Simulation of the diffusion equation on a type-II quantum computer

G. P. Berman,[1] A. A. Ezhov,[2] D. I. Kamenev,[1] and J. Yepez[3]
[1]*Theoretical Division and CNLS, Los Alamos National Laboratory, Los Alamos, New Mexico 87545*
[2]*Troitsk Institute of Innovation and Fusion Research, Troitsk, Russia 142092*
[3]*Air Force Research Laboratory, Hanscom Field, Massachusetts 01731*
(Received 20 February 2002; published 24 July 2002)

A lattice-gas algorithm for the one-dimensional diffusion equation is realized using radio frequency pulses in a one-dimensional spin system. The model is a large array of quantum two-qubit nodes interconnected by the nearest-neighbor classical communication channels. We present a quantum protocol for implementation of the quantum collision operator and a method for initialization and reinitialization of quantum states. Numerical simulations of the quantum-classical dynamics are in good agreement with the analytic solution for the diffusion equation.

DOI: 10.1103/PhysRevA.66.012310 PACS number(s): 03.67.Lx, 47.11.+j, 05.60.Gg

I. INTRODUCTION

Recently a quantum computer of type II [1] has been proposed to solve complex gas and fluid dynamics [2–4]. In a simplest implementation, this type of a quantum computer is an array of a few-qubit elementary nodes that are organized in the discrete lattice. The important feature of the type-II quantum computer is that different nodes do not interact quantum mechanically. The operation of the type-II quantum computer includes the sequential repetition of the three main steps.

(1) Initialization of the quantum computer: creation of the quantum-mechanical initial state that corresponds to the initial probability distribution for a partial differential equation (PDE) to be solved.

(2) Application of the quantum unitary transformation that acts on all nodes in parallel.

(3) Measurement: reading out the quantum states of all nodes. The results of the measurement are used to reinitialize (step I) the quantum computer in the state that corresponds to the new probability distribution.

The type-II quantum computers have many attractive features including the following:

(1) This computer can operate on a macroscopically large number of microscopic nodes. Analogous simulations of the PDE on a digital computer would require an enormous amount of memory and time.

(2) The identical (in time and space) and relatively simple quantum logic operations are implemented on the whole microscopic array of elementary nodes.

(3) The type-II quantum computer should not maintain the quantum coherence for a long period of time, since the quantum logic operations are relatively simple, and each time after implementation of the quantum logic the quantum states are collapsed by measurement procedure and reinitialized.

The disadvantage of the type-II quantum computer is that it can be relatively slow, since each time step requires measurement and reinitialization based on the results of the measurement. As well, before reinitialization the system should relax to the ground state.

Simulations of the dynamics of different physical systems require different quantum logic. We consider in this paper the realization of one-dimensional (1D) diffusion equation in the system of two-qubit nodes interconnected by the classical channels [5]. The word ''classical channels'' means that the states of qubits can be shifted along the chain of the nodes, in spite of the fact that these nodes do not interact quantum mechanically. Technically, classical communication between the nodes can be realized by measurement of quantum states of the nodes of the chain (or in an ensemble of the identical chains) and reinitialization of the spin chain in the new state. We present in this paper the quantum protocol that realizes the quantum logic required to implement the simulation of 1D diffusion equation.

The paper is organized as follows. The formal procedure for simulation of a 1D diffusion equation in the type-II quantum computer is discussed in Sec. II. In Sec. III we discuss a form of the collision operator. The quantum dynamics of a single node that consists of two coupled qubits placed in an external magnetic field, is considered in Sec. IV. In Sec. V we use the solution discussed in Sec. IV to build the protocol (the sequence of pulses) that allows us to initialize our system and to simulate the quantum logic in our computer. The parameters required for simulations are analyzed in Sec. VI. In Sec. VII we show numerically that the quantum logic correctly simulates the diffusion equation. Some general remarks are presented in Sec. VIII.

II. TYPE-II QUANTUM COMPUTER FOR SIMULATION A 1D DIFFUSION EQUATION

Our type-II quantum computer represents a 1D chain of L nodes placed in an external magnetic field, as shown in Fig. 1. Each node consists of two coupled spins (qubits) that remain phase coherent for some short time. Different nodes are interconnected with each other by the classical communication channels as indicated in Fig. 1 by dashed lines.

First, we derive the formal relation between the observables for the quantum-mechanical model presented in Fig. 1 and the probability distribution for the 1D diffusion equation. The Hilbert space for one node consists of four basis states,

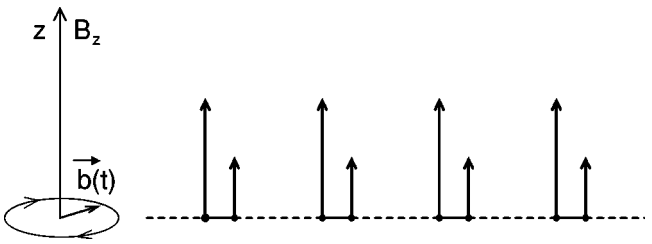

FIG. 1. A schematic illustration of the type-II quantum computer. Each node of the computer consists of two coupled quantum bits (qubits) connected with each other. (These connections are shown by solid lines.) Only four nodes are shown. Different nodes are interconnected by the classical communication channels indicated by dashed lines.

$$|0_2 0_1\rangle = |0\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad |0_2 1_1\rangle = |1\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix},$$

$$|1_2 0_1\rangle = |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |1_2 1_1\rangle = |3\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{1}$$

The operators of the number of particles, $\hat{n}_1$ and $\hat{n}_2$, for qubits, $|q_1\rangle$ and $|q_2\rangle$, are represented by the following matrices,

$$\hat{n}_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad \hat{n}_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{2}$$

All nodes in our 1D chain are characterized by the coordinate x. The occupancy probability of lth qubit at site x at time t is defined as

$$f_l(x,t) = \langle \psi(x,t) | \hat{n}_l | \psi(x,t) \rangle, \tag{3}$$

where $l = 1,2$. The wave function $|\psi(x,t)\rangle$ at each node with the coordinate x can be expanded over the eigenstates $|p\rangle$ [see Eq. (1)] of this node as

$$|\psi(x,t)\rangle = \sum_{p=0}^{3} C_p(x,t) |p\rangle \exp(-iE_p t), \tag{4}$$

where E_p is the energy of the state $|p\rangle$, and we suppose that the Planck's constant is $\hbar = 1$. Since all nodes are identical, we do not indicate the dependences of $|p\rangle$ and E_p on x. The mass density at the node with the coordinate x at time t is defined as the sum of the occupancy probabilities,

$$\begin{aligned} \rho(x,t) &= f_1(x,t) + f_2(x,t) \\ &= |C_1(x,t)|^2 + |C_3(x,t)|^2 + |C_2(x,t)|^2 + |C_3(x,t)|^2, \end{aligned} \tag{5}$$

where

$$f_1(x,t) = |C_1(x,t)|^2 + |C_3(x,t)|^2,$$

$$f_2(x,t) = |C_2(x,t)|^2 + |C_3(x,t)|^2. \tag{6}$$

If an appropriate sequence of quantum gate operations and classical shift operations as described below is applied to the quantum computer, the function ρ in Eq. (5) evolves in time as a solution of the diffusion equation [5],

$$\frac{\partial \rho(x,t)}{\partial t} = \frac{D}{2} \frac{\partial^2 \rho(x,t)}{\partial x^2}, \tag{7}$$

where D is the diffusion constant.

Factorized quantum lattice-gas algorithm

The factorized quantum lattice-gas algorithm for the 1D diffusion equation can be implemented in the following three steps: a collision, a measurement, and a reinitialization (shifting). We assume that the initial state of a node with the coordinate x is set in the form $|q_1(x,t_0)\rangle \otimes |q_2(x,t_0)\rangle$, where the symbol $\otimes$ represents the tensor product, $|q_l(x,t)\rangle = \sqrt{f_l(x,t)}|1\rangle + \sqrt{1-f_l(x,t)}|0\rangle$. [Here and in Eq. (10) below we do not indicate the phases of the wave functions.]

Step 1. One applies a collision operator $\hat{U}$, simultaneously to all nodes,

$$|\psi'(x,t)\rangle = \hat{U} |\psi(x,t)\rangle. \tag{8}$$

The structure of the collision operator is discussed below. This step accounts for the quantum part of the algorithm that is accomplished in parallel fashion across all nodes of the array.

Step 2. One measures (reads out) all occupancy probabilities,

$$f_1'(x,t) = \langle \psi'(x,t) | \hat{n}_1 | \psi'(x,t) \rangle,$$

$$f_2'(x,t) = \langle \psi'(x,t) | \hat{n}_2 | \psi'(x,t) \rangle. \tag{9}$$

In practice, f_1 and f_2 must be determined by either repeated measurement of a single realization of the system or by a single measurement over a statistical ensemble of the systems.

Step 3. One reinitializes (rewrites) the state of the quantum computer as a separable state where each qubit is set as follows:

$$|q_1(x,t+T)\rangle = \sqrt{f_1'(x-l,t)}|1\rangle + \sqrt{1-f_1'(x-l,t)}|0\rangle,$$

$$|q_2(x,t+T)\rangle = \sqrt{f_2'(x+l,t)}|1\rangle + \sqrt{1-f_2'(x+l,t)}|0\rangle, \tag{10}$$

for all x. Note that the state of the qubit $|q_1\rangle$ is shifted to its neighboring node at the left, and the state of the qubit $|q_2\rangle$ is shifted to its neighboring node to the right. This step requires nearest-neighbor ''classical'' communication between all lattice nodes.

III. COLLISION OPERATOR

The collision operator U ''mixes'' the occupancy probabilities,

$$f_1' = \langle\psi|\hat{U}^+\hat{n}_1\hat{U}|\psi\rangle = \frac{1}{2}(f_1+f_2),$$

$$f_2' = \langle\psi|\hat{U}^+\hat{n}_2\hat{U}|\psi\rangle = \frac{1}{2}(f_1+f_2), \tag{11}$$

so that the probability is conserved,

$$f_1'+f_2' = f_1+f_2. \tag{12}$$

The collision operator $\hat{U}$ can be written in the following symmetric form [5]:

$$\hat{U} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}}e^{-i\pi/4} & \frac{1}{\sqrt{2}}e^{i\pi/4} & 0 \\ 0 & \frac{1}{\sqrt{2}}e^{i\pi/4} & \frac{1}{\sqrt{2}}e^{-i\pi/4} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{13}$$

Then, direct calculation yields us the following formulas:

$$f_1'(x,t) = |C_3(x,t)|^2 + \frac{1}{2}[|C_1(x,t)|^2+|C_2(x,t)|^2] + \frac{i}{2}[C_1^*(x,t)C_2 - C_2^*(x,t)C_1(x,t)],$$

$$f_2'(x,t) = |C_3(x,t)|^2 + \frac{1}{2}[|C_1(x,t)|^2+|C_2(x,t)|^2] - \frac{i}{2}[C_1^*(x,t)C_2(x,t) - C_2^*(x,t)C_1(x,t)]. \tag{14}$$

One can see that in order to satisfy Eq. (11), where $f_1(x,t)$ and $f_2(x,t)$ are defined by Eq. (6), one should have

$$C_1^*(x,t)C_2(x,t) = C_2^*(x,t)C_1(x,t) \tag{15}$$

In order to satisfy this condition, $C_1(x,t)$ and $C_2(x,t)$ must be real or one of them should be zero, i.e., $C_1(x,t)=0$ or $C_2(x,t)=0$. One can see from Eq. (11) that the collision operator can have a more general form,

$$\hat{U}_1 = e^{i\Phi}\begin{pmatrix} e^{i\Phi_1} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}}e^{-i\pi/4} & \frac{1}{\sqrt{2}}e^{i\pi/4} & 0 \\ 0 & \frac{1}{\sqrt{2}}e^{i\pi/4} & \frac{1}{\sqrt{2}}e^{-i\pi/4} & 0 \\ 0 & 0 & 0 & e^{i\Phi_2} \end{pmatrix}, \tag{16}$$

where Φ, Φ_1, and Φ_2 are arbitrary phases. In this case and under the condition (15), the relations (11) and (14) do not change.

If one of the coefficients, C_1 or C_2, is equal to zero before the collision then Eq. (11) can be satisfied by the collision operator of a more general form,

$$\hat{U}_2 = \begin{pmatrix} e^{i\Phi_1} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}}e^{i\phi_1} & \frac{1}{\sqrt{2}}e^{i\phi_2} & 0 \\ 0 & \frac{1}{\sqrt{2}}e^{i\phi_3} & \frac{1}{\sqrt{2}}e^{i\phi_4} & 0 \\ 0 & 0 & 0 & e^{i\Phi_2} \end{pmatrix}, \tag{17}$$

where $\phi_1-\phi_3 = \phi_2-\phi_4+\pi \bmod(2\pi)$ and $\phi_1-\phi_2 = \phi_3-\phi_4+\pi \bmod(2\pi)$, since the matrix $\hat{U}$ is unitary. These relations for phases are automatically satisfied for any physical quantum Hamiltonian system provided the corresponding relations for the amplitudes are satisfied. In order to illustrate the action of the collision operator $\hat{U}_2$, we choose $C_2(x,t)=0$ and $C_1(x,t)\neq 0$ and directly calculate the unitary transformation,

$$f_1'(x,t) = \langle\psi|\hat{U}_2^+\hat{n}_1\hat{U}_2|\psi\rangle = |C_3(x,t)|^2 + \frac{1}{2}|C_1(x,t)|^2,$$

$$f_2'(x,t) = \langle\psi|\hat{U}_2^+\hat{n}_2\hat{U}_2|\psi\rangle = |C_3(x,t)|^2 + \frac{1}{2}|C_1(x,t)|^2. \tag{18}$$

This equation has the same form as Eq. (14) with the substitution $C_2(x,t)=0$. Note, however, that the evolution operator (17), providing the transformation (11), has a very general form unlike that in Eq. (13), which allows us to implement the quantum protocol by the radio frequency pulses with arbitrary initial phases of these pulses (see Sec. IV below).

As a result of mixing (11) the probabilities to find each of the spins in the state $|1\rangle$ become equal to each other,

$$f_1'(x,t) = f_2'(x,t)$$

or

$$|C_1'(x,t)|^2+|C_3'(x,t)|^2 = |C_2'(x,t)|^2+|C_3'(x,t)|^2 = \frac{1}{2}\rho(x,t), \tag{19}$$

where ρ is defined in Eq. (5) and prime in $C_i'(x,t)$, $i=0,\ldots,3$ indicates that the probability amplitudes are taken after action of the collision operator. In the next step (step 3 in Sec. II A) the state $|q_1(x,t)\rangle$ of the first qubit shifts to the left, and the state $|q_2(x,t)\rangle$ of the second qubit shifts to the right,

$$\rho(x,t+T)=|C_1'(x+l,t)|^2+|C_3'(x+l,t)|^2+|C_2'(x-l,t)|^2+|C_3'(x-l,t)|^2$$
$$=\frac{1}{2}[\rho(x+l,t)+\rho(x-l,t)]. \quad (20)$$

Finally, we obtain the finite-difference diffusion equation in the form,

$$\rho(x,t+T)-\rho(x,t)=\frac{1}{2}[\rho(x+l,t)-2\rho(x,t)+\rho(x-l,t)]. \quad (21)$$

In the continuous limit, Eq. (21) is reduced to Eq. (7) with the diffusion coefficient $D=l^2/T$ [5].

IV. QUANTUM DYNAMICS FOR TWO-QUBIT QUANTUM SYSTEM

In this section, we show how to initialize (and reinitialize) the initial state of our system and how to implement the collision operator. By the term ''(re)initialization'' we mean that each node of our computer is excited to the quantum state that corresponds to a given profile, $\rho(x,t)$ in Eq. (5). All nodes are equivalent, hence for our purposes it is enough to consider the quantum dynamics only for a single node.

Each node consists of two qubits placed in a magnetic field,

$$\mathbf{B}(t)=[b\cos(\nu t+\varphi),-b\sin(\nu t+\varphi),B_z], \quad (22)$$

where B_z is a uniform permanent magnetic field oriented in the positive z direction, and b, ν, and φ are, respectively, the amplitude, the frequency, and the initial phase of the circularly polarized x-y plane magnetic field. This magnetic field has the form of rectangular pulses of the length (time duration) τ. The one-node Hamiltonian of the spin chain in the magnetic field is

$$H=-\omega_1 I_1^z-\omega_2 I_2^z-2JI_1^zI_2^z-\sum_{l=1}^{2}(\Omega_l/2)\times\{I_l^-\exp[-i(\nu t+\varphi)]+I_l^+\exp[i(\nu t+\varphi)]\}$$
$$=H_0+V(t), \quad (23)$$

where the index l labels the spins at the node, J is the Ising interaction constant, $\Omega_l=\gamma_l b$ is the precession (Rabi) frequency, $\omega_l=\gamma_l B_z$ is the Larmor frequency, γ_l is the gyromagnetic ratio for the lth spin, I_l^z is the z projection of the lth spin, and $I_l^+=I_l^x+iI_l^y$ and $I_l^-=I_l^x-iI_l^y$ are the one-spin-flip operators. Schematically the two-spin system is illustrated in Fig. 2. Below we write the solution for this system and use it in the following section for simulation of the diffusion equation.

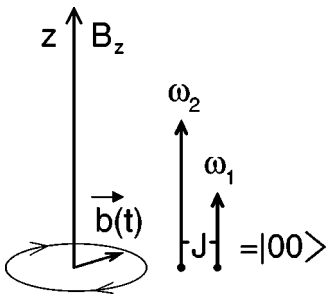

FIG. 2. A schematic illustration of a single node—a two-qubit system in an external permanent magnetic field B_z and in a circularly polarized radio frequency field.

In the interaction representation the Schrödinger equation for the coefficients $C_p(t)$ in Eq. (4) [here $C_p(t)$ is $C_p(x,t)$ at fixed x] has the form [6],

$$i\dot{C}_p(t)=\sum_{m'=0}^{3}V_{pm'}\exp[i(E_p-E_{m'})t+ir_{pm'}(\nu t+\varphi)]C_{m'}(t), \quad (24)$$

where $r_{pm'}=\pm 1$ for $E_p>E_{m'}$ and $E_p<E_{m'}$, respectively. $V_{pm'}=-\Omega_{l'}/2$ for the states $|p\rangle$ and $|m'\rangle$ connected by a flip of l'th spin, and $V_{pm'}=0$ for all other states. Since the Hamiltonian (23) provides only one-spin-flip transitions, there are two nonzero terms in the right-hand side of Eq. (24), so that the state $|m'\rangle$ (for which $V_{pm'}\neq 0$) is related to the state $|p\rangle$ by the flip of only one spin. For example, $V_{pm'}=-\Omega_1/2$ for the transition between the state $|p\rangle=|1_2 0_1\rangle$ with the energy $E_p=(1/2)(-\omega_1+\omega_2+J)$ [see Eq. (23)] and the state $|m'\rangle=|1_2 1_1\rangle$ with the energy $E_p=(1/2)\times(\omega_1+\omega_2-J)$. In another example, $V_{pm'}=0$ for the transition between the states $|p\rangle=|1_2 0_1\rangle$ and $|m'\rangle=|0_2 1_1\rangle$ since these states are related to each other by a two-spin-flip transition.

When the difference $\delta\omega=\omega_1-\omega_0$ between the Larmor frequencies of the spins is large, and when the Rabi frequencies Ω_l are small, $\Omega_l\ll J\ll\delta\omega$, $l=1,2$, one can flip a particular spin (without flip of the other spin) choosing the frequency of the external pulse to be resonant to this particular transition. In this case, the system of four differential equations (24) splits into two independent (in some approximation) parts [6]. Each part consists of two coupled differential equations with only one term on the right-hand side,

$$i\dot{C}_p(t)=V_{pm}\exp[i(E_p-E_m)t-i(\nu t+\varphi)]C_m(t),$$
$$i\dot{C}_m(t)=V_{mp}\exp[-i(E_p-E_m)t+i(\nu t+\varphi)]C_p(t), \quad (25)$$

where we suppose $E_p>E_m$ and the states $|p\rangle$ and $|m\rangle$ are related to each other by the flip of the lth spin with the resonant $(E_p-E_m-\nu=0)$ or near-resonant $(E_p-E_m-\nu\sim J)$ transition frequency, $V_{pm}=-\Omega_l/2$.

In the case where the system is initially in the state $|m\rangle$, i.e., when $C_m(t_0)=1$ and $C_p(t_0)=0$, the solution has the form [6]

$$C_m(t)=\left[\cos(\lambda_{pm}^l\tau/2)+i\frac{\Delta_{pm}}{\lambda_{pm}^l}\sin(\lambda_{pm}^l\tau/2)\right]\exp\left(-\frac{i\tau\Delta_{pm}}{2}\right),$$

$$C_p(t)=i\frac{\Omega_l}{\lambda_{pm}^l}\sin(\lambda_{pm}^l\tau/2)\exp\left[it_0\Delta_{pm}+i\left(\frac{\tau\Delta_{pm}}{2}-\varphi\right)\right], \tag{26}$$

where $\tau=t-t_0$ is the duration of the pulse, $\Delta_{pm}=E_p-E_m-\nu$ is the detuning from exact resonance, $\lambda_{pm}^l=\sqrt{\Omega_l^2+(\Delta_{pm})^2}$ is the precession frequency of lth qubit in the frame rotating with the frequency ν. If the system is initially in the state $|p\rangle$, i.e., when $C_p(t_0)=1$ and $C_m(t_0)=0$, the solution has the form [6]

$$C_p(t)=\left[\cos(\lambda_{pm}^l\tau/2)-i\frac{\Delta_{pm}}{\lambda_{pm}^l}\sin(\lambda_{pm}^l\tau/2)\right]\exp\left(\frac{i\tau\Delta_{pm}}{2}\right),$$

$$C_p(t)=i\frac{\Omega_k}{\lambda_{pm}^l}\sin(\lambda_{pm}^l\tau/2)\exp\left[-it_0\Delta_{pm}-i\left(\frac{\tau\Delta_{pm}}{2}-\varphi\right)\right]. \tag{27}$$

Equation (27) can be derived from Eq. (26) by substituting $C_p\rightarrow C_m$, $C_m\rightarrow C_p$, $\Delta_{pm}\rightarrow-\Delta_{pm}$, $\varphi\rightarrow-\varphi$.

In order to optimize the work of our computer we choose the frequencies of the pulses, which realize the logic operations in our computer to be resonant ($\Delta_{pm}=0$, $\lambda_{pm}^l=\Omega_l$) for the corresponding transitions. In this case, and under the condition $\Omega_l\tau=\pi$ (a π pulse), Eq. (26) describes the complete transition from the state $|m\rangle$ to the state $|p\rangle$,

$$|m\rangle\rightarrow ie^{-i\varphi}|p\rangle, \tag{28}$$

and Eq. (27) describes the complete transition from the state $|p\rangle$ to the state $|m\rangle$,

$$|p\rangle\rightarrow ie^{i\varphi}|m\rangle. \tag{29}$$

One can see that the π pulse can be used for the swap operation between the states $|p\rangle$ and $|m\rangle$. The result of the swap operation is independent of the phase of the wave function.

If the duration of the pulse is $\Omega_l\tau=\pi/2$ (a $\pi/2$ pulse), then according to Eq. (26) the state $|p\rangle$ transforms to the superposition of the states, $|p\rangle$ and $|m\rangle$, with equal probabilities,

$$|m\rangle\rightarrow\frac{1}{\sqrt{2}}(|m\rangle+ie^{-i\varphi}|p\rangle), \tag{30}$$

and according to Eq. (27) the state $|p\rangle$ transforms to the superposition

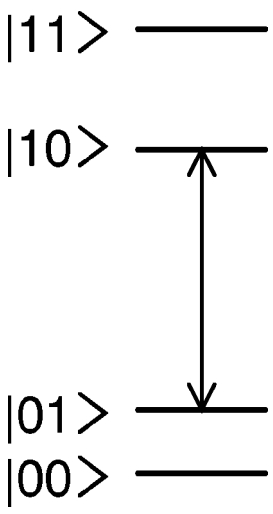

FIG. 3. A schematic illustration of the action of the collision operator. This operator mixes the states $|01\rangle$ and $|10\rangle$ in equal proportions, while only the phases of the states $|00\rangle$ and $|11\rangle$ change.

$$|p\rangle\rightarrow\frac{1}{\sqrt{2}}(|p\rangle+ie^{i\varphi}|m\rangle). \tag{31}$$

If the system before the pulse is in a superposition of the states, $|p\rangle$ and $|m\rangle$, then in the general case the $\pi/2$ pulse does not mix the states in equal proportions, $|C_p'|^2\neq(1/2)\times(|C_p|^2+|C_m|^2)$ and $|C_m'|^2\neq(1/2)(|C_p|^2+|C_m|^2)$. The probabilities after a $\pi/2$ pulse are equal,

$$|C_m'|^2=|C_p'|^2=\frac{1}{2}(|C_p|^2+|C_m|^2), \tag{32}$$

only when the wave function has a definite phase, for example, when C_p and C_m before the pulse are pure real or pure imaginary. In the situation when before the pulse only one level is populated, $C_p=0$ or $C_m=0$, Eq. (32) is satisfied independently of the phase of the initial wave function.

V. PROTOCOL FOR REALIZATION OF THE COLLISION OPERATOR

The energy levels for the system shown in Fig. 2 are illustrated in Fig. 3. The action of the collision operator $\hat{U}$ results in mixing of the states $|01\rangle$ and $|10\rangle$. As follows from the preceding section, mixing can be implemented by a $\pi/2$ pulse. However, since our Hamiltonian (23) provides only one-spin-flip transitions, mixing cannot be implemented by a single pulse. Instead, we propose to use the protocol that consists of three pulses as shown in Fig. 4. The first π pulse [see Eqs. (28) and (29)] of our protocol transfers the state $|01\rangle$ to the state $|11\rangle$, and the state $|11\rangle$ to the state $|01\rangle$ (swaps the states $|01\rangle$ and $|11\rangle$). The second $\pi/2$ pulse mixes the states $|10\rangle$ and $|11\rangle$. The third π pulse again swaps the states $|01\rangle$ and $|11\rangle$. In brief, using two additional π pulses we shift the swap operation shown in Fig. 3 to upper levels, so that it could be implemented in our Hamiltonian (23) that provides only one-spin-flip transitions. From Fig. 4 one can

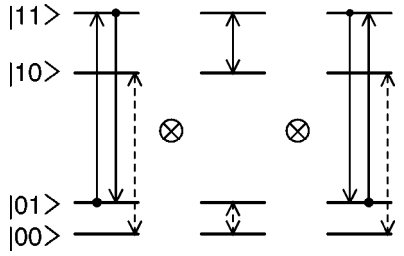

FIG. 4. The results of action of a sequence of pulses (the protocol) that realizes the collision operator. Each diagram indicates the action of one pulse. The whole protocol implements the operation shown in Fig. 3. The dashed lines indicates the near-resonant transitions that are suppressed by the $2\pi k$ method discussed in Sec. VI. The symbol $\otimes$ means that the transformations follow after each other from the left to the right. The solid lines with arrows at both ends indicate mixing of the states in equal proportions. The solid lines with one arrow indicate the swap operation. Before the collision only the states $|00\rangle$ and $|01\rangle$ are populated ($C_2=C_3=0$).

see that the states $|11\rangle$ and $|00\rangle$ effectively remain unchanged (they change only their phases).

Now we discuss in detail the procedure outlined above.

Step I: Initialization. The first step is the initialization or creation of the initial state with the probability $\rho(t=0,x)$. The initial state of each node is supposed to be the ground state. Physically, initialization of our system is the excitation of each node from the ground state to the state $|01\rangle$. We assume here that we can initialize each node independently as might be possible with an array of micro-NMR coils [7]. From Eq. (26) we have

$$\rho(x,t)=|C_1(x,t)|^2=\sin^2[\Omega_1\tau(x,t)/2], \tag{33}$$

where the initial profile at $t=0$ is $\rho(x,0)=\rho_0(x)$. The profile of the probability distribution in our model is controlled by the duration of the pulse,

$$\Omega_1\tau(x,t)=2\arcsin[\sqrt{\rho(x,t)}], \tag{34}$$

where t and x are the time and the coordinate in the diffusion equation (7).

Step II: Collision. After the initialization, the π pulse transforms the state $|01\rangle$ to the state $|11\rangle$, as shown in Fig. 4. The second $\pi/2$ pulse mixes the states $|10\rangle$ and $|11\rangle$. These states are mixed in equal proportions, since before the $\pi/2$ pulse only the state $|11\rangle$ is populated [and the state $|10\rangle$ is empty, see Eq. (32)]. The third π pulse swaps between the states $|11\rangle$ and $|01\rangle$. The parameters of this pulse are the same as the parameters of the first one. Using Eqs. (26) and (27) one can present the evolution operator $\hat{U}$ explicitly. It has the form (17). The matrix elements of the collision operator of the real physical system slightly differs from those in Eq. (17) by the values of the order $\Omega/\delta\omega$ due to the nonresonant transitions (flips of nonresonant spins). Since the probabilities of the nonresonant transitions are very small [$\sim(\Omega/\delta\omega)^2$ [8]], the deviations of the matrix elements from those in Eq. (17) are small. The matrix elements of the exact matrix $\hat{U}$ in Eq. (11) can be obtained by numerical integration of the system of differential equations (24) (see also Ref. [8]). In our numerical simulations presented below we used the exact form of the collision operator calculated numerically. Since our system was initialized in one state $|01\rangle$ (but not in the superposition of the states $|01\rangle$, $|10\rangle$, and $|11\rangle$), our protocol is phase independent, i.e., it works for any initial phase of the pulses, φ_i.

Step III: Measurement and reinitialization. After measurement we define a new distribution using Eq. (20), at each node. The reinitialization is the same procedure like the initialization (step I) but with the new probability $\rho(x,t+T)$. This step can also be implemented using an array of micro-NMR coils [7]. Note, that we assume that after each measurement all nodes of our system relax to the ground state.

VI. PARAMETERS

Now we discuss the parameters of the pulses, which allow us to implement the collision operator. Since all pulses of our protocol are resonant, the frequency of the pulse used for (re)initialization (the transition $|00\rangle\leftrightarrow|01\rangle$) is [see Eq. (23) for the values of the energies E_i],

$$\nu_0=E_1-E_0=\frac{1}{2}(\omega_1-\omega_2+J)-\frac{1}{2}(-\omega_1-\omega_2-J)=\omega_1+J. \tag{35}$$

The frequency of the first pulse required for implementation of the collision operator (the transition $|01\rangle\leftrightarrow|11\rangle$ in Fig. 4) is

$$\nu_1=E_3-E_1=\frac{1}{2}(\omega_1+\omega_2-J)-\frac{1}{2}(\omega_1-\omega_2+J)=\omega_2-J. \tag{36}$$

The frequency of the second pulse (the transition $|10\rangle\leftrightarrow|11\rangle$) is,

$$\nu_2=E_3-E_1=\frac{1}{2}(\omega_1+\omega_2-J)-\frac{1}{2}(-\omega_1+\omega_2+J)=\omega_1-J, \tag{37}$$

and the frequency of the third pulse is equal to the frequency of the first one, $\nu_3=\nu_1$.

In order to suppress the probabilities of flips of nonresonant spins we choose $\omega_2-\omega_1\gg J\gg\Omega_l$, $l=1,2$ (see Ref. [8]). In order to suppress the near-resonant transitions (illustrated in Fig. 4 by the dashed lines) for which $|\Delta|=J$, we apply the $2\pi k$ method [6]. As follows from Eqs. (26) and (27) the probability of the near-resonant transitions generated by the first or third π pulse is,

$$\varepsilon_2=\left\{\frac{\Omega_2}{\lambda^2}\sin\left[\frac{\lambda^2\pi}{2\Omega_2}\right]\right\}^2, \tag{38}$$

where the superscript 2 indicates the number of the spin $l=2$ (see Fig. 2), and $\lambda^l=\sqrt{\Omega_l^2+J^2}$. This probability is equal to zero if $\lambda^2\pi/(2\Omega_2)=\pi k$, $k=1,2,\ldots$. This gives for Ω_2 the following values:

$$\Omega_2^k=J/\sqrt{4k^2-1}\quad(k=1,2,\ldots). \tag{39}$$

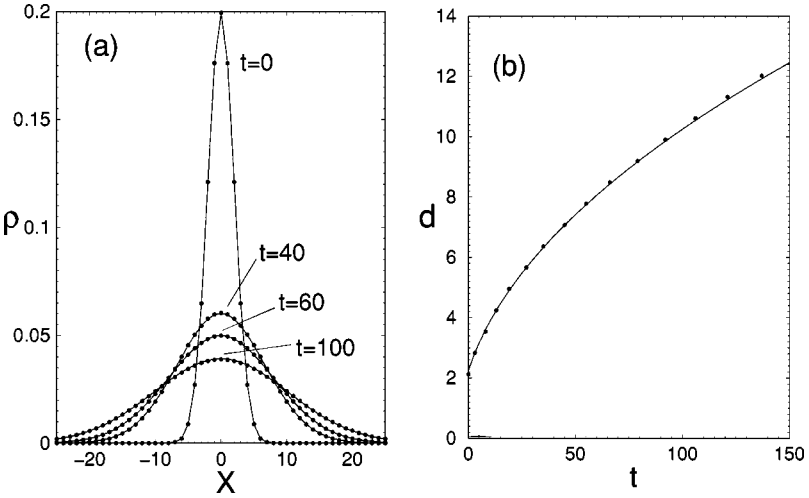

FIG. 5. (a) Dynamics of the profile, $\rho(x,t)$, and (b) broadening of the dispersion $d(t)$, simulated using the quantum-mechanical system (filled circles) and the analytical solution of the diffusion equation (solid lines) with the same parameters. The values of parameters are presented in the text.

If $\Omega_2=\Omega_2^k$, the near-resonant transitions indicated in the left and the right diagrams in Fig. 4 are completely suppressed. Using the same arguments for the second $\pi/2$ pulse, we obtain

$$\Omega_1^{k'}=J/\sqrt{16k'^2-1}. \tag{40}$$

The total time required to implement the collision operator is,

$$\mathcal{T}=\frac{\pi}{\Omega_2^k}+\frac{\pi}{2\Omega_1^{k'}}+\frac{\pi}{\Omega_2^{k''}}.$$

In our simulations we choose $k=k''=10$ and $k'=5$, so the values of Ω are the same for all pulses ($\Omega\approx 0.05$). We also used the same Ω for initialization and reinitialization. We put all initial phases of all pulses [including that required for (re)initialization] equal to zero, $\varphi_i=0, \quad i=1,2,3$, since our protocol is completely insensitive to them.

VII. NUMERICAL SIMULATIONS

In our simulations, we assume that $T=1$, $l=1$, Ω, and ω are dimensionless, and are measured in units of J; $\delta\omega=1000$, $\omega_1=\delta\omega$, $\omega_2=2\delta\omega$. We simulate a 1D diffusion of the Gaussian wave packet, and compare the numerical results with the analytic solution. The initial profile is

$$\rho(x,0)=\frac{1}{\sqrt{2\pi d_0^2}}\exp\left(-\frac{x^2}{2d_0^2}\right),$$

where d_0 is the width of the initial packet, $-300<x<300$. The time evolution is given by the equation

$$\rho(x,t)=\frac{1}{\sqrt{2\pi d^2(t)}}\exp\left(-\frac{x^2}{2d^2(t)}\right), \tag{41}$$

where $d^2(t)=d_0^2+Dt, \quad D=l^2/T=1$. In Figs. 5(a) and 5(b) we compare the profile $\rho(t)$ and the dispersion $d(t)$, obtained by simulating the dynamics of our quantum-mechanical system with those given by the analytical solution (36). One can see that our model correctly simulates the diffusive behavior of the system.

VIII. CONCLUSION

We simulated a 1D diffusion equation in the system that consists of quantum two-qubit nodes interconnected by the classical channels. The initialization and reinitialization are simulated by a different sequence of the radio frequency pulses applied independently to each node of the 1D chain. The collision operator is simulated by a single pulse sequence applied to the entire bulk of the sample. In order to realize the described protocol, the pulses should have the definite (resonant) frequencies, amplitudes (Rabi frequencies Ω), and durations. All these parameters are discussed in the paper. The protocol is insensitive to the initial phases of the pulses. The 1D diffusion equation is the simplest equation that describes the fluid dynamics. On the other hand, until now there were no proposals for implementation of this equation in the real type-II quantum computer using electromagnetic pulses. Our results can be used to develop quantum protocols for simulations of quantum logic in more complicated systems, such as a 1D Burgers equation [9], 2D diffusion or 2D fluid dynamics.

ACKNOWLEDGMENTS

We thank G. D. Doolen for useful discussions. This work was supported by the Department of Energy under the Contract No. W-7405-ENG-36 and DOE Office of Basic Energy Sciences. The work of G.P.B. was partly supported by the National Security Agency (NSA) and by the Advanced Research and Development Activity (ARDA). A.A.E. is thankful to the Center for Nonlinear Studies at the Los Alamos National Laboratory for hospitality.

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