Computational Physics Course 17104 Lecture 9

Hartmut Ruhl, Nils Moschüring, and Nina Elkina
LMU, Theresienstrasse 37, Munich, Room C113

Dec 4 and 6, 2012

Topics

Literature

Schrödinger equation

Hartmut Ruhl, Nils Moschüring, and Nina Elkina
LMU, Theresienstrasse 37, Munich, Room C113

Topics

- Higher order Schrödinger equation integrators.

Hartmut Ruhl, Nils Moschüring, and Nina Elkina
LMU, Theresienstrasse 37, Munich, Room C113

Useful literature

- Dennis M. Sullivan, *Electromagnetic Simulation Using The FDTD Method*, IEEE Press Series on RF and Microwave Technology, Poger D. Pollard and Richard Booton, ISBN: 0-7803-4747-1.
- Frederick Ira Moxley III, Fei Zhu, and Weizhong Dai, *A Generalized FDTD Method with Absorbing Boundary Condition for Solving a Time-Dependent Linear Schrödinger Equation*, American J. of Comp. Math. **2**, 163-172 (2012).

The generalized FDTD method

To derive a generalized FDTD scheme we write

$$\partial_t \psi_{Re}(x,t) = \left(-\frac{\hbar}{2m} A + \frac{V(x)}{\hbar} \right) \psi_{Im}(x,t) \,, \quad (1)$$

$$\partial_t \psi_{Im}(x,t) = \left(+\frac{\hbar}{2m} A - \frac{V(x)}{\hbar} \right) \psi_{Re}(x,t) \,. \quad (2)$$

Next we expand $\psi_{Re}(x,t_n)$ and $\psi_{Re}(x,t_{n-1})$ about $t_{n-0.5}$

$$\begin{aligned} \psi_{Re}(x,t_n) = \psi_{Re}(x,t_{n-0.5}) &+ \frac{\Delta t}{2} \partial_t \psi_{Re}(x,t_{n-0.5}) \\ &+ \frac{1}{2!} \left(\frac{\Delta t}{2} \right)^2 \partial_t^2 \psi_{Re}(x,t_{n-0.5}) \\ &+ \frac{1}{3!} \left(\frac{\Delta t}{2} \right)^3 \partial_t^3 \psi_{Re}(x,t_{n-0.5}) \pm \dots \end{aligned} \quad (3)$$

$$\begin{aligned} \psi_{Re}(x,t_{n-1}) = \psi_{Re}(x,t_{n-0.5}) &- \frac{\Delta t}{2} \partial_t \psi_{Re}(x,t_{n-0.5}) \\ &+ \frac{1}{2!} \left(\frac{\Delta t}{2} \right)^2 \partial_t^2 \psi_{Re}(x,t_{n-0.5}) \\ &- \frac{1}{3!} \left(\frac{\Delta t}{2} \right)^3 \partial_t^3 \psi_{Re}(x,t_{n-0.5}) \pm \dots \end{aligned} \quad (4)$$

The generalized FDTD method

Subtracting $\psi_{Re}(x,t_{n-1})$ from $\psi_{Re}(x,t_n)$ yields

$$\psi_{Re}(x,t_n) = \psi_{Re}(x,t_{n-1}) + 2\sum_{p=0}^{\infty}\left(\frac{\Delta t}{2}\right)^{2p+1}\frac{1}{(2p+1)!}\,\partial_t^{2p+1}\psi_{Re}(x,t_{n-0.5})\,. \tag{5}$$

With the help of the Schrödinger equation the time derivatives can be evaluated. We obtain up to order N

$$\begin{aligned}\psi_{Re}(x,t_n) &= \psi_{Re}(x,t_{n-1}) \\ &\quad +2\sum_{p=0}^{N}\left(\frac{\Delta t}{2}\right)^{2p+1}\frac{(-1)^{p+1}}{(2p+1)!}\left(\frac{\hbar A}{2m}-\frac{V}{\hbar}\right)^{2p+1}\psi_{Im}(x,t_{n-0.5}) \\ &\quad +O\left(\Delta t^{2N+3}\right)\,.\end{aligned} \tag{6}$$

Expanding $\psi_{Im}(x,t_{n+0.5})$ and $\psi_{Im}(x,t_{n-0.5})$ about $\psi_{Im}(x,t_n)$ and applying the Schrödinger equation yields

$$\begin{aligned}\psi_{Im}(x,t_{n+0.5}) &= \psi_{Im}(x,t_{n-0.5}) \\ &\quad +2\sum_{p=0}^{N}\left(\frac{\Delta t}{2}\right)^{2p+1}\frac{(-1)^{p}}{(2p+1)!}\left(\frac{\hbar A}{2m}-\frac{V}{\hbar}\right)^{2p+1}\psi_{Re}(x,t_n) \\ &\quad +O\left(\Delta t^{2N+3}\right)\,.\end{aligned} \tag{7}$$

The generalized FDTD method

The discrete Schrödinger equation becomes

$$\psi^{n}_{j,Re} = \psi^{n-1}_{j,Re} + 2\sum_{p=0}^{N} \left(\frac{\Delta t}{2}\right)^{2p+1} \frac{(-1)^{p+1}}{(2p+1)!} \left(\frac{\hbar A}{2m} - \frac{V}{\hbar}\right)^{2p+1} \psi^{n-0.5}_{j,Im} \,, \tag{8}$$

$$\psi^{n+0.5}_{j,Im} = \psi^{n-0.5}_{j,Im} + 2\sum_{p=0}^{N} \left(\frac{\Delta t}{2}\right)^{2p+1} \frac{(-1)^{p}}{(2p+1)!} \left(\frac{\hbar A}{2m} - \frac{V}{\hbar}\right)^{2p+1} \psi^{n}_{j,Re} \,. \tag{9}$$

Next a specific discrete representation of the operator A has to be given. For

$$A\,\psi^{n}_{j,Re} = \frac{\psi^{n}_{j+1,Re} - 2\psi^{n}_{j,Re} + \psi^{n}_{j-1,Re}}{\Delta x^2} \tag{10}$$

we obtain

$$A\,\psi^{n}_{j,Re} = \frac{1}{\Delta x^2}\left(-4\sin^2\frac{k\Delta x}{2}\right)\lambda^{n}_{Re}\,e^{i(jk\Delta x)} \,, \tag{11}$$

$$A\,\psi^{n+0.5}_{j,Im} = \frac{1}{\Delta x^2}\left(-4\sin^2\frac{k\Delta x}{2}\right)\lambda^{n}_{Im}\,e^{i(jk\Delta x)} \,, \tag{12}$$

where the ansatz

$$\psi^{n}_{j,Re} = \lambda^{n}_{Re}\,e^{i(jk\Delta x)} \,, \quad \psi^{n+0.5}_{j,Im} = \lambda^{n}_{Im}\,e^{i(jk\Delta x)} \tag{13}$$

has been made.

The generalized FDTD method

The discrete Schrödinger equation becomes

$$\lambda_{Re}^{n} = \lambda_{Re}^{n-1} + 2\sum_{p=0}^{N} \frac{(-1)^p}{(2p+1)!} \left(\frac{\hbar \Delta t}{m \Delta x^2} \sin^2 \frac{k \Delta x}{2} + \frac{V \Delta t}{2\hbar} \right)^{2p+1} \lambda_{Im}^{n-1} \,, \tag{14}$$

$$\lambda_{Im}^{n} = \lambda_{Im}^{n-1} + 2\sum_{p=0}^{N} \frac{(-1)^{p+1}}{(2p+1)!} \left(\frac{\hbar \Delta t}{m \Delta x^2} \sin^2 \frac{k \Delta x}{2} + \frac{V \Delta t}{2\hbar} \right)^{2p+1} \lambda_{Re}^{n} \,. \tag{15}$$

Alternatively, this can be writen as

$$\lambda_{Re}^{n} = \lambda_{Re}^{n-1} + \alpha \, \lambda_{Im}^{n-1} \,, \tag{16}$$

$$\lambda_{Im}^{n} = \lambda_{Im}^{n-1} - \alpha \, \lambda_{Re}^{n} \,, \tag{17}$$

where

$$\alpha = 2\sum_{p=0}^{N} \frac{(-1)^p}{(2p+1)!} \left(\frac{\hbar \Delta t}{m \Delta x^2} \sin^2 \frac{k \Delta x}{2} + \frac{V \Delta t}{2\hbar} \right)^{2p+1} \,. \tag{18}$$

We find

$$\lambda_{Re}^{n+1} - \lambda_{Re}^{n} = \lambda_{Re}^{n} - \lambda_{Re}^{n-1} + \alpha \left(\lambda_{Im}^{n} + \lambda_{Im}^{n-1} \right) \,, \quad \lambda_{Im}^{n} = \lambda_{Im}^{n-1} - \alpha \, \lambda_{Re}^{n} \,. \tag{19}$$

Hartmut Ruhl, Nils Moschüring, and Nina Elkina
LMU, Theresienstrasse 37, Munich, Room C113

The generalized FDTD method

Finally, we find

$$\lambda_{Re}^{n+1} - \left(2 - \alpha^2\right)\ \lambda_{Re}^{n} + \lambda_{Re}^{n-1} = 0 \tag{20}$$

or

$$\lambda_{Re}^{2} - \left(2 - \alpha^2\right)\ \lambda_{Re} + 1 = 0\,. \tag{21}$$

The solution of this equation is

$$\lambda_{Re} = e^{i\omega\Delta t} \rightarrow 2 - e^{i\omega\Delta t} - e^{-i\omega\Delta t} = \alpha^2 \tag{22}$$

$$1 - \ cos\,\omega\Delta t = \frac{\alpha^2}{2} \rightarrow \sin^2\frac{\omega\Delta t}{2} = \frac{\alpha^2}{4}\ . \tag{23}$$

This leads to

$$\sin^2\frac{\omega\Delta t}{2} = \left(\sum_{p=0}^{N}\frac{(-1)^p}{(2p+1)!}\,\left(\frac{\hbar\Delta t}{m\Delta x^2}\sin^2\frac{k\Delta x}{2} + \frac{V\Delta t}{2\hbar}\right)^{2p+1}\right)^2\ . \tag{24}$$

The generalized FDTD method

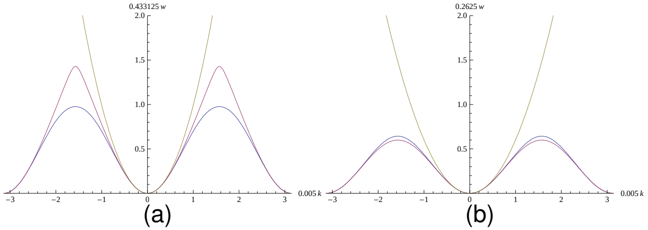
Hartmut Ruhl, Nils Moschüring, and Nina Elkina LMU, Theresienstrasse 37, Munich, Room C113

Topics
Literature
Schrödinger equation

For vanishing potential we obtain for the $\Delta t^4 \Delta x^2$ order approximation

$$\sin^2 \frac{\omega \Delta t}{2} = \left(\frac{\hbar \Delta t}{m \Delta x^2} \sin^2 \frac{k \Delta x}{2} - \frac{1}{3!} \left(\frac{\hbar \Delta t}{m \Delta x^2} \sin^2 \frac{k \Delta x}{2} \right)^3 \right)^2 . \tag{25}$$

The plots below compare analytical (yellow) , $\Delta t^2 \Delta x^2$ order FDTD (red), and $\Delta t^4 \Delta x^2$ order FDTD (blue) dispersion relations for (a) a Courant factor of 0.99 and (b) a Courant factor 0.6. For the Courant factor 0.6 the second and first orders are almost identical implying that the higher order FDTD scheme is much more stable than the lowest order one.



The generalized FDTD method: Comparison

For the classical FDTD method we have found

$$2i\,\psi_{0,Re}\ \sin\left(\frac{\omega\Delta t}{2}\right) = -\psi_{0,Im}\frac{2\hbar\Delta t}{m\Delta x^2}\ \sin^2\left(\frac{k\Delta x}{2}\right)\ , \tag{26}$$

$$2i\,\psi_{0,Im}\ \sin\left(\frac{\omega\Delta t}{2}\right) = +\psi_{0,Re}\frac{2\hbar\Delta t}{m\Delta x^2}\ \sin^2\left(\frac{k\Delta x}{2}\right) \tag{27}$$

or alternatively

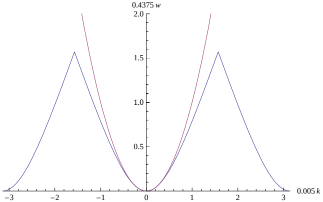
$$\begin{pmatrix} 2i\ \sin\left(\frac{\omega\Delta t}{2}\right) & \frac{2\hbar\Delta t}{m\Delta x^2}\ \sin^2\left(\frac{k\Delta x}{2}\right) \\ -\frac{2\hbar\Delta t}{m\Delta x^2}\ \sin^2\left(\frac{k\Delta x}{2}\right) & 2i\ \sin\left(\frac{\omega\Delta t}{2}\right) \end{pmatrix} \begin{pmatrix} \psi_{Re} \\ \psi_{Im} \end{pmatrix} = 0\ . \tag{28}$$

This yields the lowest order dispersion contribution of the generalized FDTD scheme

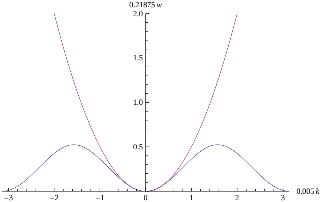
$$\sin^2\left(\frac{\omega\Delta t}{2}\right) = \left(\frac{\hbar\Delta t}{m\Delta x^2}\right)^2\ \sin^4\left(\frac{k\Delta x}{2}\right)\ . \tag{29}$$

Schrödinger equation: Dispersion

Plot of the discrete dispersion relation of the Schrödinger equation for (c) $\Delta x = 0.01\mu$m and $\Delta t = m_e\, \Delta x^2/\hbar$ and (d) $\Delta t = 0.5\, m_e\, \Delta x^2/\hbar$.



(c)



(d)

The generalized FDTD method

If we make use of a 4th order discrete representation of the operator A

$$A\,\psi^n_{j,Re} = \frac{-\psi^n_{j+2,Re} + 16\psi^n_{j+1,Re} - 30\psi^n_{j,Re} + 16\psi^n_{j-1,Re} - \psi^n_{j-2,Re}}{12\,\Delta x^2} \tag{30}$$

we obtain

$$A\,\psi^n_{j,Re} = -\frac{4}{3\Delta x^2}\sin^2\frac{k\Delta x}{2}\left(3+\sin^2\frac{k\Delta x}{2}\right)\lambda^n_{Re}\,e^{i(jk\Delta x)}\,, \tag{31}$$

$$A\,\psi^{n+0.5}_{j,Im} = -\frac{4}{3\Delta x^2}\sin^2\frac{k\Delta x}{2}\left(3+\sin^2\frac{k\Delta x}{2}\right)\lambda^n_{Im}\,e^{i(jk\Delta x)}\,, \tag{32}$$

where the ansatz

$$\psi^n_{j,Re} = \lambda^n_{Re}\,e^{i(jk\Delta x)}\,,\quad \psi^{n+0.5}_{j,Im} = \lambda^n_{Im}\,e^{i(jk\Delta x)} \tag{33}$$

has been made. The discrete Schrödinger equation becomes

$$\psi^n_{j,Re} = \psi^{n-1}_{j,Re} + 2\sum_{p=0}^{N}\left(\frac{\Delta t}{2}\right)^{2p+1}\frac{(-1)^{p+1}}{(2p+1)!}\left(\frac{\hbar A}{2m} - \frac{V}{\hbar}\right)^{2p+1}\psi^{n-0.5}_{j,Im}\,, \tag{34}$$

$$\psi^{n+0.5}_{j,Im} = \psi^{n-0.5}_{j,Im} + 2\sum_{p=0}^{N}\left(\frac{\Delta t}{2}\right)^{2p+1}\frac{(-1)^{p}}{(2p+1)!}\left(\frac{\hbar A}{2m} - \frac{V}{\hbar}\right)^{2p+1}\psi^{n}_{j,Re}\,. \tag{35}$$

The generalized FDTD method

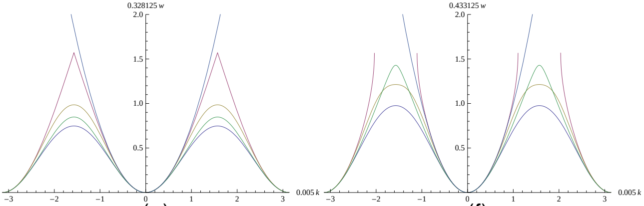
For vanishing potential we obtain for the $\Delta t^2 \Delta x^4$ order FDTD dispersion

$$\sin^2 \frac{\omega \Delta t}{2} = \left(\frac{\hbar \Delta t}{3 m \Delta x^2} \sin^2 \frac{k \Delta x}{2} \left(3 + sin^2 \frac{k \Delta x}{2} \right) \right)^2 \tag{36}$$

and for the $\Delta t^4 \Delta x^4$ order dispersion

$$\begin{aligned} \sin^2 \frac{\omega \Delta t}{2} = \Bigg(& \frac{\hbar \Delta t}{3 m \Delta x^2} \sin^2 \frac{k \Delta x}{2} \left(3 + sin^2 \frac{k \Delta x}{2} \right) \\ & - \frac{1}{3!} \left(\frac{\hbar \Delta t}{3 m \Delta x^2} \sin^2 \frac{k \Delta x}{2} \left(3 + sin^2 \frac{k \Delta x}{2} \right) \right)^3 \Bigg)^2 . \end{aligned} \tag{37}$$

The plots below compare analytical (blue) , $\Delta t^2 \Delta x^4$ order FDTD (red), $\Delta t^2 \Delta x^2$ order FDTD (green), $\Delta t^4 \Delta x^4$ order FDTD (yellow), and $\Delta t^4 \Delta x^2$ order (blue) dispersion relations for (e) a Courant factor of 0.75 and (f) 0.99. The $\Delta t^4 \Delta x^4$ scheme is stable for 0.99 and approximates dispersion better.



(e) (f)

Schrödinger equation: Exercises

Hartmut Ruhl, Nils Moschüring, and Nina Elkina
LMU, Theresienstrasse 37, Munich, Room C113

Exercise: Write a *C*-program for the $\Delta t^4 \Delta x^2$ and $\Delta t^4 \Delta x^4$ order FDTD solvers of the free Schrödinger equation with periodic boundary conditions in 3D. Assume that

$$\psi(\vec{x}, 0) = e^{-\frac{x^2}{w_x^2}} \, e^{-\frac{y^2}{w_y^2}} \, e^{-\frac{z^2}{w_z^2}} \, e^{ik_{x0} x} \tag{38}$$

holds, where w_x, w_y, and w_z determine the widths of the Gaussian wave packet and k_{x0} is the initial momentum of the wave. Obtain the $\Delta t^4 \Delta x^2$ and $\Delta t^4 \Delta x^4$ order dispersion relations of the free Schrödinger equation in 3D. Compare the speed of integration with the $\Delta t^2 \Delta x^2$ order scheme.

Schrödinger equation: Dispersion in 3D

Hartmut Ruhl, Nils Moschüring, and Nina Elkina
LMU, Theresienstrasse 37, Munich, Room C113

In 3D we obtain

$$\sin^2\left(\frac{\omega\Delta t}{2}\right) = \left(\frac{\hbar\Delta t}{m\Delta x^2}\right)^2 \sin^4\left(\frac{k_x\Delta x}{2}\right) + \left(\frac{\hbar\Delta t}{m\Delta y^2}\right)^2 \sin^4\left(\frac{k_y\Delta y}{2}\right) + \left(\frac{\hbar\Delta t}{m\Delta z^2}\right)^2 \sin^4\left(\frac{k_z\Delta z}{2}\right) \tag{39}$$

or

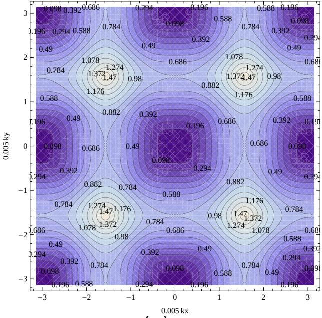
$$\frac{\omega\Delta t}{2} = \arcsin\left(\left[\left(\frac{\hbar\Delta t}{m\Delta x^2}\right)^2 \sin^4\left(\frac{k_x\Delta x}{2}\right) + \left(\frac{\hbar\Delta t}{m\Delta y^2}\right)^2 \sin^4\left(\frac{k_y\Delta y}{2}\right) + \left(\frac{\hbar\Delta t}{m\Delta z^2}\right)^2 \sin^4\left(\frac{k_z\Delta z}{2}\right)\right]^{\frac{1}{2}}\right) , \tag{40}$$

where the more general expressions from above have to be inserted for higher order integrators.

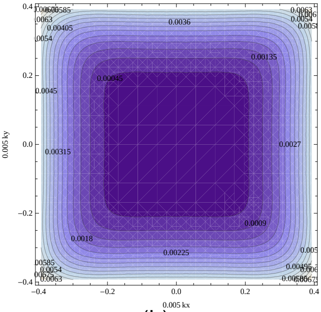
Schrödinger equation: Dispersion 2D

Plot of (g) the discrete dispersion relation of the Schrödinger equation for $\Delta x = \Delta y = 0.01\mu$m and (h) the difference between the analytical and the discrete dispersion relations for

$$\Delta t = \frac{1}{\sqrt{\left(\frac{\hbar}{m_e\,\Delta x^2}\right)^2 + \left(\frac{\hbar}{m_e\,\Delta y^2}\right)^2}} \tag{41}$$



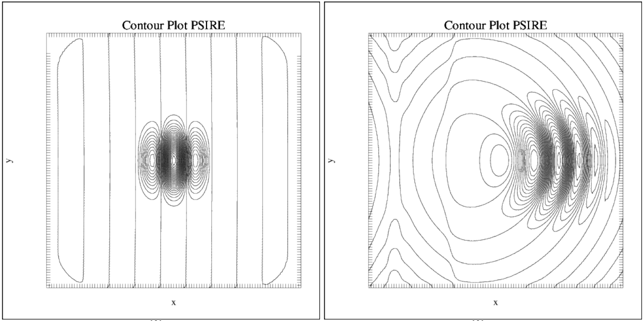
(g)



(h)

Schrödinger equation

Plot of the real part of a Gaussian wave packet propagating to the right with $\hbar = m_e = 1$, box dimensions $L_x = L_y = L_z = 1.0$, resolution $\Delta x = \Delta y = \Delta z = 0.01$, $\Delta t = 2.3 \cdot 10^{-5}$, Gaussian packet widths $w_x = w_y = w_z = 0.1$. Plot (i) gives the real part of the wave packet at $t = 0$ and plot (j) at $t = 300\,\Delta t$ with the $\Delta t^2 \Delta x^2$ order scheme.

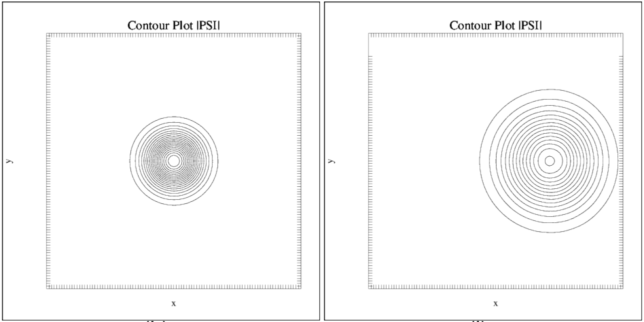


(i) (j)

Hartmut Ruhl, Nils Moschüring, and Nina Elkina LMU, Theresienstrasse 37, Munich, Room C113

Schrödinger equation

Plot of the absolute value of a Gaussian wave packet propagating to the right with $\hbar = m_e = 1$, box dimensions $L_x = L_y = L_z = 1.0$, resolution $\Delta x = \Delta y = \Delta z = 0.01$, $\Delta t = 2.3 \cdot 10^{-5}$, Gaussian packet widths $w_x = w_y = w_z = 0.1$. Plot (k) gives the absolute value of the wave packet at $t = 0$ and plot (l) at $t = 300\,\Delta t$ with the $\Delta t^2 \Delta x^2$ order scheme.



(k) (l)

Schrödinger equation: Exercises

Hartmut Ruhl, Nils Moschüring, and Nina Elkina
LMU, Theresienstrasse 37, Munich, Room C113

Exercise: Write a *C*-program for the $\Delta t^2 \Delta x^2$ order FDTD solver of the Schrödinger equation with an attractive and repulsive harmonic potential with periodic boundary conditions in 3D. Assume that

$$\psi(\vec{x}, 0) = e^{-\frac{x^2}{L_x^2}} \, e^{-\frac{y^2}{L_y^2}} \, e^{-\frac{z^2}{L_z^2}} \, e^{ik_{x0} x} \tag{42}$$

and

$$V(\vec{x}) = V_0 \, e^{-\frac{x^2}{r_x^2}} \, e^{-\frac{y^2}{r_y^2}} \, e^{-\frac{z^2}{r_z^2}} \tag{43}$$

holds, where w_x, w_y, and w_z determine the widths of the Gaussian wave packet and k_{x0} is the initial momentum of the wave, while r_x, r_y, and r_z represent the widths of the potential.