Quantum lattice-gas models
for the many-body Schrödinger equation

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A general class of discrete unitary models are described whose behavior in the continuum limit corresponds to a many-body Schrödinger equation. On a quantum computer, these models could be used to simulate quantum many-body systems with an exponential speedup over analogous simulations on classical computers. On a classical computer, these models give an explicitly unitary and local prescription for discretizing the Schrödinger equation. It is shown that models of this type can be constructed for an arbitrary number of particles moving in an arbitrary number of dimensions with an arbitrary interparticle interaction.

1. Introduction

In this paper we describe a class of algorithms for simulating quantum mechanical systems. These algorithms are very similar to the lattice-gas automata and lattice Boltzmann models for hydrodynamics which were discussed in many of the other talks at this conference. In the models we will be discussing, however, the microscopic dynamics is defined by a time-development rule which is unitary, rather than probability-conserving as in traditional lattice-gas automata or lattice Boltzmann models.

There are several reasons for believing that these discrete models for quantum mechanics are interesting. First, they give an explicitly unitarity way of discretizing the Schrödinger equation, so they might be better behaved numerically than standard finite-difference methods. Second, they are particularly well suited to im-

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In fact, if someone could build a general purpose quantum computer, it would be possible to use these algorithms to simulate systems of many interacting quantum particles in exponentially less time than it would take on a classical computer.

David Meyer, who first suggested the term “quantum lattice-gas automata”, discussed some aspects of these systems in his talk, but for completeness we begin by reviewing briefly what a quantum lattice-gas automaton is, and how such a system is different from a classical lattice-gas automaton. We then consider a fairly generic 1-dimensional quantum lattice system which obeys the Schrödinger equation in the continuum limit. By extending the system in various ways, we show how multiple particles, higher dimensionality and interparticle interactions can naturally be incorporated into the system, so that we end up with a simple microscopic lattice model which describes an arbitrary system of interacting nonrelativistic quantum particles. Finally, we discuss how these models can be used on a quantum computer to achieve exponential performance enhancement over an analogous system on a classical computer.

2. Quantum lattice-gas automata

The idea of a quantum lattice-gas automaton (QLGA) was first suggested by David Meyer, who considered such systems in the context of a multiple-particle Dirac equation in one dimension. Essentially, a quantum lattice-gas automaton is very similar to a classical lattice-gas automaton. At each vertex of some lattice $\Lambda$ there are $m$ quantum bits ($q$-bits), which represent particle occupation numbers. In a classical lattice-gas automaton (LGA), there would be $m$ classical bits with values 0 or 1 indicating the absence or presence of particles with velocities $v_i$, $1 \leq i \leq m$ (see Fig. 1). The state space for a classical LGA contains $2^m$ discrete states, where

Fig. 1. A state in a 2-dimensional classical LGA with $m = 4$ particle sites at each lattice site. Arrows indicate occupied sites. In a quantum lattice-gas automaton, this state would be a basis vector in a Hilbert space of dimension $2^4$. 
$l = |\Lambda|$ is the number of lattice sites. In a QLGA, on the other hand, the space of allowed states of the system at a fixed point in time corresponds to a Hilbert space of $lm$ independent two-state quantum components. The state space for a single q-bit is a continuous space parameterized by two complex numbers $\psi_+, \psi_-$ satisfying $|\psi_+|^2 + |\psi_-|^2 = 1$. These numbers correspond to amplitudes for the presence or absence of a particle in the QLGA, respectively. For a system of $n$ q-bits, the Hilbert space is parameterized by $2^n$ complex numbers $\psi_{\sigma_1, \cdots, \sigma_n}$ where $\sigma_i \in \{+, -\}$. All states are normalized so that $\sum_\sigma |\psi_\sigma|^2 = 1$. In a quantum lattice-gas system, a natural basis for the Hilbert space is given by the $2^{lm}$ classical configurations corresponding to definite particle occupation numbers; the parameters $\psi_\sigma$ correspond to the amplitudes for each state in this basis.

Thus, we see that while the state space for a classical LGA is defined by an element of a set of $2^{lm}$ states, the state space for a QLGA is a complex linear vector space of dimension $2^{lm}$, where the state is restricted to have unit norm. We now consider the time development rule for a QLGA. In a (deterministic) classical LGA, the time development rule is defined in two steps. First each particle advects forward in the direction of its associated velocity vector. Then, the bits associated with particles at each lattice site are transformed by acting on the set of $2^m$ possible local states by a permutation matrix. Generally, this “collision rule” is defined in such a way as to conserve particle number and/or momentum, to achieve the desired hydrodynamic equations in the continuum limit. In a QLGA, we break the time development rule into two parts in the same way. First, we advect the particles by exchanging pairs of q-bits between adjacent lattice sites in the manner indicated by the velocity vectors associated with each q-bit. Next, we act on the set of q-bits at each lattice site with a fixed collision operator. Because the Hilbert space of q-bits at each site is $2^m$-dimensional, this involves acting on the state space with a $2^m \times 2^m$ unitarity matrix. We will restrict attention to collision operators which conserve particle number.

We have thus given a general formulation of the state space and dynamics of a quantum lattice-gas automaton. There is a very natural parallel between the evolution of a single state of a QLGA and the evolution of an ensemble of states in a stochastic (nondeterministic) classical LGA. In a stochastic LGA, the collision rule acting on the states at a given lattice site is only defined probabilistically. We can define an ensemble of states by associating a probability $p_\sigma$ with every state $\sigma$. In a stochastic LGA, the advection part of the time evolution rule permutes the probabilities $p_\sigma$ by permuting the individual bits. The collision rule has the effect of acting on the vector of probabilities $p_\sigma$ by a matrix which is probability-conserving, in the sense that the columns as well as the rows of the matrix sum to unity. The only difference between this dynamics on an ensemble and the definition given above of a QLGA is that the collision matrix for a QLGA is unitary rather than probability-conserving. Thus, we see that at the expense of having exponentially more information contained in each state, the QLGA naturally contains the complete dynamics of an ensemble rather than those of a single instance. As
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will be discussed later, a QLGA can naturally be implemented on a quantum computer with an exponential increase in performance. In this case, the measurements which must be performed to calculate results on the quantum computer correspond to single instances of measurements in the physical system being simulated. This highlights one of the essential distinctions between a classical probabilistic system and a quantum system, which is that the quantum system contains information about all possible trajectories until such a time as the system is measured.

3. A simple example: the free particle in 1D

Let us now begin by considering the simplest nontrivial QLGA we can think of. Consider a 1-dimensional lattice of size $l$ where each lattice site has two possible occupation sites for particles ($m = 2$), corresponding to left- and right- moving particles. At each time step, the q-bits representing the particles at each lattice site will hop one step to the left or right, and then the q-bits associated with the new pair of particles at each lattice site will interact through a collision matrix $T$. If we restrict $T$ to conserve particle number and we insist that $T$ be invariant under reflection, then in the basis $-\rightarrow, +\rightarrow, -\leftarrow, +\leftarrow$ the matrix $T$ will be given (up to an irrelevant overall phase) by

$$T = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & q & p & 0 \\ 0 & p & q & 0 \\ 0 & 0 & 0 & \phi \end{pmatrix} \quad (1)$$

where the parameters $q, p$ and $\phi$ satisfy $|q|^2 + |p|^2 = 1$, $p\bar{q} + \bar{p}q = 0$ and $|\phi|^2 = 1$. Graphically, the parameters $q$ and $p$ correspond to the amplitudes that a single particle entering a lattice site will continue forward or bounce back (see Fig. 2). The phase factor $\phi$ affects multiple particle collisions, and will be discussed further later.

In order to understand the dynamics of this simple QLGA, let us first restrict
attention to the subspace of the total Hilbert space of the system in which there is only a single occupied state. Since the collision rule conserves particle number, this subspace remains invariant under the action of the time-development rule. This subspace is a $2^l$-dimensional complex vector space, parameterized by complex numbers $\psi_r(x)$, $\psi_l(x)$ where $1 \leq x \leq l$. The QLGA dynamics defined above gives the equations of motion

$$
\begin{align*}
\psi_r(x,t+1) &= q\psi_r(x-1,t) + p\psi_l(x+1,t) \\
\psi_l(x,t+1) &= q\psi_l(x+1,t) + p\psi_r(x-1,t)
\end{align*}
$$

(2)

It is worth noting that the 1-particle system described here is very similar to a discrete formulation of the 1+1D Dirac equation discussed long ago by Feynman. In Feynman’s model a similar dynamics is considered, however the parameter $p$ is taken to scale as $\epsilon$. The Dirac system was taken as the starting point in the work of Meyer. The emergent Schrödinger behavior of the system with fixed $p$ was also discussed by Succi and Benzi.

Just as the continuum behavior of a classical LGA can be determined by performing a power series expansion of the equations of motion and applying the Chapman-Enskog procedure, we can take the continuum limit of the equations of motion (2) and determine a set of differential equations satisfied by $\psi_r$ and $\psi_l$ in the continuum limit. Scaling $x$ as $\epsilon$ and $t$ as $\epsilon^2$, we take the limit $\epsilon \to 0$. Factoring out a time-dependent phase factor from the total amplitude

$$
\Psi(x,t) = (p + q)^{-t}(\psi_l(x,t) + \psi_r(x,t))
$$

(3)

we find that the total amplitude satisfies the Schrödinger equation

$$
\frac{\partial}{\partial t} \Psi(x,t) = \frac{i}{2m} \frac{\partial^2}{\partial x^2} \Psi(x,t)
$$

(4)

for a free particle of mass $m = ip/q$. Note that the mass is real because of the restriction $p\bar{q} + \bar{p}q = 0$. The equation (4) can also be derived by mode analysis.

4. The free particle in $D$ dimensions

We have seen that in the single-particle sector of a general 1D QLGA the continuum limit gives a free Schrödinger particle moving on a line. Let us now consider a QLGA in an arbitrary number of dimensions, still restricting to the single-particle sector. Let us assume that we have a Cartesian lattice in $D$ dimensions, with $m = 2^D$ q-bits at each lattice site, corresponding to particles moving along any of the lattice vectors. In the single-particle sector, the collision rule is defined by a unitary $2^D \times 2^D$ matrix. If we assume that the collision rule is invariant under the symmetry group of the lattice, we find that the set of allowed collision rules is parameterized by 3 complex phases $\mu, \nu, \lambda$. These phases correspond to the eigenvalues of vectors in the 3 irreducible representations of the discrete rotation group. In particular, $\mu$ is the eigenvalue associated with the constant vector $(1,1,\ldots,1)$ and $\nu$ is the
eigenvalue of vectors which change sign under a parity transformation. Just as in the 1D case, a systematic analysis shows that as long as $\mu \neq \nu$ and $\mu \neq \lambda$, the total amplitude after removing a phase

$$\Psi(x, t) = \mu^{-1} \sum_i \psi_i(x, t)$$

satisfies the Schrödinger equation

$$\frac{\partial}{\partial t} \Psi(x, t) = \frac{i}{2m} \sum_i \frac{\partial^2}{\partial x_i^2} \Psi(x, t)$$

where the mass $m$ is related to $\mu$ and $\nu$ through

$$\frac{i}{2m} = \frac{1}{d} \left( \frac{\nu}{\mu - \nu} + \frac{1}{2} \right).$$

As a simple concrete example of this general result, we can define a collision rule in the single-particle sector of a $D$-dimensional QLGA to have $\nu = 1, \lambda = -1$ with $\mu$ an arbitrary complex phase. With these phases, the amplitude for a particle to completely reverse direction in the collision phase is given by

$$\alpha = \frac{\mu + 1 - D^2 - D}{D^2 + D}$$

while the amplitude for a particle to “bounce” in any other direction is given by

$$\beta = \frac{\mu + 1}{D^2 + D}$$

These collision rules are described graphically in the case $D = 2$ in Figure 3.

Fig. 3. A QLGA collision rule in the single-particle sector giving a Schrödinger equation in 2D
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With this choice of collision rule, in any dimension $D$ the total amplitude $\Psi$ satisfies the Schrödinger equation (6) with mass

$$m = i \frac{\mu - 1}{d(\mu + 1)}.$$  

(10)

5. Adding an external potential

Thus far, the models we have considered describe in the single-particle sector the propagation of a free Schrödinger particle. We now consider the addition of an external potential. In order to incorporate the effects of a potential function $V(x)$ we need only multiply the wave function at each time step by an overall phase factor of $\exp(-i\epsilon^2 V(x))$ when there is a particle at position $x$. In the QLGA framework, this corresponds to transforming each q-bit by an operator which acts on the Hilbert space (in the basis $-, +$) by the matrix

$$U = \begin{pmatrix} 1 & 0 \\ 0 & e^{-i\epsilon^2 V(x)} \end{pmatrix}$$

(11)

where $x$ is the position associated with the given q-bit. If we modify the time-development rule for the QLGA so that after each collision step each q-bit is acted on with this operator, the resulting Schrödinger equation in the single-particle sector is

$$\frac{\partial}{\partial t} \Psi(x, t) = \frac{i}{2m} \sum_i \frac{\partial^2}{\partial x_i^2} \Psi(x, t) - iV(x, t)\Psi(x, t).$$

(12)

As an example of this type of system, let us consider a single particle moving in one dimension in a harmonic oscillator potential $V(x) = \frac{x^2}{2}$. We can combine the advection operator, the collision matrix $T$ from (1), at each point, and the external potential (11) at each point into a single time-development matrix which acts on the Hilbert space. Diagonalizing this matrix gives the eigenstates of the time-development equation, which should approximate the energy eigenfunctions of the corresponding quantum system in the limit as the lattice spacing becomes small. As a test of the method, we have analyzed this system numerically on small lattices (a similar analysis for a square well potential was performed by Meyer). Even for very small lattices, we find that the first few eigenfunctions are extremely close to the wavefunctions of the continuous theory. In Figures 4 and 5 we have graphed the ground state and first excited states for lattices with 8 and 16 lattice sites (we have only included effects of every second site since particles at sites of opposite parity never interact). As can be readily seen in the graphs, even with only 8 lattice sites the first two eigenstates are reproduced very accurately by this discretization. As the size of the lattice increases, the number of eigenstates of the continuum system which are correctly reproduced increases proportionally.

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Fig. 4. Ground state in quadratic potential with 8 and 16 lattice sites

Fig. 5. First excited state in quadratic potential with 8 and 16 lattice sites
Now that we understand the behavior of the single-particle sector of a QLGA, let us return to the more general situation where there are \( n \) particles in the system. As long as \( n \ll \ell \)m, the occupied particle sites will be sparse in the system. At most lattice sites where particles are present there will only be a single particle, so that each particle will independently satisfy a Schrödinger equation. Only when several particles arrive at a lattice site at the same time will the particles interact. In this case, the part of the collision rule in the multiple particle sector will define a local (delta function) interaction between the particles. Thus, in the \( n \)-particle sector of the QLGA, the continuum limit of the dynamics will be a system of \( n \) particles moving according to the \( n \)-body Schrödinger equation with delta function interactions.

As an example of this type of system, we can describe the collision matrix for a gas of nonrelativistic particles interacting by local (\( \delta(x - y) \)) interactions in an external quadratic potential \( V(x) = ax^2 \) in one dimension. Incorporating the potential term into the collision matrix, we have

\[
T = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & \frac{\mu+1}{2} & \frac{\mu-1}{2}e^{-ia\epsilon x^2} & 0 \\
0 & \frac{\mu-1}{2}e^{-ia\epsilon x^2} & \frac{\mu+1}{2} \phi e^{-2ia\epsilon x^2} & 0 \\
0 & 0 & 0 & \phi e^{-2ia\epsilon x^2}
\end{pmatrix}
\]

where \( \phi \) is a complex phase determining the effects of the delta function interaction between particles.

Just as we can incorporate an external potential by rotating each q-bit by an appropriate phase, we can incorporate an arbitrary interparticle potential by acting on each pair of q-bits. Given an arbitrary function \( V(x, y) \) describing an interaction potential between particles at positions \( x, y \), we can act on each pair of q-bits at each time step with the matrix

\[
U = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & e^{-i\epsilon V(x, y)}
\end{pmatrix}
\]

By including such an interaction in the time development of the QLGA, we can model any interacting nonrelativistic quantum many-body system of interest.

It is worth noting that the systems we have described are most easily used to simulate a system of nonrelativistic bosons, despite the apparent use of exclusionary statistics. The simulation of fermions is also possible, however some extra overhead is necessary for keeping track of relative phases.

7. Computational complexity

We have described a class of algorithms which can be used to simulate an arbitrary system of interacting nonrelativistic quantum particles. We will now discuss briefly
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Let us consider a system of \( n \) particles moving on a \( D \)-dimensional lattice of size \( l = q^D \), with \( m = 2D \) allowed particle positions per lattice site. Assuming that \( n \ll lm \), the number of complex variables needed to describe the state of the system at a point in time is

\[
\frac{(lm)!}{n!(lm-n)!} \approx \frac{(lm)^n}{n!}.
\]

To simulate a system with this number of variables on a classical computer would take at the very least on the order of the number of variables for each time step. The number of time steps needed scales as \( q^2 \) (because \( t \) scales as \( q^2 \)), so the total time needed for a computation on a classical computer would be

\[
T_c \approx O\left(\frac{q^{2+D}m^nn^n}{n!}\right).
\]

For a typical calculation of physical interest, we might have \( n = 100, q = 20, D = 3 \). For such a calculation, the number of operations needed on a classical computer would be on the order of \( T_c \approx 10^{312} \). This is clearly impractical. Note that a standard finite difference method would eliminate the factor of \( m^n \) in (16), however this would not make such a calculation any more accessible. Only when the number of particles \( n \) is extremely small is it conceivable that these algorithms might be a useful approach for simulating quantum systems on a classical computer.

Now let us consider the computational complexity of the same algorithms on a quantum computer. For the quantum simulation, we need \( m \cdot l \) q-bits. The local advection and collision steps can be accomplished with on the order of \( m \cdot l \) quantum operations per time step. Thus, a system of quantum particles which affect one another only through local delta function interactions can be simulated on a quantum computer in time on the order of

\[
T_q \approx O(2^{Dq^{2+D}}).
\]

Note that this time is independent of the number of particles \( n \) being simulated. In fact, this algorithm will simultaneously simulate the system for all allowed numbers of particles \( n \leq lm \) in the same time it takes to simulate a system with only a single particle. With the numbers used in the example above on a classical machine, the number of operations needed to perform the simulation is a much more tractable \( T_q \approx 19.2 \cdot 10^6 \). The idea that it might be possible to simulate quantum mechanical systems exponentially faster on a quantum computer than on a classical computer was first suggested by Feynman\[10\]; a general argument for this conclusion was given more recently by Lloyd\[12\]. The algorithms discussed in this talk represent a concrete instantiation of the general principles discussed by those authors.

An additional factor appears in the computational complexity of the algorithm when we have an arbitrary interparticle potential. Because in this case at every...
time step we must include an operation for every pair of q-bits, the complexity on a quantum computer becomes

\[ T_q \approx O(4D^2q^{2+2D}). \]  

(18)

In the example discussed above, this increases the computational complexity to \( T_q \approx 10^{12} \) operations. Clearly, a fairly sizable quantum computer would be needed to carry out such a calculation. Note, however, that by comparison a standard home PC can currently perform this number of operations in about 15 minutes.

8. Conclusions

In this paper we have described a class of discrete algorithms for simulating the many-body Schrödinger equation. Under fairly simple conditions of isotropy and genericity, the behavior of a general quantum lattice-gas automaton which preserves particle number is to simulate a many-body Schrödinger equation with pointlike interactions. By adding a nonlocal interaction term, we can simulate any interacting nonrelativistic quantum system of interest using quantum lattice-gas automata models.

Because the number of degrees of freedom in the quantum system is so large, it is impractical to use the algorithms described here on a classical computer to simulate more than a handful of interacting particles. Because simulating quantum systems is such a difficult problem, however, these algorithms may be useful in certain situations even on a classical computer, due to their inherent unitarity.

The real utility of these algorithms will be realized only if they can be implemented on quantum computers. At the moment, it is rather unclear whether a general purpose quantum computer capable of performing millions or billions of coherent quantum operations can be constructed, even in principle. There are a number of serious technical challenges to be overcome in constructing such a system. There are also possible theoretical obstacles due to decoherence problems. Recent work has indicated that decoherence and imprecision problems can be overcome by clever use of quantum error correction codes. Nonetheless it will be many years before a working quantum computer of reasonable size will be available, even if all the technical problems can be solved.

If, however, there ever are general purpose quantum computers available for use in scientific research, the algorithms described here would allow for the simulation of a wide range of quantum systems of physical interest which are inaccessible to simulation on classical computers. Using quantum lattice-gas automata, any interacting nonrelativistic quantum many-body system could be simulated. This would allow for the study of systems including electron gases, metals, plasmas, nuclear matter, Fermi gases, and many other phenomena of physical and industrial interest.

In this paper we have only discussed simulations of nonrelativistic Schrödinger systems using QLGA. There are other more complicated physical systems which may also be accessible using these same methods. Some work has been done on
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Simulating a many-body Dirac equation using QLGA. A class of systems for which it would be particularly interesting to find QLGA models are abelian and nonabelian gauge theories. In particular, there is a fairly large research effort devoted to the numerical study of quantum chromodynamics (QCD), the nonabelian gauge theory coupled to fermions which describes the interaction of quarks. If it were possible to simulate QCD using a simple QLGA lattice model, this would indicate that quantum computers could be used to simulate QCD in the Hamiltonian framework with an exponential speedup, possibly making accessible to numerical experiment a number of poorly understood aspects of this important theory.

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