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Quantum gate arrays as coherent sums over classical logic gate arrays

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Abstract. Quantum spin systems may provide physical realizations of quantum gate arrays. It is shown that certain natural unitary time evolution matrices for spin-$\frac{1}{2}$ quantum spins, interpreted in this context as quantum gate arrays, can be represented as coherent sums, with appropriate phases, over classical logic gate arrays, in a direct analogy with the Feynman path integral representation of quantum mechanics. On the other hand, it is shown that a natural quantum gate obtained by analytically continuing the transfer matrix of the anisotropic nearest-neighbour Ising model to imaginary time, does not admit such a representation.

Shor's discovery [1] of polynomial time quantum algorithms for prime factorization and discrete logarithm has resulted in an upsurge of interest in the properties of quantum computation [2]. Significant results have been obtained concerning the physical realizability of quantum gates, and the realizability of classical universal 3-bit gates such as the Fredkin and Toffoli [3] gates in terms of quantum 2-bit logic. Furthermore, Barenco *et al* [4] have shown that all quantum gates can be expressed as compositions of all 1-bit quantum gates and the 2-bit exclusive-or gate. The problems of error correction [5] and decoherence [6] in quantum computation have also been addressed.

Our aim here is to consider the properties of quantum-computational devices in a different light. Instead of constructing classical computational devices in terms of quantum gate arrays, we want to represent some rather general quantum gate arrays in terms of coherent sums over classical gate arrays, much as Feynman represented quantum-mechanical amplitudes in terms of sums over paths, including paths which are not necessarily solutions of the classical equations of motion [7]. There are obvious reasons for wanting such a representation. An intuition for the efficiency of quantum computation is that quantum computers sum coherently over many classical computations, and it is important to understand quantitatively how this works, and how it can be exploited. After this paper first appeared, related ideas were discussed in detail in [14].

Further, it is likely that the true power of quantum computation will come from massively parallel computation, a point that has been considered from the very beginnings of the subject, and recently re-emphasized [8]. A possible physical realization of such massively parallel quantum computers might be in terms of quantum spin systems (such as spin chains or spin arrays), and *it is the interplay between the dynamics and quantum logic*

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of these spin systems that we will focus on in this paper. An intuition for the behaviour of quantum gate arrays, in terms of classical logic gate arrays, is of great interest in this context, just as in the case of the Feynman path integral. Consider, for example, the quantum phenomenon of tunnelling—one would like to know what the classical computational analogue of this might be, and how it should be used in the design of quantum computers and quantum programming.

Indeed, programming quantum computers on the basis of what classical logic it replaces, is likely to be inefficient. It may be more efficient to program according to the properties of quantum computers, much as with a writing code for parallel processors, and for this purpose it is again important to gain some classical intuition for the properties of quantum gate arrays. Such classical logic representations also allow for a new type of simulation of quantum computers by classical parallel processors, rather obviously.

We present two independent insights into classical representations of quantum logic gate arrays. First, we show that for a natural set of Hamiltonians governing quantum spin-$\frac{1}{2}$ degrees of freedom, there is a simple representation of the unitary time evolution operator, in other words, the quantum logic gate array, in terms of appropriately weighted sums over classical logic gate arrays [9]. We describe properties of these 'logic integrals' (adapting the term 'path integrals' to the present context) which can be deduced from the physical properties of the spin systems, and we suggest some uses for such quantum logic gate arrays. There is extensive literature on path integrals for spin (see, for example, [13]), but the 'logic integrals' we describe are at some remove from such representations, as will be clear in the following. Certain general properties of such quantum gate arrays for a one-dimensional chain of spins could be inferred by finite-size scaling calculations around conformal field theories in two dimensions [10].

In the first part of this paper we have established that for certain natural quantum computers, such as quantum spin chains, there is a 'logic integral' representation, we then want to show that not every unitary evolution matrix that occurs in a physical context need have such classical logic representations. Therefore, we consider an anisotropic Ising model on a two-dimensional square lattice. We show that the transfer matrix of this model, analytically continued, is unitary at a unique value of the 'time' coupling, and we show that this unitary quantum gate *cannot* be represented as a sum over classical logic gates in general. Thus, 'logic integrals' do not necessarily exist as representations of quantum logic gate arrays, to be compared with the result of [11].

For our first problem, we consider quantum spin-$\frac{1}{2}$ degrees of freedom defined on a finite set of sites Γ. The unitary matrix governing the time evolution of the wavefunction of these spins is a quantum gate array found in nature, for example, arrays of interacting magnetic atoms as they occur in magnetic materials. The Hilbert space at each site is $\mathcal{H}_x \cong \mathbb{C}^2$, and observables are elements of the bounded operators on this Hilbert space, just the set of 2×2 complex matrices $M(2, \mathbb{C})$. The Hamiltonian H for such a system can be written in general as $H = -\sum_{b \in \mathcal{B}} J_b h_b$ where $\mathcal{B}$, the set of 'bonds', is a collection of subsets of Γ, h_b is an arbitrary element in $\otimes_{x \in b} M(2, \mathbb{C})$, with obvious restrictions to ensure that H is Hermitian, and the J_b, $b \in \mathcal{B}$ are coupling constants. For much of our discussion, it will suffice to take Γ as a subset of the integers, say $\{0, \ldots, L\}$, and $\mathcal{B} = \{\{0, 1\}, \ldots, \{L-1, L\}\}$, which is the easiest case to visualize, that of a one-dimensional quantum spin chain, but it is important to observe that our approach holds in all generality. Physically important observables are usually expressed in terms of the spin matrices S^1, S^2, S^3 which are the generators of the fundamental representation of SU(2). They satisfy the commutation relations $[S^\alpha, S^\beta] = i \sum_\gamma \epsilon_{\alpha\beta\gamma} S^\gamma$ where $\alpha, \beta, \gamma \in \{1, 2, 3\}$ and $\epsilon_{\alpha\beta\gamma}$ is the completely antisymmetric tensor with $\epsilon_{123} = 1$.

Our logic integral representation of the time evolution generated by H is based on the 'quasistate' decomposition introduced by Aizenman and Nachtergaele [9] in a statistical mechanics context. The starting point is the following identity derived in [9]:

$$\exp(-\mathrm{i}tH) = \int D_t\omega\ K(\omega) \tag{1}$$

where, up to normalization, $D_t\omega$ is the integration measure given by

$$D_t\omega = \prod_b \sum_{n_b=0}^{\infty} (\mathrm{i}J_b)^{n_b} \int_{0\leqslant t_1<\cdots<t_{n_b}<t} \prod_{j=1}^{n_b} \mathrm{d}t_j \tag{2}$$

where ω is a set of time-labelled bonds $\{(b_1, t_1), \ldots, (b_n, t_n)\}$, with $t_1 < t_2 < \cdots t_n$, and $K(\omega)$ is the time-ordered product of operators, one for each bond in ω:

$$K(\omega) = \prod{}^{*} h_{b_n} h_{b_{n-1}} \ldots h_{b_1}. \tag{3}$$

Here, $\prod^{*}$ indicates a time-ordered product. The time ordering is necessarily due to the fact that the different h_b typically do not commute. If they do, i.e. $[h_b, h_{b'}] = 0$, (1) and (2) reduce to the trivial identity $\exp(\mathrm{i}t\sum_b J_b h_b) = \prod_b \sum_{n_b=0}^{\infty} \frac{1}{n_b!}(\mathrm{i}tJ_b h_b)^{n_b}$. In (1) it can be seen as the Dyson series known from perturbation theory, but where the entire Hamiltonian is considered as a perturbation of $H = 0$. This formula was used in [9] to study antiferromagnetic isotropic quantum spin chains. These systems are not at all in a perturbative regime, yet (1) is the starting point for a powerful description of these systems in terms of Feynman-type diagrams.

The interpretation of the logic integral is simply that the time evolution of the system governed by H can be written as a coherent superposition of classical logic gates determined by the sequence of operators h_{b_i} that act on the state of the system at times t_i. This is illustrated in figure 1, in the case that Γ is a one-dimensional lattice and $\mathcal{B}$ are the nearest-neighbour bonds on this lattice.

The next step is to pick special decompositions of the Hamiltonian as a sum of the form $H = -\sum_b J_b h_b$ such that each term h_b can be interpreted as a classical logic gate. In such a case the logic integral becomes an integral over classical logic gates, and we believe that this may give a good starting point for developing effective intuitions about the functioning of quantum computing devices.

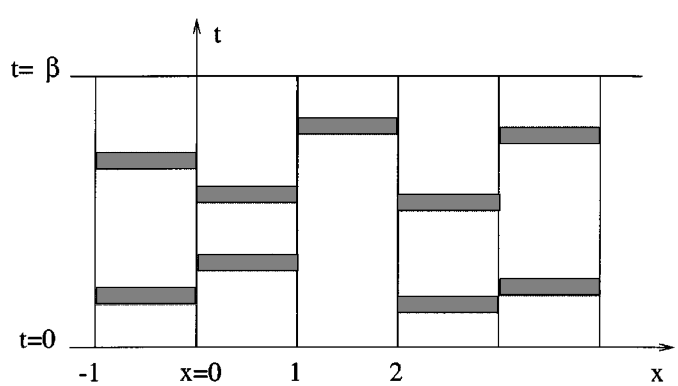

Figure 1. A space-time configuration ω for a general Hamiltonian. Each grey bar represents a quantum gate acting on two quantum bits at time t_i given by its vertical coordinate.

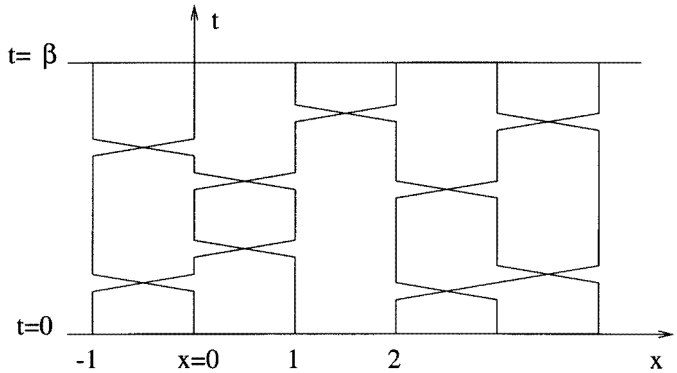

Figure 2. A configuration ω for the one-dimensional Heisenberg spin-$\frac{1}{2}$ ferromagnet. The grey bar in this case is an exchange gate, depicted in standard notation.

We illustrate with two examples that such special decompositions exist for physically interesting Hamiltonians. Consider, for example, h to be the operator that interchanges the states of the two sites,

$$h\phi \otimes \psi = \psi \otimes \phi \tag{4}$$

for any two vectors $\phi, \psi \in \mathbb{C}^2$. This is the exchange gate on two bits,

$$E \equiv \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{5}$$

which, as $E = (\frac{1}{4}) - \boldsymbol{S}_1 \cdot \boldsymbol{S}_2$, is equivalent to the Heisenberg spin-$\frac{1}{2}$ ferromagnet! Figure 2 shows a configuration ω in this model.

From expressions equations (1)–(3) it is obvious that the quantum-evolution operator can be decomposed as a linear superposition of classical logic gate arrays of the form $K(\omega)$. For concreteness, consider a 3-spin system (equivalently, a 3-bit gate). By performing the integrals in (2), for the example given in equations (4) and (5), we obtain series expansions for the coefficients of the various classical logic gate arrays appearing in the decomposition:

$$\begin{aligned} \exp(-\mathrm{i}tH) = {} & (1 - t^2J^2 + \cdots)\mathbf{1} + (\mathrm{i}tJ + \cdots)E_{12} + (\mathrm{i}tJ + \cdots)E_{23} + (-\tfrac{1}{2}t^2J^2 + \cdots)E_{123} \\ & + (-\tfrac{1}{2}t^2J^2 + \cdots)E_{123}^2 + (-\tfrac{1}{3}\mathrm{i}t^3J^3 + \cdots)E_{13}. \end{aligned}$$

In the case of the example given in equations (4) and (5), E_{ij} is the exchange gate on the i and j bits, and

$$E_{123} = E_{23}E_{12} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

is the matrix that permutes the three bits cyclically. This example illustrates the utility of classical logic representations of quantum gate arrays—by varying t, one can single out

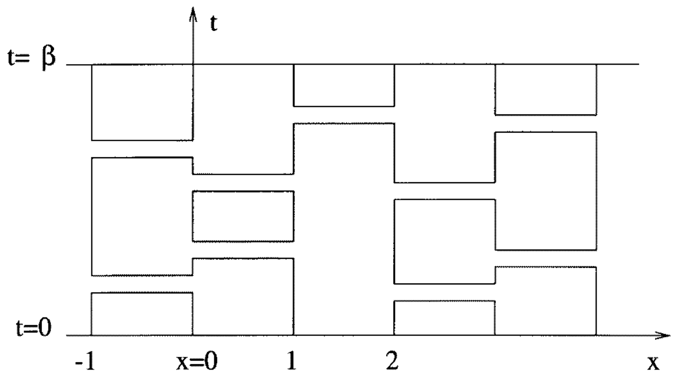

Figure 3. A configuration ω for the one-dimensional Heisenberg antiferromagnet, showing virtual loops. Each horizontal pair of lines represents the sum of the identity (or do nothing) gate on two bits and (minus) the exchange gate ($1-E$, in the notation used in this paper).

contributions of different classical logic gate arrays from the quantum gate array. t is just the time of evolution of the quantum system, so no external classical 'switches' are needed, which helps in minimizing the effects of decoherence [6].

If $\Gamma = \Gamma_A \cup \Gamma_B$ is a bipartite lattice, and $\mathcal{B}$ is a set with elements of the form $\{a, b\}, a \in \Gamma_A$ and $b \in \Gamma_B$, then we consider

$$h = \sum_{m,m'=\pm 1/2} (-1)^{m-m'} |m, -m\rangle\langle m', -m'|.$$

This is the Heisenberg antiferromagnet. In terms of classical logic, this operator h corresponds to $\mathbf{1} - E$, and is shown in figure 3. In this case, a new phenomenon that contributes to the quantum gate array, but would not appear in classical logic, becomes apparent in the quasistate representation. Notice that $1 - E$ is proportional to a projection of rank 1: $(1-E)^2 = 2(1-E)$. The factor of 2 corresponds to the fact that there are *closed loops* in a typical ω, as shown in figure 3. The sum over classical configurations that gives the quantum amplitude therefore includes sums over 'virtual' states of the classical logic.

Such logic-integral decompositions of quantum gate arrays can be extended to a much wider class of Hamiltonians with ease [9], providing simple classical logic representations with component classical gates that are n-bit gates. In the one-dimensional case, with $\Gamma = \{0, \ldots, L\}$, this amounts to taking $\mathcal{B} = \{\{0, \ldots, n\}, \{1, \ldots, n+1\}, \ldots\}$. Quasistate decompositions for such cases have been reported in detail elsewhere [9].

Simple properties of such quantum gate arrays can be extracted from physical properties of these systems. The original quasistate decomposition introduced in [9] was formulated for $\beta \leftrightarrow \mathrm{i}t$ real, as appropriate for studying quantum-statistical mechanics. Under rather general conditions (see e.g. [12]), the correlation functions of quantum-statistical mechanics, analytically continued, become the correlation functions of the quantum spin system under unitary time evolution. Of interest from the present point of view are the following.

(1) Some quantum spin systems exhibit phase transitions at real values of β in the infinite volume limit. This implies that the analytically continued real time correlation functions exhibit different characteristics, for long-time versus short-time evolution, effectively behaving as two different quantum gate arrays. With *very* naive assumptions about the analytic continuation, one could have a situation such that for long-time evolution, one would have algebraically decaying correlations between the input and output, but for short-time evolution one would have oscillations in the correlation between output and input.

(2) At finite lattice sizes, one can still get a good handle on properties of quantum gate arrays for β close to β_c by calculating finite-size corrections to the correlation functions at criticality [10], and then continuing to imaginary β, to obtain the required correlation of the quantum gate array. This will be reported on in detail elsewhere.

For the converse of our first problem, we now turn to the anisotropic Ising model in two dimensions, to exhibit another aspect to representations of quantum gate arrays as 'logic integrals' of classical logic gate arrays. In contrast to the first part of this paper, where we dealt with quantum spin chains or arrays which are found (or can be fabricated) in nature, we do not know of a physical realization of the Ising model continued as we do below. Nevertheless, we present this formal example to indicate possible limits to the logic integral approach that we have formulated in this paper.

Recall that this model is a classical statistical mechanics model, with spins taking values ± 1 living on the sites of a square two-dimensional lattice. For our purposes, we take the system to be of finite extent in the space direction. The time direction's extent will not be relevant for us, but for the nonce we assume periodic boundary conditions in the time direction. The partition function of this model is

$$\mathcal{Z} \equiv \sum_{\{\sigma\}} \exp\left(- \beta_1 \sum_{i=0}^{N} \sum_{t} \sigma_{i,t}\sigma_{i,t+1} - \beta \sum_{t} \sum_{i=0}^{N-1} \sigma_{i,t}\sigma_{i+1,t} \right)$$

where the sum over t is a sum over the time slices of the lattice. Introduce a transfer matrix T, defined by

$$\langle \tilde{\sigma}_0, \ldots \tilde{\sigma}_N | T | \sigma_0, \ldots \sigma_N \rangle \equiv 2^{-N/2} \exp\left(- \beta_1 \sum_{i=0}^{N} \tilde{\sigma}_i \sigma_i - \beta \sum_{i=0}^{N-1} \sigma_i \sigma_{i+1} \right).$$

For a lattice of time extent τ, the partition function can now be written as $\mathcal{Z} \propto \operatorname{tr} T^{\tau}$. This transfer matrix T essentially allows one to interpret the Ising model as a discrete-time one-dimensional quantum system, with $T \equiv \exp(-H)$. We can now analytically continue this matrix to imaginary time, and ask if there are imaginary values of β and β_1 such that T is a unitary matrix.

To this end, we evaluate

$$\langle \tilde{\sigma} | T T^{\dagger} | \sigma \rangle = 2^{-N} \sum_{\sigma'} \exp\left(- \sum_{i=0}^{N} [\beta_1 \tilde{\sigma}_i + \beta_1^* \sigma_i] \sigma_i' - (\beta + \beta^*) \sum_{i=0}^{N-1} \sigma_i' \sigma_{i+1}' \right).$$

It follows then that if $\beta = \mathrm{i}\gamma$, and $\beta_1 = \pm \mathrm{i}\pi/4$, T is a unitary matrix for any value of γ.

For $N = 2$, this matrix is

$$T = \begin{pmatrix} \mathrm{i} & 1 & 1 & -\mathrm{i} \\ 1 & \mathrm{i} & -\mathrm{i} & 1 \\ 1 & -\mathrm{i} & \mathrm{i} & 1 \\ -\mathrm{i} & 1 & 1 & \mathrm{i} \end{pmatrix} \times \operatorname{diag}(\Delta, \Delta^*, \Delta^*, \Delta)$$

where $\Delta \equiv \exp(-\mathrm{i}\gamma)$. If $\Delta = 1$, it is clear that T can be written as

$$T(\gamma = 0) = \mathrm{i} \left[\mathbf{1} - \mathrm{i} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} - \mathrm{i} \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \right]$$

which is readily recognizable as a sum over classical logic gates, with appropriate phase factors. Here, we have restricted ourselves to decompositions with coefficients of modulus 1. It is easy to see that there are two such decompositions.

However, when $\Delta \neq 1$, such a decomposition is not possible in general. Indeed, there is no reason to suppose that such a decomposition must exist. Classical logic gates on N bits are matrices in the $2^N \times 2^N$ permutation representation of the permutation group on 2^N letters. By Schur's lemma, the complex linear span of the permutation representation on n letters is a strict subalgebra of the algebra of complex $n \times n$ matrices, since the permutation representation is reducible, but the defining representation of $\mathrm{U}(n)$ is certainly irreducible, so its complex linear span is all of the algebra of complex $n \times n$ matrices.

In conclusion, we have shown there is a natural representation of quantum-gate arrays that occur in nature in the form of spin chains in terms of sums over classical logic gate arrays, analogous to the Feynman sum over paths representation of quantum-mechanical amplitudes. We have pointed out that this viewpoint on quantum logic gate arrays allows a whole host of tools from statistical mechanics and quantum spin chains to be used to obtain a better intuition for their characteristics. We have explicitly shown that such representations may not always be possible, indicating some of the limits of this approach.

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