability* does not hold generally for separable states.

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[40] Some authors have been careful about advancing claims for the quantum nature of NMR quantum-information processing. For example, Cory *et al.*, in a paper [8] outlining the principles of NMR quantum computation, comment (in the abstract) that "nuclear magnetic resonance spectroscopy is capable of *emulating* (our emphasis) many of the capabilities of quantum computers, including unitary evolution and coherent superpositions, but without attendant wave-function collapse." Others have been less cautious. Gershenfeld and Chuang, in their original paper on NMR [2], remark, "Because the N spins in each molecule may be in entangled quantum superposition states, our computer can be a quantum one," and Chuang *et al.* [11], in describing the experiment referred to at the end of Sec. III, which implements a single 2-qubit gate (a controlled-NOT), note, "Perhaps the most interesting aspect of this experiment is that the experimental results cannot be explained by a classical model of two interacting spins (of spin $\frac{1}{2}$)."