Quantum lattice gas algorithm for the telegraph equation

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The telegraph equation combines features of both the diffusion and wave equations and has many applications to heat propagation, transport in disordered media, and elsewhere. We describe a quantum lattice gas algorithm (QLGA) for this partial differential equation with one spatial dimension. This algorithm generalizes one previously known for the diffusion equation. We present an analysis of the algorithm and accompanying simulation results. The QLGA is suitable for simulation on combined classical-quantum computers.

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I. INTRODUCTION

Quantum lattice gas algorithms (QLGAs) are well known to be versatile in simulating a wide range of physical phenomena. Like their relatives cellular automata, from simple local rules, complex dynamics may emerge [1,2].

Lattice gas algorithms are attractive due to their relative simplicity, physical foundations, and suitability for implementation on parallel computing architectures. Lattice gas algorithms may incorporate conservation of mass, momentum, and energy, and in the quantum context, probability. Lattice gas algorithms have proven successful in a range of applications including fluid dynamics, plasma physics, and other multiparticle simulations [3,4].

Recent experiments and proposals for combined classical-quantum computing (e.g., [5–7]) further motivate the development of quantum lattice gas methods. For instance, a QLGA for the linear diffusion equation has been demonstrated in a liquid-state NMR system [7]. In addition, a detailed design for executing a QLGA for the linear diffusion equation with superconducting qubits has been given [5]. Such implementations could allow the exploitation of quantum entanglement well before large-scale purely quantum computers are constructed.

In this paper we present a QLGA for simulation of the telegraph equation. This hyperbolic partial differential equation (PDE) combines aspects of both the wave and diffusion equations. As such, our algorithm subsumes some earlier works that are restricted to the diffusion equation. We present representative numerical results verifying the algorithm and its analysis.

Classical connections between random walk and the telegraph equation have been known for quite some time [8–12]. In such a model on a one-dimensional (1D) lattice, a walker steps a distance Δx in time increment τ randomly to the left or right, with additionally a probability $a\tau$ to reverse direction. In the simultaneous limit that $a \to \infty$ as well as the speed v, such that the ratio $2a/v^2 \equiv 1/D$ remains constant, the diffusion equation results

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}. \tag{1}$$

Another situation for which this equation results is when $a\tau = 1/2$. Then there is equal probability for a move to the left or right. In a sense, we seek a quantum version of this stochastic model.

We also mention a connection of the telegraph equation with relativistic quantum mechanics and the point of view of a Dirac particle as moving at the speed of light c with random reversals of direction. If we write the telegraph equation in the form $(\partial_t^2 - 2a\partial_t - c^2\partial_x^2)P = 0$, then the change of dependent variable $P(x,t) = e^{-at}\psi(x,t)$ shows that ψ satisfies the Klein-Gordon equation $(\partial_t^2 - c^2\partial_x^2 - a^2)\psi = 0$. Both the telegraph and Klein-Gordon equations may be factored into a pair of equations first order in time, with the latter instance giving the well known Dirac equation. In the case of a Dirac particle, we identify the frequency of probability of reversal $a = m_0c^2/i\hbar$, with m_0c^2 as the rest mass energy [10]. This can provide, for example, an interpretation for the *Zitterbewegung* phenomena of Dirac theory.

Classically or quantum mechanically, lattice gas dynamics may be thought of in terms of scattering due to local potentials. There is an associated scattering matrix, leading to transmission and reflection coefficients. Building on such an approach, recent work has used quantum random walk to examine diffusion in 1D crystalline nanostructures [13]. The telegraph equation results in the continuum limit for an irreversible *second-order* Markov process.

A QLGA includes the sequential repetition of four main steps [4,14,15]. First, initialization creates the quantum-mechanical initial state that corresponds to the initial probability distribution for a partial differential equation to be solved. Second, in the collision step, a unitary transformation is applied in parallel to all the local Hilbert spaces in the lattice. Next, in the measurement step, the quantum states of all the nodes are read out. Lastly, these results are shifted or "streamed" to neighboring lattices sites, providing reinitialization of the lattice in the state that corresponds to the updated probability distribution.

QLGAs have been shown to solve the diffusion, Burgers, Boltzmann, Schrödinger, and Dirac equations [4,15–17]. In some QLGAs (e.g., [16,17]) the measurement step is omitted and the generally entangled quantum states are streamed. This places much stronger requirements on the quantum computing hardware, but it gives an exponential speed up over classical simulation. We present an algorithm with intermediate-time measurements.

There is much application interest in both classical and QLGAs. Elsewhere [18], we have demonstrated that hybrid computing, running versions of diffusion processing, could be useful for the enhancement of digital images. In particular, diffusion of intensities, with a constraint on the difference of pixel iterate values, gives selective smoothing within an image. In another very recent scenario, we have developed QLGAs for the Maxwell equations by starting from a Dirac formulation [19]. The algorithms may be executed with measurement only at the final time, resulting in an exponential speed up over classical simulation.

Very recently, a telegraph-diffusion operator has been proposed for purposes of image restoration and denoising [20]. This approach requires the solution of a nonlinear telegraph equation with diffusivity dependent on the gradient of the intensity function. Our results now indicate the possibility to apply a QLGA with a signal strength constraint for a 1D telegraph equation for obtaining the denoising of digital signals.

A drawback of the ordinary diffusion equation for many applications is that the associated propagation speed is infinite. For any positive time t, there can be diffusion, albeit usually very small, to arbitrarily large distances. The telegraph equation offers one way of correcting this aspect: it models diffusion with a finite propagation speed. This can be very important for modeling diffusion in a variety of contexts including turbulent fluids, biological processes, and ecological problems (e.g., [12]). The search for a fully special relativistic diffusion equation remains an open and important problem for statistical physics and other areas, but the telegraph equation provides an improvement over Eq. (1).

Whereas parabolic Eq. (1) has a number of well known properties, including satisfying a maximum principle, the behavior of solutions of the telegraph equation is generally more complicated. We relegate to Appendix A a brief discussion of a Fourier series solution of the telegraph equation with special zero Dirichlet or Neumann boundary conditions. Already these special cases hint at the varied behavior of the solutions.

The QLGA has a significant numerical advantage inherent in its formulation. This is the guaranteed stability due to the use of a unitary collision operator. For a hyperbolic equation as we are dealing with here, this is not a small matter. We recall that in comparison an explicit finite difference scheme for a wave equation must satisfy the Courant-Friedrichs-Levy (CFL) condition [21] as a *necessary* constraint. Roughly described, the CFL condition arises from ensuring that the domain of dependence of the numerical method contains the domain of dependence of the partial differential equation being solved. It has the direct consequence of limiting how large the time step may be taken in relation to the size of the spatial discretization. The severity of the CFL condition can be reduced only at substantial computational cost. Either the time step is drastically reduced or another method such as an implicit scheme is required. In the latter event, there is significant additional computational cost in solving a set of coupled equations at each time iteration. Even then, if the boundary conditions are not treated fully implicitly also the CFL constraint will manifest.

A QLGA also offers a significant advantage as far as realizing a hybrid architecture. This is because if the nodal qubits have sufficiently long coherence time, no quantum error correction is required. In contrast, many other methods require quantum error correction, and this is typically a tremendous increase in resource. Typical error correcting techniques encode one logical qubit in either five or seven physical qubits. On top of this, several levels of concatenation are used.

In the following, we describe the QLGA for the telegraph equation, with accompanying analysis. We then present numerical results on certain test cases that verify this equation and its parameter-dependent coefficients.

II. QLGA FOR THE TELEGRAPH EQUATION

We consider a 1D lattice of L nodes, with two qubits per node, $|q_a(x,t)\rangle = \sqrt{f_a(x,t)}|1\rangle + \sqrt{1-f_a(x,t)}|0\rangle$, $a=1,2$, where the occupancy probability f_a is the probability for qubit a to be in the $|1\rangle$ state. The Hilbert space for one node has four basis states, taken as $|0_1 0_2\rangle = |0\rangle = (0,0,0,1)^T, \ldots, |1_1 1_2\rangle = |3\rangle = (1,0,0,0)^T$. The local wave function at each node is given as the tensor product $|\psi(x,t)\rangle = |q_1(x,t)\rangle \otimes |q_2(x,t)\rangle$. The number operators n_1 and n_2 for the two qubits are given by

$$n_1 = \mathrm{diag}(1,1,0,0),$$

$$n_2 = \mathrm{diag}(1,0,1,0). \tag{2}$$

The occupancy probability of the jth qubit at position x at time t is defined as

$$f_j(x,t) = \langle \psi(x,t)|n_j|\psi(x,t)\rangle, \tag{3}$$

where $j=1,2$. A nodal density is defined as the sum of the occupancy probabilities,

$$\rho(x,t) = f_1(x,t) + f_2(x,t). \tag{4}$$

We describe an appropriate sequence of quantum gate and classical shift operations applied across the lattice so that the function ρ is made to evolve in time as a solution of the linear telegraph equation

$$\frac{\partial^2 u}{\partial t^2} + \frac{2\sin^2\theta}{\tau}\frac{\partial u}{\partial t} = \cos 2\theta \frac{\Delta x^2}{\tau^2}\frac{\partial^2 u}{\partial x^2}. \tag{5}$$

The local collision operator U_θ is given by

$$U_\theta = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{-i\pi/4}\cos\theta & e^{i\pi/4}\sin\theta & 0 \\ 0 & e^{i\pi/4}\sin\theta & e^{-i\pi/4}\cos\theta & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \tag{6}$$

where θ is taken as a free parameter. As a result of the operation $|\psi'(x,t)\rangle = U_\theta|\psi(x,t)\rangle$, we find

$$f_1' = f_1 f_2 + \cos^2\theta f_1(1-f_2) + \sin^2\theta f_2(1-f_1), \tag{7a}$$

$$f_2' = f_1 f_2 + \sin^2\theta f_1(1-f_2) + \cos^2\theta f_2(1-f_1), \tag{7b}$$

satisfying the conservation condition $\rho' = f_1' + f_2' = f_1 + f_2 = \rho$. We can rewrite Eqs. (7) in a standard form,

$$f_j'(x,t) = f_j(x,t) - (-1)^j \Omega(x,t), \quad j = 1,2, \tag{8}$$

where the collision term $\Omega(x,t)=[f_2(x,t)-f_1(x,t)]\sin^2\theta$.

Equation (7) or (8) is akin to a random walk model with probability of reversal of direction given by $\sin^2\theta$. Building on this interpretation, we consider streaming the state of qubit 1 to the right and that of qubit 2 to the left. Then after a combination of collision followed by such streaming, we have

$$f_1(x,t+\tau) = f_1'(x-\Delta x,t) = \cos^2\theta f_1(x-\Delta x,t) + \sin^2\theta f_2(x-\Delta x,t), \tag{9a}$$

$$f_2(x,t+\tau) = f_2'(x+\Delta x,t) = \sin^2\theta f_1(x+\Delta x,t) + \cos^2\theta f_2(x+\Delta x,t). \tag{9b}$$

If we Taylor expand Eqs. (9) to first order in Δx and τ, suppressing the (x,t) arguments, we have

$$f_1 + \tau\frac{\partial f_1}{\partial t} \approx \cos^2\theta\left[f_1 - \Delta x\frac{\partial f_1}{\partial x}\right] + \sin^2\theta\left[f_2 - \Delta x\frac{\partial f_2}{\partial x}\right], \tag{10a}$$

$$f_2 + \tau\frac{\partial f_2}{\partial t} \approx \sin^2\theta\left[f_1 + \Delta x\frac{\partial f_1}{\partial x}\right] + \cos^2\theta\left[f_2 + \Delta x\frac{\partial f_2}{\partial x}\right]. \tag{10b}$$

Adding and simplifying both of these equations gives

$$\tau\frac{\partial(f_1+f_2)}{\partial t} \approx -\Delta x\cos 2\theta\frac{\partial(f_1-f_2)}{\partial x}, \tag{11a}$$

while subtracting Eq. (10b) from Eq. (10a) gives

$$\tau\frac{\partial(f_1-f_2)}{\partial t} \approx -2\sin^2\theta(f_1-f_2) - \Delta x\frac{\partial(f_1+f_2)}{\partial x}. \tag{11b}$$

Differentiating Eq. (11a) with respect to time and using Eq. (4) yields

$$\tau\frac{\partial^2\rho}{\partial t^2} \approx -\Delta x\cos 2\theta\frac{\partial^2(f_1-f_2)}{\partial t\,\partial x}, \tag{12a}$$

while differentiating Eq. (11b) with respect to x and using Eq. (4) yields

$$\tau\frac{\partial^2(f_1-f_2)}{\partial x\,\partial t} \approx -2\sin^2\theta\frac{\partial(f_1-f_2)}{\partial x} - \Delta x\frac{\partial^2\rho}{\partial x^2}. \tag{12b}$$

We next substitute Eq. (12b) into Eq. (12a), eliminating the mixed derivative term,

$$\tau\frac{\partial^2\rho}{\partial t^2} \approx \frac{\Delta x}{\tau}\cos 2\theta\left[2\sin^2\theta\frac{\partial(f_1-f_2)}{\partial x} + \Delta x\frac{\partial^2\rho}{\partial x^2}\right]. \tag{13}$$

Finally, substituting Eq. (11a) into this equation gives a PDE only involving the density ρ and the telegraph [Eq. (5)] results.

In summary, for the QLGA we first initialize with $\rho(x,0)=g(x)$, the initial density, providing the initial nodal wave functions. We apply collision operator (6) to the local wave functions $|\psi\rangle$ across the lattice. We then measure the states of both qubits across the lattice, giving the local occupancy probabilities f_1 and f_2. Lastly, the values f_1 are streamed to the right neighboring lattice sites and those of f_2 are streamed to the left neighboring sites, providing reinitialization of the nodal wave functions.

In Eq. (5), we have the speed $v=\sqrt{\cos 2\theta}\Delta x/\tau$. In the special case that $\theta\to 0$, the collision operator becomes diagonal, and the telegraph equation reduces to the wave equation. Suppose that we multiply Eq. (5) by τ and take $\tau\to 0$. The diffusion equation results, assuming that $\Delta x^2/2\tau=D$ remains constant.

III. SIMULATION RESULTS

We illustrate the above algorithm for the 1D linear telegraph equation with various initial conditions. Unless described otherwise, we take a lattice of stated size with unit lattice spacing, $\Delta x=1$.

We have verified our algorithm in the special case $\theta=0$ when the wave equation results and we have periodic boundary conditions. In this circumstance the QLGA provides the correct solution. More challenging is when $\theta\neq 0$.

As a first example for the telegraph equation, we consider on the half line $x\geq 0$ the initial condition (IC) $u(0,0)=1$, with $u(0,t)=1$ maintained for all later times, $u(x,0)=0$ for $x>0$, and

$$\left.\frac{\partial u}{\partial t}\right|_{t=0} = 0. \tag{14}$$

This then will generate a Green's functionlike solution. In fact, the spatially integrated Green's function is essentially the solution we seek. Writing Eq. (5) in the form

$$u_{tt} + \frac{1}{A}u_t = v^2 u_{xx}, \tag{15}$$

corresponding to $A=\tau/2\sin^2\theta$ and $v^2=\cos 2\theta\Delta x^2/\tau^2$, the solution for $0<x<vt$ is given by [8] (pp. 147–149),

$$u(x,t) = 1 - \int_0^x \sigma(x,t)dx, \tag{16}$$

where

$$\sigma(x,t) = \frac{e^{-t/2A}}{2Av}\left[I_0(y) + \frac{t}{2A}\frac{I_1(y)}{y}\right], \tag{17a}$$

$$y(x,t) = \frac{\sqrt{v^2t^2 - x^2}}{2Av}, \tag{17b}$$

and I_ν is the modified Bessel function of the first kind. For $x>vt$, the solution is 0. An alternative form of the solution is given in Ref. [22]. When the speed $v\to\infty$, the solution reduces to a complementary error function solution appropriate for the diffusion equation.

For this model problem we are obviously presented with nonperiodic initial and boundary conditions, and we need the

QLGA to at least approximately satisfy these. Initially we put $f_1 = f_2 = 0$ across the entire lattice except for $f_1 = 1$ on the leftmost node. Since f_1 is the occupancy probability that gets streamed to the right, initially we can look at the system as an empty lattice, with a flux of particles to the right at the left boundary and no particles moving to the left (since f_2 is zero).

Now to satisfy the boundary condition we need to set the leftmost node to have a total occupancy probability $f_1 + f_2$ always equal to 1, and we would also like the solution's derivative to be continuous. One way to keep the derivative approximately continuous is to maintain the f_2 values and set $f_1 = 1 - f_2$. This way the density of left and right going particles at the boundary depends on the node to the right, node 2, and will allow the slope at the boundary to change appropriately. This also fixes the total occupancy probability to one at the left boundary. We expect this method to be most successful when $\sin^2 \theta$ is small, and thus there is a small chance of reversal, the primary factor in the solution being the small occupancy probability in f_2, which represents the reversed particles moving to the left.

Although the collision operator conserves the density, the overall algorithm cannot on the domain of nodes 1 to L since initially there are no particles and no "signal" on the lattice. Rather, the total density over the lattice is constantly increasing due to the fixed source on the left.

In Fig. 1 we graphically compare the numerical and exact solutions for $\theta = 5\pi/180$ and $L = 128$. The two solutions are shown at 32, 64, and 96 multiples of τ. Given the approximations described above in implementing the initial-boundary conditions, the very near agreement is remarkable.

In the exact solution (16), σ acts like an un-normalized line density of particles, with the property [8]

$$\int_0^{vt} \sigma(x,t)dx = 1 - e^{-t/2A}. \tag{18}$$

This relation may be verified by using a change of variable and the integrals,

$$\int_0^b \frac{xI_0(cx)}{\sqrt{b^2 - x^2}}dx = \frac{\sinh(bc)}{c} \tag{19a}$$

and

$$\int_0^b \frac{I_1(cx)}{\sqrt{b^2 - x^2}}dx = \frac{\cosh(bc) - 1}{c}. \tag{19b}$$

The PDE (15) is the limit of the finite difference equation,

$$\sigma(x,t+dt) = \left(1 - \frac{dt}{2A}\right)[\sigma(x - dx/2,t) + \sigma(x + dx/2,t)] - \left(1 - \frac{dt}{A}\right)\sigma(x,t - dt), \tag{20}$$

with $v = dx/2dt$.

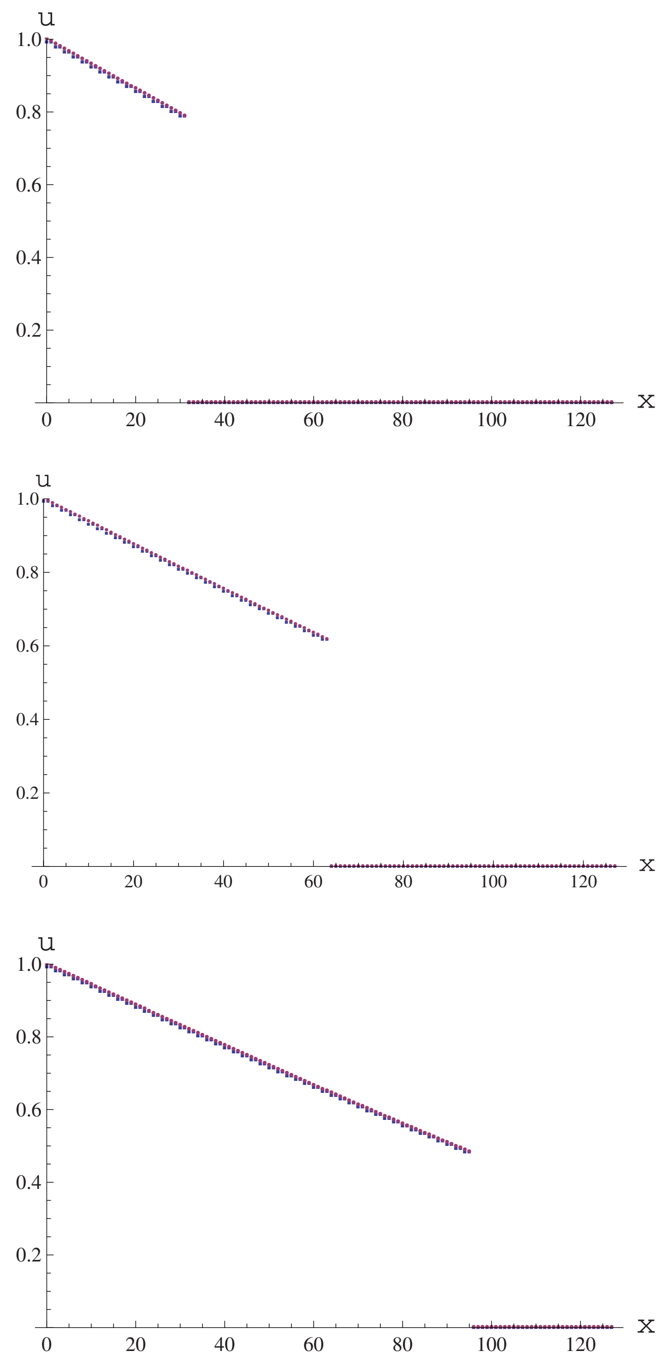

FIG. 1. (Color online) Plot of the QLGA (blue, dark gray) and exact (red, light gray) solutions of Eq. (15) with $\theta = 5\pi/180$ after (a) 32, (b) 64, and (c) 96 time steps.

Concerning solutions (16) and (17), we observe that

$$\frac{\partial}{\partial t}\int_0^x I_0[y(x,t)]dx = \frac{t}{4A^2}\int_0^x \frac{I_1[y(x,t)]}{y(x,t)}dx. \tag{21}$$

Therefore, if either integral in Eq. (16) may be determined in closed form, the other can be found from it.

Similarly, we have been able to use the QLGA to solve the related initial-boundary value problem on a finite interval $u(x,0) = 0$ for $0 < x < L$, Eq. (14), and $u(0,t) = u(L,t) = 1$ for

$t>0$. Now at the boundary $x=L$ we impose $f_2=1-f_1$. We have obtained good agreement with the known analytic solution [23].

We have solved a case of the telegraph equation with elementary functions comprising the solution [11]. Here, we have initial condition (14) and

$$F(x,0)=\frac{1}{4}\sin\left(\frac{2\pi x}{L}\right)+\frac{1}{2} \tag{22}$$

along with periodic boundary conditions. To write the exact solution we put $v^2=\cos 2\theta(4\pi/L)^2/\tau^2$, $a=\sin^2\theta/\tau$, $w_1=(v^2-a^2)^{1/2}$, and $w_2=(a^2-v^2)^{1/2}$. Then the solution is given by

$$F(x,t)=e^{-at}\left[\frac{a}{w_1}\sin(w_1 t)+\cos(w_1 t)\right]\frac{1}{4}\sin\left(\frac{2\pi x}{L}\right)+\frac{1}{2},$$

$$v\geq a, \tag{23a}$$

$$F(x,t)=e^{-at}\left[\frac{a}{w_2}\sinh(w_2 t)+\cosh(w_2 t)\right]\frac{1}{4}\sin\left(\frac{2\pi x}{L}\right)+\frac{1}{2},$$

$$v<a. \tag{23b}$$

This solution can also be deduced from the separation of variables approach given in Appendix A.

We are also able to solve problems with the zero Neumann boundary condition

$$\left.\frac{\partial u}{\partial x}\right|_{x=0}=\left.\frac{\partial u}{\partial x}\right|_{x=L}=0. \tag{24}$$

In this case, we employ reflective boundary conditions for the QLGA. At the left boundary, we put $f_1(1,t+\tau)=f_2'(1,t)$ and $f_2(1,t)=f_2(2,t)$, and at the right boundary we put $f_2(L,t+\tau)=f_1'(L,t)$ and $f_1(L,t+\tau)=f_1(L-1,t)$, assuming that the node indices run from 1 to L. This enables the solution of a variety of other boundary value problems.

For problems with a Dirac delta function initial condition [24,25], the algorithm must be modified. This is because the initial condition is localized at a single node.

IV. ALTERNATIVE COLLISION OPERATOR

In place of Eq. (6) we have found a unitarily equivalent collision operator. We put

$$V_\theta=\frac{1}{2}\begin{bmatrix}2 & 0 & 0 & 0\\ 0 & 1+e^{i\theta} & 1-e^{i\theta} & 0\\ 0 & 1-e^{i\theta} & 1+e^{i\theta} & 0\\ 0 & 0 & 0 & 2\end{bmatrix}. \tag{25}$$

By the method in, for instance, Ref. [26], one can show that both U_θ and V_θ have controlled-NOT (CNOT) complexity 3. Thus, up to single-qubit gates, these two two-qubit gates are equivalent to triple CNOT (or the SWAP gate) and therefore to one another. We have verified the symmetry $H^{\otimes 2}V_\theta H^{\otimes 2}=V_\theta$, where H is the Hadamard gate.

We give canonical decompositions of V_ϕ and U_θ that verify their CNOT complexity. We put

$$a_1=\frac{1}{2}\begin{bmatrix}1+i & -1-i\\ 1-i & 1-i\end{bmatrix},\quad c_1=\frac{1}{2}\begin{bmatrix}1-i & 1+i\\ -1+i & 1+i\end{bmatrix}. \tag{26}$$

Then with σ_j, the standard Pauli matrices, we may write

$$V_\phi=e^{i\phi/4}(a_1\otimes a_1)e^{-i\phi(\sigma_x^{\otimes 2}+\sigma_y^{\otimes 2}+\sigma_z^{\otimes 2})/4}(c_1\otimes c_1). \tag{27}$$

Similarly, we may write

$$U_\theta=e^{-i\pi/8}(\sigma_x\otimes\sigma_y)e^{-i[(\theta/2)\sigma_x^{\otimes 2}+(\theta/2)\sigma_y^{\otimes 2}-(\pi/8)\sigma_z^{\otimes 2}]}(\sigma_x\otimes\sigma_y). \tag{28}$$

The explicit decompositions of the central operator factors of Eqs. (27) and (28) are given in Appendix B.

Following from $|\psi'(x,t)\rangle=V_\theta|\psi(x,t)\rangle$ we have the update rules

$$f_1'=\tfrac{1}{2}(1+\cos\theta)f_1+\tfrac{1}{2}(1-\cos\theta)f_2 \tag{29a}$$

and

$$f_2'=\tfrac{1}{2}(1-\cos\theta)f_1+\tfrac{1}{2}(1+\cos\theta)f_2. \tag{29b}$$

Thus we obtain for the frequency of probability of reversal and velocity, respectively, $a=(1-\cos\theta)/2$ and $v=\sqrt{\cos\theta}$.

We have verified these results on the model problems of Eqs. (15), (16), (17a), and (17b) [8] and Eqs. (22) and (23) [11] and obtained excellent agreement. An advantage of the $a(\theta)$ and $v(\theta)$ parameters is that the period is longer, so that the algorithm is not as sensitive to small changes in θ.

V. CONCLUDING REMARKS

The 1D telegraph equation arises as the probability density function (PDF) for the displacement at time t for persistent random walk on a 1D lattice in the continuum limit. With a form of momentum introduced into the random walk, persistent random walk has applications in describing scattering and diffusion in disordered media. As we have mentioned, the telegraph equation has solutions with a finite velocity of propagation, and this can provide an advantage for describing heat propagation, light dispersion in turbid media, or in biological modeling.

We have presented a QLGA for the 1D telegraph equation that subsumes one for the diffusion equation while complementing that for the 1D Dirac equation. Both the telegraph and Dirac equations may be developed from microscopic models with particles undergoing random reversals of direction. The resulting QLGA for the 1D telegraph equation is highly parallelizable and well founded on physical principles including conservation laws. This algorithm offers the prospect for simulation on combined classical-quantum computing architectures. In such a computing environment, local nodes with two qubits each are connected to nearest neighbors with classical communication.

We have verified our QLGA on model problems that take into account the boundary conditions and the initial conditions on both the solution and its first-order time derivative. Despite using an approximation to implement nonperiodic boundary conditions for some test problems, we are still able to find accurate solutions. The incorporation of further types of boundary conditions is an area for future research.

We have described the computational stability advantage given by constructing a QLGA with a unitary collision operator. The stability requirement alone, as evidenced by the tangible CFL condition, is a serious matter for conventional computing schemes. This condition can only be mitigated at a significant computational cost. For a traditional finite difference scheme using a regular lattice, an order of magnitude increase in cost is typical in going from an explicit to an implicit method. This change also increases the complexity of implementation, including the treatment of the boundary conditions.

As we have mentioned, there have been initial nuclear magnetic resonance (NMR) system implementations of quantum lattice gas methods, one of these being for linear diffusion. This is a fascinating combination of quantum computing with classical molecular computing. If one could sufficiently sample from the computing ensemble, then Markov chain problems could be solved that are outside the capability of classical digital computers. With current liquid-state NMR computing using 10^{18} molecules, Markov chain problems with up to 2^{60} states could, in principle, be addressed. This in turn implies that there is a range of NMR-computable problems of size 2^{30}–2^{60} that lie beyond the capabilities of conventional digital computers.

Moreover, we anticipate that our QLGAs may be generalized to the broader context of such Markov chain problems. This is a general framework in which one assumes a number of states and their corresponding transition probabilities to other states. As particular and important cases, this would enable the simulation of quantum random walk and quantum search. In particular, we recall that quantum search may be derived as a form of quantum random walk on a hypercube or other n-dimensional regular lattice [27]. A hybrid architecture provides a pathway to approaching the quadratic speed up that is optimal for quantum search. This is achieved as the streaming of entangled nodal states becomes available and intermediate-time measurements are eliminated.

In the continuum limit for dimensions greater than 1, the PDF for persistent random walk does not satisfy a higher dimensional telegraph equation nor does the projection of the motion of persistent random walk on a given axis satisfy a higher dimensional telegraph equation [28]. The partial differential equations for the PDF are of order in time $2d$ for dimensions $d \geq 2$ and are more complicated. It is thus intriguing that there should exist QLGAs for these other partial differential equations. These QLGAs would be expected to have applications to transport in disordered media in dimensions higher than 1.

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APPENDIX A: FOURIER SINE SERIES SOLUTION OF A TELEGRAPH EQUATION

Suppose that the partial differential equation of interest is given by

$$au_t + bu_{tt} - Du_{xx} = 0, \tag{A1}$$

with a, b, and D being given constants and subscripts denoting partial differentiation. Suppose for simplicity the boundary conditions $u(0,t)=u(L,t)=0$. Then we first assume a separation of variables form

$$u(x,t) = \sin\left(\frac{n\pi x}{L}\right)e^{\lambda t}, \tag{A2}$$

with λ to be determined as a function of a, b, and D. Substituting Eq. (A2) into Eq. (A1) we find

$$b\lambda^2 + a\lambda + \frac{n^2\pi^2}{L^2}D = 0, \tag{A3a}$$

i.e., λ is given by

$$\lambda_n^{(\pm)} = \frac{1}{2b}\left(-a \pm \sqrt{a^2 - 4b\frac{n^2\pi^2}{L^2}D}\right). \tag{A3b}$$

Then we take a Fourier sine series solution,

$$u(x,t) = \sum_{n=1}^{\infty} [A_n^{(+)}e^{\lambda_n^{(+)}t} + A_n^{(-)}e^{\lambda_n^{(-)}t}]\sin\left(\frac{n\pi x}{L}\right). \tag{A4}$$

If the IC is $u(x,0)=f(x)$, then as usual by orthogonality we have the relation

$$A_n^{(+)} + A_n^{(-)} = \frac{2}{L}\int_0^L f(x)\sin\left(\frac{n\pi x}{L}\right)dx. \tag{A5}$$

Similarly, from the initial time derivative condition (14), we find

$$\lambda_n^{(+)}A_n^{(+)} + \lambda_n^{(-)}A_n^{(-)} = 0. \tag{A6}$$

Therefore, we have obtained solution (A4) with

$$A_n^{(+)} = \frac{2}{L}\frac{\lambda_n^{(-)}}{(\lambda_n^{(-)} - \lambda_n^{(+)})}\int_0^L f(x)\sin\left(\frac{n\pi x}{L}\right)dx \tag{A7a}$$

and

$$A_n^{(-)} = -\frac{2}{L}\frac{\lambda_n^{(+)}}{(\lambda_n^{(-)} - \lambda_n^{(+)})}\int_0^L f(x)\sin\left(\frac{n\pi x}{L}\right)dx. \tag{A7b}$$

For the diffusion equation with $b=0$ in Eq. (A1), $\lambda_n = -n^2\pi^2 D/L^2 a < 0$ for $D>0$ and $a>0$. In contrast, for the telegraph equation, $\lambda_n^{(\pm)}$ in Eq. (A3b) may be complex. For large bD/L^2 and large enough n, an oscillatory factor enters the solution.

If instead we have the zero Neumann boundary condition $\partial u/\partial x=0$ at *both* end points $x=0$ and $x=L$, we may replace the sine with the cosine function in the above solution. The frequencies $\lambda_n^{(\pm)}$ of Eq. (A3b) remain the same.

For the initial condition (22), only the coefficients $A_2^{(\pm)}$ are nonvanishing. Then the solution (23) is obtained from the sole term with $n=2$ in the sum of Eq. (A4).

APPENDIX B: COLLISION OPERATORS IN TERMS OF THREE CNOT GATES

Here we complete the decompositions of Eqs. (27) and (28). In the following, CNOT denotes the gate with control qubit the first qubit,

$$\mathrm{CNOT} = \begin{bmatrix} I & 0 \\ 0 & \sigma_x \end{bmatrix}, \tag{B1}$$

wherein I denotes the 2×2 identity matrix and 0 denotes a 2×2 matrix of zeros. Again, σ_k denote the single-qubit Pauli gates and H denotes the Hadamard gate. We let $S=\mathrm{diag}(1,i)$, $A_3=HS$, and $C=e^{i\pi\sigma_x/4}$.

In order to write the central factors of Eqs. (27) and (28) we use the results in Ref. [29]. We have for Eq. (27)

$$e^{-i\phi(\sigma_x^{\otimes 2}+\sigma_y^{\otimes 2}+\sigma_z^{\otimes 2})/4} = (C\otimes C^\dagger)\mathrm{CNOT}(A_3\otimes B_3)\mathrm{CNOT}(A_2\otimes B_2)\mathrm{CNOT}, \tag{B2}$$

with

$$A_2 = He^{-i\phi\sigma_x/4}, \quad B_2 = e^{-i\phi\sigma_z/4}, \quad B_3 = e^{i\phi\sigma_z/4}. \tag{B3}$$

Similarly, we write for Eq. (28)

$$e^{-i[(\theta/2)\sigma_x^{\otimes 2}+(\theta/2)\sigma_y^{\otimes 2}-(\pi/8)\sigma_z^{\otimes 2}]} = (C\otimes C^\dagger)\mathrm{CNOT}(A_3\otimes B_3)\mathrm{CNOT}(A_2\otimes B_2)\mathrm{CNOT}, \tag{B4}$$

where now

$$A_2 = He^{-i\theta\sigma_x/2}, \quad B_2 = e^{i\pi\sigma_z/8}, \quad B_3 = e^{i\theta\sigma_z/2}. \tag{B5}$$

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