Quantum lattice-gas model for the many-particle Schrödinger equation in *d* dimensions

Bruce M. Boghosian*
Center for Computational Science, Boston University, 3 Cummington Street, Boston, Massachusetts 02215

Washington Taylor IV†
Department of Physics, Princeton University, Princeton, New Jersey 08544
(Received 8 May 1996; revised manuscript received 16 January 1997)

We consider a general class of discrete unitary dynamical models on the lattice. We show that generically such models give rise to a wave function satisfying a Schrödinger equation in the continuum limit, in any number of dimensions. There is a simple mathematical relationship between the mass of the Schrödinger particle and the eigenvalues of a unitary matrix describing the local evolution of the model. Second quantized versions of these unitary models can be defined, describing in the continuum limit the evolution of a nonrelativistic quantum many-body theory. An arbitrary potential is easily incorporated into these systems. The models we describe fall in the class of quantum lattice-gas automata and can be implemented on a quantum computer with a speedup exponential in the number of particles in the system. This gives an efficient algorithm for simulating general nonrelativistic interacting quantum many-body systems on a quantum computer. [S1063-651X(97)06808-6]

PACS number(s): 64.60.Cn

I. INTRODUCTION

There are many situations in physics where a continuous system obeying a particular set of equations at a macroscopic scale can be modeled by a discrete microscopic system obeying a very simple set of local rules. For example, in equilibrium statistical mechanics, simple lattice models such as the Ising model capture the behavior of generic classes of critical systems at large scales. Another interesting class of discrete systems are lattice-gas automata [1–3]; these models describe systems of particles moving about on a lattice, obeying simple collision rules that conserve quantities such as mass and momentum. In the macroscopic limit, these systems obey Navier-Stokes or other hydrodynamic equations of interest.

In the quantum domain, there are also examples of discrete microscopic systems that capture interesting macroscopic behavior. Lattice-gauge theories (see, for example, [4]) give an approach to studying the partition function and spectra of quantum field theories by mapping these theories to statistical mechanical ensembles. There are, however, few discrete models for describing the dynamical evolution of quantum systems that preserve important features such as unitarity. An example of a quantum system for which a unitary discrete model is known is the Dirac equation describing a relativistic particle moving in one spatial dimension. As shown by Feynman [5,6], this system can be described by a simple microscopic model of a particle moving on a one-dimensional (1D) lattice according to a simple local rule that essentially corresponds to a unitary form of random walk. A straightforward attempt to realize a Dirac equation in more than one spatial dimension as a form of unitary random walk cannot succeed. By using operator splitting methods, however, it was shown by Succi and Benzi [7] that a sequence of random moves along single axes, alternating with transformations that diagonalize each of the Dirac matrices in turn, can give an analogous construction in higher dimensions. The discrete model for the (1+1)-dimensional Dirac equation has been of renewed interest recently [7–9], due partly to the possibility of simulating such unitary microscopic discrete systems by quantum computers. In particular, recently it has been suggested [9] that a simple quantum lattice model can be constructed that describes the motion of a system of many particles moving according to the one-dimensional Dirac equation.

In this paper we consider a class of models closely related to the 1D Dirac lattice model, which give rise to a nonrelativistic single-particle Schrödinger equation in an arbitrary number of dimensions. In these models, the time development rule is given by a single local, unitary transformation matrix. Thus we are essentially considering the motion of a single particle under a unitary random walk process. For this class of models we show that the macroscopic equation of motion satisfied by the wave function corresponding to particle density is the Schrödinger equation. We show that such nonrelativistic models can be constructed for an arbitrary number of spatial dimensions. We also show that an arbitrary potential can easily be included in these models.

It is natural to generalize from the single-particle models to a second quantized many-body system. Such a model could be implemented very efficiently on a quantum computer, so that the number of computational steps necessary to simulate a single time step would depend only upon the size of the lattice and would not depend upon the number of particles in the system being simulated. Thus our results could be used to efficiently simulate an arbitrary nonrelativistic interacting quantum many-body system on a quantum computer exponentially faster than the same calculation could be performed on a classical computer. Such a system would be an ideal example of quantum computing since the

*Electronic address:bruceb@bu.edu
†Electronic address:wati@princeton.edu

computing elements could be built from a system of spin-1/2 particles on a lattice obeying simple local unitary time evolution rules.

The principal difference between our models and the 1D Dirac lattice model (and its generalization by Succi and Benzi [7]) is that in the Dirac model, the unitary evolution rule satisfied by the wave function or particle at each time step is infinitesimally close to the identity transformation. As the lattice spacing ϵ goes to 0, the unitary transition matrix is of the form $S=1+i\epsilon M$, where M is Hermitian. In our models, we take the transition matrix to be independent of the lattice spacing. This form of a time development equation makes the system nonrelativistic, but allows for a formulation in an arbitrary number of dimensions. A closely related model was considered recently in one spatial dimension [10], where simulations were shown to be consistent with emergent behavior corresponding to a Schrödinger equation. In this paper we prove that this is the general behavior of such models, giving a simple algebraic relation between the transition matrix and the mass of the nonrelativistic particle. We develop such models for the Schrödinger equation in an arbitrary number of dimensions.

In the first part of this paper we will consider lattice models for single-particle motion. These models are essentially unitary lattice Boltzmann models [11]. In the latter part of the paper we generalize to many-body systems and discuss how a lattice of quantum computing elements could be used to describe the motion of a large number of nonrelativistic quantum particles. We conclude with a simple numerical check of the analytic description of a sample model.

As a simple example of the type of system considered in this paper, consider the lattice Boltzmann model with a configuration space defined by two complex fields $\psi_1(x,t)$ and $\psi_2(x,t)$, taking independent values on a lattice with one spatial dimension x and one temporal dimension t. Define the dynamics of this model to obey the equations

$$\psi_1(x+1,t)=\frac{1}{2}[(1-i)\psi_1(x,t-1)-(1+i)\psi_2(x,t-1)],$$

$$\psi_2(x-1,t)=\frac{1}{2}[(1-i)\psi_2(x,t-1)-(1+i)\psi_1(x,t-1)].$$

These equations give a unitary time evolution to ψ. To understand how ψ evolves in a continuum limit, we can expand the equations of motion through four time steps, giving for example

$$\psi_1(x,t+4)=\frac{1}{4}[-\psi_1(x-4,t)+3\psi_1(x-2,t)+\psi_1(x,t)+\psi_1(x+2,t)]+\frac{i}{4}[\psi_2(x-2,t)-\psi_2(x,t)-\psi_2(x+2,t)+\psi_2(x+4,t)].$$

Taking a continuous limit as the lattice spacing scales as ϵ in the x direction and ϵ^2 in the t direction, we find the differential equation

$$\partial_t\psi_1(t)=\frac{i}{2}\partial_x^2\psi_2(t).$$

A similar equation holds for ψ_2, and so it follows that

$$\partial_t(\psi_1+\psi_2)=\frac{i}{2}\partial_x^2(\psi_1+\psi_2).$$

Thus we see that the total amplitude $\Psi(x,t)=\psi_1(x,t)+\psi_2(x,t)$ satisfies a Schrödinger equation. As we shall demonstrate, this is the generic behavior of a unitary Boltzmann model with a fixed time development rule.

We introduce the Schrödinger model in Sec. II by presenting the one-dimensional case. The model is generalized to Cartesian lattices of arbitrary dimension in Sec. III; in this section we also discuss the inclusion of a potential. In Sec. IV we discuss how the one-particle models can be generalized to construct a quantum lattice-gas model of many nonrelativistic particles. In Sec. V we give the results of a simulation of a single free nonrelativistic particle in two dimensions, comparing numerical results with the theoretical framework presented here. The Appendixes give explicit formulas for models in two and three dimensions on a Cartesian lattice.

II. SCHRÖDINGER EQUATION IN ONE DIMENSION

In this section we consider unitary lattice Boltzmann models describing the evolution of a single particle in one dimension. Keeping the collision operator fixed in the scaling limit, we show that a very general class of microscopic models gives rise in the continuum limit to a Schrödinger equation.

We define the model on a lattice given by points $x=\epsilon n$, where n is an integer. The lattice can be taken to either have periodic boundary conditions or to be of infinite extent. The state of the system at a fixed value of the time parameter t is described by a wave function $\psi_k(x,t)$ that depends upon the discrete position x and an ''internal'' index k taking values from 1 to m, labeling possible particle velocities at the lattice site x. As in lattice Boltzmann models, at each discrete time step the various components of the field at each site undergo a local unitary ''collision'' and then the jth component of $\psi(x,t)$ propagates along the jth lattice vector c_j to the new site $x+c_j$ to yield the new state of the system at time $t+\Delta t$. We consider only linear processes, so this interaction can be specified by an $m\times m$ scattering matrix S.

We take the continuum limit of the theory by scaling $\epsilon\to 0$, where $\Delta t\sim\epsilon^2$. In this limit we will find that the discrete equation describing the dynamics of ψ becomes a continuous differential equation, which we identify as the Schrödinger equation.

In this section we will assume that each lattice site has two associated possible particle velocities, corresponding to right- and left-moving particles. We will also assume that the dynamics is symmetric under right-left reflection. More general models can easily be analyzed using a similar formalism.

The equation of motion for the model reads

$$\psi_k(x+\epsilon c_k,t)=S_{kj}\psi_j(x,t-\Delta t),$$

where $k=1,2$ correspond to right- and left-moving particles, so that $c_1=+1, c_2=-1$. The quantum wave function $\psi_k(x,t)$ is normalized so that

$$\sum_{x,k} |\psi_k(x,t)|^2 = 1 \tag{1}$$

for all t. The matrix S_{kj} is a 2×2 matrix that is unitary so as to preserve the condition (1).

We begin our analysis by transforming to the wave function

$$\psi(x,t) = S^{\tau}\phi(x,t),$$

where $\tau \equiv t/\Delta t$. We can then expand the difference $\phi(t)-\phi(t-1)$ in the infinitesimal parameter ϵ to get

$$\phi(t)-\phi(t-1) = -\epsilon S^{-\tau} C S^{\tau}\partial_x\phi - \frac{\epsilon^2}{2} S^{-\tau} C^2 S^{\tau}\partial_x^2\phi + O(\epsilon^3),$$

where C is the 2×2 matrix

$$C = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Because we are assuming that the interaction described by the matrix S is invariant under reflection, S must be of the form

$$S = \begin{pmatrix} a & b \\ b & a \end{pmatrix},$$

where a and b are complex numbers. Because of unitarity we have $|a|^2+|b|^2=1$. S can be put in diagonal form by writing

$$S = X^{-1} D X,$$

where

$$X = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

We can redefine S and ψ up to a phase, so that without loss of generality we can take

$$D = \begin{pmatrix} \mu & 0 \\ 0 & 1 \end{pmatrix},$$

where μ is a complex number with magnitude 1 ($\mu\mu^*=1$). We then have

$$S = \frac{1}{2} \begin{pmatrix} \mu+1 & \mu-1 \\ \mu-1 & \mu+1 \end{pmatrix}.$$

If we write $X\phi = \eta$, then we have

$$\eta(t)-\eta(t-1) = -\epsilon D^{-\tau}(XCX^{-1}) D^{\tau}\partial_x\eta - \frac{\epsilon^2}{2} D^{-\tau}(XC^2X^{-1}) D^{\tau}\partial_x^2\eta + O(\epsilon^3).$$

At this point we would like to scale the time step as a power of ϵ so that this equation can be written as a differential equation in time. However, there is a difficulty that arises due to the fact that there are two relevant time scales involved in the dynamics of η. There is an order-ϵ change to η at every time step; however, this order-ϵ term has a phase angle that rotates at every time step. Thus the order-ϵ dynamics average out after a large number of time steps, so that the time-averaged rate of change of η actually goes as ϵ^2. The dynamics we are interested in are independent of the short-term order-ϵ fluctuations, so we must perform another transformation to remove these effects. With this goal in mind, we write

$$\eta(t) = \zeta(t) + \epsilon\rho(t),$$

where

$$\rho(t)-\rho(t-1) = -D^{-\tau}(XCX^{-1}) D^{\tau}\partial_x\zeta.$$

This equation is solved by

$$\rho(t) = D^{-\tau} G D^{\tau}\partial_x\zeta,$$

where

$$G - DGD^{-1} = -B = -(XCX^{-1}).$$

This can be solved for G as long as the only nonzero entries B_{ij} appear where the i and j eigenvalues of D are different. We can now write a final dynamical equation for ζ,

$$\zeta(t)-\zeta(t-1) = -\epsilon^2 D^{-\tau} B G D^{\tau}\partial_x^2\zeta - \frac{\epsilon^2}{2} D^{-\tau}(XC^2X^{-1}) D^{\tau}\partial_x^2\zeta + O(\epsilon^3).$$

If we assume that the unit of time scales as ϵ^2, we have the continuous dynamical equation

$$\partial_t\zeta = -D^{-\tau} B G D^{\tau}\partial_x^2\zeta - \frac{1}{2} D^{-\tau}(XC^2X^{-1}) D^{\tau}\partial_x^2\zeta.$$

We can now substitute the known matrices X, C, D to compute

$$B = XCX^{-1} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$XC^2X^{-1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$G = \begin{pmatrix} 0 & \dfrac{-1}{1-\mu} \\ \dfrac{-1}{1-\mu^*} & 0 \end{pmatrix}.$$

Using these matrices we have

$$BG+\frac{1}{2}XC^2X^{-1}=\begin{pmatrix}\frac{1}{2}-\frac{1}{1-\mu^*} & 0\\ 0 & \frac{1}{2}-\frac{1}{1-\mu}\end{pmatrix}.$$

Writing $\mu=\cos\theta+i\sin\theta$, we have

$$\frac{1}{1-\mu}=\frac{1-\cos\theta+i\sin\theta}{(1-\cos\theta)^2+\sin^2\theta}=\frac{1}{2}+i\frac{\sin\theta}{2(1-\cos\theta)}.$$

Thus the dynamical equation for ζ becomes

$$\partial_t\zeta=i\begin{pmatrix}\frac{1}{2m} & 0\\ 0 & -\frac{1}{2m}\end{pmatrix}\partial_x^2\zeta,$$

where

$$m=\cot\theta-\csc\theta.$$

The equation for the first component of ζ is thus precisely a Schrödinger equation for a particle moving in one dimension with mass m. To leading order, $\zeta(t)$ is related to ψ through the sequence of transformations described above, so that

$$\zeta(t)=D^{-\tau}X\psi(t)+O(\epsilon).$$

The first component of $\zeta(t)$ is therefore given by

$$\Psi=\zeta_1(t)=\frac{\mu^{-\tau}}{\sqrt{2}}[\psi_1(t)+\psi_2(t)];$$

this satisfies the Schrödinger equation in the continuum limit,

$$\partial_t\Psi=i\frac{1}{2m}\partial_x^2\Psi.$$

Note that by taking $\mu=-i$ we get $m=1$, giving precisely the example discussed in Sec. I. We shall demonstrate in Sec. III that, in an analogous fashion, in higher-dimensional theories the sum of the wave function components forms a scalar quantity that satisfies a Schrödinger equation.

III. SCHRÖDINGER EQUATION IN DIMENSIONS $d\geqslant 1$

In this section we derive the general form for the continuum limit of the dynamics for a unitary lattice Boltzmann model with fixed collision matrix on a lattice with any number of dimensions. Specializing to the case where the lattice is Cartesian and the collision rule is invariant under discrete rotations, we find that a generic collision rule gives a Schrödinger equation in any dimension d.

A. General form of the dynamical equation

The analysis of the continuous equations of motion in d dimensions proceeds in a fashion very similar to the discussion in the preceding section. We assume that the lattice contains a set of points $\mathbf{x}$ and that at each lattice site there are particle velocities labeled by k, corresponding to velocity vectors $\mathbf{c}_k$ in the lattice. Denoting spatial indices by α, we denote the αth component of the kth velocity vector by c_k^α. The dynamics of the lattice Boltzmann model are described by the equation of motion

$$\psi_k(\mathbf{x}+\epsilon\mathbf{c}_k,t)=S_{kj}\psi_j(\mathbf{x},t-1),$$

where S is unitary. Transforming as before

$$\psi(t)=S^\tau\phi(t),$$

we have

$$\phi(t)-\phi(t-1)=-\epsilon S^{-\tau}C^\alpha S^\tau\partial_\alpha\phi-\frac{\epsilon^2}{2}S^{-\tau}C^\alpha C^\beta S^\tau\partial_\alpha\partial_\beta\phi+O(\epsilon^3),$$

where the diagonal matrices C^α are given by

$$C^\alpha\equiv\mathrm{diag}(c_1^\alpha,\ldots,c_n^\alpha),$$

with c_j^α being the αth spatial component of the jth lattice vector. Writing $S=X^{-1}DX$, $X\phi=\eta$ we have

$$\eta(t)-\eta(t-1)=-\epsilon D^{-\tau}(XC^\alpha X^{-1})D^\tau\partial_\alpha\eta-\frac{\epsilon^2}{2}D^{-\tau}(XC^\alpha C^\beta X^{-1})D^\tau\partial_\alpha\partial_\beta\eta+O(\epsilon^3).$$

We write

$$\eta(t)=\zeta(t)+\epsilon\rho(t),$$

where

$$\rho(t)-\rho(t-1)=-D^{-\tau}(XC^\alpha X^{-1})D^\tau\partial_\alpha\zeta.$$

This is solved, as before, by

$$\rho(t)=D^{-\tau}G^\alpha D^\tau\partial_\alpha\zeta,$$

where

$$G-DGD^{-1}=-(XCX^{-1})=-B.$$

Again, this can be solved for G as long as the only nonzero entries B_{ij} appear where the i and j eigenvalues of D are different. The resulting continuum equation for η is

$$\partial_t\eta=-D^{-\tau}B^\alpha G^\beta D^\tau\partial_\alpha\partial_\beta\eta-\frac{1}{2}D^{-\tau}(XC^\alpha C^\beta X^{-1})D^\tau\partial_\alpha\partial_\beta\eta.$$

This is the general form of the dynamical equation for a unitary lattice Boltzmann model.

B. Schrödinger equation in d dimensions

We now specialize to the case where the lattice is Cartesian, so that there are $2d$ possible particle velocities at each lattice site, corresponding to vectors of magnitude $+\epsilon,-\epsilon$ in each of the d directions. We choose the collision matrix S to

be invariant under the symmetry group of the lattice. We will show that generically the continuum limit of the equation of motion is a Schrödinger equation, just as we found for a general collision matrix in one dimension on the Cartesian lattice.

The constraint that S is invariant under discrete rotations and reflections is actually quite a strong condition. The $2d$ dimensional space of velocity vectors transforms under a linear representation of this discrete group. This representation contains only three irreducible representations, which allows us to determine D up to three distinct eigenvalues. Because of the symmetry constraint, we can always diagonalize S by the matrix

$$X=\begin{pmatrix} \frac{1}{\sqrt{2d}} & \frac{1}{\sqrt{2d}} & \frac{1}{\sqrt{2d}} & \cdots & \frac{1}{\sqrt{2d}} & \frac{1}{\sqrt{2d}} & \frac{1}{\sqrt{2d}} & \frac{1}{\sqrt{2d}} & \cdots & \frac{1}{\sqrt{2d}} & \frac{1}{\sqrt{2d}} \\ \frac{1}{\sqrt{2}} & 0 & 0 & \cdots & 0 & -\frac{1}{\sqrt{2}} & 0 & 0 & \cdots & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & \cdots & 0 & 0 & -\frac{1}{\sqrt{2}} & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \cdots & 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & -\frac{1}{2} & 0 & \cdots & 0 & \frac{1}{2} & -\frac{1}{2} & 0 & \cdots & 0 & 0 \\ \frac{1}{2\sqrt{3}} & \frac{1}{2\sqrt{3}} & -\frac{2}{2\sqrt{3}} & \cdots & 0 & \frac{1}{2\sqrt{3}} & \frac{1}{2\sqrt{3}} & -\frac{2}{2\sqrt{3}} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots & \vdots \\ \frac{1}{2\sqrt{d_2}} & \frac{1}{2\sqrt{d_2}} & \frac{1}{2\sqrt{d_2}} & \cdots & \frac{1-d}{2\sqrt{d_2}} & \frac{1}{2\sqrt{d_2}} & \frac{1}{2\sqrt{d_2}} & \frac{1}{2\sqrt{d_2}} & \cdots & \frac{1}{2\sqrt{d_2}} & \frac{1-d}{2\sqrt{d_2}} \end{pmatrix},$$

where $d_2=d(d-1)/2$. The rows of this matrix consist of the three groups of vectors in the irreducible representations of the rotation group mentioned above. The first row is the normalized vector $(1,1,\ldots,1)$. The next d rows are normalized versions of the vectors $\mathbf{c}^\alpha$ with $+1$ in position i and -1 in position $i+d$. The last $d-1$ rows are vectors with equal components i and $i+d$, subject to the condition that the sum of the components vanishes. This matrix puts S in the diagonal form

$$D=XSX^{-1}=\begin{pmatrix} \mu & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & \nu & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & & \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \nu & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 & \lambda & \cdots & 0 \\ \vdots & \vdots & & \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & 0 & 0 & \cdots & \lambda \end{pmatrix},$$

where the eigenvalue ν appears d times and the eigenvalue λ appears $d-1$ times. By a simple phase redefinition we can choose $\nu=1$. We will furthermore set $\lambda=-1$, which as we shall see will give rise to a Schrödinger equation in the continuum limit. As we shall discuss later, however, any value of $\lambda\neq\mu$ gives a Schrödinger equation; we use the $\lambda=-1$ condition merely to simplify the presentation.

With the stated conditions on D, we can compute S. We find that all elements of S are equal to $(1+\mu)/2d$, except the matrix elements $S_{i,i+d}$ and $S_{i+d,i}$, which are equal to $(1+\mu)/2d-1$. Thus

$$S_{ij}=\frac{1+\mu}{2d}-\delta_{0,|i-j|-d}.$$

At a microscopic level, this collision matrix gives an equal amplitude for a particle to move in every direction other than directly backward. To check the unitarity condition, we verify

$$(2d-1)\frac{(1+\mu)(1+\mu^*)}{4d^2}+\frac{(1+\mu-2d)(1+\mu^*-2d)}{4d^2}=1$$

and

$$(2d-2)\frac{(1+\mu)(1+\mu^*)}{4d^2}+\frac{(1+\mu)(1+\mu^*-2d)}{4d^2}$$
$$+\frac{(1+\mu-2d)(1+\mu^*)}{4d^2}=0.$$

We can now proceed to calculate the other matrices needed for the dynamics. There are d matrices B^α. For a particular value of α, we find that all matrix entries vanish except those in the $(\alpha+1)$th row and the $(\alpha+1)$th column, which are given by

$$(B^\alpha)_{\alpha+1,i}=(B^\alpha)_{i,\alpha+1}=\left(\frac{1}{\sqrt{d}},0^{d+\alpha-2},-\frac{\sqrt{\alpha-1}}{\sqrt{\alpha}},r(\alpha),\right.$$
$$\left.r(\alpha+1),\ldots,r(d-1)\right)_i,$$

where by 0^k we denote a sequence of k 0's and we have defined

$$r(\alpha)=\frac{1}{\sqrt{\alpha(\alpha+1)}}.$$

We can now immediately compute G^α, which has nonzero elements in the same positions, given by

$$(G^\alpha)_{\alpha+1,i}=\left(\frac{-1}{(1-\mu^*)\sqrt{d}},0^{d+\alpha-2},\frac{\sqrt{\alpha-1}}{2\sqrt{\alpha}},-\frac{1}{2}r(\alpha),\right.$$
$$\left.-\frac{1}{2}r(\alpha+1),\ldots,-\frac{1}{2}r(d-1)\right)_i,$$

$$(G^\alpha)_{i,\alpha+1}=\left(\frac{-1}{(1-\mu)\sqrt{d}},0^{d+\alpha-2},\frac{\sqrt{\alpha-1}}{2\sqrt{\alpha}},-\frac{1}{2}r(\alpha),\right.$$
$$\left.-\frac{1}{2}r(\alpha+1),\ldots,-\frac{1}{2}r(d-1)\right)_i.$$

We are now interested in computing the differential equation describing the continuum limit of the dynamics of the first component of ζ, which we will denote by Ψ. As before, we define

$$\Psi(\mathbf{x},t)=\zeta_1=\frac{\mu^{-\tau}}{\sqrt{2d}}\left(\sum_i \psi_i(\mathbf{x},t)\right)+O(\epsilon).$$

To compute the dynamics of Ψ, we need to know only the first rows of the matrices $B^\alpha G^\beta$ and $XC^\alpha C^\beta X^{-1}$. From the above expressions, we find that the first row of $B^\alpha G^\beta$ is given by

$$(B^\alpha G^\beta)_{0i}=\frac{1}{\sqrt{d}}\delta^{\alpha\beta}\left(-\frac{1}{\sqrt{d}(1-\mu^*)},0^{d+\alpha-2},\frac{\sqrt{\alpha-1}}{2\sqrt{\alpha}},\right.$$
$$\left.-\frac{1}{2}r(\alpha),-\frac{1}{2}r(\alpha+1),\ldots,-r(d-1)\right)_i.$$

From the above form of X, we see that the first row of $XC^\alpha C^\beta X^{-1}$ is given by

$$(XC^\alpha C^\beta X^{-1})_{0i}=\delta^{\alpha\beta}\frac{1}{\sqrt{d}}\left(\frac{1}{\sqrt{d}},0^{d+\alpha-2},-\frac{\sqrt{\alpha-1}}{\sqrt{\alpha}},\right.$$
$$\left.r(\alpha),r(\alpha+1),\ldots,r(d-1)\right)_i.$$

Thus the first row of the combined matrix is

$$\left(-B^\alpha G^\beta-\frac{1}{2}XC^\alpha C^\beta X^{-1}\right)_{0i}=\left(i\frac{1}{2m},0^{2d-1}\right)_i,$$

where

$$m=d(\cot\theta-\csc\theta), \tag{2}$$

with

$$\mu=\cos\theta+i\sin\theta. \tag{3}$$

As a result, we obtain the differential equation describing the dynamical evolution of Ψ in the continuum limit,

$$\partial_t\Psi(\mathbf{x},t)=i\frac{1}{2m}\sum_\alpha \partial_\alpha^2\Psi(\mathbf{x},t), \tag{4}$$

which we recognize as Schrödinger evolution in d dimensions. In Appendixes A and B we work out the specific cases of $d=2$ and $d=3$ in detail.

Note that had we chosen the eigenvalue λ differently, the difference would have appeared in the last $d-1$ rows and columns of G. Following through the computation, we find that the only change would be that new terms would appear on the right-hand side of Eq. (4), proportional to the eigenvectors of S with eigenvalue λ. However, these terms would have had a phase $(\mu\lambda^*)^\tau$ and thus would have averaged out in the continuum limit as long as $\mu\neq\lambda$, making no change to the final result Eq. (4). Thus we reach the conclusion that for any collision rule invariant under the lattice symmetry group, as long as μ is distinct from the other eigenvalues of the collision matrix, the resulting continuum dynamics for the total amplitude Ψ are governed by a Schrödinger equation.

C. Inclusion of a potential

In general, we can easily include an arbitrary potential $V(\mathbf{x})$ by including a position-dependent phase in the transition matrix S. If we perform the above analysis for a model with transition matrix

$$\widetilde{S}(\mathbf{x})=\exp[-i\epsilon^2V(\mathbf{x})]S,$$

where S is a spatially invariant matrix such as discussed above, then the general form of the dynamical equation becomes

$$\partial_t \eta(\mathbf{x},t) = -D^{-\tau} B^{\alpha} G^{\beta} D^{\tau} \partial_{\alpha}\partial_{\beta}\eta(\mathbf{x},t) - \frac{1}{2} D^{-\tau}(X C^{\alpha} C^{\beta} X^{-1}) D^{\tau} \partial_{\alpha}\partial_{\beta}\eta(\mathbf{x},t) - iV(\mathbf{x})\,\eta(\mathbf{x},t).$$

This becomes, for the total amplitude Ψ, the Schrödinger equation in an external potential

$$\partial_t \Psi(\mathbf{x},t) = i\frac{1}{2m}\sum_{\alpha} \partial_{\alpha}^2 \Psi(\mathbf{x},t) - iV(\mathbf{x},t)\Psi(\mathbf{x},t).$$

IV. MANY PARTICLES: QUANTUM LATTICE-GAS AUTOMATA

We now consider models in which multiple particles move independently according to the Schrödinger equation in d dimensions. One way of simulating the motion of n particles in d dimensions is to introduce extra degrees of freedom for each particle. Thus, for example, we could model the motion of two particles in one dimension by the lattice Boltzmann model

$$\psi_{ik}(x+\epsilon c_i, y+\epsilon c_k, t) = S_{il} S_{kj} \psi_{lj}(x,y,t-1), \qquad (5)$$

where x,y are the positions of the two particles, i,k are the internal indices specifying their directions, and S is a 2×2 matrix for unitary Schrödinger evolution in one dimension, as discussed in Sec. II. Notice that this dynamics is equivalent to that of a single particle moving in two dimensions.

In a similar fashion we can describe models where n particles move in d dimensions, by constructing a unitary lattice Boltzmann model in nd dimensions. It is straightforward to incorporate an arbitrary interparticle potential in this formulation; the potential is a function of the particle positions and can be included as discussed in Sec. III C.

This gives a procedure for simulating an interacting nonrelativistic quantum many-body system on a classical computer. Although this may give a useful algorithm for systems containing only a few particles, if we wish to simulate the motion of a large number of particles using the method just described it is clear that the number of calculations needed to perform even one time step of the evolution become rapidly intractable. For example, simulating the motion of 20 particles in three dimensions on a lattice of side length 100 would take on the order of 10^{120} calculations per time step, beyond the capacity of any imaginable classical computer.

However, the technology of *quantum computing* [12] presents a paradigm in which such calculations can be done. We will now describe a way in which the above algorithm can be implemented on a quantum computer with a speedup exponential in the number of particles. In fact, it is natural to perform simultaneously the calculation for all numbers of particles that will fit on the lattice, essentially performing a discrete simulation of nonrelativistic quantum many-body theory. The resulting model falls in the class of quantum lattice-gas automata, which were recently defined by Meyer [9] in the context of the $(1+1)$-dimensional Dirac model. The exponential speedup of this algorithm on a quantum computer is a specific example of the general observation by Feynman [13] and Lloyd [14] that quantum-mechanical systems can be simulated more efficiently on a quantum computer than on a classical computer.

A quantum-computing device is composed of simple quantum elements such as particles with spin 1/2 (quantum bits, or q-bits). The state space of the system at any fixed time is the tensor product of the Hilbert spaces of the states of the elementary computational elements. Thus, for example, a system with m q-bits has a state space of dimension 2^m. At each time step, some small number of q-bits (usually 2 or 3 [16]) are subjected to a unitary time evolution, described by acting with a unitary matrix on the Hilbert space of the affected elements. Quantum computers have recently become of great interest because of the result due to Shor [15] that it is possible to factor large integers on a quantum computer in polynomial time, a procedure thought to be impossible on a classical computer.

In order to implement the many-body simulation described in the beginning of this section on a quantum computer, it is necessary to make some restrictions on the behavior of the many-body wave function under exchange of particles. The example system in Eq. (5) describes two particles moving in one dimension without interacting. In this model, both particles can be moving in the same direction from the same lattice site at a given point in time. We can modify this model slightly to give the particles exclusionary (Fermi) statistics by making the transition matrix at $x=y$ force the two particles to move in different directions. This corresponds to introducing a contact interaction between the two particles when they move within a single lattice distance. By making the initial conditions antisymmetric under exchange of x and y, we have a simulation of two nonrelativistic fermions moving in one dimension. Alternatively, we could symmetrize the wave function and we would have a simulation of ''hard bosons'' that obey Bose statistics, but cannot occupy the same lattice site. Either of these approaches naturally generalize to arbitrary numbers of particles and arbitrary dimensions. For the remainder of the discussion we assume that the particles obey Bose statistics. The issue of implementing fermionic systems on a quantum computer is more subtle [13] and has been addressed recently by Abrams and Lloyd [17].

In previous sections we discussed the motion of a single particle, with a wave function $\psi_k(\mathbf{x},t)$. Now, we would like to consider the state space for a quantum system of many particles. A natural basis for the Hilbert space of such a system is the set of states in the fermionic Fock space associated with the spatial lattice; such states are identified by a set of occupation numbers $s_k(\mathbf{x})$ (taking values 0 or 1) for each possible particle position $\mathbf{x}$ and internal index k. The Hilbert space of the model is thus 2^{ml^d} dimensional, where m is the number of possible values of the internal index and l^d is the number of lattice sites. For example, a basis vector of the state space for a one-dimensional system with four lattice sites $x=1,2,3,4$ might be given by

$$|s\rangle = |(s_2(1),s_1(1)), \ldots, (s_2(4),s_1(4))\rangle = |(0,1),(0,0),(0,0),(1,1)\rangle \qquad (6)$$

where each ordered pair corresponds to the occupation numbers at a given lattice site. Thus this state corresponds to the

configuration where a single particle is at $x=1$, with $k=1$, and both particle positions at $x=4$ are filled.

The state of the quantum system at any given value of the discrete time parameter t is given by a vector

$$|\psi(t)\rangle=\sum_s C_s(t)|s\rangle,$$

where the sum is taken over all basis vectors of the Hilbert space. This state is defined by the coefficients $C_s(t)$. In the quantum computing paradigm, this corresponds to the state space of ml^d independent q-bits.

We will now define a quantum lattice-gas automaton by defining a dynamics on the quantum state space. The dynamics of the quantum lattice gas will be described in two steps, just as in classical lattice-gas automaton models. First there is a collision step in which the particles at each lattice site interact. Then there is an advection step, describing the propagation of the particles in the directions associated with the vectors $\mathbf{c}_k$. Each of these steps is described in the quantum system by a unitary transfer matrix acting on the state space of the system. The total dynamics can then be described by the equation

$$|\psi(t+\Delta t)\rangle=AK|\psi(t)\rangle.$$

The advection step simply corresponds to a permutation matrix A on the basis vectors described above, where each bit is moved forward in the direction corresponding to the appropriate vector $\mathbf{c}_k$. For example, acting on the state in Eq. (6), the result of applying the advection operator would be

$$A|s\rangle=|(0,1),(0,1),(1,0),(0,0)\rangle$$

where we assume periodic boundary conditions on the lattice. The particle that was at lattice site $x=1$ has been advected to $x=2,k=1$ and the two particles that were at $x=4$ have moved to $x=3$ and $x=1$.

We now consider the collision part of the time development rule. The collision process is defined by a single unitary $2^m\times 2^m$ matrix T, which acts separately on the quantum bits associated with each lattice site. Thus the state of the system is transformed by the unitary matrix

$$K=T\otimes T\otimes\cdots\otimes T,$$

given by the l^d-fold tensor product of T. We would like the collision matrix T to have the property that it conserves particle number. Thus this matrix is block diagonal in the subspaces of the Hilbert space at each lattice site corresponding to a fixed particle number.

We have now defined a discrete model for quantum many-particle systems. To understand the behavior of this model in the continuum limit, let us consider the behavior when the number of particles in the system is relatively small compared to the number of lattice sites. In this case, at most lattice sites the number of particles present will be either 0 or 1. This part of the dynamics, which describes the free propagation of single particles, is described by the part of T in the single-particle Hilbert space. However, because this is a unitary matrix, generically the dynamics described by this transition matrix is precisely that which we studied in the previous sections and corresponds to a nonrelativistic particle propagating according to the Schrödinger equation. Thus, for relatively sparse systems, this quantum lattice-gas model simulates a system of many nonrelativistic particles whose free propagation is given by the Schrödinger equation. The remaining parts of the collision matrix T describe a contact interaction between the various particles.

Let us now discuss the computational complexity of the quantum algorithm. To implement the advection transformation by using quantum computing elements, it is only necessary to perform a series of exchanges of the values of the quantum bits representing the particle occupation numbers. The number of such exchanges is essentially equal to the number of bits ml^d (recall that on a Euclidean lattice of dimension d, $m=2d$, so that for example, if $d=3$, the advection operation can be implemented in approximately $6l^3$ quantum operations).

The matrix T acts on the Hilbert space associated with a subset of m of the q-bits in the system. Counting degrees of freedom, generically such a matrix can be implemented with approximately $2^{2m}/15$ elementary quantum operations on pairs of q-bits. For example, in a 3D system, it would take on the order of 300 quantum operations to implement each T matrix, so that the number of computational steps needed to perform the transformation by K would be around $300l^3$. Note, however, that the part of T that acts on the multiple-particle Hilbert space simply changes the phases of a δ-function-type interaction between the particles. Since these phases may not affect the results in most problems of physical interest, these components of T can be arbitrary. Thus, in practice we need only find a combination of operations on q-bits that will give a matrix T that preserves particle number and gives the desired symmetry properties and eigenvalues, reducing the number of steps needed significantly below 300.

Combining these observations, we see that this model can be simulated with on the order of l^d elementary quantum computations at each time step (or on the order of 1 if we are using a quantum computing system that allows parallel computation). Since this system automatically contains the multiparticle wave function for all possible particle numbers, we have achieved an exponential increase in speed over what was possible on a classical computer.

The system as defined so far includes only interactions between the particles in the form of δ-function interactions parametrized by the components of T in the multiple-particle space. We can introduce an arbitrary interparticle potential $V(\mathbf{x},\mathbf{y})$ by hand, by multiplying the wave function at each time step by the tensor product over all pairs of q-bits

$$U=\otimes U_{i,j,\mathbf{x},\mathbf{y}},$$

where the matrix

$$U_{i,j,\mathbf{x},\mathbf{y}}=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&e^{-i\epsilon^2V(\mathbf{x},\mathbf{y})}\end{pmatrix}$$

acts on the Hilbert space associated with the q-bits $s_i(\mathbf{x})$ and $s_j(\mathbf{y})$, changing the phase of the wave function only in the

component where both q-bits have the value 1. Implementing this interparticle potential will take on the order of $m^2 l^{2d}$ quantum computations for each time step. Although this significantly increases the computational complexity of the quantum algorithm this is still exponentially faster than the analogous classical algorithm, since the particle number n does not affect the complexity. Note that, unlike the rest of the algorithm, the implementation of interparticle potentials involves nonlocal interactions on the lattice.

To clarify the discussion, we consider a simple example of a collision matrix T. For a many-body system in one dimension, at each lattice site the collision matrix T is a 4×4 matrix, acting on the Hilbert space with basis $|(0,0)\rangle$, $|(0,1)\rangle$, $|(1,0)\rangle$, $|(1,1)\rangle$. Since we are assuming that particle number is conserved and that the dynamics is symmetric under left-right reflection, the matrix T is of the form

$$T=\begin{pmatrix} \alpha & 0 & 0 & 0 \\ 0 & a & b & 0 \\ 0 & b & a & 0 \\ 0 & 0 & 0 & \beta \end{pmatrix},$$

where α,β,a,b are complex numbers satisfying $|\alpha|^2=|\beta|^2=|a|^2+|b|^2=1$ and $a\overline{b}+\overline{a}\,b=0$. By a simple global phase redefinition, we can choose $\alpha=1$. The part of T in the single-particle Hilbert space is precisely the form of the collision matrix S from Sec. II. From the eigenvalues of this matrix we can determine the mass of the free particles in the model. Finally, there is a single parameter β that describes the phase with which two particles ''bounce.'' In this simple one-dimensional model, there is therefore little freedom in choosing the particle interaction. In higher dimensions there would be nontrivial phases describing δ function interactions between up to $2d$ particles.

One major concern in the implementation of any algorithm is the issue of precision. This problem is particularly acute on a quantum computer, where each quantum operation involves acting on the state with a unitary transformation that can only be controlled up to some finite precision. Furthermore, on a quantum computer there is the related but distinct problem of decoherence that must be addressed in order for any quantum computation to be feasible. There has been a great deal of work recently describing how these problems can be solved using dynamical quantum error correction methods [18]. Without going into this issue in depth, we make the simple observation that even without error correction, if the precision of each quantum operation is $1-1/t$, then at each time step the error in the wave function will take a random step in the Hilbert space with size $1/t$. Only after on the order of t^2 operations will this error become significant. Thus, if we could achieve a precision better than 10^{-5}, we could perform 10^{10} quantum operations successfully, which would allow us to simulate, for example, an interacting 3D system on a lattice with size of order 20^3. With the error correction schemes described in [18], there is in principle no upper bound on how large a system could be simulated, other than the size of the quantum computer that could be built to perform the simulation.

Finally, we consider the issue of measurement in quantum lattice gases. In a classical lattice gas, hydrodynamic quantities, such as mass and momentum density, are obtained by averaging particles' mass and momentum over blocks in space and/or time. In a typical lattice-gas simulation, this is done from time to time to obtain the macroscopic variables of interest. The process of measuring these quantities is purely passive, that is, their measurement does not affect the subsequent dynamical evolution at all. In contrast, the analogous operation for a quantum lattice gas would involve occasionally measuring the state of some subset of the q-bits in the system, thus collapsing the quantum wave function onto the eigenstates of the (space and/or time) block number operator. The set of quantities that are accessible through this type of simulation are rather different from those accessible through simulation methods on a classical computer. For example, the dynamics of the system defines an effective Hamiltonian that is an approximation to the Hamiltonian of the many-body quantum system being simulated; however, the spectrum of this Hamiltonian is not directly amenable to measurement. Instead, the types of observables that can be measured in the simulation are precisely equivalent to the types of observables that can be measured in an actual interacting quantum system. For example, a typical experiment might be to initialize the system in a particular known state at time $t=0$ and to ask for the probability p at time t that there is a particle in a region of space dx^3. Just as in the physical quantum system, we can ask such a question of our simulation; we can perform the experiment a number of times and each time we will find a particle with probability p. To actually compute p to some degree of accuracy requires repeating the experiment a number of times.

V. NUMERICAL RESULTS

To test the algorithm, we consider the dispersion relation of plane waves in periodic geometry in two dimensions. We consider a periodic grid with dimensions $N\times N$, and initialize it with a plane wave of the form

$$\psi_j(\mathbf{x},0)=\frac{1}{4}\exp(i\mathbf{k}\cdot\mathbf{x}-i\omega t)$$

for $j=1,\ldots,4$, where

$$\mathbf{k}=2\pi(l_x\hat{\mathbf{x}}+l_y\hat{\mathbf{y}}),$$

where l_x and l_y are integers. Choosing units where the spatial dimensions are of unit length, we have $\epsilon=1/N$ and $\Delta t=\epsilon^2=1/N^2$

We evolve this initial condition in time, using Eq. (A1) with $\mu=-i$ (hence $m=2$) for the collisions. Every four time steps, we measure the inner product of the wave function with its initial condition

$$S(t)\equiv\frac{1}{N^2}\sum_{\mathbf{x}}\Psi^*(\mathbf{x},0)\Psi(\mathbf{x},t).$$

The result should go like $\exp(-i\omega t)$, so the ratio of two successive values of this quantity is

$$\frac{S(t+4\Delta t)}{S(t)}=\exp(-4i\omega\Delta t)$$

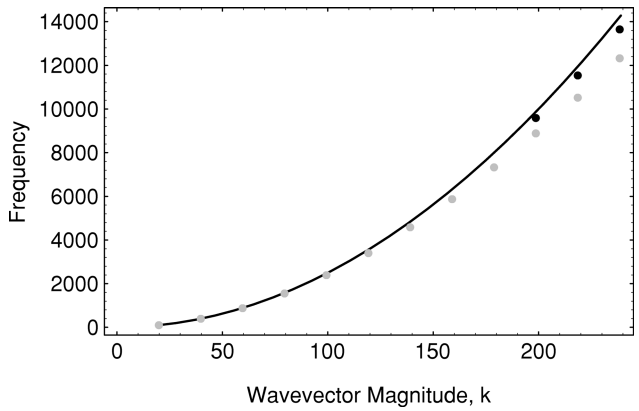

FIG. 1. Plane-wave dispersion relation shown for $N_x=256$ (gray points) and $N_x=512$ (black points).

and hence the frequency is given by

$$\omega=\frac{i}{4\Delta t}\ln\left(\frac{S(t+4\Delta t)}{S(t)}\right).$$

For a given wave vector $\mathbf{k}$, we measure this frequency at many time steps t and take an average.

We expect the evolution of the system to be governed by the Schrödinger equation

$$\partial_t\Psi=\frac{i}{2m}\partial^2\Psi.$$

Since $m=2$, this leads to the dispersion relation

$$\omega=\frac{k^2}{4}.$$

We performed a series of simulations where we considered wave numbers $l_x=3l$ and $l_y=l$, where $l\in\{1,\ldots,12\}$. The points plotted in Fig. 1 show the measured frequency ω as a function of $|\mathbf{k}|=2\pi\sqrt{l_x^2+l_y^2}$. The solid curve is $|\mathbf{k}|^2/4$. It is evident that the agreement is excellent in the ''hydrodynamic'' limit of small $|\mathbf{k}|$, but degrades due to lattice artifacts of order $|\mathbf{k}|\Delta x$ at higher wave-vector magnitudes. To demonstrate this, we include data for $N=256$ (gray points) and $N=512$ (black points). It is evident that the dispersion relation is valid for higher wave numbers on the larger lattice.

VI. CONCLUSION

We have considered a very general class of lattice models satisfying unitary time-evolution rules. We have shown that generic models of this type describe the evolution of a nonrelativistic particle according to the Schrödinger equation in an arbitrary number of dimensions. These models can naturally be used to construct quantum lattice gases describing nonrelativistic many-body physics in an arbitrary number of dimensions. It is straightforward to include an arbitrary interparticle potential into these models.

There are many ways in which this work could be extended. Numerical simulations could be performed in an arbitrary number of dimensions with multiple particles and with nontrivial spatially dependent potentials and the results checked in analytically tractable cases. Further analysis is needed to understand the behavior of the system in the regime where particles are dense. It might also be interesting to consider more general collision rules that create and destroy particles, possibly including antiparticles with separate quantum numbers.

Of course, the actual implementation of quantum lattice-gas models on quantum computing devices is something that may not be possible for many years, if ever. However, these lattice models give a simple framework with which to study problems in many-body theory. Furthermore, the methods described here are also quite practical for simulating systems of a few particles on a classical computer. It may be that the exact unitarity of these models at a microscopic level will make them more stable and possibly more useful than currently used discrete methods such as finite-difference approaches.

ACKNOWLEDGMENTS

We would like to acknowledge helpful conversations with Francis Alexander, Peter Coveney, Eddie Farhi, and Jeffrey Yepez. B.M.B. was supported in part by Phillips Laboratories and by the United States Air Force Office of Scientific Research under Grant No. F49620-95-1-0285. W.T. was supported in part by the division of Applied Mathematics of the U.S. Department of Energy under Contracts Nos. DE-FG02-88ER25065 and DE-FG02-88ER25066, in part by the U.S. Department of Energy under cooperative agreement No. DE-FC02-94ER40818, and in part by the National Science Foundation under Contract No. PHY90-21984.

APPENDIX A: SCHRÖDINGER EQUATION IN TWO DIMENSIONS

We now present the formalism described above explicitly in two dimensions. The matrices D and X are given by

$$D=\begin{pmatrix}\mu&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&-1\end{pmatrix},$$

$$X=\begin{pmatrix}1/2&1/2&1/2&1/2\\\frac{1}{\sqrt{2}}&0&-\frac{1}{\sqrt{2}}&0\\0&\frac{1}{\sqrt{2}}&0&-\frac{1}{\sqrt{2}}\\1/2&-1/2&1/2&-1/2\end{pmatrix}.$$

This gives us the collision matrix

$$S=X^{-1}DX=\frac{1}{4}\begin{pmatrix}\mu+1&\mu+1&\mu-3&\mu+1\\\mu+1&\mu+1&\mu+1&\mu-3\\\mu-3&\mu+1&\mu+1&\mu+1\\\mu+1&\mu-3&\mu+1&\mu+1\end{pmatrix}. \tag{A1}$$

We can compute

$$B^1 = XC^1X^{-1} = \begin{pmatrix} 0 & \frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 \end{pmatrix}, \quad B^2 = XC^2X^{-1} = \begin{pmatrix} 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & -\frac{1}{\sqrt{2}} \\ 0 & 0 & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix},$$

and thus

$$G^1 = XC^1X^{-1} = \begin{pmatrix} 0 & -\frac{1}{(1-\mu)\sqrt{2}} & 0 & 0 \\ -\frac{1}{(1-\mu^*)\sqrt{2}} & 0 & 0 & -\frac{1}{2\sqrt{2}} \\ 0 & 0 & 0 & 0 \\ 0 & -\frac{1}{2\sqrt{2}} & 0 & 0 \end{pmatrix},$$

$$G^2 = XC^2X^{-1} = \begin{pmatrix} 0 & 0 & -\frac{1}{(1-\mu)\sqrt{2}} & 0 \\ 0 & 0 & 0 & 0 \\ -\frac{1}{(1-\mu^*)\sqrt{2}} & 0 & 0 & \frac{1}{2\sqrt{2}} \\ 0 & 0 & \frac{1}{2\sqrt{2}} & 0 \end{pmatrix}.$$

Combining these matrices together we find

$$\partial_t \zeta = \begin{pmatrix} \frac{i}{2m} & 0 & 0 & 0 \\ 0 & -\frac{i}{2m} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{i(-\mu)^\tau}{2m} & 0 & 0 & 0 \end{pmatrix} \partial_x^2 \zeta + \begin{pmatrix} \frac{i}{2m} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{i}{2m} & 0 \\ \frac{i(-\mu)^\tau}{2m} & 0 & 0 & 0 \end{pmatrix} \partial_y^2 \zeta + \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{i}{2m} & 0 \\ 0 & -\frac{i}{2m} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \partial_x \partial_y \zeta,$$

with m described as in Eqs. (2) and (3), with $d=2$.

As predicted by the general discussion above, the total amplitude contained in the first component of ζ satisfies a Schrödinger equation

$$\partial_t \Psi(\mathbf{x},t) = i \frac{1}{2m} (\partial_x^2 + \partial_y^2) \Psi(\mathbf{x},t),$$

where

$$\Psi(\mathbf{x},t) = \frac{\mu^{-\tau}}{2} [\psi_1(\mathbf{x},t) + \psi_2(\mathbf{x},t) + \psi_3(\mathbf{x},t) + \psi_4(\mathbf{x},t)].$$

It is interesting to note that while the variation of the fourth component of ζ contains an oscillating phase, and thus has no interesting behavior on the time scale of interest, the second and third components obey separate second-order differential equations analogous to the Schrödinger equation, but without rotational invariance.

APPENDIX B: SCHRÖDINGER EQUATION IN THREE DIMENSIONS

Using the above formalism in three dimensions, we have

$$X=\begin{pmatrix} \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} \\ \frac{1}{\sqrt{2}} & 0 & 0 & -\frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 & -\frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 & 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & -\frac{1}{2} & 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ \frac{1}{2\sqrt{3}} & \frac{1}{2\sqrt{3}} & -\frac{1}{\sqrt{3}} & \frac{1}{2\sqrt{3}} & \frac{1}{2\sqrt{3}} & -\frac{1}{\sqrt{3}} \end{pmatrix},$$

$$D=\begin{pmatrix} \mu & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}, \quad S=\frac{1}{6}\begin{pmatrix} \mu+1 & \mu+1 & \mu+1 & \mu-5 & \mu+1 & \mu+1 \\ \mu+1 & \mu+1 & \mu+1 & \mu+1 & \mu-5 & \mu+1 \\ \mu+1 & \mu+1 & \mu+1 & \mu+1 & \mu+1 & \mu-5 \\ \mu-5 & \mu+1 & \mu+1 & \mu+1 & \mu+1 & \mu+1 \\ \mu+1 & \mu-5 & \mu+1 & \mu+1 & \mu+1 & \mu+1 \\ \mu+1 & \mu+1 & \mu-5 & \mu+1 & \mu+1 & \mu+1 \end{pmatrix},$$

$$B^1=\begin{pmatrix} 0 & \frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{3}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$G^1=\begin{pmatrix} 0 & -\frac{1}{\sqrt{3}(1-\mu)} & 0 & 0 & 0 & 0 \\ -\frac{1}{\sqrt{3}(1-\mu^*)} & 0 & 0 & 0 & \frac{-1}{2\sqrt{2}} & \frac{-1}{2\sqrt{6}} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{-1}{2\sqrt{2}} & 0 & 0 & 0 & 0 \\ 0 & \frac{-1}{2\sqrt{6}} & 0 & 0 & 0 & 0 \end{pmatrix}.$$

$$B^2=\begin{pmatrix} 0 & 0 & \frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{3}} & 0 & 0 & 0 & -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{6}} & 0 & 0 & 0 \end{pmatrix}, \quad G^2=\begin{pmatrix} 0 & 0 & -\frac{1}{\sqrt{3}(1-\mu)} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{\sqrt{3}(1-\mu^*)} & 0 & 0 & 0 & \frac{1}{2\sqrt{2}} & \frac{-1}{2\sqrt{6}} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2\sqrt{2}} & 0 & 0 & 0 \\ 0 & 0 & \frac{-1}{2\sqrt{6}} & 0 & 0 & 0 \end{pmatrix},$$

$$B^3=\begin{pmatrix} 0 & 0 & 0 & \frac{1}{\sqrt{3}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{3}} & 0 & 0 & 0 & 0 & -\sqrt{\frac{2}{3}} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\sqrt{\frac{2}{3}} & 0 & 0 \end{pmatrix}, \quad G^3=\begin{pmatrix} 0 & 0 & 0 & -\frac{1}{\sqrt{3}(1-\mu)} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ -\frac{1}{\sqrt{3}(1-\mu^*)} & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{6}} \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{6}} & 0 & 0 \end{pmatrix}.$$

From these matrices we find that the total amplitude

$$\Psi(\mathbf{x},t)=\frac{\mu^{-\tau}}{\sqrt{6}}[\psi_1(\mathbf{x},t)+\psi_2(\mathbf{x},t)+\psi_3(\mathbf{x},t)+\psi_4(\mathbf{x},t)+\psi_5(\mathbf{x},t)+\psi_6(\mathbf{x},t)]$$

satisfies the Schrödinger equation

$$\partial_t\Psi(\mathbf{x},t)=i\frac{1}{2m}(\partial_x^2+\partial_y^2+\partial_z^2)\Psi(\mathbf{x},t),$$

where as usual m is related to μ through Eqs. (2) and (3), with $d=3$.

[1] U. Frisch, B. Hasslacher, and Y. Pomeau, Phys. Rev. Lett. **56**, 1505 (1986).

[2] U. Frisch, D. d'Humières, B. Hasslacher, P. Lallemand, Y. Pomeau, and J.-P. Rivet, Complex Syst. **1**, 648 (1987).

[3] S. Wolfram, J. Stat. Phys. **45**, 471 (1986).

[4] M. Creutz, *Quarks, Gluons, and Lattices* (Cambridge University Press, Cambridge, 1983).

[5] R. P. Feynman (unpublished) [reproduced in S. S. Schweber, Rev. Mod. Phys. **58**, 449 (1986)].

[6] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965), pp. 35–36.

[7] S. Succi and R. Benzi, Physica D **69**, 327 (1993).

[8] L. Kauffman and H. Noyes, Phys. Lett. A **218**, 139 (1996).

[9] D. Meyer, J. Stat. Phys. **85**, 551 (1996).

[10] S. Succi, Phys. Rev. E **53**, 1969 (1996).

[11] R. Benzi, S. Succi, and M. Vergassola (unpublished).

[12] See, e.g., [13] and D. Deutsch, Proc. R. Soc. London, Ser. A **400**, 96 (1985); **425**, 73 (1989); C. H. Bennett, Phys. Today **48**, 24 (1995).

[13] R. Feynman, Int. J. Theor. Phys. **21**, 467 (1982); Found. Phys. **16**, 507 (1986);

[14] S. Lloyd, Science **273**, 1073 (1996).

[15] P. W. Shor, in *Algorithms for Quantum Computation: Discrete Log and Factoring*, Proceedings of the 35th Annual Symposium on the Foundations of Computer Science, edited by S. Goldwasser (IEEE Computer Society, Los Alamitos, CA, 1994), p. 124.

[16] S. Lloyd, Phys. Rev. Lett. **75**, 346 (1995); A. Barenco, C. H. Bennett, R. Cleve, D. DiVincenzo, N. H. Margolus, P. Shor, T. Sleator, J. Smolin, and H. Weinfurter, Phys. Rev. A **52**, 3457 (1995).

[17] D. S. Abrams and S. Lloyd (unpublished).

[18] P. W. Shor, in *Proceedings of the 37th Annual Symposium on the Foundations of Computer Science* (IEEE Comput. Soc. Press, Los Alamitos, CA, 1996), pp. 56–65, and references therein.