

COMMENT

On cellular automata models for quantum systems

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Received 22 April 1996

Abstract. We analyse a recent approach to quantum systems based on some recent cellular automata models. It is shown that, although mass and probability conservation holds, non-physical behaviour is typically obtained.

Recent studies [1–3] have shown the interest of cellular automata (CA) models as an adequate approximation to quantum systems. A CA model can be constructed with a unitary evolution operator [1] and several generalizations lead, under some natural assumptions, to, for example, the Weyl equation [2]. A recent study by Kostin [3] has used this CA approach to the Schrödinger and Dirac equations. Kostin claimed that such methods have some advantages over local conventional numerical methods. These advantages are that, because they conserve mass and probability, they can never give solutions that grow without bound. In some local conventional numerical methods, meaningless solutions can be obtained that grow with no bounds if the spatial step is too small or if the time step is too large.

Though mass and probability conservation certainly hold in Kostin's approach, this is no guarantee for the discrete system to be physically meaningful, as we will show in this comment.

Let us consider our system as being discrete in space and time, on a uniformly distributed grid, Δx being the spatial step between lattice points, and Δt the corresponding time step. If only local (nearest-neighbour) rules are considered, information propagates at a finite speed $v < \Delta x/\Delta t$. Kostin's CA model is a discrete approximation to the Schrödinger wave equation (SWE), that is to say, to a wave equation where information propagates with a group velocity v_g . So if the spatial discretization Δx is too small or the time discretization Δt is too large, information will never propagate with group velocity v_g . In other words, the discretized system is unable to reproduce the dynamic behaviour of the continuous counterpart. This is a physical constraint for any local discrete system, but numerical constraints are generally stronger.

According to Kostin's CA model, the following rules for time evolution of the local mass m_j at a given lattice point are obtained:

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

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

with:

$$\begin{aligned} m_j &= a_j^2 & n_j &= b_j^2 \\ \kappa &= \frac{\hbar \Delta t}{m(\Delta x)^2} \\ \lambda_j &= 2\kappa + \frac{2V_j \Delta t}{\hbar} \end{aligned}$$

where the amplitudes a_j and b_j are the real and imaginary parts of the wavefunction at site j , i.e. $\psi_j = a_j + ib_j$, and V_j is the potential at j . Here upper case letters hold for updated quantities.

Now let us see that meaningless, non-physical time evolutions are obtained by following the previous equations (1), (2). Let us consider a small perturbation of the wavefunction ψ_j by a value $\epsilon > 0$, i.e. $\tilde{\psi}_j \equiv (a_j + \epsilon) + ib_j = \psi_j + \epsilon$ (in the following, we use the notation $\tilde{\cdot}$ to indicate a perturbed quantity). Then the time evolution for the probability density \tilde{p}_j obtained from $\tilde{\psi}_j$ (using Kostin's equations) will be

$$\begin{aligned} \tilde{P}_j &= M_j + N_j = (a_j + \epsilon)^2 - \kappa(a_j + \epsilon) \left(b_{j+1} + b_{j-1} - \frac{\lambda_j}{\kappa} b_j \right) \\ &\quad + b_j^2 + \kappa b_j \left(a_{j+1} + a_{j-1} - \frac{\lambda_j}{\kappa} (a_j + \epsilon) \right) \\ &= a_j^2 - \kappa a_j \left(b_{j+1} + b_{j-1} - \frac{\lambda_j}{\kappa} b_j \right) + b_j^2 + \kappa b_j \left(a_{j+1} + a_{j-1} - \frac{\lambda_j}{\kappa} a_j \right) \\ &\quad + (2a_j + \epsilon - \kappa(b_{j+1} + b_{j-1}))\epsilon \\ &\approx P_j + (2a_j - \kappa(b_{j+1} + b_{j-1}))\epsilon \end{aligned}$$

where P_j is the updated probability density obtained for the non-perturbed wavefunction ψ_j . If a_j and b_j are both positive, then the following implication

$$\tilde{p}_j > p_j \Rightarrow \tilde{P}_j < P_j \quad (3)$$

holds for

$$\frac{\Delta t}{\Delta x^2} > \frac{m}{\hbar} \frac{2a_j}{b_{j+1} + b_{j-1}}. \quad (4)$$

One can see that this implication is physically meaningless. Let us consider two identical initial states, only differing by ϵ at a given point j . Then, following Kostin's arguments, the state with higher probability at j , once updated, will have the lowest probability at j .

Moreover, the time evolution of the probability depends strongly on the quotient $\Delta t/\Delta x^2$. Given a time step Δt , there exists Δx such that the probability behaves as

$$\tilde{p}_j > p_j \Rightarrow \tilde{P}_j < P_j$$

and there exists Δx such that

$$\tilde{p}_j > p_j \Rightarrow \tilde{P}_j > P_j$$

and, when Δx goes to zero, \tilde{P}_j goes to $-\infty$.

Finally it can be pointed out that in the limit when both Δx and Δt go to zero, the discretization does not reduce to the SWE, because κ is undefined. In order to guarantee that the discretized system reduces to SWE we must require that κ goes to zero (which makes the method impracticable), or that the numerical scheme is stable, i.e. given a continuous solution it remains continuous through the time evolution.

Acknowledgments

This work has been supported by grants UPC PR9407 and DGYCIT PB94-1195. One of the authors (JMGV) wishes to thank the Generalitat de Catalunya for its financial support.

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