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LETTER TO THE EDITOR

Cellular automata for quantum systems

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Abstract. Cellular automata for modelling quantum systems are presented. The mass at each site is updated according to rules that depend on the masses of neighbouring sites. An essential feature of these local rules is that mass and probability are conserved. In the limit of small spatial and time steps it is shown that the equation defining one class of automata reduces to the Schrödinger equation and the equation defining another class of automata reduces to the Dirac equation. Advantages of these methods are discussed.

Cellular automata have been defined as discrete space and time mathematical models of physical systems. The state of each site of the cellular automaton changes with each time step according to local rules of updating which require only the values of states of the nearest neighbouring sites at the previous time. Cellular automata, which were first considered by von Neumann and Ulam, have recently been used to model numerous physical phenomena including diffusion, sound waves, hydrodynamics and phase transitions [1–3]. A cellular automaton for modelling the Schrödinger equation of quantum theory has also been presented, but the local updating rules do not conserve probability [4]. It is the purpose of this research to present cellular automata for solving the time-dependent equations of quantum theory which use local rules for updating and which conserve probability and mass. The methods presented here have significant advantages over conventional methods. Most if not all local three-dimensional conventional methods for solving the time-dependent quantum equations numerically give meaningless solutions that grow without bound if the spatial step is too small or the time step is too large. However, the methods presented here, because they conserve mass and probability, can never give solutions that grow without bound. In addition, it is well known that the time-dependent Schrödinger and Dirac equations, which are continuum equations in space and time, conserve mass and probability. If it should turn out that space or time or both are quantized and discrete, it is possible that the discrete equations presented here, which also conserve mass and probability, may give more accurate results than the continuum equations.

First we will treat cellular automata for one-dimensional quantum systems and then we will generalize the results to three spatial dimensions. Each spatial site j consists of two independent subsites with the numbers m_j and n_j, which denote the mass at each subsite. The total mass at spatial site j of the quantum system is the sum of m_j and n_j. Mass is transferred between the subsite with mass m_j and the subsite with mass n_{j+1}. The amount of mass transferred at each update is given by

$$T_{j,j+1} = \kappa(m_j n_{j+1})^{1/2} \tag{1}$$

$$\kappa = \frac{\hbar \Delta t}{\mu(\Delta x)^2} \tag{2}$$

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where $\hbar$ and μ are the constants of the Schrödinger equation, Δt is the time step and Δx is the spatial distance between lattice points. The amount of mass transferred between the subsite with mass m_j and the subsite with mass n_{j-1} is given by

$$T_{j,j-1} = \kappa(m_j n_{j-1})^{1/2}. \tag{3}$$

Finally, the amount of mass transferred between the subsite with mass n_j and the subsite with mass m_j is

$$T_{j,j} = \lambda_j(n_j m_j)^{1/2} \tag{4}$$

$$\lambda_j = 2\kappa + \gamma_j \tag{5}$$

$$\gamma_j = 2V_j \Delta t/\hbar \tag{6}$$

where V_j is the potential at site j. The initial subsite masses m_j and n_j are obtained from the initial wavefunction ψ_j at site j

$$\psi_j = a_j + ib_j \tag{7}$$

$$m_j = a_j^2 \tag{8}$$

$$n_j = b_j^2 \tag{9}$$

where the amplitudes a_j and b_j are the real and imaginary parts of the wavefunction at site j. The directions of transfer are determined by the signs of the amplitudes

$$T_{j,j+1} = \kappa a_j b_{j+1} \tag{10}$$

$$T_{j,j-1} = \kappa a_j b_{j-1} \tag{11}$$

$$T_{j,j} = \lambda_j b_j a_j. \tag{12}$$

Thus if the amplitudes a_j and b_{j+1} are both positive or both negative, the transfer of mass will take place from the subsite with mass m_j to the subsite with mass n_{j+1}. The rules (1), (3) and (4) determine the mass distribution at any later time when combined with the rule that all transfer directions at a subsite are reversed when the mass at that subsite approaches zero. This reversal corresponds to a change in the sign of the amplitude at that subsite. We add the condition that the mass at any subsite cannot be less than zero. Once the initial conditions have been given, the amplitudes themselves do not need to be calculated. Since mass is transferred from one subsite to another, mass and probability are conserved.

Next we will show that in the limit of small time and spatial steps, the finite difference equation of the cellular automaton converges to the Schrödinger equation. According to the automaton rules (1), (3) and (4) the updated mass M_j at site j is given by

$$M_j = m_j - \kappa(m_j n_{j-1})^{1/2} - \kappa(m_j n_{j+1})^{1/2} + \lambda_j(m_j n_j)^{1/2}. \tag{13}$$

This equation can also be expressed in terms of the amplitudes

$$M_j = m_j - \kappa a_j b_{j-1} - \kappa a_j b_{j+1} + \lambda_j a_j b_j. \tag{14}$$

In the limit of small time and spatial steps we have

$$M_j - m_j = 2\Delta t\, a(x, t)\frac{\partial a}{\partial t} \tag{15}$$

$$b_{j-1} - 2b_j + b_{j+1} = (\Delta x)^2 \frac{\partial^2 b}{\partial x^2}. \tag{16}$$

Combining (2), (5), (6), (14), (15) and (16), we obtain the partial differential equation

$$\frac{\hbar \partial a}{\partial t} = -\frac{\hbar^2}{2\mu}\frac{\partial^2 b}{\partial x^2} + Vb(x, t). \tag{17}$$

Similarly the equation for the updated mass N_j at site j

$$N_j = n_j + \kappa(m_{j-1}n_j)^{1/2} + \kappa(m_{j+1}n_j)^{1/2} - \lambda_j(m_j n_j)^{1/2} \tag{18}$$

gives us the partial differential equation

$$\frac{\hbar \partial b}{\partial t} = \frac{\hbar^2}{2\mu}\frac{\partial^2 a}{\partial x^2} - Va(x, t). \tag{19}$$

Finally noting that the wavefunction $\psi(x, t)$ can be expressed in terms of real and imaginary amplitudes

$$\psi(x, t) = a(x, t) + ib(x, t) \tag{20}$$

we see that (17) and (19) are equivalent to the Schrödinger equation

$$i\hbar\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2\mu}\frac{\partial^2 \psi}{\partial x^2} + V\psi(x, t). \tag{21}$$

In order to determine how the discretization in space and time affected the results, a truncation error analysis was carried out on the update equations (14) and (18). Using Taylor series expansions, we found that the truncation error in time is $O(\Delta t)$ and the truncation error in space is $O((\Delta x)^2)$.

The rules for the cellular automaton were easily programmed. In order to eliminate the effect that occurs when the mass at a subsite is exactly zero, the average local mass was used in the transfer expressions. For example the transfer expressions (1) becomes

$$T_{j,j+1} = \kappa(\bar{m}_j \bar{n}_{j+1})^{1/2} \tag{22}$$

$$\bar{m}_j = (1-3\zeta)m_j + \zeta m_{j-1} + \zeta m_{j+1} + \zeta m_j^* \tag{23}$$

$$\bar{n}_{j+1} = (1-3\zeta)n_{j+1} + \zeta n_j + \zeta n_{j+2} + \zeta n_{j+1}^* \tag{24}$$

where the averaging parameter ζ is much less than one and the starred quantities are the masses at the previous time step. Excellent results were obtained from this algorithm, which conserved mass and probability.

The results are easily generalized to treat three spatial dimensions. The amount of mass transferred in the x-direction between the subsite with mass m_{ijk} and the subsite with mass n_{i+1jk} is

$$T_{ijk,i+1jk} = \kappa_x(m_{ijk}n_{i+1jk})^{1/2} \tag{25}$$

and the amount of mass transferred in the x-direction between the subsite with mass m_{ijk} and the subsite with mass n_{i-1jk} is

$$T_{ijk,i-1jk} = \kappa_x(m_{ijk}n_{i-1jk})^{1/2} \tag{26}$$

$$\kappa_x = \frac{\hbar \Delta t}{\mu(\Delta x)^2}. \tag{27}$$

Similar expressions apply for the y- and z-directions

$$T_{ijk,ij+1k} = \kappa_y (m_{ijk} n_{ij+1k})^{1/2} \tag{28}$$

$$T_{ijk,ij-1k} = \kappa_y (m_{ijk} n_{ij-1k})^{1/2} \tag{29}$$

$$T_{ijk,ijk+1} = \kappa_z (m_{ijk} n_{ijk+1})^{1/2} \tag{30}$$

$$T_{ijk,ijk-1} = \kappa_z (m_{ijk} n_{ijk-1})^{1/2} \tag{31}$$

$$\kappa_y = \frac{\hbar \, \Delta t}{\mu (\Delta y)^2} \tag{32}$$

$$\kappa_z = \frac{\hbar \, \Delta t}{\mu (\Delta z)^2}. \tag{33}$$

The amount of mass transferred between the subsite with mass n_{ijk} and the subsite with mass m_{ijk} is

$$T_{ijk,ijk} = \lambda_{ijk} (n_{ijk} m_{ijk})^{1/2} \tag{34}$$

$$\lambda_{ijk} = 2(\kappa_x + \kappa_y + \kappa_z) + \gamma_{ijk} \tag{35}$$

$$\gamma_{ijk} = 2 V_{ijk} \, \Delta t / \hbar. \tag{36}$$

The automaton rules for calculating the updated masses M_{ijk} and N_{ijk} from the current masses m_{ijk} and n_{ijk} are

$$M_{ijk} = m_{ijk} - T_{ijk,i-1jk} - T_{ijk,i+1jk} - T_{ijk,ij-1k} - T_{ijk,ij+1k} - T_{ijk,ijk-1} - T_{ijk,ijk+1} + T_{ijk,ijk} \tag{37}$$

$$N_{ijk} = n_{ijk} + T_{i-1ijk,ijk} + T_{i+1jk,ijk} + T_{ij-1k,ijk} + T_{ij+1k,ijk} + T_{ijk-1,ijk} + T_{ijk+1,ijk} - T_{ijk,ijk}. \tag{38}$$

As before, the actual directions of transfer are determined by the signs of the amplitudes. In the limit of small time and spatial steps it can be shown by using the method discussed for the one-dimensional case that (37) and (38) reduce to the three-dimensional Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2\mu} \left[\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right] + V\psi(x, y, z, t). \tag{39}$$

If these automaton rules correspond in some sense to a law of nature then it should be possible to find automaton rules which conserve mass and which reduce to the Dirac equation in the limit of small step sizes. Since the wavefunction of the Dirac equation has four complex components, we consider an automaton where each spatial site ijk consists of eight independent subsites with the mass numbers $m_{\nu,ijk}$ and $n_{\nu,ijk}$, where $\nu = 1, 2, 3, 4$. The total mass at the spatial site ijk is the sum of these eight numbers. The essential feature of the automaton corresponding to the Schrödinger equation is the update rule that the amount of mass transferred between adjacent subsites is proportional to the square root of the product of the masses of the two adjacent subsites. We have found that a Dirac automaton can be formulated by using similar update rules that specify eight mass transfers between eight pairs of adjacent

subsites. These discretization rules can be regarded as representing coupled maps. For the x-direction the eight transfer rules for subsites at positions ijk and $1+1jk$ are

$$\begin{aligned}
&T_{m4,i+1jk,m1,ijk} = K(m_{4,i+1jk}m_{1,ijk})^{1/2}\\
&T_{n4,i+1jk,n1,ijk} = K(n_{4,i+1jk}n_{1,ijk})^{1/2}\\
&T_{m3,i+1jk,m2,ijk} = K(m_{3,i+1jk}m_{2,ijk})^{1/2}\\
&T_{n3,i+1jk,n2,ijk} = K(n_{3,i+1jk}n_{2,ijk})^{1/2}\\
&T_{m2,i+1jk,m3,ijk} = K(m_{2,i+1jk}m_{3,ijk})^{1/2}\\
&T_{n2,i+1jk,n3,ijk} = K(n_{2,i+1jk}n_{3,ijk})^{1/2}\\
&T_{m1,i+1jk,m4,ijk} = K(m_{1,i+1jk}m_{4,ijk})^{1/2}\\
&T_{n1,i+1jk,n4,ijk} = K(n_{1,i+1jk}n_{4,ijk})^{1/2}\\
&K = c\,\Delta t/\Delta x.
\end{aligned} \tag{40}$$

For example the mass transfer term $T_{m4,i+1jk,m1,ijk}$ gives the amount of mass transferred from the subsite with mass m_4 at position $i+1jk$ to the subsite with mass m_1 at position ijk in the time interval Δt. As before, if the initial amplitudes are positive at both subsites, the direction of transfer is from the first subsite to the second. All directions of transfer at a particular subsite are reversed as the mass at that subsite tends to zero. The eight transfer rules for the y-direction between subsites at position ijk and position $ij+1k$ are

$$\begin{aligned}
&T_{n4,ij+1k,m1,ijk} = K(n_{4,ij+1k}m_{1,ijk})^{1/2}\\
&T_{n1,ijk,m4,ij+1k} = K(m_{4,ij+1k}n_{1,ijk})^{1/2}\\
&T_{m2,ijk,n3,ij+1k} = K(n_{3,ij+1k}m_{2,ijk})^{1/2}\\
&T_{m3,ij+1k,n2,ijk} = K(m_{3,ij+1k}n_{2,ijk})^{1/2}\\
&T_{n2,ij+1k,m3,ijk} = K(n_{2,ij+1k}m_{3,ijk})^{1/2}\\
&T_{n3,ijk,m2,ij+1k} = K(m_{2,ij+1k}n_{3,ijk})^{1/2}\\
&T_{m4,ijk,n1,ij+1k} = K(n_{1,ij+1k}m_{4,ijk})^{1/2}\\
&T_{m1,ij+1k,n4,ijk} = K(m_{1,ij+1k}n_{4,ijk})^{1/2}.
\end{aligned} \tag{41}$$

For simplicity we have taken $\Delta x = \Delta y = \Delta z$. Each of the above mass transfer terms connects a subsite at position ijk with another subsite at position $ij+1k$. The eight transfer rules for the z-direction are

$$\begin{aligned}
&T_{m3,ijk+1,m1,ijk} = K(m_{3,ijk+1}m_{1,ijk})^{1/2}\\
&T_{n3,ijk+1,n1,ijk} = K(n_{3,ijk+1}n_{1,ijk})^{1/2}\\
&T_{m2,ijk,m4,ijk+1} = K(m_{4,ijk+1}m_{2,ijk})^{1/2}\\
&T_{n2,ijk,n4,ijk+1} = K(n_{4,ijk+1}n_{2,ijk})^{1/2}\\
&T_{m1,ijk+1,m3,ijk} = K(m_{1,ijk+1}m_{3,ijk})^{1/2}\\
&T_{n1,ijk+1,n3,ijk} = K(n_{1,ijk+1}n_{3,ijk})^{1/2}\\
&T_{m4,ijk,m2,ijk+1} = K(m_{2,ijk+1}m_{4,ijk})^{1/2}\\
&T_{n4,ijk,n1,ijk+1} = K(n_{2,ijk+1}n_{4,ijk})^{1/2}.
\end{aligned} \tag{42}$$

In addition, mass transfers can occur between subsites at the same position. These transfer terms are

$$\begin{aligned} T_{m1,ijk,n1,ijk} &= \Xi(n_{1,ijk}m_{1,ijk})^{1/2} \\ T_{m2,ijk,n2,ijk} &= \Xi(n_{2,ijk}m_{2,ijk})^{1/2} \\ T_{n3,ijk,m3ijk} &= \Xi(n_{3,ijk}m_{3,ijk})^{1/2} \\ T_{n4,ijk,m4ijk} &= \Xi(n_{4,ijk}m_{4,ijk})^{1/2} \\ \Xi &= 2\Delta t\mu c^2/\hbar. \end{aligned} \tag{43}$$

With these mass transfer terms the automaton rules for updating the masses at the eight subsites at position ijk become

$$\begin{aligned} M_{1,ijk} &= m_{1,ijk} + T_{m4,i+1jk,m1,ijk} - T_{m1,ijk,m4,i-1jk} + T_{n4,ij+1k,m1,ijk} - T_{m1,ijk,n4,i-1jk} \\ &\quad + T_{m3,ijk+1,m1,ijk} - T_{m1,ijk,m3,ijk-1} - T_{m1,ijk,n1,ijk} \\ N_{1,ijk} &= n_{1,ijk} + T_{n4,i+1jk,n1,ijk} - T_{n1,ijk,n4,i-1jk} - T_{n1,ijk,m4,ij+1k} + T_{m4,ij-1k,n1,ijk} \\ &\quad + T_{n3,ijk+1,n1,ijk} - T_{n1,ijk,n3,ijk-1} + T_{m1,ijk,n1,ijk} \\ M_{2,ijk} &= m_{2,ijk} + T_{m3,i+1jk,m2,ijk} - T_{m2,ijk,m3,i-1jk} - T_{m2,ijk,n3,ij+1k} + T_{n3,ij-1k,m2,ijk} \\ &\quad - T_{m2,ijk,m4,ijk+1} + T_{m4,ijk-1,m2,ijk} - T_{m2,ijk,n2,ijk} \\ N_{2,ijk} &= n_{2,ijk} + T_{n3,i+1jk,n2,ijk} - T_{n2,ijk,n3,i-1jk} + T_{m3,ij+1k,n2,ijk} - T_{n2,ijk,m3,ij-1k} \\ &\quad - T_{n2,ijk,n4,ijk+1} + T_{n4,ijk-1,n2,ijk} + T_{m2,ijk,n2,ijk} \\ M_{3,ijk} &= m_{3,ijk} + T_{m2,i+1jk,m3,ijk} - T_{m3,ijk,m2,i-1jk} + T_{n2,ij+1k,m3,ijk} - T_{m3,ijk,n2,ij-1k} \\ &\quad + T_{m1,ijk+1,m3,ijk} - T_{m3,ijk,m1,ijk-1} + T_{n3,ijk,m3ijk} \\ N_{3,ijk} &= n_{3,ijk} + T_{n2,i+1jk,n3,ijk} - T_{n3,ijk,n2,i-1jk} - T_{n3,ijk,m2,ij+1k} + T_{m2,ij-1k,n3,ijk} \\ &\quad - T_{n1,ijk+1,n3,ijk} - T_{n3,ijk,n1,ijk-1} - T_{n3,ijk,m3,ijk} \\ M_{4,ijk} &= m_{4,ijk} + T_{m1,i+1jk,m4,ijk} - T_{m4,ijk,m1,i-1jk} - T_{m4,ijk,n1,ij+1k} + T_{n1,ij-1k,m4,ijk} \\ &\quad - T_{m4,ijk,m2,ijk+1} + T_{m2,ijk-1,m4,ijk} + T_{n4,ijk,m4,ijk} \\ N_{4,ijk} &= n_{4,ijk} + T_{n1,i+1jk,n4ijk} - T_{n4,ijk,n1,i-1jk} + T_{m1,ij+1k,n4ijk} - T_{n4,ijk,m1,ij-1k} \\ &\quad - T_{n4,ijk,n2ijk+1} + T_{n2,ijk-1,n4,ijk} - T_{n4,ijk,m4,ijk}. \end{aligned} \tag{44}$$

Expressing the four component wavefunction in terms of real and imaginary amplitudes

$$\psi_\nu(x, y, z, t) = a_\nu(x, y, z, t) + ib_\nu(x, y, z, t) \qquad \nu = 1, 2, 3, 4 \tag{45}$$

relating mass terms to the amplitudes

$$m_\nu(x, y, z, t) = [a_\nu(x, y, z, t)]^2 \qquad n_\nu(x, y, z, t) = [b_\nu(x, y, z, t)]^2 \tag{46}$$

and letting the spatial and time steps tend to zero, we can show by repeating the procedure of the previous case that the update equations (44) for the automaton reduce to the coupled set of partial differential equations

$$\begin{aligned} [(1/c)\partial_t + mc/i\hbar]\psi_1 - \partial_x\psi_4 + i\partial_y\psi_4 - \partial_z\psi_3 &= 0 \\ [(1/c)\partial_t + mc/i\hbar]\psi_2 - \partial_x\psi_3 - i\partial_y\psi_3 + \partial_z\psi_4 &= 0 \\ [(1/c)\partial_t - mc/i\hbar]\psi_3 - \partial_x\psi_2 + i\partial_y\psi_2 - \partial_z\psi_1 &= 0 \\ [(1/c)\partial_t - mc/i\hbar]\psi_4 - \partial_x\psi_1 - i\partial_y\psi_1 + \partial_z\psi_2 &= 0 \end{aligned} \tag{47}$$

which is a form of the Dirac equation

$$ih\,\partial_t\psi + mc^2\beta\psi - i\hbar c(\alpha_x\partial_x + \alpha_y\partial_y + \alpha_z\partial_z)\psi = 0 \tag{48}$$

where α_x, α_y, α_z, and β are the Dirac matrices.

Both the vector and scalar potentials can easily be incorporated into the discretation rules of the Dirac equation. The inclusion of these potentials involves additional mass transfers between subsites at the same position, which is a straight-forward modification of (43).

In summary, cellular automata have been presented for modelling quantum systems. After the initial masses and directions of mass flows at each site have been specified, spatially local updating rules, which depend on the masses of neighbouring sites, determine the masses of the sites at future times. A significant feature of these spatially local updating rules is that they conserve mass and probability. In the limit of small spatial and time steps, the equations defining the automata reduce to the Schrödinger and Dirac equations. Most if not all other local numerical methods for solving the time-dependent three-dimensional Schrödinger and Dirac equations give solutions that increase without bound for too small spatial steps or too large time steps. In contrast, the solutions given by the methods presented here never increase without bound.

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