We propose to design multispin quantum gates in which the input and output two-state systems (spins) are not necessarily identical. We describe the motivations for such studies and then derive an explicit general two-spin interaction Hamiltonian which accomplishes the quantum XOR gate function for a system of three spins: two input and one output.
1. Introduction

Dimensions of semiconductor computer components will soon reach\(^1\) about 0.25 \(\mu m = 2500 \text{ Å}\), still well above the sizes at which quantum-mechanical effects are important. However, it is generally expected that as the miniaturization continues, atomic dimensions will be reached, perhaps, with technology different from today’s semiconductors. The physics of quantum-mechanical computation has attracted much attention recently.\(^2\) Quantum computer is a quantum-coherent system that functions as a programmable calculational apparatus, quite unlike its classical counterparts. It can perform certain tasks\(^2\) much faster than the classical computer: the quantum interference property yields\(^2\) the fast-factoring (Shor’s), as well as certain other fast algorithms. Recent theoretical results have included identification of universal reversible two-bit gates\(^3\) and advances in error correction.\(^4\) There have also been experiments and proposals for experiments,\(^5\) realizing the simplest gates. However, the actual construction of a macroscopic computer out of a large number of quantum bits (two-state systems, qubits) is elusive\(^6\) at the present stage of technology. The main obstacle is the sensitivity of coherent quantum evolution and interference to undesirable external interactions such as noise or other failures in operation,\(^2,6,7\) even though a number of error correction schemes have been proposed.\(^4\)

We therefore propose an alternative approach along the lines of the “classical” analog computer design, of operating the computer as a single unit performing in one shot a complex logical task instead of a network of simple gates each performing a simple “universal-set” logical function. The computer as a whole will still be subject to errors. However, these will not be magnified by proliferation of sub-steps each of which must be exactly controlled.

Indeed, quantum (and more generally reversible) computation must be externally timed: the time scale of the operation of each gate is determined by the interactions rather than by the relaxation processes as in the ordinary computer. Furthermore, gate interactions must be externally switched\(^2\) on and off because the gates affect each other’s operation. Time dependence smoother than the on/off protocol is possible: see Ref. 8.

In fact, we consider it likely that technological advances might first allow design and manufacturing of limited size units, based on several tens of atomic two-level systems, operating in a coherent fashion over sufficiently large time interval to function as parts of a larger classical (dissipative) computer. We would like these to function as single units rather than being composed of many gates.

While in principle in a reversible computational unit input and output spins (qubits) need not be different, for larger units interacting with the external world it may be practically useful to consider input and output separate (or at least not identical). Indeed, the interactions that feed in the input need not necessarily be identical to those interactions/measurements that read off the output.

We consider in this work a spatially extended XOR gate based on three spins: two input and one output. Generally, we have to address a complicated set of
problems: can multispin computational units be designed with short-range, two-particle interactions? Can they accomplish logical functions with interactions of the form familiar in condensed-matter or other experimental systems? These and similar questions can only be answered by multispin-unit calculations which will have to be numerical. Analytical results are limited to the simplest gates such as NOT and XOR, the former studied in Ref. 8, and they provide only a partial picture.

We emphasize that the XOR function is used only as a solvable example of a gate with more than two spins, in which one can seek to accomplish a useful logical function solely with two-spin interactions. The XOR function can be also realized with two spins (one of the inputs serving as the output), for instance as the sub-result of the controlled-NOT gate. It is also important to emphasize that while moving from two spins to three spins brings in the issue of the two-body interactions, the other important aspect of multispin gates: having the interactions short-range, can only be explored with larger systems.

In Section 2, we define the problem and introduce some notation. In Section 3, we analyze the matrix forms of the unitary evolution operator and Hamiltonian operator. The latter is explicitly calculated in Section 4 and then further refined in Sections 4 and 5 to yield a two-spin-interaction result.

2. The Three-Spin XOR Gate

We will use the term “spin” to describe a two-state system, and we will represent spin-$\frac{1}{2}$ particle spin-components (measured in units of $\hbar/2$) by the standard Pauli matrices $\sigma_{x,y,z}$. We denote by $A$, $B$, $C$ the three two-state systems, i.e., three spins, involved. We are particularly interested in such initial conditions, at time $t$, that the input spins $A$ and $B$ are in one of the basis states $|AB\rangle = |11\rangle$, $|10\rangle$, $|01\rangle$, or $|00\rangle$, where 1 and 0 refer to the eigenstates of the $z$-component of the spin operator, with 1 referring to the “up” state and 0 referring to the “down” state. We use this convention for consistency with the classical “bit” notion. The initial state of $C$ is arbitrary.

We would like to have a quantum evolution which, provided $A$ and $B$ are initially in those basis states, mimics the XOR function:

\[
\begin{array}{ccc}
A & B & \text{output} \\
1 & 1 & 0 \\
1 & 0 & 1 \\
0 & 1 & 1 \\
0 & 0 & 0 \\
\end{array}
\]

(1)

where the output is at time $t + \Delta t$. As already mentioned, one way to accomplish this is to produce the output in $A$ or $B$, i.e., work with a two-spin system. The Hamiltonian for such a system is not unique. Explicit examples can be found in Refs. 2, 5, 9. In the case of two spins involved, the interactions can be single- and two-spin only.
An important question is whether multispin systems can produce useful logical operations with only two-spin and, for larger systems, short-range interactions. Indeed, two-particle short-range interactions are much better studied and accessible to experimental probe than multiparticle interactions. As a solvable example that addresses the former issue, here we require that the XOR result be put in C at time \( t + \Delta t \). The final states of A and B, as well as the phase of C are arbitrary. In fact, there are many different unitary transformations, \( U \), that correspond to the desired evolution in the eight-state space with the basis \(|ABC\rangle = |111\rangle, |110\rangle, |101\rangle, |100\rangle, |011\rangle, |010\rangle, |001\rangle, |000\rangle\), which we will use in this order. The choice of the transformation determines what happens when the initial state is a superposition of the reference states, what are the phases in the output, etc.

Let us consider first, for illustration, the following Hamiltonian, which elludes to our more general results below,

\[
H = \frac{\pi \hbar}{4 \Delta t} \left( \sqrt{2}\sigma_z A \sigma_y B + \sqrt{2}\sigma_z B \sigma_y C - \sigma_y B \sigma_x C \right),
\]

It is written here in terms of the spin components; the subscripts \( A, B, C \) denote the spins. In the eight-state basis specified earlier, its matrix can be obtained by direct product of the Pauli matrices and unit 2 \( \times \) 2 matrices \( I \). For instance, the first interaction term is proportional to

\[
\sigma_z A \otimes \sigma_y B \otimes I_C,
\]

etc. This Hamiltonian involves only two-spin-component interactions. In fact, in this particular example A and C only interact with B.

One can show that the Hamiltonian (2) corresponds to the XOR result in C at \( t + \Delta t \) provided A and B where in one of the superpositions of the appropriate “binary” states at \( t \) (we refer to superposition here because C is arbitrary at \( t \)). There are two ways to verify this. Firstly, one can diagonalize \( H \) and then calculate the unitary evolution operator (matrix) \( U \) in the diagonal representation by using the general relation (valid for Hamiltonians which are constant during the time interval \( \Delta t \); see Ref. 8 for a formulation that introduces a multiplicative time dependence in \( H \)),

\[
U = \exp \left( -iH \Delta t / \hbar \right),
\]

and then reverse the diagonalizing transformation. The calculation is quite cumbersome.

The second, more general approach adopted here is to “design” a whole family of two-spin-interaction Hamiltonians of which the form (2) is but a special case, by analyzing generally a family of 8 \( \times \) 8 unitary matrices corresponding to the XOR evolution. This “design” program is carried out in the following sections.

3. The Structure of the Unitary Matrix and Hamiltonian

We require any linear combination of the states \(|111\rangle\) and \(|110\rangle\) to evolve into a linear combination of \(|110\rangle, |100\rangle, |010\rangle, \) and \(|000\rangle\), compare the underlined quantum
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numbers with the first entry in (1), with similar rules for the other three entries in (1).

In the matrix notation, and in the standard basis introduced earlier, namely, $|ABC\rangle = |111\rangle, |110\rangle, |101\rangle, |100\rangle, |011\rangle, |010\rangle, |001\rangle, |000\rangle$, the most general XOR evolution operator corresponding to the Boolean function (1), with the output in $C$, is, therefore

$$U = \begin{pmatrix}
0 & 0 & U_{13} & U_{14} & U_{15} & U_{16} & 0 & 0 \\
U_{21} & U_{22} & 0 & 0 & 0 & 0 & U_{27} & U_{28} \\
0 & 0 & U_{33} & U_{34} & U_{35} & U_{36} & 0 & 0 \\
U_{41} & U_{42} & 0 & 0 & 0 & 0 & U_{47} & U_{48} \\
0 & 0 & U_{53} & U_{54} & U_{55} & U_{56} & 0 & 0 \\
U_{61} & U_{62} & 0 & 0 & 0 & 0 & U_{67} & U_{68} \\
0 & 0 & U_{73} & U_{74} & U_{75} & U_{76} & 0 & 0 \\
U_{81} & U_{82} & 0 & 0 & 0 & 0 & U_{87} & U_{88}
\end{pmatrix}. \tag{5}$$

The condition of unitarity, $UU^\dagger = 1$, reduces the number of independent parameters. Still they are too numerous for the problem to be manageable analytically; recall that each nonzero element $U_{kn}$ is complex and therefore involves two real parameters. Thus, we are going to consider a subset of operators of the form (5).

From our earlier work\(^8\) we know that one convenient way to reduce the number of parameters and at the same time ensure unitarity is to have a single phase factor in each column and row of the matrix. Furthermore, we choose a form which is diagonal in the states of the $A$-spin,

$$U = \begin{pmatrix}
V_{4\times4} & 0_{4\times4} \\
0_{4\times4} & W_{4\times4}
\end{pmatrix}. \tag{6}$$

Thus, $A$ and $B$ are not treated symmetrically. Here $0_{4\times4}$ denotes the $4 \times 4$ matrix of zeros. The $4 \times 4$ matrices $V$ and $W$ are parametrized as follows:

$$V = \begin{pmatrix}
0 & 0 & e^{i\delta} & 0 \\
e^{i\alpha} & 0 & 0 & 0 \\
0 & 0 & 0 & e^{i\beta} \\
0 & e^{i\gamma} & 0 & 0
\end{pmatrix}, \tag{7}$$

$$W = \begin{pmatrix}
0 & e^{i\rho} & 0 & 0 \\
e^{i\xi} & 0 & 0 & 0 \\
0 & 0 & 0 & e^{i\omega} \\
0 & 0 & e^{i\eta} & 0
\end{pmatrix}. \tag{8}$$

The reasons for this choice of an 8-parameter unitary matrix $U$ will become apparent in the course of the calculation. Some of the features can be explained at this stage as follows. We note that, omitting the direct-product symbols and replacing unit matrices by $1$, etc., the matrix $U$ in (6) has the structure

$$2U = (1 + \sigma_z A) V + (1 - \sigma_z A) W = V + W + \sigma_z A (V - W), \tag{9}$$
where $V$ and $W$ are operators in the space of $B$ and $C$. Since $U$ was chosen diagonal in the space of $A$, the Hamiltonian $H$ will have a similar structure,

$$2H = P + Q + \sigma_z A(P - Q),$$

(10)

with the appropriate $(B \otimes C)$-space Hamiltonians $P$ and $Q$. Now in order to avoid three-spin interactions, $P - Q$ must be linear in Pauli matrices. On the other hand, we also prefer to avoid single-spin (external-field) interactions. Thus, $P + Q$ must contain only terms of the second order in the spin components while $P - Q$ must contain only terms of the first order in the spin components. This suggests avoiding putting phase factors on the diagonal, which would lead to matrices similar to those encountered in the NOT-gate calculations\(^8\) that are known to be of a structure undesirable here: they contain a mixture of first-order and second-order terms. The off-diagonal choices remaining are considerably limited; the forms (7) and (8) are thus nearly unique.

In summary, while the arguments are admittedly vague and they do involve a certain level of guess, trial and error, the presented parametrization offers a good chance that with further restrictions on the parameters a two-spin interaction Hamiltonian can be obtained. As will be seen later, five conditions are imposed so that the resulting Hamiltonian depends on three (real) parameters.

4. The Hamiltonian Matrix

Let us define

$$\mu = \frac{\alpha + \beta + \gamma + \delta}{4},$$

$$\nu = \frac{\rho + \omega + \xi + \eta}{4},$$

and also introduce the reduced operators $p$ and $q$ according to

$$P = -\frac{\hbar}{\Delta t} p \quad \text{and} \quad Q = -\frac{\hbar}{\Delta t} q.$$ (13)

Then (4) reduces to

$$V = \exp(ip) \quad \text{and} \quad W = \exp(iq).$$ (14)

The following calculations are rather cumbersome. Only the results will be presented. The algebraic steps omitted are straightforward. First, we diagonalize $V$ and $W$: we calculate their eigenvalues and also the matrices of their normalized eigenvectors. The latter can be used to transform to the diagonal representations.

Specifically, the eigenvalues of $V$ are $e^{i\mu}$, $ie^{i\mu}$, $-e^{i\mu}$, $-ie^{i\mu}$. The appropriate eigenvalues of $p$ then follow form (14) as $\mu$, $\mu + \frac{1}{2}\pi$, $\mu + \pi$, $\mu + \frac{3}{2}\pi$. Arbitrary multiples of $2\pi$ can be added to these choices. However, there are certain nonrigorous arguments\(^8\) for generally keeping the spread of eigenvalues of the Hamiltonian as small as possible. Thus, we choose the simplest expressions. The eigenvalues of $q$ are determined identically, with $\mu$ replaced by $\nu$ throughout.
The next step is to apply the inverse of the diagonalizing transformations for \( V \) and \( W \) to the diagonal \( 4 \times 4 \) matrices for, respectively, \( p \) and \( q \). The latter contain the eigenvalues of \( p \) and \( q \) as the diagonal elements. The results are the matrix forms of the operators \( p \) and \( q \) in the original representation:

\[
\frac{4}{\pi} p = \begin{pmatrix}
\frac{4}{\pi} + 3 & -(1 + i) e^{i(\mu - \alpha)} & -(1 - i) e^{i(\delta - \mu)} & -e^{i(2\mu - \alpha - \gamma)} \\
-(1 - i) e^{i(\alpha - \mu)} & \frac{4}{\pi} + 3 & -e^{i(2\mu - \beta - \gamma)} & -(1 + i) e^{i(\mu - \gamma)} \\
-(1 + i) e^{i(\mu - \delta)} & -e^{i(\beta + \gamma - 2\mu)} & \frac{4}{\pi} + 3 & -(1 - i) e^{i(\beta - \mu)} \\
-e^{i(\alpha + \gamma - 2\mu)} & -(1 - i) e^{i(\gamma - \mu)} & -(1 + i) e^{i(\mu - \beta)} & \frac{4}{\pi} + 3
\end{pmatrix}
\]  
\label{15}

\[
\frac{4}{\pi} q = \begin{pmatrix}
\frac{4}{\pi} + 3 & -(1 - i) e^{i(\rho - \nu)} & -(1 + i) e^{i(\nu - \xi)} & -e^{i(\rho + \omega - 2\nu)} \\
-(1 + i) e^{i(\nu - \rho)} & \frac{4}{\pi} + 3 & -e^{i(\omega + \eta - 2\nu)} & -(1 - i) e^{i(\omega - \nu)} \\
-(1 - i) e^{i(\xi - \nu)} & -e^{i(2\nu - \omega - \eta)} & \frac{4}{\pi} + 3 & -(1 + i) e^{i(\nu - \eta)} \\
-e^{i(2\nu - \rho - \omega)} & -(1 + i) e^{i(\nu - \omega)} & -(1 - i) e^{i(\eta - \nu)} & \frac{4}{\pi} + 3
\end{pmatrix}
\]  
\label{16}

5. The Two-Spin-Interaction XOR Hamiltonian

Thus far we decreased the number of independent parameters in the general unitary transformation and chose it to be diagonal in the \( A \)-space. We now “refine” our design of the Hamiltonian to favor interactions of the second order in the Pauli matrices. First, we note that both \( P \) and \( Q \) are constant-diagonal matrices. In terms of the Pauli matrices, then, both their sum and difference in (10) will involve constant terms. These are undesirable because in \( \sigma_z A (P - Q) \) they lead to terms of order one (instead of the desired two), in \( H \), while in \( P + Q \) they lead to an additive constant in \( H \) which only affects the overall phase of the unitary transformation and is of no interest otherwise. Therefore, we put

\[
\mu = \nu = \frac{3}{4} \pi ,
\]  
\label{17}
in order to nullify these diagonal elements in both \( P \) and \( Q \).

Let us now focus our attention on \( P - Q \) which, by (17), is now a matrix with zero diagonal. We must impose conditions on the parameters to make \( P - Q \) of order exactly one in the Pauli matrices. We note, however, that due to zero-diagonal, it cannot contain \( \sigma_z \) terms. The general form linear in \( \sigma_x, \sigma_y \) is

\[
P - Q = \mathcal{I}_B \otimes \begin{pmatrix} 0 & X \\ X^* & 0 \end{pmatrix}_C + \begin{pmatrix} 0 & Y \\ Y^* & 0 \end{pmatrix}_B \otimes \mathcal{I}_C = \begin{pmatrix} 0 & X & Y & 0 \\ X^* & 0 & 0 & Y \\ Y^* & 0 & 0 & X \\ 0 & Y^* & X^* & 0 \end{pmatrix},
\]  
\label{18}

where the stars denote complex conjugation, \( X \) and \( Y \) are arbitrary (complex) numbers, and \( \mathcal{I} \) stands for the unit matrix as before. Thus we require that \( P - Q \) be
of the form suggested by (18). This imposes several rather cumbrous algebraic conditions: two above-diagonal elements of the difference must be equal to zero while the remaining four elements must be equal pairwise. After a lengthy but straightforward algebra not reproduced here, we conclude that these conditions can be satisfied if \( \alpha, \beta, \gamma \) are kept as three independent (real) parameters while the remaining angles are given by

\[
\delta = -3\pi - \alpha - \beta - \gamma , \quad (19)
\]

\[
\rho = -\pi + \beta , \quad (20)
\]

\[
\omega = -2\pi - \alpha - \beta - \gamma , \quad (21)
\]

\[
\xi = -\pi + \gamma , \quad (22)
\]

\[
\eta = \pi + \alpha . \quad (23)
\]

These conditions take care of the form of \( P - Q \). Interestingly, our results below also show that \( P + Q \) contains only two-spin interactions with this choice of parameters. We have no simple explanation of this property (of the absence of first-order terms in \( P + Q \)). It is probably related to the fact that the structure pattern of the original matrices \( V \) and \( W \) is quite similar even though the precise positioning of nonzero elements in them is different. Note that (17) is built into (19)-(23). The explicit expressions are obtained by a lengthy calculation,

\[
P + Q = -\frac{\sqrt{2}hi}{4\Delta t} \times \begin{pmatrix}
0 & e^{-i\alpha} + e^{i\beta} & e^{-i(\alpha + \beta + \gamma)} - e^{-i\gamma} & -\sqrt{2}e^{-i(\alpha + \gamma)} \\
-e^{i\alpha} - e^{-i\beta} & 0 & -\sqrt{2}e^{-i(\beta + \gamma)} & e^{-i(\alpha + \beta + \gamma)} - e^{-i\gamma} \\
e^{i\gamma} - e^{i(\alpha + \beta + \gamma)} & \sqrt{2}e^{i(\beta + \gamma)} & 0 & e^{-i\gamma} - e^{-i(\alpha + \beta + \gamma)} \\
\sqrt{2}e^{i(\alpha + \gamma)} & e^{i(\alpha + \beta + \gamma)} - e^{i\gamma} & e^{i\alpha} + e^{-i\beta} & 0 
\end{pmatrix},
\]

\[
P - Q = -\frac{\sqrt{2}hi}{4\Delta t} \times \begin{pmatrix}
0 & e^{-i\alpha} - e^{i\beta} & e^{-i(\alpha + \beta + \gamma)} + e^{-i\gamma} & 0 \\
-e^{i\alpha} + e^{-i\beta} & 0 & 0 & e^{-i(\alpha + \beta + \gamma)} + e^{-i\gamma} \\
e^{i(\alpha + \beta + \gamma)} - e^{i\gamma} & 0 & 0 & e^{-i\alpha} - e^{i\beta} \\
0 & -e^{i(\alpha + \beta + \gamma)} - e^{i\gamma} & -e^{i\alpha} + e^{-i\beta} & 0 
\end{pmatrix}.
\]

Finally, we expand these matrices in terms of products of the Pauli matrices and collect terms according to (10) to get
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\[ H = -\frac{\hbar}{2\sqrt{2}} \left\{ \sqrt{2} (\sin \alpha + \sin \beta) \sigma_z A \sigma_z C - \sqrt{2} (\cos \alpha - \cos \beta) \sigma_z A \sigma_y C \\
+ \sqrt{2} (\sin \gamma + \sin(\alpha + \beta + \gamma)) \sigma_z A \sigma_y B - \sqrt{2} (\cos \gamma + \cos(\alpha + \beta + \gamma)) \sigma_z A \sigma_z B \\
+ \sqrt{2} (\sin \alpha - \sin \beta) \sigma_z B \sigma_z C - \sqrt{2} (\cos \alpha + \cos \beta) \sigma_z B \sigma_y C \\
- \sqrt{2} (\sin \gamma - \sin(\alpha + \beta + \gamma)) \sigma_z B \sigma_z C + \sqrt{2} (\cos \gamma - \cos(\alpha + \beta + \gamma)) \sigma_y B \sigma_y C \\
- [\sin(\alpha + \gamma) + \sin(\beta + \gamma)] \sigma_x B \sigma_x C + [\cos(\alpha + \gamma) - \cos(\beta + \gamma)] \sigma_x B \sigma_y C \\
+ [\cos(\alpha + \gamma) + \cos(\beta + \gamma)] \sigma_y B \sigma_x C + [\sin(\alpha + \gamma) - \sin(\beta + \gamma)] \sigma_y B \sigma_y C \right\}. \tag{26} \]

Note that (2) corresponds to the parameter choice \(\alpha = \beta = \gamma = 0\). The Hamiltonian (26) describes the three-spin XOR for arbitrary parameter values. All the interactions involved are two-spin as desired.

The result, however, is not symmetric in any obvious way. It seems to correspond to complicated tensor interactions involving expressions of order two in the components of the three spins involved. No rotational or other symmetry in the three-component spin space, or planar symmetry, or uniaxial coupling, are apparent. These would correspond to the familiar Heisenberg, XY, and Ising couplings in condensed matter physics. Thus, in order to realize interaction (26) in materials, a rather anisotropic medium with highly nonsymmetric tensorial magnetic interactions will be required.

In this respect our analytical attempt to “design” a multispin quantum gate in this work may indicate that different results to the derivation of Hamiltonians should be also explored. One could start with the more conventional magnetic interactions, isotropic (Heisenberg), planar (XY), uniaxial (Ising), write down general-parameter Hamiltonians, and then adjust the coupling parameters numerically in search of those values for which useful Boolean gate operations are carried out. There is no guarantee that such a program will succeed. We intend to pursue both approaches in our future work.

In summary, we derived a three-parameter family of Hamiltonians that correspond to the three-spin XOR gate. While our calculation demonstrates that multispin gates can accomplish quantum-logic operations with two-particle interactions, our results seem also to call for further work seeking improvement in two ways. Firstly, our derivation is not general and it has involved a good deal of guess work. Secondly, the terms in the resulting Hamiltonians have no obvious grouping by symmetries.

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