A Solution of Time Dependent Schrödinger Equation by Quantum Walk

Hideo Sekino, Masayuki Kawahata and Shinji Hamada

1Toyohashi University of Technology

Toyohashi Aichi 441-8580, Japan

sekino@tut.jp

Abstract. Time Dependent Schrödinger Equation (TDSE) with an initial Gaussian distribution, is solved by a discrete time/space Quantum Walk (QW) representing consecutive operations corresponding to a dot product of Pauli matrix and momentum operators. We call it as Schrödinger Walk (SW). Though an Hadamard Walk (HW) provides same dynamics of the probability distribution for delta-function-like initial distributions as that of the SW with a delta-function-like initial distribution, the former with a Gaussian initial distribution leads to a solution for advection of the probability distribution; the initial distribution splits into two distinctive distributions moving in opposite directions. Both mechanisms are analysed by investigating the evolution of the both amplitude components. Decoherence of the oscillating amplitudes in central region is found to be responsible for the splitting of the probability distribution in the HW.

1. Introduction
Quantum information is propagated by unitary transformations of the quantum states which is called q-bit. Expectation value of a particle to be in position $x$ at time $t$ is evaluated by the spatial evolution of the probability amplitude for the particle given at initial time $t_0$. Conventional technology to provide such evolution of the probability amplitude is to solve Time Dependent Schrödinger Equation (TDSE) for the quantum particle in a Hilbert space composed by real-space and internal degree of freedom $H_p \otimes H_c$. TDSE is a partial differential equation which is equivalent to a finite difference equation with the difference of infinitesimal length. As is understood, however, infinitesimal length is not allowed as any meaningful size of quantum particles which carry information. That is, the measure of propagation of the quantum information by the solution of the differential equation with finite difference approximation is bounded by the finite length used. The any simulation with finite momentum (the ratio of physical space interval to time interval times mass) is meaningful for evaluating the transportation of information contained in a space of finite size. With this in mind, we introduce a quantum walk (QW) which leads to a solution of the TDSE with an initial Gaussian distribution and further analyze the solution by comparison with Hadamard Walk (HW) which leads to a solution for advection of the probability distribution.

2. Theoretical method
QW is typically used in the context of quantum computation where time-progression of quantum state is simulated using consecutive application of unitary operations to the initial state. Natural
interpretation of wavefunction represented in physical space is the probability amplitude distribution of a quantum particle on physical space. A dynamics of quantum information within a space smaller than the minimum length allowed for quantum mechanics cannot be simulated using techniques based on the finite difference approximation where the unit length is smaller than the quantum minimum. More precisely, we cannot simulate the dynamics of the probability amplitude within an area smaller than the area of $\Delta x \cdot \Delta p$. We focus the dynamics of quantum information and simulate it using QW techniques. A typical QW is performed by consecutive application of unitary operation to a state from which we evaluate an observable quantum property at later time. We introduce a QW to generate a wavefunction at time $t$ by consecutively applying a unitary operation in the composite Hilbert space $H_p \otimes H_c$ to the initial probability distribution of a quantum particle at $t_0$. Here $H_p$ is physical space and the probability amplitude is represented on a set of discrete grid and $H_c$ is a space spanned by internal degree of freedom. The latter can be spin of electron or chirality of photon for example and often called as coin space. Since we focus on the TDSE, it is probably more appropriate to interpret the internal degree of freedom considered here as spin of electron. Since the physical space is represented on grid point $s$, an initial distribution at a single grid point mimics delta function. However it is impossible to describe a quantum dynamics within the area smaller than $\Delta x \cdot \Delta p$ by the simulation using such initial distribution. In order to provide appropriate solutions of TDSE by such discrete time/space QW, we take a QW of regular strategy but with an initial probability amplitude distribution of Gaussian instead.

2.1 Lévy-Leblond Equation

Schrödinger Equation (SE) usually does not contain spin coordinate and it is commonly understood that the notion of spin arises from consideration of relativity beyond SE. However, we could formulate an equation which has a coordinate for extra degree of freedom than physical space for a non-relativistic particle which obeys TDSE. The equation was introduced and is called Lévy-Leblond Equation (LLE).

\[
H_{LL} \equiv \begin{pmatrix} V & \sigma \cdot p \\ \sigma \cdot p & -2m \end{pmatrix} \begin{pmatrix} \phi \\ \chi \end{pmatrix} = E \begin{pmatrix} \phi \\ 0 \end{pmatrix}
\]

(1)

Where $\phi$ and $\chi$ are upper and lower components of wavefunction spinors and each of them has two components. Here $m$ is a mass of the particle and $p$ and $V$ are momentum and potential energy operators and $\sigma$ stands for Pauli matrix vector. Eliminating the lower component from the time-dependent version of the LLE, we have a solution for the upper component.

\[
\phi(r,t) = \exp\left[ -\frac{i}{2m} (\sigma \cdot p)^2 + V \right] \phi(r) = \exp\left[ -\frac{i}{2m} p^2 + V \right] \phi(r)
\]

(2)

Typically numerical solution of the TDSE is achieved by consecutively applying the operation $-ip^2/2m + V$ as in the last expression of Eq. (2), to the wavefunction using certain approximation scheme for the exponential ansatz with sufficiently small time step for guaranteeing the precision of the approximation. We have identical solutions for the upper and lower components of the spinor $\phi$ and therefore the equation reduces to a solution of scalar wavefunction. We here employ the first expression in Eq. (2) for solving the TDSE by QW. For a particle which has a definite spin along a direction, the corresponding component of the $\sigma$ operator is diagonalized and the operation $\sigma \cdot p$ provides momenta $-p$ and $+p$ for the lower and upper components.
\[(\sigma \cdot p)\phi(r) = -i\sigma_z \frac{\partial}{\partial z} \phi(r) = \begin{pmatrix} -i \frac{\partial}{\partial z} & 0 \\ 0 & +i \frac{\partial}{\partial z} \end{pmatrix} \phi(r) \] (3)

However, the spin is not always aligned along certain axis without imposing an external perturbation to enforce it and thus \(\sigma\) is not diagonalized all the time even started with a definite spin state. Indeed, any spin component is smaller than the absolute value of spin itself, meaning that no spin is aligned completely parallel to any axis. A spin with a definite value of a component to an axis can be interpreted to be rotating around the axis with certain angle kept. When we simulate the dynamics of a quantum particle by QW in a combined Hilbert space using a finite time step, the spin state should be altered during the boost corresponding to a momentum operation in Eq. (3). For the second operation of \(\sigma \cdot p\), the spin is not aligned along the axis even if it was before the first operation of \(\sigma \cdot p\). Therefore we employ two different components of the Pauli matrix together with the diagonal component \(\sigma_z\) in order to investigate the effect of the rotation during the walk.

\[
\exp(i\sigma_x \cdot p) = \begin{pmatrix} \cos p & i \sin p \\ i \sin p & \cos p \end{pmatrix} \] (4a)
\[
\exp(i\sigma_y \cdot p) = \begin{pmatrix} \cos p & \sin p \\ -i \sin p & \cos p \end{pmatrix} \] (4b)

We refer (4a) to TDSE walk (SW) and (4b) to Hadamard walk (HW). The operation corresponding the \(\sigma_z p\) is performed by a QW as in the typical QW where shift operators corresponding to \(-p\) and \(+p\) momenta are applied to the wavefunction represented on a grid in the discrete physical space, together with the spin rotating operations \(P\) and \(Q\) which correspond to the upper and lower components of (4a) or (4b) respectively.

### 2.2 Numerical method

For the preliminary study of the QW for solving TDSE by the above walks, we set \(p = \pi / 4\) for (4a) and (4b) operations. For investigating the basic behaviour of the QW defined above, we execute QWs with an initial distribution where only one grid has a value with all the others zero. We call the initial condition as delta-function (DF) distribution. Next, we execute QWs with a Gaussian distribution as an initial condition.

### 3. Results and discussion

It is known that HWs result in non-symmetric evolution of the probability for certain initial condition. We study here a symmetric HW with an initial condition \((1/\sqrt{2}, i/\sqrt{2})^T\) and SW with an initial condition \((1/\sqrt{2}, 1/\sqrt{2})^T\). We investigate the evolution of each component of the amplitude together with the evolution of the probability distribution. Those are shown in the pictures of second- and third-rows in Fig.1. The ones indicated by alpha and beta in the figures mean the upper and lower components of the amplitudes. The corresponding results of SW are summarized in Fig 2. Both walks provide identical probability evolution and the peaks of consisting amplitudes moves similarly. Namely the peaks of upper and lower components of the amplitudes move in an opposite direction with same speed. However careful observation provides significant information on the difference between those walks. While each component of the HW has gradients in the magnitude (opposite signs to each other) of their amplitudes, there seems no spatial inhomogeneity in their oscillatory behaviour. On the other hand, while the magnitudes of the SW amplitudes evolve non-symmetrically as those of the HW amplitudes, spatial inhomogeneity of the oscillatory behaviour is observed for the
case. There is finer structure of the oscillation in the central region than in the peripheral front area of the SW amplitudes distribution where the peaks are.

Fig. 1 Symmetric Hadamard Walk with delta-function initial distribution at 99th step

Fig. 2. Symmetric Schrödinger Walk with delta-function initial distribution at 99th step

We show the results of the two QWs with an initial Gaussian distribution in Fig. 3 and Fig. 4. In the HW, the initial Gaussian peak of the probability distribution splits into two and each peak moves in opposite directions with same speed (Fig. 3). On the contrary, the SW with the initial Gaussian distribution provides an evolution of the original single Gaussian shape kept. The widening of the probability distribution is quite slow and the evolution of the probability seems stable along the walk (Fig. 4). The remarkable difference of the two walks is explained by the difference in the oscillatory
structures of the amplitudes. The spatial averaging of the amplitudes results in a cancelation in magnitude for oscillating amplitudes. Two oscillating components of the HW spread in opposite directions and cancelation of the magnitude by the Gaussian superposition is enhanced in the central region. Consequently the original Gaussian peak splits to two distinct distributions which move in opposite directions. The spatial decoherence of amplitudes in the central region is responsible for the distinctive dynamics of the probability distribution in the HW.

As is seen in Fig 2, the two amplitudes of SW evolve also non-symmetrically with the peaks moving in opposite directions, but the oscillation wavelength of the amplitudes is longer in central region than in the peripheral region where the peaks of components are. The Gaussian superposition of the amplitudes results in much lesser cancelation of the magnitudes in the central region. Consequently the initial Gaussian probability distribution evolves without splitting the original single peak shape. The evolution of the initial Gaussian distribution obtained by the SW is exact and identical to the solution by the method based on finite difference approximation for the TDSE partial differential equation.
4. Conclusion

We perform a QW which leads to a solution for the TDSE with an initial Gaussian distribution by introducing a Pauli matrix component which mixes the upper and lower components of the coin space (rotation of spin) together with a boost of the quantum information in the real discrete space. The QW reproduces the exact results and the one by a conventional finite difference method. Another Pauli matrix component with certain delta-function like initial distribution leads to symmetric HW. Although two walks provide identical evolutions of probability distribution, the spatial oscillatory structures of amplitudes in the two walks are different. Consequently the probability distributions of the two walks evolve in markedly different ways: the SW evolves with the single peak structure of the initial Gaussian distribution shape kept while the HW results in splitting of the initial Gaussian distribution into two distinctive distributions moving in opposite directions. The latter evolution is considered as advection process.

We introduce Lévy-Leblond Equation which is identical to Schrödinger Equation with multi-components in order to interpret the QW in the combined Hilbert space. While LLE can be derived without any consideration of relativity, it can be considered as zero\textsuperscript{th} order approximation of Dirac equation\textsuperscript{3}. Preliminary study\textsuperscript{4} was done for a one-dimensional Dirac equation where the width of the wave packet is referred in connection with the velocity of quantum information. Wide wave packets evolved as a single peaked distribution while narrow wave packets provided an evolution of two peak structure for the probability distribution. Similar observation is done in our SW based upon the LLE formulation.
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