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Solution of the Time Dependent Schrödinger Equation Using the Higher Order Trotter-Suzuki Method

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Abstract

We solve the solution of the Time-Dependent Schrödinger Equation (TDSE) using the higher-order Trotter-Suzuki Decomposition. We use The Gaussian function as a stationary state in a linear potential system. The TDSE solution using Baker-Campbell-Hausdorff was used to validate the results and to measure the accuracy of the Trotter-Suzuki decomposition. So that the difference between the Baker-Campbell-Hausdorff result and the Suzuki-Trotter decomposition is considered an error. The error of the TDSE solution by the Trotter - Suzuki second-order decomposition was lower than the first order. Meanwhile, the error of the TDSE solution by second-order hybrid will be lower than the second-order Trotter - Suzuki decomposition when the value of $dx = 0.1$ and 0.05 with $dt \leq 0.0001$. The error comparison of these three methods is only valid when time $t < 1$.

Keywords: Time-Dependent Schrödinger Equation; Trotter – Suzuki decomposition high order; Baker – Campbell – Hausdorff

1 INTRODUCTION

In quantum mechanics, the wave equation can explain the behavior of particle systems. The information obtained from the wave equation is the probability of a particle's position and the particle's energy. We can find the wave equation by solving the Schrödinger equation. Solution of the Time-dependent Schrödinger Equation (TDSE) contains a lot of dynamic information. Schrödinger's equation for one dimension can be written as follows

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x,y)\Psi(x,t) \quad (1)$$

The solution of equation (1) for a dynamic system can be written as

$$\Psi(x,t) = e^{it\widehat{H}}\Psi(x,0) = \widehat{U}(t)\Psi(x,0) \quad (2)$$

$\widehat{U}(t)$ the time evolution operator, $\Psi(x,0)$ the initial state when time $t = 0$ and $\widehat{H}$ the Hamiltonian operator. Hamiltonian operators have unitary properties that must be maintained [1]. So that to complete the TDSE, a unitary numerical solution is needed [2].

There have been many attempts to solve the time-dependent Schrödinger's equation. One and two-dimensional solutions of the Time Dependent Schrödinger Equation (TDSE) have been carried out by Becerril et al., (2008) using the finite difference method. However, this method cannot maintain the unitary properties of the Hamiltonian Operator. There is a unitary algorithm such as Crank-Nicholson, but this algorithm involves a large matrix size[2]. The TDSE solution has found by Soto-Eguibar and Moya-Cessa [3] with the extended Baker - Campbell - Hausdorff method. The TDSE solution obtained from this method is explicit, so this method requires precision in mathematical derivation.

Suzuki [4] introduced the generalized Trotter equation (1959). Which is now known as the Trotter-Suzuki equation. The advantage of the Trotter - Suzuki decomposition is that it can maintain the unitary properties of the Hamiltonian operator. So we can use this method to solve dynamic quantum and Hamilton dynamic problems [1]. Trotter-Suzuki decomposition has implemented a lot. Among them are [5] and [2]. In general, the Trotter - Suzuki decomposition equation can be written with the

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following equation [6].

$$e^{x(A+B)} = e^{p_1 xA} e^{p_2 xB} e^{p_3 xA} e^{p_4 xB} ... e^{p_m xB} + \mathcal{O}(x^{m+1}) \tag{3}$$

To solve the TDSE with the Trotter - Suzuki decomposition we construct the Hamiltonian operator in the form of a matrix. First, we need to discretize equation (1) by replacing the second derivative with respect to x with the finite-difference approach [7]. By assuming $-\frac{1}{\Delta x^2} = w$ and $V(l\Delta x) + \frac{2}{\Delta x^2} = v_l$, Hamiltonian operators in the form of a tri-diagonal matrix can be written as

$$\widehat{H} = \begin{bmatrix} v_1 & w & 0 & 0 & \cdots & 0 \\ w & v_2 & w & 0 & \cdots & \vdots \\ 0 & w & v_3 & w & 0 & \vdots \\ 0 & \cdots & w & \ddots & w & 0 \\ \vdots & \vdots & 0 & w & v_{l-1} & w \\ 0 & 0 & \cdots & 0 & w & v_l \end{bmatrix} \tag{4}$$

Hamiltonian matrix can be decomposed into 3 matrices $H = H_0 + H_1 + H_2$. The diagonal matrix H_0 is written as

$$H_0 = \begin{bmatrix} v_1 & 0 & \cdots & \\ 0 & v_2 & 0 & \cdots \\ \vdots & 0 & \ddots & 0 \\ & \cdots & 0 & v_l \end{bmatrix} \tag{5}$$

The block diagonal Matrices H_1 and H_2 are written as [2]

$$H_1 = \begin{bmatrix} 0 & w & & & & & \\ w & 0 & 0 & & & & \\ & 0 & 0 & w & & & \\ & & w & 0 & & & \\ & & & \ddots & \ddots & & \\ & & & & & & 0 \end{bmatrix} \tag{6}$$

and

$$H_2 = \begin{bmatrix} 0 & 0 & & & & \\ 0 & 0 & w & & & \\ & w & 0 & & & \\ & & & \ddots & & \\ & & & & 0 & w \\ & & & & w & 0 \end{bmatrix} \tag{7}$$

H_1 and H_2 contains a matrix containing a block matrix 2×2. The exponent of the 2×2 matrices are written as [2]

$$\exp\left(-i\tau \begin{bmatrix} w & o \\ 0 & w \end{bmatrix}\right) = M = \begin{bmatrix} \cos\tau|w| & -i\sin\tau|w| \\ -i\sin\tau|w| & \cos\tau|w| \end{bmatrix} \tag{8}$$

Matric decomposition makes it easy to solve the TDSE with the Trotter - Suzuki method.

Form of the Trotter - Suzuki first order decomposition is given by [?]

$$e^{x(A+B)} = e^{xA} e^{xB} + \mathcal{O}\left(x^2\right) \tag{9}$$

So that the solution of the time evolution operator with the Trotter - Suzuki first-order decomposition is written as

$$e^{-i\tau\widehat{H}} = e^{-i\tau\widehat{H_0}} e^{-i\tau\widehat{H_1}} e^{-i\tau\widehat{H_2}} \tag{10}$$

The higher order Suzuki – Trotter decomposition can be constructed in various ways, including fractal decomposition and Trotter – Suzuki Hybrid decomposition. Constructing a Trotter-Suzuki higher order from the symmetrized Trotter-Suzuki lower order [6]. The approximation equation for the second-order exponential operator can be written as [?]

$$e^{x(A+B)} = e^{\frac{x}{2}A} e^{xB} e^{\frac{x}{2}A} + \mathcal{O}(x^3) \tag{11}$$

So that the solution of the time evolution operator with the second-order Trotter-Suzuki decomposition can be written as

$$e^{-i\tau\widehat{H}} = e^{-\frac{i\tau}{2}\widehat{H_0}} e^{-\frac{i\tau}{2}\widehat{H_1}} e^{-\imath\tau\widehat{H_2}} e^{-\frac{i\tau}{2}\widehat{H_1}} e^{-\frac{i\tau}{2}\widehat{H_0}} \tag{12}$$

The second-order hybrid Trotter-Suzuki decomposition is a second-order Trotter-Suzuki decomposition involving the exponential of the commutator matrix in its correction term [?]. In general, the second-order hybrid Trotter – Suzuki decomposition equation can be written as [1].

$$e^{xA} e^{xB} e^{\frac{x^2}{2}[A,B]} = e^{x(A+B)+\mathcal{O}(x^3)} \tag{13}$$

From the explanation above, we can implement the Trotter – Suzuki decomposition method to solve TDSE and see the effect of higher-order on the TDSE solution. With the higher correction term of this method, we expect the stability and the accuracy to complete the TDSE will be higher.

2 EXPERIMENTAL METHOD

From equation(12), we can construct the Trotter–Suzuki second order to solve the Time-dependent Schrödinger Equation (TDSE). The equation of Trotter-Suzuki second order to solve TSDE written as:

$$|\psi(x,t)\rangle = e^{-\frac{i\tau}{2}\widehat{H_0}}e^{-\frac{i\tau}{2}\widehat{H_1}}e^{-1\tau\widehat{H_2}}e^{-\frac{i\tau}{2}\widehat{H_1}}e^{-\frac{i\tau}{2}\widehat{H_0}}|\psi(x,0)\rangle \quad (14)$$

From equation (14), the Time-dependent Schrödinger Equation (TDSE) solution using the second-order approach can be expressed by the flowchart in Figure 1. We illustrate the TDSE solution by plotting the probability $|\psi(x,t)|^2$ as a function of position x and as a function of time t.

To get Trotter – Suzuki hybrid formula for three operators $H = H_0 + H_1 + H_2$, first, write a Trotter – Suzuki hybrid decomposition for $H_0 + H_1$.

$$\begin{aligned}\exp\left(-i\tau(H_0+H_1)\right) &= \exp\left(-i\tau D\right) \\ &= \exp\left(-i\tau H_0\right)\exp\left(-i\tau H_1\right)\times \\ &\quad \exp\left(-\frac{1}{2}(-i\tau)^2[H_0,H_1]\right)\end{aligned} \quad (15)$$

After obtaining the formula for exp $(-i\tau(H_0 + H_1))$ then finding the Trotter - Suzuki hybrid decomposition for $\exp\left(-i\tau(H_0 + H_1 + H_2)\right)$

$$\exp\left(-i\tau(H_0+H_1+H_2)\right) = \exp(-i\tau(D+H_2)) \quad (16)$$

$$\exp(-i\tau(D+H_2)) = \exp(-i\tau D)\exp(-i\tau H_2)\times \exp\left(-\frac{1}{2}(-i\tau)^2[D,H_2]\right) \quad (17)$$

Substitute $\exp(-i\tau D)$ in the above equation with equation (14). The equation of Trotter-Suzuki hybrid second order to solve TSDE written as:

$$\begin{aligned}|\psi(x,t)\rangle &= \exp(-i\tau H_0)\exp(-i\tau H_1)\times \\ &\quad \exp\left(-\frac{1}{2}(-i\tau)^2[H_0,H_1]\right)\cdots\times \\ &\quad \exp(-\tau H_2)\times \\ &\quad \exp\left(-\frac{1}{2}(-i\tau)^2[H_0+H_1,H_2]\right)|\psi(x,0)\rangle\end{aligned} \quad (18)$$

The TDSE solution using the second-order hybrid approach can be expressed by the flowchart in Figure 2.

The TDSE solution using the Baker – Campbell – Hausdorff method has been described by Soto-Eguibar and Moya-Cessa as an explicit solution, so it tends to be easy to recalculate. Therefore, to validate and measure the accuracy, the TDSE solutions using second order method and the second order hybrid method compared with TDSE solutions using the Baker – Campbell – Hausdorff method. The difference between the two methods and the Baker – Campbell – Hausdorff method will be considered an error. The accuracy of both methods measured by Root Mean Square Error (RMSE). The RMSE equation is written as in the following equation

$$RMSE = \sqrt{\frac{1}{N}\left(\psi_{TS} - \psi_{BCH}\right)^2} \quad (19)$$

where ψ_{TS} is the result of Trotter – Suzuki decomposition and ψ_{BCH} is the result of Baker – Campbell – Hausdorff.

3 RESULTS AND DISCUSSIONS

The TDSE solution affect by dx and dt. The smaller the value of dx, the larger the size of the Hamiltonian matrix used and the value of dt affects the number of iterations. The values of dx are varied to $dx = 0,1$, $dx = 0,05$ and $dx = 0,02$, with the values of dt are varied to $dt = 0,01$, $dt = 0,001$, $dt = 0,0005$, $dt = 0,0001$ dan $dt = 0,00005$. The accuracy of the Trotter–Suzuki first order, second order, and second order hybrids is compared in the RMSE table.

The TDSE solution from Baker – Campbell – Hausdorff with a value of $dx = 0,1$ in a three-dimensional graph can be seen in Figure 3. The TDSE solution from Trotter – Suzuki decomposition with $dx = 0,1$ and $dt = 0,01$ can be seen in Figure 4. There is a relatively significant difference between the solutions by the Baker–Campbell–Hausdorff method with the Trotter–Suzuki decomposition of second order and second order hybrid. Especially when time $t > 1$. In Table 1, we show an errors comparison of Trotter – Suzuki decomposition first order, second order, and second order hybrid. The RMSE of the second order is smaller than the first order but the RMSE second order hybrid is greater than the first order. When the value of dt is reduced to $0,001$, then the TDSE solution can be seen in Figure 5. If the solution by second order with $dt = 0,001$ is compared with the solution by second order with $dt = 0.01$, then there is no significant difference between the two. However, if the second order hybrid with $dt = 0,001$ is compared to the second order hybrid with $dt = 0,01$ then there will be differences, especially at $t > 1$. In Table 2, RMSE second order with $dt = 0,001$ is smaller than

RMSE second order with $dt = 0,01$, This also applies to second order hybrids. When the RMSE second order and second order hybrids are compared, the second-order hybrid gives more accurate results than the second order at state $t < 1$. Likewise, when the value of dt continues to be reduced, the RMSE of the first order, second order, and second order hybrid is getting smaller. Although the error reduction is not significant. This RMSE comparison can be seen in Table 3, Table 4, and Table 5.

When value of dx is $0,05$ and $dt = 0,01$, the TDSE solution by the Baker – Campbell – Hausdorff method can be seen in Figure 6 and the TDSE solution by the Trotter – Suzuki decomposition can be seen in Figure 7. The TDSE solution by the Trotter–Suzuki decomposition second order in Figure 7(b) has not yet produced a solution that fits to the comparison method. When the value of $dt \leq 0.01$, the solutions by second order and second order hybrids look the same on the three-dimensional graph. This solution can be seen at Figure 8. If we compared the RMSE second order to the RMSE second order hybrid, then the TDSE solution by second order is more accurate than the second order hybrid when the $dt = 0,01$,$dt = 0,001$, and $dt = 5 \times 10^{-4}$. We show this RMSE comparison in Table 6, Table 7, and Table 8. Meanwhile, when we reduce the value of dt to 1×10^{-4} and 5×10^{-5}, the TDSE solution by second-order hybrid is more accurate than the second order. We show RMSE comparison in Table 9 and Table 10.

We show the TDSE solution by the Baker – Campbell - Hausdorff method with the value of $dx = 0,02$ and $dt = 0,01$ in Figure 9 and the TDSE solution by the Trotter – Suzuki second-order and second-order hybrid method in Figure 10. In Figure 10(a) and 10(b), the solution has not fitted with the comparison method. Figure 11 is a TDSE solution when the value of $dt = 0,001$, the TDSE solution by the Trotter-Suzuki second order and second order hybrid still has a relatively large error. We show the TDSE solution when the value of $dt = 0,0005$ in Figure 12. We present the RMSE table to show the magnitude of the error when when $dt = 0,001$ and $dt = 5 \times 10^{-4}$ in Table 11 and Table 12. Both tables show relatively large error. so, when we use $dx = 0,02$ and $dt = 0,001$ and $dt = 5 \times 10^{-4}$, that both methods cannot be used to solve the TDSE. However, if we reduce the value of dt to 1×10^{-4} and 5×10^{-5}, the TDSE solution by the Trotter-Suzuki second order and second-order hybrid at state $t < 1,5$ will be more accurate. We can see it in Figure 13. To compare the RMSE second order and second-order hybrid, we present the RMSE table in Table 14 and Table 15. RMSE value is smaller than the RMSE with the previous dt, which means the accuracy of the Trotter - Suzuki second order and second order hybrid increases with a small dt value. If we compare the RMSE of the second order and second order hybrid when $dx = 0,02$, the TDSE solution by second order will be more accurate than the TDSE solution by a second order hybrid approach.

In this paper, we also consider the time required for the calculation process. The time comparison for the second order and second-order hybrid to process the calculation is presented in Table 16. The time to process the calculation depends on the selection of dx and dt. When the value of dx is large, the size of the Hamiltonian matrix is small so that the time needed to process calculations is shorter. When $dx = 0,1$, the size of Hamiltonian matrix is 100×100 so that the processing time required for both approaches is relatively short. When dx is reduced to $0,05$, the Hamiltonian matrix size is doubled from the matrix size when $dx = 0,1$ so that the processing time required is longer. From the comparison of Trotter–Suzuki second order and second order hybrid, the time to process the calculation by the Trotter – Suzuki second-order hybrid is almost twice the processing time for the first order approach. Likewise, when the value of dx continues to be reduced, the time required to process the calculation will be longer.

Of the three methods, the second-order hybrid takes longer to process the calculations. This method takes a long time to process the calculations because it involves a commutator matrix. So that the exponential matrix involves a large matrix size.

4 CONCLUSION

In summary, we can use Trotter-Suzuki decomposition first-order, second-order or second-order hybrid to solve the Time Dependent Schrödinger Equation (TDSE) equation with the condition $t < 1$. Meanwhile, when $t > 1$, there is instability in the three methods. Because of this instability, the three tested methods have the same error size in the condition $t > 1$. The accuracy of the second order Trotter-Suzuki decomposition is more accurate than the first order for each selection of the tested dx and dt values. Meanwhile, the second-order hybrid Trotter-Suzuki decomposition will be more accurate than the second-order Trotter-Suzuki decomposition only if the value of $dx = 0,1$ and $0,05$ with $dt \leq 1 \times 10^{-4}$. The second order hybrid Trotter-Suzuki Decomposition calculation process takes longer than the second order.

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LIST OF TABLES AND FIGURE

Table 1: RMSE of Trotter–Suzuki decomposition first-order, second-order, and second-order hybrids with values of $dx = 0.1$ and $dt = 0.01$ at a certain time

time (t)	RMSE 1st order approach	RMSE 2nd order approach	RMSE 2nd order hybrid approach
0,5	1,5723,E-03	7,4891,E-04	3,7357,E-03
1	1,5797,E-03	1,0096,E-03	4,4561,E-03
1,5	1,5434,E-03	1,0424,E-03	4,5917,E-03
2	2,7772,E-03	2,5787,E-03	6,9277,E-03
2,5	6,2799,E-03	6,3180,E-03	8,8812,E-03
3	8,8526,E-03	8,9728,E-03	8,9069,E-03

Table 2: RMSE of Trotter–Suzuki decomposition first-order, second-order, and second-order hybrids with values of $dx = 0.1$ and $dt = 0.001$ at a certain time

time (t)	RMSE 1st order approach	RMSE 2nd order approach	RMSE 2nd order hybrid approach
0,5	1,3584,E-04	4,0846,E-05	2,0787,E-05
1	1,2776,E-04	4,7364,E-05	3,5441,E-05
1,5	1,7679,E-04	1,3756,E-04	1,3827,E-04
2	1,8679,E-03	1,8670,E-03	1,8947,E-03
2,5	6,0134,E-03	6,0177,E-03	6,0543,E-03
3	9,2677,E-03	9,2716,E-03	9,2850,E-03

Table 3: RMSE of Trotter–Suzuki decomposition first-order, second-order, and second-order hybrids with values of $dx = 0.1$ and $dt = 5 \times 10^{-4}$ at a certain time

time (t)	RMSE 1st order approach	RMSE 2nd order approach	RMSE 2nd order hybrid approach
0,5	7,9600,E-05	4,6093,E-05	4,0844,E-05
1	7,9330,E-05	5,2585,E-05	4,7360,E-05
1,5	1,5021,E-04	1,3956,E-04	1,3871,E-04
2	1,8796,E-03	1,8799,E-03	1,8868,E-03
2,5	6,0537,E-03	6,0558,E-03	6,0650,E-03
3	9,3045,E-03	9,3062,E-03	9,3095,E-03

Table 4: RMSE of Trotter–Suzuki decomposition first-order, second-order, and second-order hybrids with values of $dx = 0.1$ and $dt = 1 \times 10^{-4}$ at a certain time

time (t)	RMSE 1st order approach	RMSE 2nd order approach	RMSE 2nd order hybrid approach
0,5	4,9566,E-05	4,7780,E-05	4,7569,E-05
1	5,5657,E-05	5,4362,E-05	5,4137,E-05
1,5	1,4125,E-04	1,4082,E-04	1,4077,E-04
2	1,8935,E-03	1,8937,E-03	1,8940,E-03
2,5	6,0904,E-03	6,0909,E-03	6,0912,E-03
3	9,3349,E-03	9,3352,E-03	9,3353,E-03

Table 5: RMSE of Trotter–Suzuki decomposition first-order, second-order, and second-order hybrids with values of $dx = 0.1$ and $dt = 5 \times 10^{-5}$ at a certain time

time (t)	RMSE 1st order approach	RMSE 2nd order approach	RMSE 2nd order hybrid approach
0,5	4,8302,E-05	4,7833,E-05	4,7780,E-05
1	5,4748,E-05	5,4418,E-05	5,4361,E-05
1,5	1,4105,E-04	1,4094,E-04	1,4093,E-04
2	1,8955,E-03	1,8956,E-03	1,8957,E-03
2,5	6,0953,E-03	6,0955,E-03	6,0956,E-03
3	9,3387,E-03	9,3389,E-03	9,3389,E-03

Table 6: RMSE of Trotter–Suzuki decomposition first-order, second-order, and second-order hybrids with values of $dx = 0{,}05$ and $dt = 0,01$ at a certain time

time (t)	RMSE 1st order approach	RMSE 2nd order approach	RMSE 2nd order hybrid approach
0,5	5,0862,E-04	8,8718,E-04	8,1583,E-03
1	1,0927,E-03	1,0755,E-03	8,7488,E-03
1,5	1,4336,E-03	6,9704,E-04	5,3455,E-03
2	1,5980,E-03	1,0888,E-03	6,8796,E-03
2,5	2,6546,E-03	2,5792,E-03	6,5830,E-03
3	3,8845,E-03	4,0020,E-03	6,4843,E-03

Table 7: RMSE of Trotter–Suzuki decomposition first-order, second-order, and second-order hybrids with values of $dx = 0{,}05$ and $dt = 0,001$ at a certain time

time (t)	RMSE 1st order approach	RMSE 2nd order approach	RMSE 2nd order hybrid approach
0,5	9,7713,E-05	5,5425,E-05	2,4765,E-04
1	1,0992,E-04	7,6011,E-05	3,2700,E-04
1,5	1,7353,E-04	1,1364,E-04	3,5731,E-04
2	1,0058,E-03	1,0013,E-03	1,2945,E-03
2,5	3,0238,E-03	3,0255,E-03	3,3294,E-03
3	4,5669,E-03	4,5703,E-03	4,6592,E-03

Table 8: RMSE of Trotter–Suzuki decomposition first-order, second-order, and second-order hybrids with values of $dx = 0{,}05$ and $dt = 5 \times 10^{-4}$ at a certain time

time (t)	RMSE 1st order approach	RMSE 2nd order approach	RMSE 2nd order hybrid approach
0,5	4,1180,E-05	9,4825,E-06	5,5276,E-05
1	4,2665,E-05	1,5708,E-05	7,6008,E-05
1,5	9,9431,E-05	7,4762,E-05	1,1502,E-04
2	9,6013,E-04	9,5920,E-04	1,0231,E-03
2,5	2,9966,E-03	2,9975,E-03	3,0742,E-03
3	4,5801,E-03	4,5813,E-03	4,6073,E-03

Table 9: RMSE of Trotter–Suzuki decomposition first-order, second-order, and second-order hybrids with values of $dx = 0{,}05$ and $dt = 1 \times 10^{-4}$ at a certain time

time (t)	RMSE 1st order approach	RMSE 2nd order approach	RMSE 2nd order hybrid approach
0,5	9,6704,E-06	5,3765,E-06	3,67073E-06
1	1,0264,E-05	1,5708,E-05	7,6008,E-05
1,5	7,1913,E-05	7,0708,E-05	7,1087,E-05
2	9,5624,E-04	9,5629,E-04	9,5872,E-04
2,5	3,0112,E-03	3,0114,E-03	3,0145,E-03
3	4,6022,E-03	4,6024,E-03	4,6035,E-03

Table 10: RMSE of Trotter–Suzuki decomposition first-order, second-order, and second-order hybrids with values of $dx = 0{,}05$ and $dt = 5 \times 10^{-5}$ at a certain time

time (t)	RMSE 1st order approach	RMSE 2nd order approach	RMSE 2nd order hybrid approach
0,5	7,0748,E-06	5,8125,E-06	5,3765,E-06
1	7,9663,E-06	6,8968,E-06	6,4780,E-06
1,5	7,1083,E-05	7,0781,E-05	7,0862,E-05
2	9,5772,E-04	9,5776,E-04	9,5837,E-04
2,5	3,0154,E-03	3,0155,E-03	3,0163,E-03
3	4,6057,E-03	4,6058,E-03	4,6061,E-03

Table 11: RMSE of Trotter–Suzuki decomposition first-order, second-order, and second-order hybrids with values of $dx = 0{,}02$ and $dt = 0,01$ at a certain time

time (t)	RMSE 1st order approach	RMSE 2nd order approach	RMSE 2nd order hybrid approach
0,5	1,4319,E-03	1,4347,E-03	4,0222,E-03
1	2,9432,E-03	2,9504,E-03	2,9134,E-03
1,5	3,7912,E-03	3,8010,E-03	2,7630,E-03
2	4,2857,E-03	4,2966,E-03	2,3926,E-03
2,5	4,6035,E-03	4,6149,E-03	2,3430,E-03
3	4,8195,E-03	4,8316,E-03	2,4858,E-03

Table 12: RMSE of Trotter–Suzuki decomposition first-order, second-order, and second-order hybrids with values of $dx = 0{,}02$ and $dt = 0,001$ at a certain time

time (t)	RMSE 1st order approach	RMSE 2nd order approach	RMSE 2nd order hybrid approach
0,5	1,8149,E-03	1,8018,E-03	3,0665,E-03
1	1,8563,E-03	1,8505,E-03	3,8772,E-03
1,5	2,1065,E-03	2,1103,E-03	1,5378,E-03
2	1,9833,E-03	1,9867,E-03	2,1407,E-03
2,5	1,6497,E-03	1,6536,E-03	2,1269,E-03
3	1,5513,E-03	1,5578,E-03	1,7617,E-03

Table 13: RMSE of Trotter–Suzuki decomposition first-order, second-order, and second-order hybrids with values of $dx = 0{,}02$ and $dt = 5 \times 10^{-4}$ at a certain time

time (t)	RMSE 1st order approach	RMSE 2nd order approach	RMSE 2nd order hybrid approach
0,5	2,7961,E-04	2,7014,E-04	1,3099,E-03
1	3,4929,E-04	3,4444,E-04	1,4156,E-03
1,5	3,6774,E-04	3,6361,E-04	1,6686,E-03
2	7,9552,E-04	7,9439,E-04	1,9776,E-03
2,5	1,5341,E-03	1,5349,E-03	1,7541,E-03
3	1,8736,E-03	1,8752,E-03	1,7503,E-03

Table 14: RMSE of Trotter–Suzuki decomposition first-order, second-order, and second-order hybrids with values of $dx = 0{,}02$ and $dt = 1 \times 10^{-4}$ at a certain time

time (t)	RMSE 1st order approach	RMSE 2nd order approach	RMSE 2nd order hybrid approach
0,5	1,5798,E-05	9,0443,E-06	3,7903,E-05
1	1,6544,E-05	1,2391,E-05	5,0788,E-05
1,5	3,4908,E-05	3,3321,E-05	6,4716,E-05
2	3,8812,E-04	3,8801,E-04	4,3049,E-04
2,5	1,2016,E-03	1,2017,E-03	1,2506,E-03
3	1,8276,E-03	1,8277,E-03	1,8433,E-03

Table 15: RMSE of Trotter–Suzuki decomposition first-order, second-order, and second-order hybrids with values of $dx = 0{,}02$ and $dt = 5 \times 10^{-5}$ at a certain time

time (t)	RMSE 1st order approach	RMSE 2nd order approach	RMSE 2nd order hybrid approach
0,5	6,7536,E-06	1,9714,E-06	9,0426,E-06
1	6,2653,E-06	3,0350,E-06	1,2391,E-05
1,5	2,9620,E-05	2,9160,E-05	3,3482,E-05
2	3,8025,E-04	3,8024,E-04	3,9015,E-04
2,5	1,1943,E-03	1,1943,E-03	1,2065,E-03
3	1,8271,E-03	1,8272,E-03	1,8313,E-03

Table 16: The time of computing the Trotter–Suzuki decomposition second-order and the Trotter–Suzuki hybrid decomposition second-order at each value of dx and dt

	dx=0,1		dx=0,05		dx=0,02	
dt	Time 2nd order (sec)	Times 2nd order hybrid (sec)	Time 2nd order (sec)	Times 2nd order hybrid (sec)	Time 2nd order (sec)	Time 2nd order hybrid (sec)
0,01	0,258287	0,295155	0,402231	0,669569	0,832481	2,738176
0,001	1,56749	1,265472	2,168436	3,107487	4,708539	8,576393
0,0005	2,229103	2,503294	3,659846	4,804617	8,849544	19,105147
0,0001	8,494141	8,269577	15,58965	22,204065	44,677553	92,593644
0,00005	16,225401	16,135152	30,553682	43,449828	81,828591	186,72913

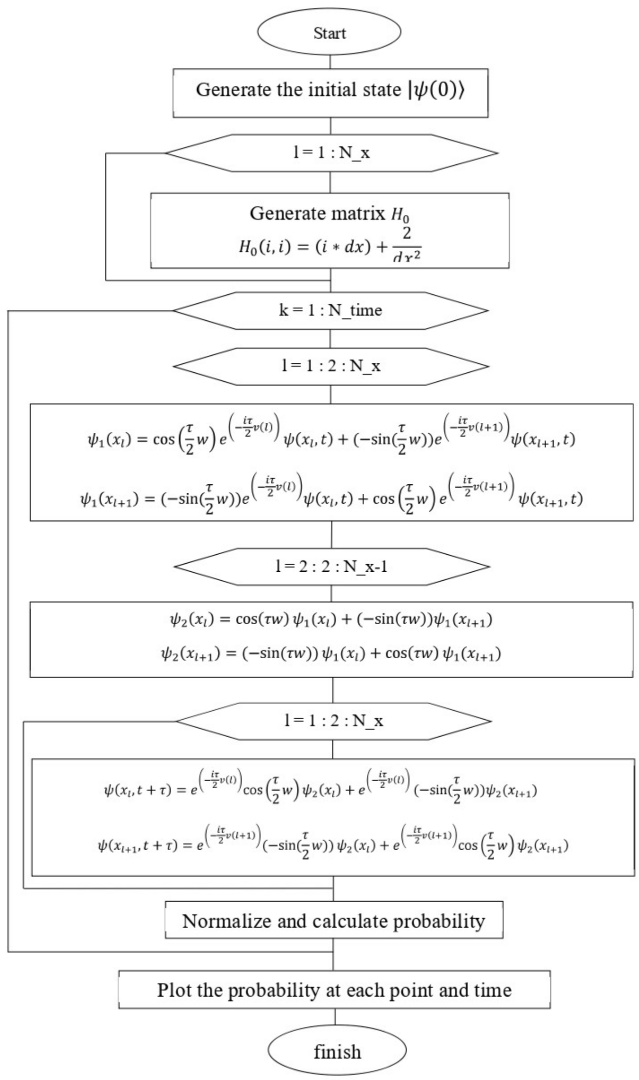

Figure 1: the flowchart of TDSE solution with Trotter – Suzuki second-order decomposition

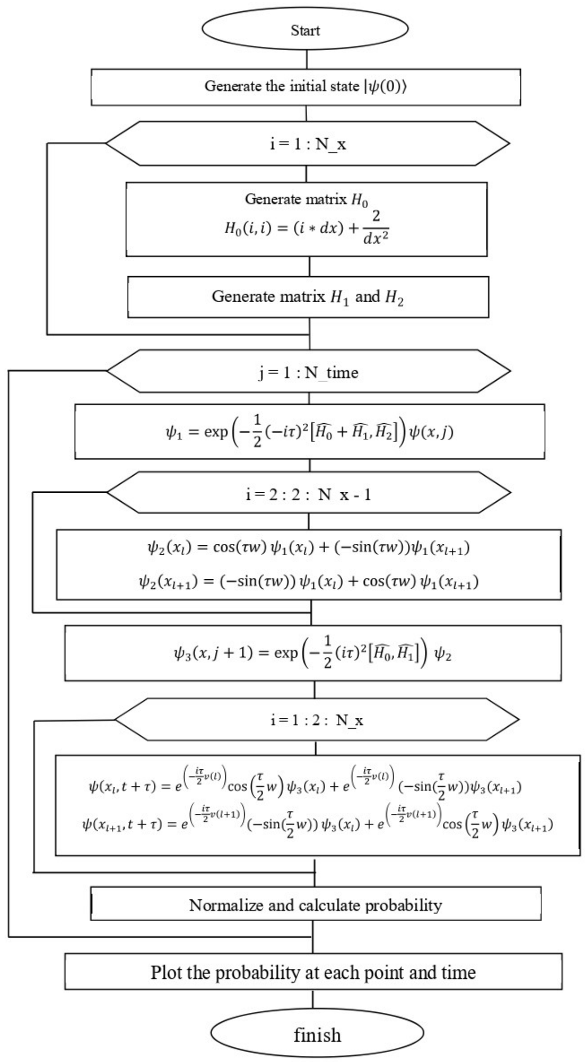

Figure 2: the flowchart of TDSE solution with Trotter – Suzuki hybrid second-order decomposition

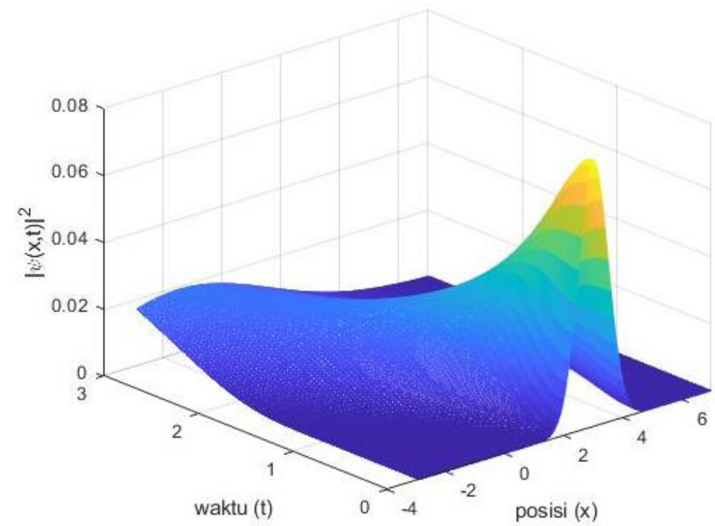

Figure 3: The solution $|\psi(x,t)|^2$ using Baker – Campbell – Hausdorff method (Soto-Eguibar and Moya-Cessa, 2015) with dx=0,1 dan dt=0,01

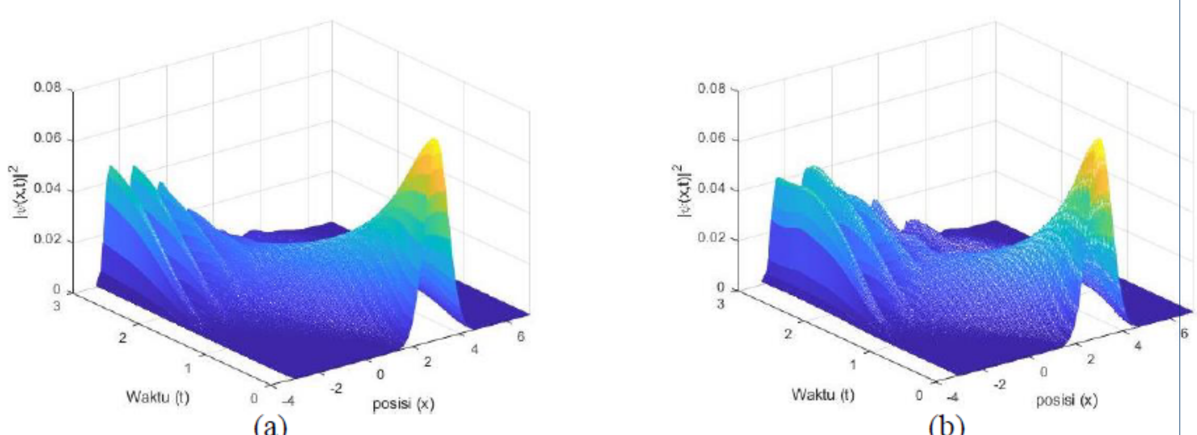

Figure 4: The solution $|\psi(x,t)|^2$ using (a) Trotter – Suzuki decomposition second order and (b) second order hybrid with dx=0,1 dan dt=0,01

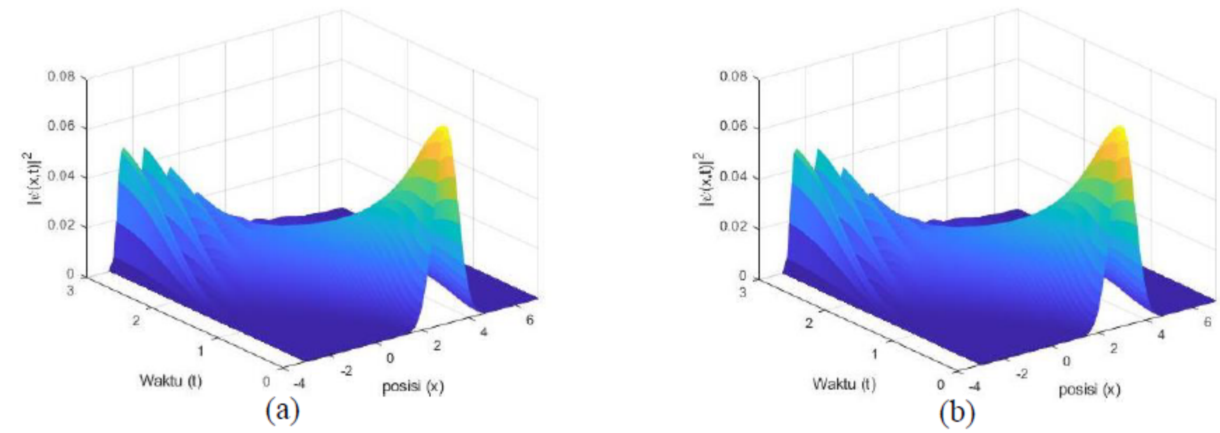

Figure 5: The solution $|\psi(x,t)|^2$ using (a) Trotter – Suzuki decomposition second order and (b) second order hybrid with dx=0,1 dan dt=0,001

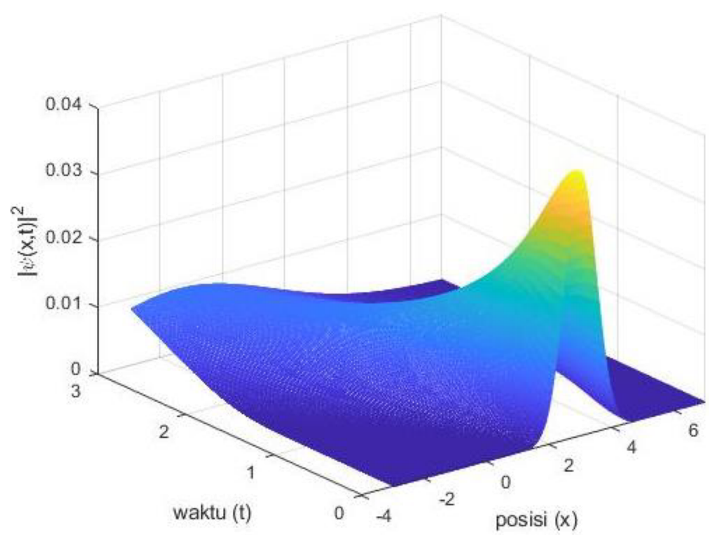

Figure 6: The solution $|\psi(x,t)|^2$ using Baker – Campbell – Hausdorff method with dx=0,05 dan dt=0,01

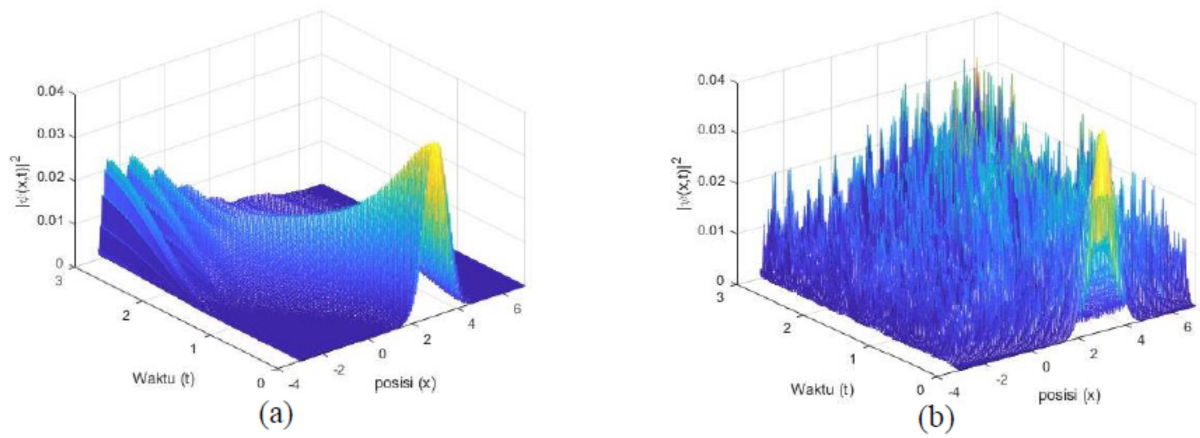

Figure 7: The solution $|\psi(x,t)|^2$ using (a) Trotter – Suzuki decomposition second order and (b) second order hybrid with dx=0,05 dan dt=0,01

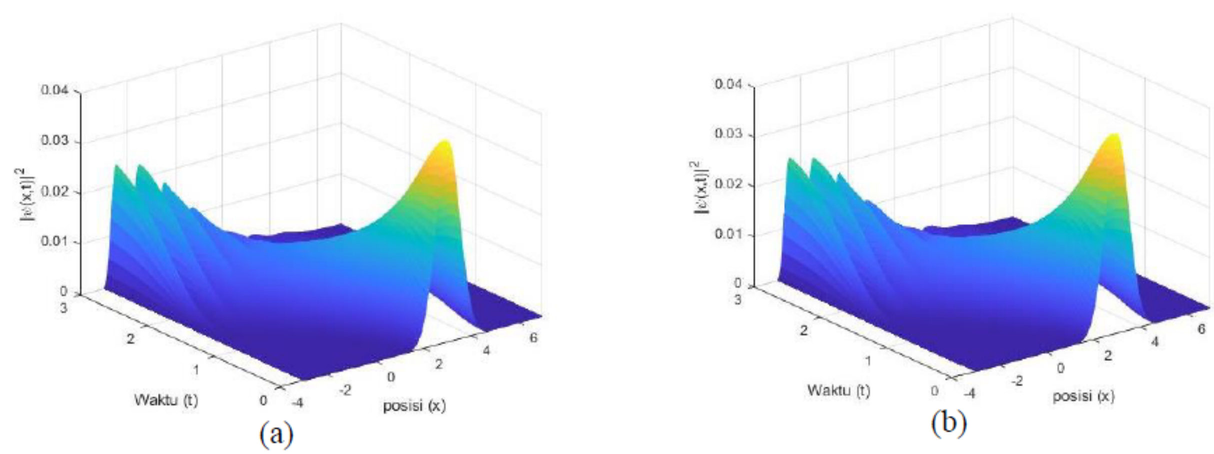

Figure 8: The solution $|\psi(x,t)|^2$ using (a) Trotter – Suzuki decomposition second order and (b) second order hybrid with dx=0,05 dan dt=0,001

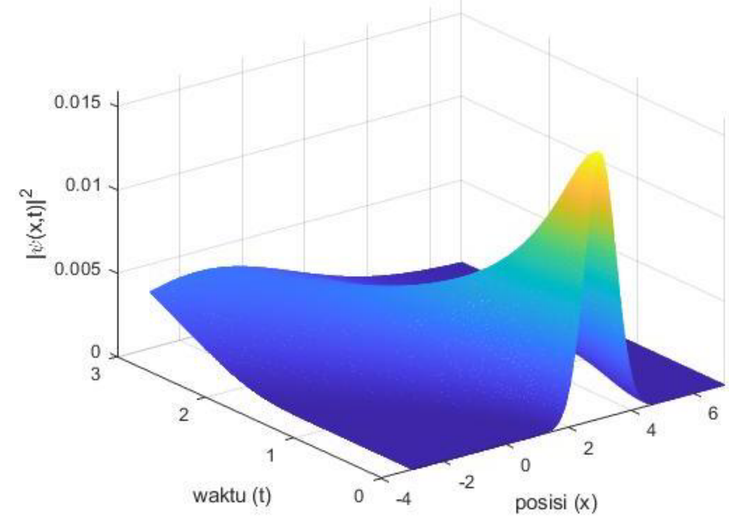

Figure 9: The solution $|\psi(x,t)|^2$ using Baker – Campbell – Hausdorff method with dx=0,02 dan dt=0,01

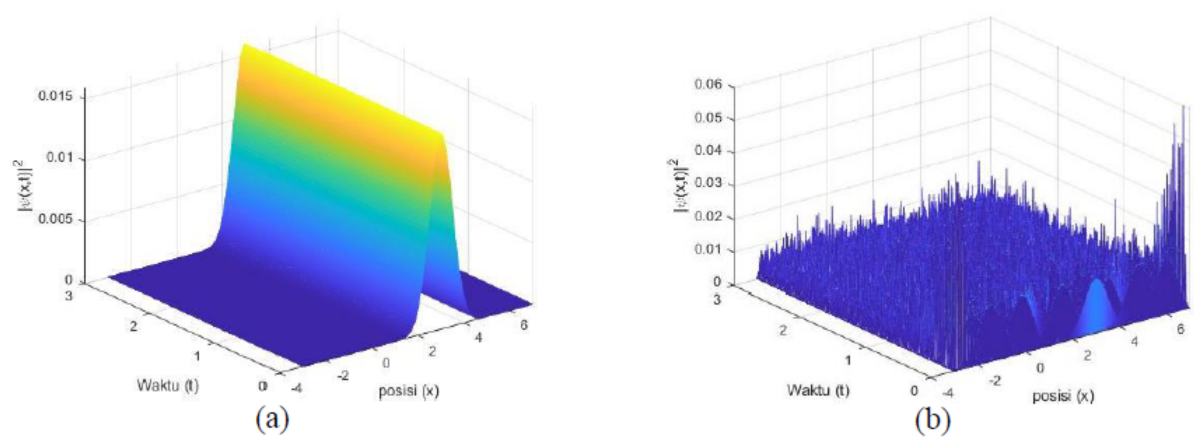

Figure 10: The solution $|\psi(x,t)|^2$ using (a) Trotter – Suzuki decomposition second order and (b) second order hybrid with dx=0,02 dan dt=0,01

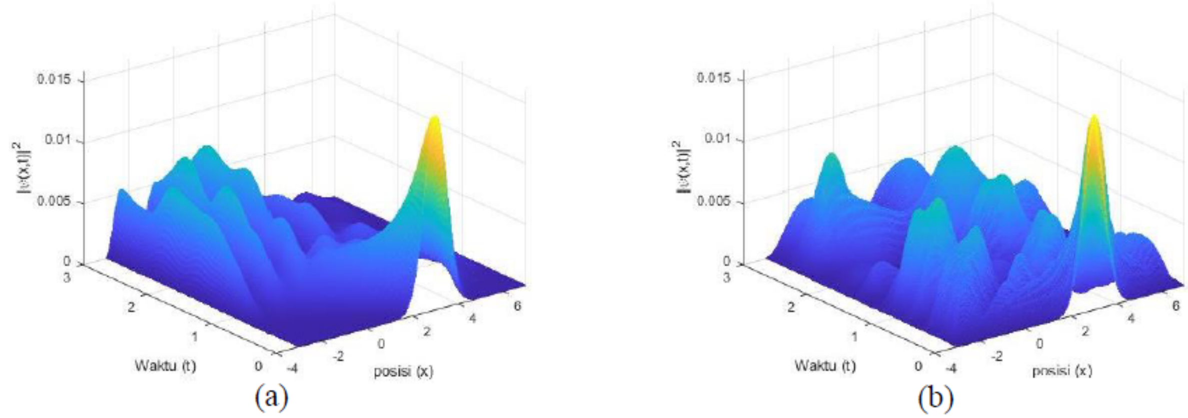

Figure 11: The solution $|\psi(x,t)|^2$ using (a) Trotter – Suzuki decomposition second order and (b) second order hybrid with dx=0,02 dan dt=0,001

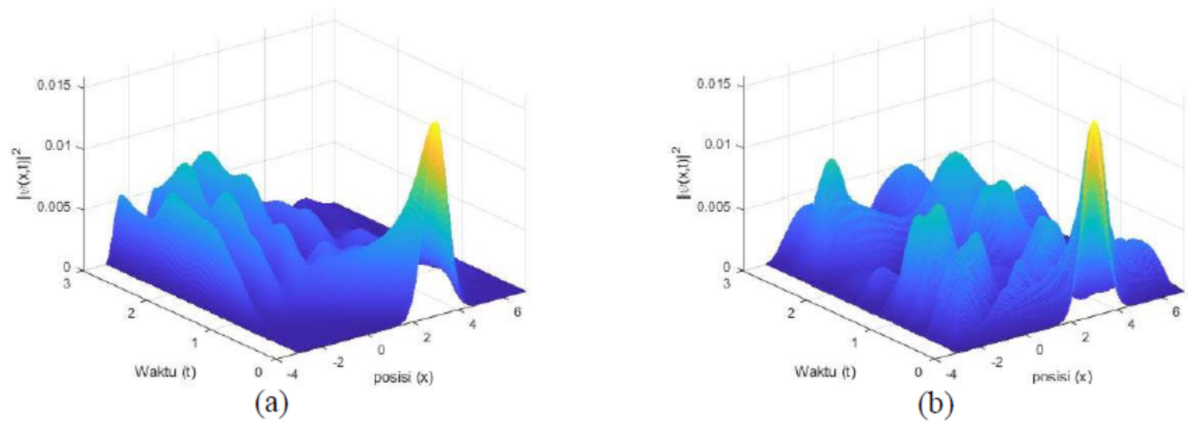

Figure 12: The solution $|\psi(x,t)|^2$ using (a) Trotter – Suzuki decomposition second order and (b) second order hybrid with dx=0,02 dan $dt = 5 \times 10^{-4}$

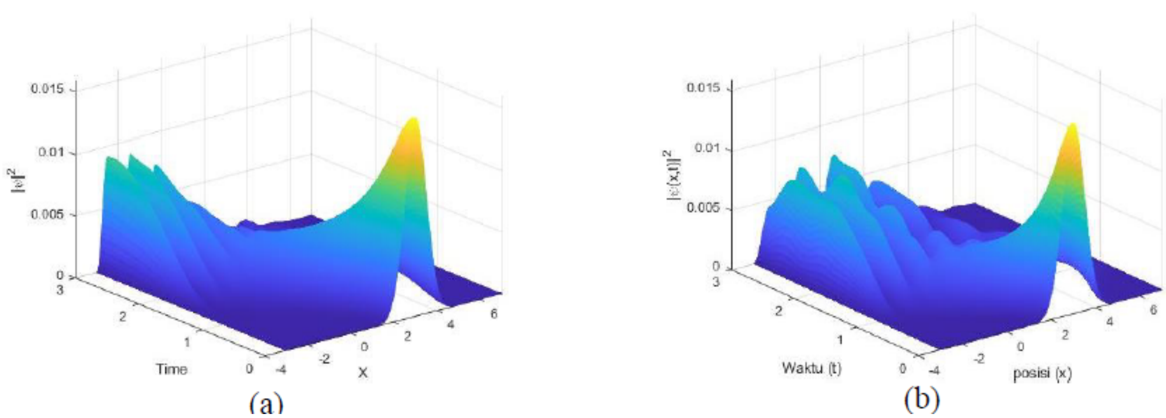

Figure 13: The solution $|\psi(x,t)|^2$ using (a) Trotter – Suzuki decomposition second order and (b) second order hybrid with dx=0,02 dan $dt = 1 \times 10^{-4}$

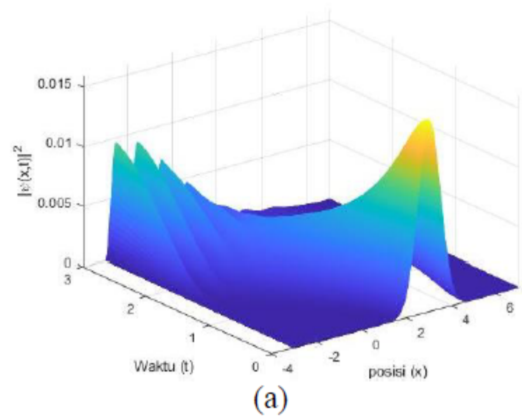

Figure 14: The solution $|\psi(x,t)|^2$ using (a) Trotter – Suzuki decomposition second order and (b) second order hybrid with dx=0,02 dan $dt = 1 \times 10^{-4}$