Simple pulses for universal quantum computation with a Heisenberg *ABAB* chain

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Recently, Levy has shown that quantum computation may be performed using an *ABAB* . . . chain of spin-1/2 systems with nearest-neighbor Heisenberg interactions. Levy notes that all necessary elementary computational ''gates'' may be achieved purely by manipulating the spin-spin interaction: he proposes using ''spin-resonance'' techniques involving modulating the interaction strength at high frequency. Here, we establish an alternative: it is possible to perform the elementary gates via simple, nonoscillatory switching of the interaction strength. This approach removes a time ''bottle neck'' in Levy's scheme, so that all elementary operations may now be performed within a time scale of order $\hbar/(E_A-E_B)$.

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The question of how to design a solid-state quantum computer has attracted tremendous interest recently. One strong possibility is to use an array of simple systems (e.g., single electron spins) coupled by the Heisenberg (or ''Exchange'') interaction [1]. It has recently been shown that in systems of this general kind, all the necessary computational building blocks may be realized purely by manipulating the interaction strengths [2,3]. If all of the component cells are physically identical systems, then this technique requires each logical qubit to be encoded into at least three physical qubits (e.g., spins). Recently, Levy has shown that this ratio may be improved to two physical qubits per logical qubit, if the single-particle (Zeeman) energies of the spins along the array alternate in an *ABABAB* . . . pattern [4]. Note that then these energies are assumed to remain fixed over time. In Levy's scheme, performing a computation involves modulating the interaction strength at high frequency, a kind of ''spin resonance.'' This resonance approach is most natural for the regime where E_A-E_B is of a greater order than the interaction strength: however, typical physical systems (e.g., quantum dots in *g*-factor ''engineered'' materials) are likely to be in the opposite limit. Here, we present a simple and efficient approach for this regime.

Consider a pair of independent (pseudo-)spin-1/2 systems, with transition energies *A* and *B*. Now suppose that these systems may be coupled by a Heisenberg-type interaction, so that the Hamiltonian is

$$\hat{H}=-\frac{A}{2}\hat{\sigma}_A^z\otimes\hat{I}_B-\frac{B}{2}\hat{I}_A\otimes\hat{\sigma}_B^z+J\underline{\hat{\sigma}}_A\otimes\underline{\hat{\sigma}}_B.$$

Here, $\hbar=1$, subscripts *A* and *B* refer to the $2\otimes2$ subspace of the corresponding system, $\{\hat{\sigma}^x,\hat{\sigma}^y,\hat{\sigma}^z\}$ are the Pauli matrices, and $\underline{\hat{\sigma}}\equiv\underline{i}\hat{\sigma}^x+\underline{j}\hat{\sigma}^y+\underline{k}\hat{\sigma}^z$. We will consider the dynamics of the system as the magnitude of *J* is abruptly switched between steady values (the square wave case). Other simple pulse shapes, such as the more realistic Gaussian form, will have comparable effects.

The dynamics of the constant-*J* system are easy to establish by diagonalizing $\hat{H}$. It is convenient to add a (physically meaningless) global energy-shift term $J\hat{I}_A\otimes\hat{I}_B$— this provides a slight simplification to the matrix form of *H*

$$\hat{H}\rightarrow\begin{pmatrix}-\Omega+K & 0 & 0 & 0\\ 0 & \omega & K & 0\\ 0 & K & -\omega & 0\\ 0 & 0 & 0 & \Omega+K\end{pmatrix}$$

in the basis $\{|00\rangle,|01\rangle,|10\rangle,|11\rangle\}$. Here, $K\equiv2J$, $\Omega\equiv1/2(A+B)$ and $\omega\equiv1/2(A-B)$. Since $\hat{H}$ is already diagonal in the $\{|00\rangle,|11\rangle\}$ subspace, we may concentrate on the $\{|01\rangle,|10\rangle\}$ subspace. Following Levy, we will identify this as the subspace of a single logical qubit, writing $|01\rangle\equiv|0\rangle_L$ and $|10\rangle\equiv|1\rangle_L$. Diagonalization is straightforward:

$$\hat{H}_L\rightarrow\begin{pmatrix}\omega & K\\ K & -\omega\end{pmatrix}=\mathbf{R}^\dagger\begin{pmatrix}\omega' & 0\\ 0 & -\omega'\end{pmatrix}\mathbf{R}=\omega'\mathbf{R}^\dagger\hat{\sigma}_z\mathbf{R}$$

in basis $\{|0\rangle_L,|1\rangle_L\}$, where $\omega'=(\omega^2+K^2)^{1/2}$ and

$$\mathbf{R}=\begin{pmatrix}\cos\frac{\theta}{2} & \sin\frac{\theta}{2}\\ -\sin\frac{\theta}{2} & \cos\frac{\theta}{2}\end{pmatrix}\quad\text{with}\quad\theta=\arctan(2J/\omega).$$

The effect on the logical qubit of applying $J=J_0$ for a period *t* is therefore given (in the basis $\{|0\rangle_L,|1\rangle_L\}$) by

$$\hat{U}(t)=\exp(-i\hat{H}_Lt)=\exp(-i\omega' t\mathbf{R}^\dagger\sigma_z\mathbf{R})$$
$$=\mathbf{R}^\dagger\begin{pmatrix}e^{-i\omega' t} & 0\\ 0 & e^{i\omega' t}\end{pmatrix}\mathbf{R}.$$

In order to understand this in terms of the Bloch sphere qubit representation [Fig. 1(a)], we employ the operator $\hat{R}_{\underline{n}}(\psi)\equiv\cos(\psi/2)\hat{I}-i\sin(\psi/2)(n_x\hat{\sigma}_x+n_y\hat{\sigma}_y+n_z\hat{\sigma}_z)$. This represents a rotation on the sphere by ψ radians about the axis specified by unit vector $\underline{n}=\underline{i}n_x+\underline{j}n_y+\underline{i}\underline{k}n_z$ [5]. Then, we find that our $\hat{U}(t)=\hat{R}_{\underline{\theta}}(2\omega' t)$ with $\underline{\theta}\equiv\cos\theta\underline{i}+\sin\theta\underline{k}$, i.e., the effect of applying $J=J_0$ for time *t* is a rotation by $2\omega' t$ about an axis

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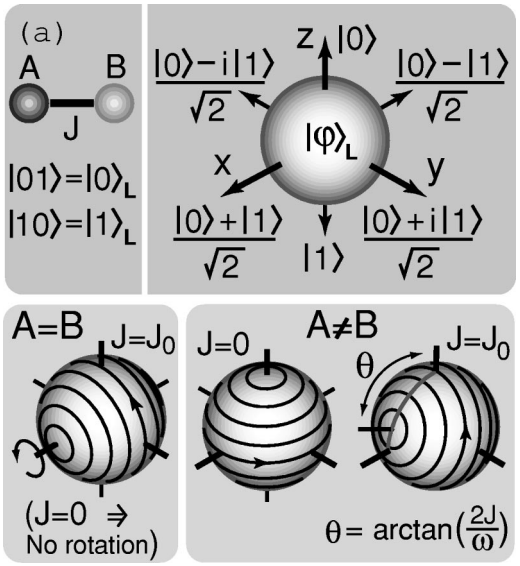

FIG. 1. (a) The two spin-1/2 systems and the corresponding Bloch sphere for the logical qubit. (b) Bloch sphere schematics showing the flow of states over time, depending on $\omega \equiv 1/2(A-B)$ and J.

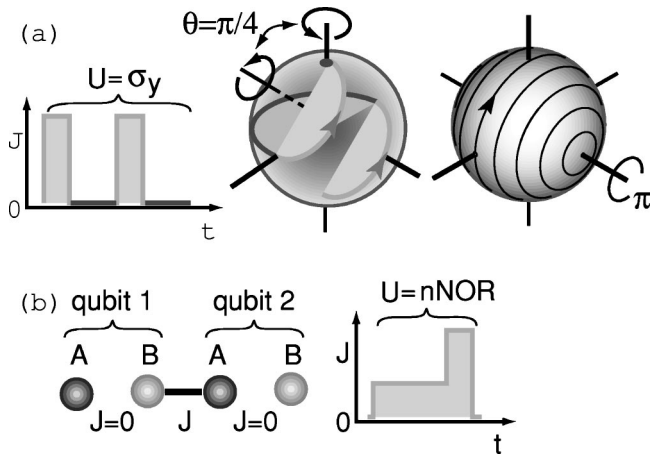

FIG. 2. (a) A sequence of four steps to synthesize $\hat{R}_{\bar{j}}(\pi)$. (b) Two steps suffice for a certain two-qubit gate.

in the z-x plane. (All rotations here are in the lab frame; the rotating frame is considered later.)

Let us assume that $\omega \equiv 1/2(A-B)$ is fixed (as in the case, for example, that our physical qubits A and B are electron spins in quantum dots of a different local g factor in a *static* global B field). We will also assume that J cannot be switched from positive right though to negative [6]. Then we may never-the-less vary the axis of rotation by choosing the magnitude of J. If $J=0$, then the rotation is $\hat{R}_{\bar{k}}(2\omega t)$, i.e., a simple rotation about the z axis. With $J>0$, we have a rotation about an axis lying in the z-x plane at an angle $\theta = \arctan(2J/\omega)$ to the z direction. To achieve a rotation about an axis close to the x direction, we would therefore require a very large J value (infinite for a pure x rotation). This is impractical, but we may instead synthesize a pure y axis rotation by a sequence of more modest rotations. For example, since $\hat{R}_{\bar{j}}(2\theta)=\hat{R}_{\bar{k}}(\pi)\hat{R}_{\theta}(\pi)$, we can generate any $\hat{R}_{\bar{j}}(0 \leqslant \psi \leqslant 2\pi/3)$ provided that the range of available J is $0 \leqslant J \leqslant \sqrt{3}\omega$. Moreover, we may concatenate such pairs of rotations in order to achieve any $\hat{R}_{\bar{j}}(0 \leqslant \psi \leqslant 2\pi)$—a maximum of three pairs will suffice. Figure 2 shows two such pairs being concatenated to produce $\hat{R}_{\bar{j}}(\pi)$.

Given that we may achieve pure z rotations and pure y rotations, we may use the sequence $\hat{R}_{\bar{k}}(\alpha)\hat{R}_{\bar{j}}(\beta)\hat{R}_{\bar{k}}(\gamma)$ to synthesize (up to a meaningless global phase) the general single-qubit transform

$$\hat{G}=\begin{pmatrix} e^{-i(\alpha/2+\gamma/2)}\cos\frac{\beta}{2} & -e^{i(-\alpha/2+\gamma/2)}\sin\frac{\beta}{2} \\ e^{i(\alpha/2-\gamma/2)}\sin\frac{\beta}{2} & e^{i(\alpha/2+\gamma/2)}\cos\frac{\beta}{2} \end{pmatrix}.$$

This formal construction therefore corresponds to a maximum of seven steps for any single-qubit gate ($1+6+1=8$, but we may amalgamate the last two, since both are z rotations). In practice, there will be shorter sequences for any given operation. For example, the important Hadamard transform corresponds to just a single step [e.g., applying $J=2\omega$ for time $t=\pi/(2\sqrt{2}\omega)$]. The time requirement for the $\hat{R}_{\bar{j}}(\pi)$ rotation shown in Fig. 2(a) is probably quite typical—it is $\pi(1+\sqrt{2})/(2\omega)$.

One might object that since the *other* qubits in the computer are also (presumably) represented by an AB pair, these qubits will have performed a z axis rotation $\hat{R}_{\bar{k}}(2\omega\tau)$ while we were performing $\hat{G}$ on our target qubit. We should take these rotations into account, i.e., we should really be working in the rotating frame of a passive qubit. A naive method (not the most efficient) for achieving this is to supplement our $\hat{G}$ sequence with a rotation $R_{\theta}(2\pi)$, which has no net effect in the lab frame but takes time $\tau'=\pi/\omega'$. With an appropriate choice of $\theta(\Rightarrow\omega')$, the total gate time τ is then such that $\omega\tau=2n\pi$, so that the "other" qubits have experienced zero net rotation. More efficiently, one would incorporate this consideration into the process of deriving the optimal short rotation sequence for $\hat{G}$.

The above analysis therefore demonstrates that any single-qubit gate may be efficiently performed on the logical qubit via by a short sequence of fixed J values. It is straightforward to extend this approach to produce a particular two-qubit gate that, together with our universal single-qubit gate, will form a complete set of gates for computation. Consider a $ABAB$ section of a quantum computer, and suppose that two logical qubits are represented in this section, one in the first AB pair and one in the second [see Fig. 2(b)]. Now suppose that the interaction is "off" between all spins except the middle BA pair (which spans the two logical qubits). With an appropriate short sequence [7] of nonzero J values, we may produce the net effect

$$\hat{U}_{gate} = -i \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \hat{U}_0$$

in the basis $\{|00\rangle,|01\rangle,|10\rangle,|11\rangle\}$ of the central two spins. Here, $\hat{U}_0$ denotes the time evolution that *would have occurred* if the interaction had simply been off for the whole period. Thus, the effect in the rotating frame (up to a meaningless global phase of $-i$) is to introduce a phase of -1 conditional on central spin-pair *BA* being in state $|10\rangle$. Remembering that the logical qubits on the two *AB* pairs are represented as $|01\rangle \equiv |0\rangle_L$ and $|10\rangle \equiv |1\rangle_L$, this condition translates to both logical qubits being in state $|0\rangle_L$. Our transformation is therefore a two-qubit gate comparable to the so-called nAND gate, which inverts the phase of the $|1\rangle_L|1\rangle_L$ component of a superposition. The difference is simply that our gate applies the inversion to the $|0\rangle_L|0\rangle_L$ component instead—we might therefore denote our gate as "nNOR."

As a final remark, it is worth noting that although the above approach does not require the $\omega \equiv (A-B)/2$ parameter to be varied, never the less, such an ability would be advantageous. In particular, it would be useful if ω could be switched to zero, because this would then allow the SWAP operation to be performed with a single pulse, and on a time scale limited only by the maximum strength of *J*. Any one-dimensional computer based on nearest-neighbor interactions must spend much of its time simply moving qubits around, therefore, efficient performance of the operation SWAP is very desirable. One might imagine a quantum dot implementation where the *B*-field has a cycle involving being "off" for a period of the time (during which qubits are moved around), before being pulsed to a large value in order to allow general one- and two-qubit gates as described above.

To conclude, we have explicitly shown that one can perform universal computation on an *ABAB* Heisenberg chain using only simple fixed values of *J*. This scheme, with its relatively modest set of physical requirements, is a strong candidate architecture for solid-state quantum computing.

As a postscript, we note that certain *J*-pulse sequences introduced in this report have now been demonstrated within a simple NMR system [8].

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[1] See, e.g., R. Vrijen *et al.*, Phys. Rev. A **62**, 012306 (2000).
[2] D.P. DiVincenzo, D. Bacon, J. Kempe, G. Burkard, and K.B. Whaley, Nature (London) **408**, 339 (2000).
[3] L.-A. Wu and D.A. Lidar, e-print quant-ph/0103039 at xxx.lanl.gov
[4] J. Levy, e-print quant-ph/0101057 at xxx.lanl.gov
[5] See, for example, Nielsen and Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, 2000).
[6] Certain physical systems *do* have this property, which would allow somewhat shorter pulse sequences in our analysis.
[7] One such sequence for the given matrix consists of just two steps as follows: for time $t = 2\pi a_+/\omega$ apply $J = \omega/2(1/a_+^2 - 1)^{1/2}$, then for time $t = 2\pi a_-/\omega$ apply $J = \omega/2(1/a_-^2 - 1)^{1/2}$. Here, $a_{+/-} = (5 +/- \sqrt{7})/8$.
[8] M. Bowdrey, J. Jones, and S. C. Benjamin (unpublished).