B Tech Project

Visualising the 1-D Schrodinger Equation

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Task

What I have done as part of my project is visualise and simulate the wave function of a particle in a box with a potential barrier, using Python.

The 1-dimensional Schrodinger equation is :

$$i\hbar\frac{\partial\psi}{\partial t} = \frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi$$

- The *wave function ψ* is a function of both position *x* and time *t*. This wave function represents a probability of measuring the particle at a position *x* at a time *t*.
- In order to visualise the wave function, the above equation will need to be solved numerically.
- One mathematical tool that comes in handy over here is the Fourier transform.

- The Fourier transform of the wave function is given by :

$$\widetilde{\psi}(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x,t) e^{-ikx} dx$$

- The corresponding inverse Fourier transform is given by :

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \widetilde{\psi}(k,t) e^{ikx} dk$$

- Using the Fourier transform in the Schrodinger equation, we get a differential equation in the k-space :

$$i\hbar \frac{\partial \widetilde{\psi}}{\partial t} = \frac{\hbar^2 k^2}{2m} \widetilde{\psi} + V(i \frac{\partial}{\partial k}) \widetilde{\psi}$$

- Solving the x-space and the k-space differential equations for a small time interval **Δ**t :

$$\psi(x,t+\Delta t) = \psi(x,t)e^{-iV(x)\Delta t/\hbar}$$

$$\widetilde{\psi}(k,t+\Delta t) = \widetilde{\psi}(k,t)e^{-i\hbar k^2\Delta t/2m}$$

- To solve this computationally, we would need to discretise this procedure. This can be done through Fast Fourier Transform (FFT), where :

$$\widetilde{F}_m = \sum_{n=0}^{N-1} F_n e^{-2\pi inm/N}$$ and $$F_n = \frac{1}{N}\sum_{m=0}^{N-1} \widetilde{F}_m e^{2\pi inm/N}$$, the inverse.

- We would, however, need to make certain approximations to follow this plan of action.

- We assume that the infinite integral in the Fourier transform can be approximated by the finite integral from a to b:

$$\tilde{\psi}(k,t) = \frac{1}{\sqrt{2\pi}} \int_a^b \psi(x,t) e^{-ikx} dx$$

- This approximation ends up being equivalent to assuming that the potential $V(x) \to \infty$ at $x \leq a$ and $x \geq b$. This integral can be further approximated as a Riemann sum of N terms, so that we can define $\Delta x = (b - a)/N$, and $x_n = a + n\Delta x$:

$$\tilde{\psi}(k,t) \simeq \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{N-1} \psi(x_n,t) e^{-ikx_n} \Delta x$$

- Further approximations in the k-space would need us to define $k_m = k_0 + m\Delta k$, with $\Delta k = 2\pi/(N\Delta x) = 2\pi/(b - a)$:

$$\tilde{\psi}(k_m,t) \simeq \frac{1}{\sqrt{2\pi}} \sum_{n=0}^{N-1} \psi(x_n,t) e^{-ik_m x_n} \Delta x$$

- Substituting the expressions for k_m and x_n, we get :

$$\left[\tilde{\psi}(k_m,t)e^{imx_0\Delta k}\right] \simeq \sum_{n=0}^{N-1}\left[\frac{\Delta x}{\sqrt{2\pi}}\psi(x_n,t)e^{-ik_0x_n}\right]e^{-2\pi imn/N}$$

, for the Fourier transform, and

$$\left[\frac{\Delta x}{\sqrt{2\pi}}\psi(x_n,t)e^{-ik_0x_n}\right] \simeq \frac{1}{N}\sum_{m=0}^{N-1}\left[\tilde{\psi}(k_m,t)e^{-imx_0\Delta k}\right]e^{2\pi imn/N}$$

, for the inverse Fourier transform.

- Therefore, we have obtained the discrete analog of the continuous Fourier transform pair.

$$\psi(x,t) \Longleftrightarrow \tilde{\psi}(k,t) \quad \equiv \quad \frac{\Delta x}{\sqrt{2\pi}}\psi(x_n,t)e^{-ik_0x_n} \Longleftrightarrow \tilde{\psi}(k_m,t)e^{-imx_0\Delta k}$$

The steps are...

1. Choose *a*, *b*, *N* and k_0 sufficient to represent the initial state of the wave function $\psi(x)$
2. Then, $\Delta x = (b - a)/N$ and $\Delta k = 2\pi/(b - a)$
3. Define, $x_n = a + n\Delta x$ and $k_m = k_0 + m\Delta k$
4. Discretise the wave function in the x-space for every *n* as :

$$\psi_n(t) = \psi(x_n, t)$$

   Discretise the wave function in the k-space for every m as :

$$\widetilde{\psi}_m = \widetilde{\psi}(k_m, t)$$

   The potential function will also have to be discretised as $V_n = V(x_n)$

5. Compute a half-step (first $\Delta t/2$) in the x-space as follows :

$$\psi_n \longleftarrow \psi_n \exp[-i(\Delta t/2)(V_n/\hbar)]$$

6. Calculate the wave function in the k-space from the wave function in the x-space using the Fast Fourier Transform.
7. Compute a full-step (*Δt)* in the k-space as follows :

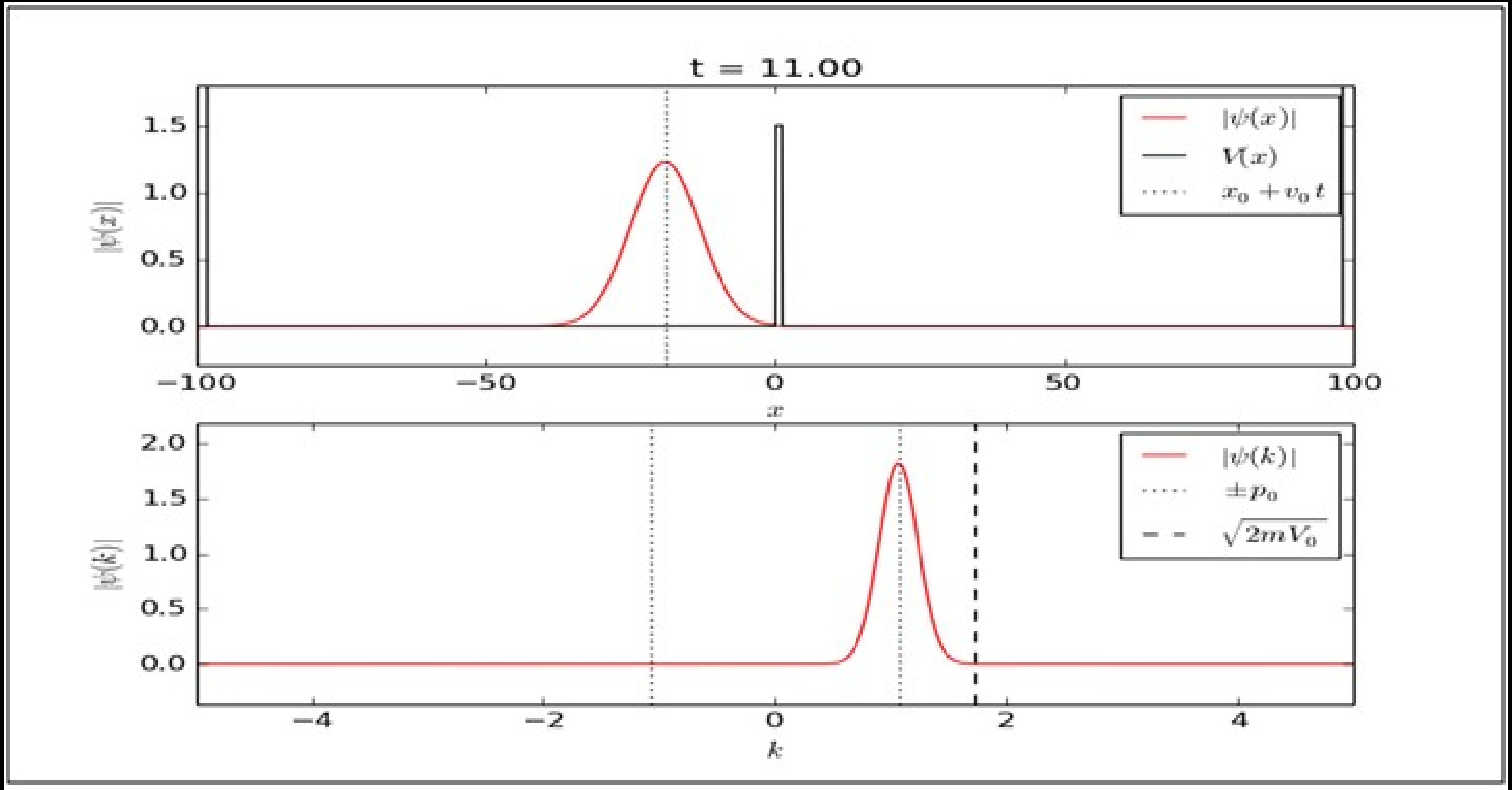
$$\widetilde{\psi}_m \longleftarrow \widetilde{\psi}_m \exp[-i\hbar(k \cdot k)\Delta t/(2m)]$$

8. Calculate the wave function in the x-space from the wave function in the k-space using the Inverse Fast Fourier Transform.
9. Compute a second half-step (second *Δt/2)* in the x-space as follows :

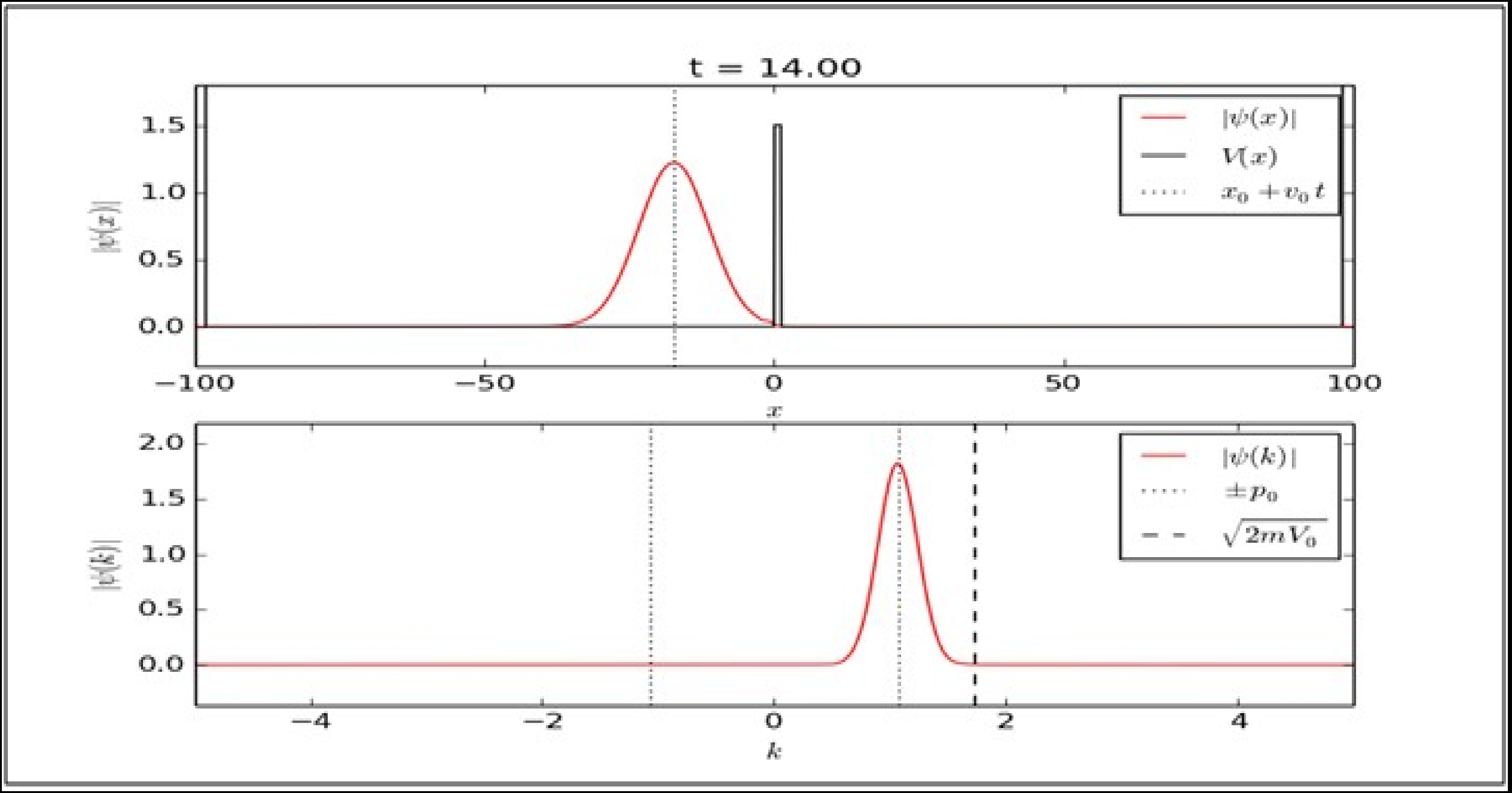
$$\psi_n \longleftarrow \psi_n \exp[-i(\Delta t/2)(V_n/\hbar)]$$

Steps 5 to 9 are repeated for all the following time intervals of *Δt*, until the desired time is reached.

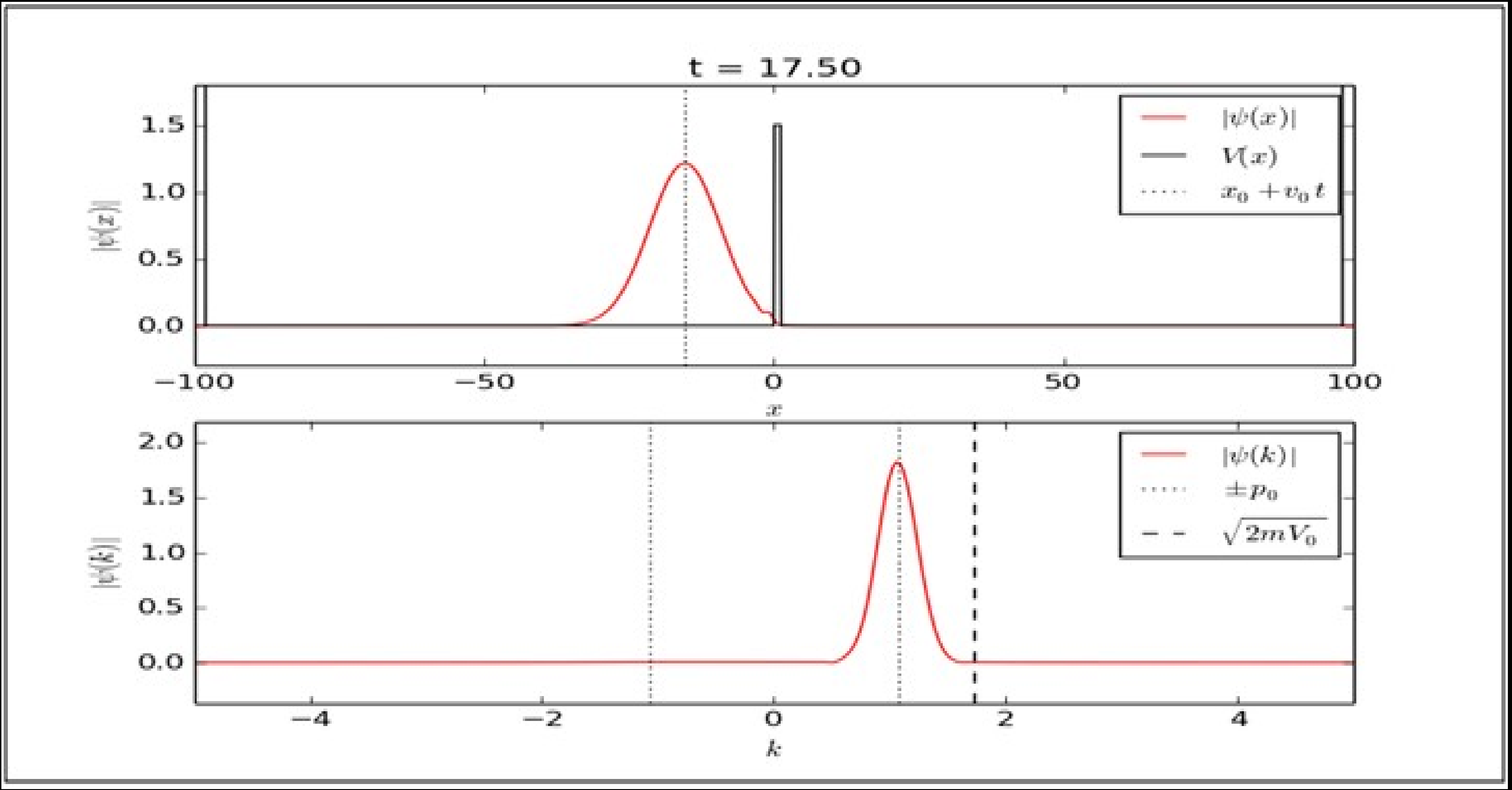
Approaching barrier...



Approaching barrier...



Approaching barrier...



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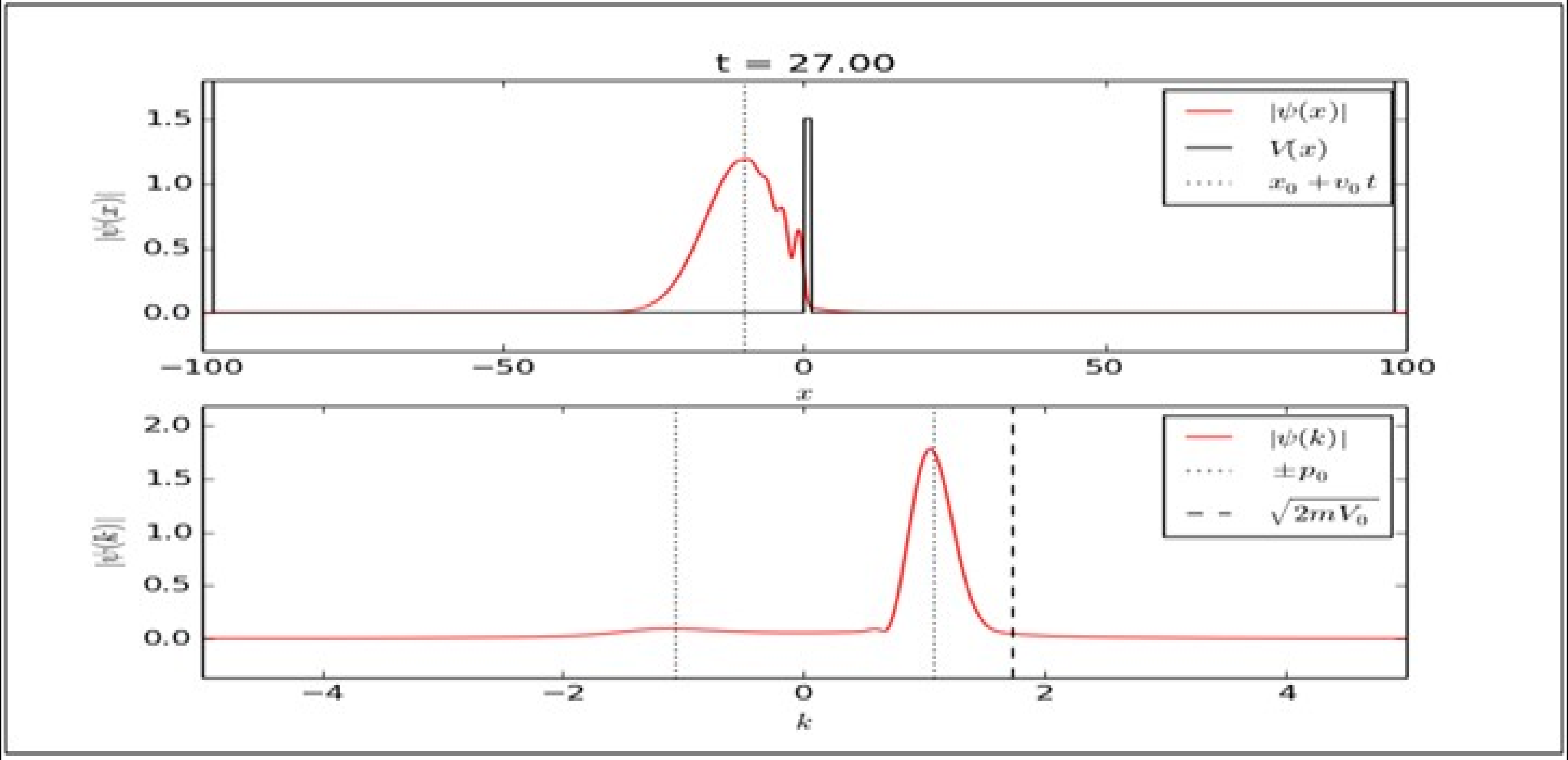
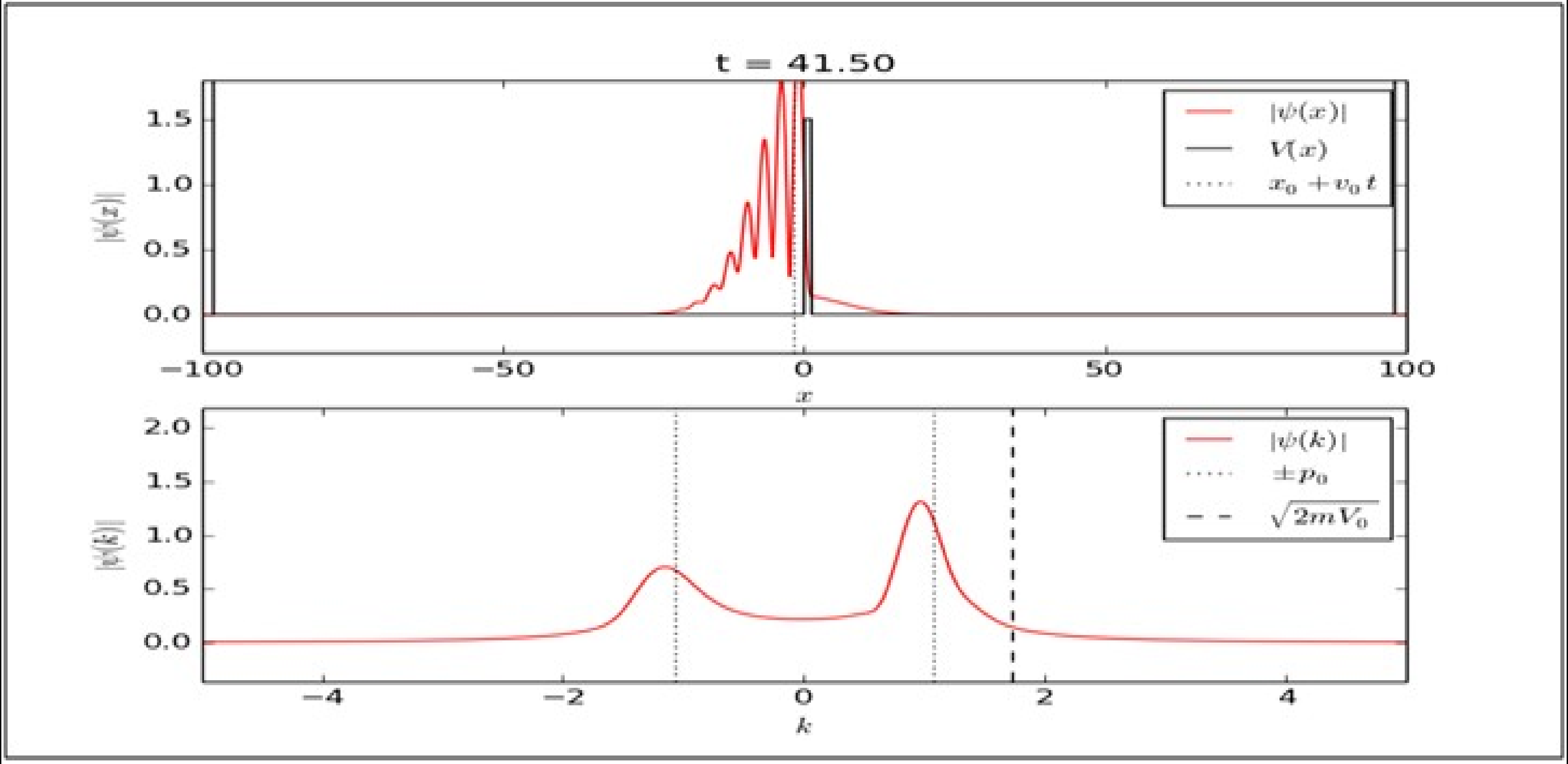
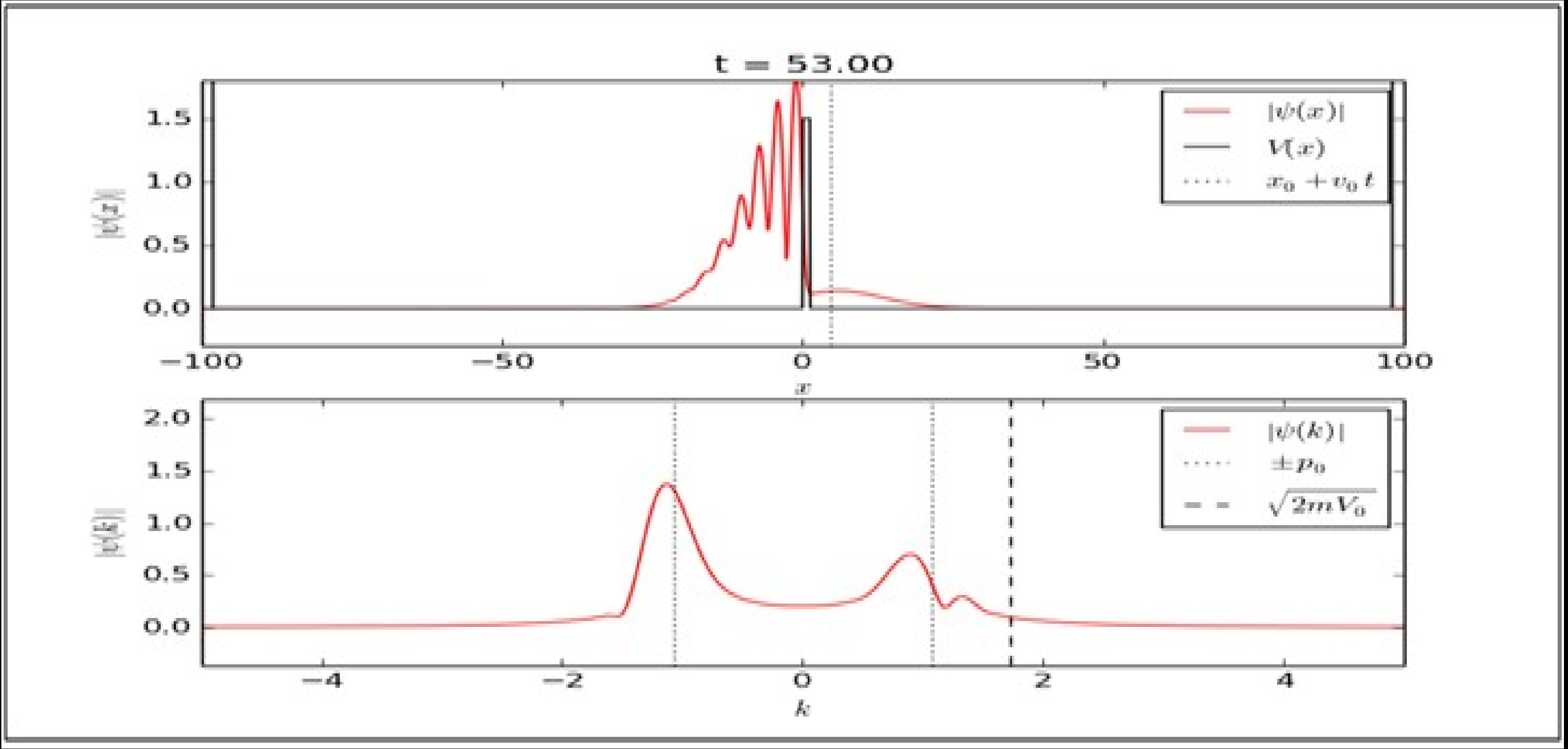


Approaching barrier...



Leaving/breaching barrier...



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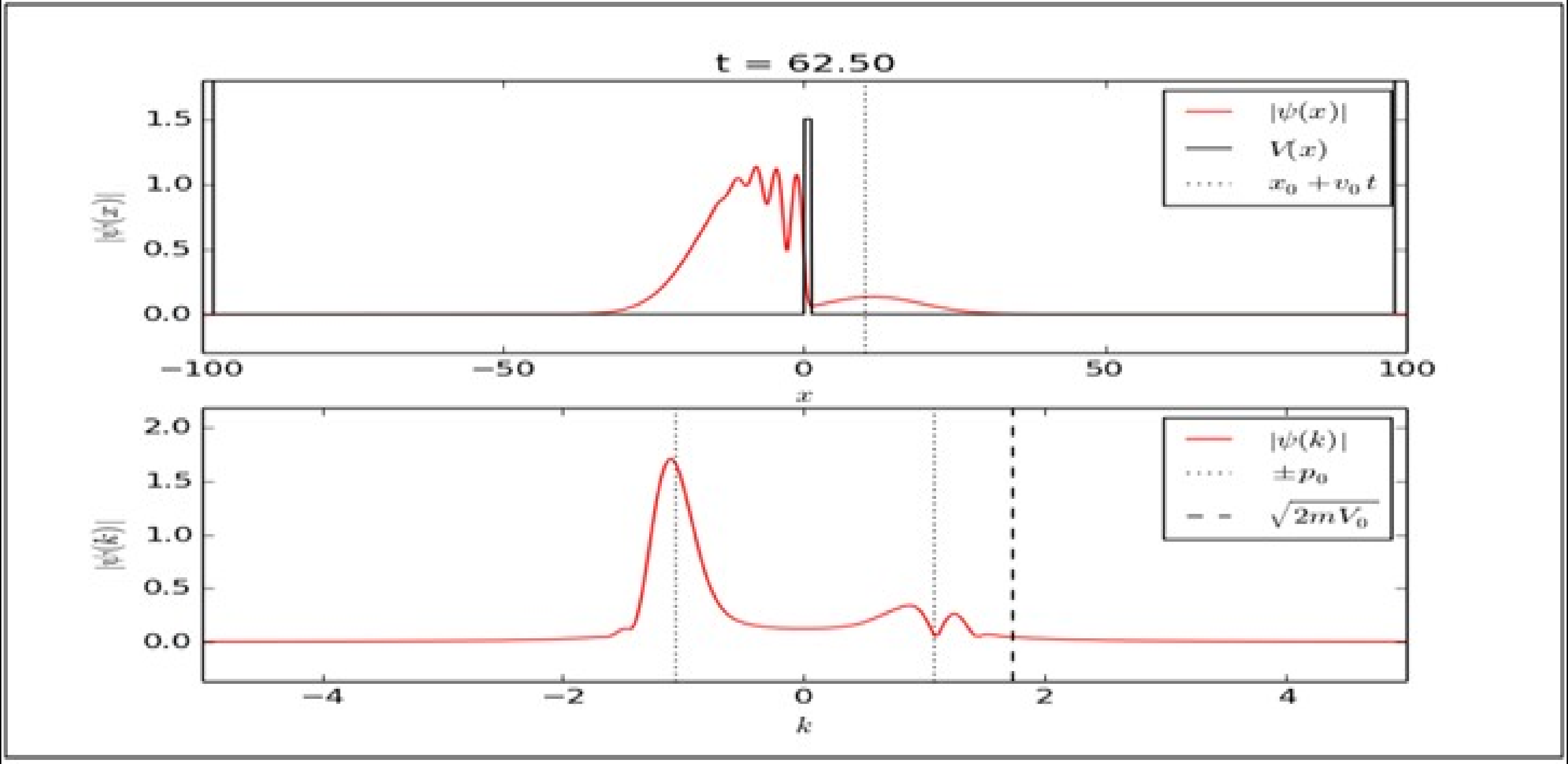
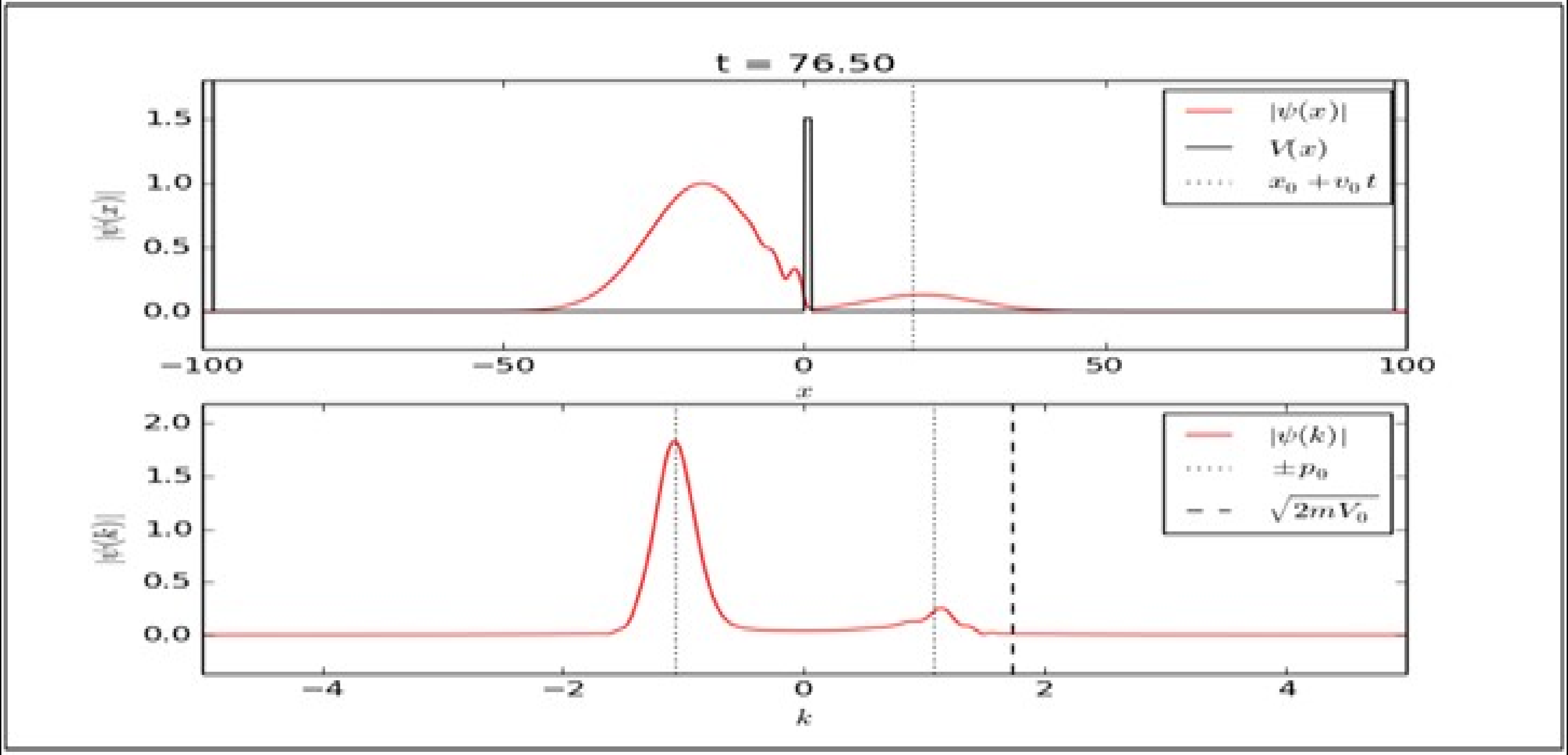


Leaving/breaching barrier…

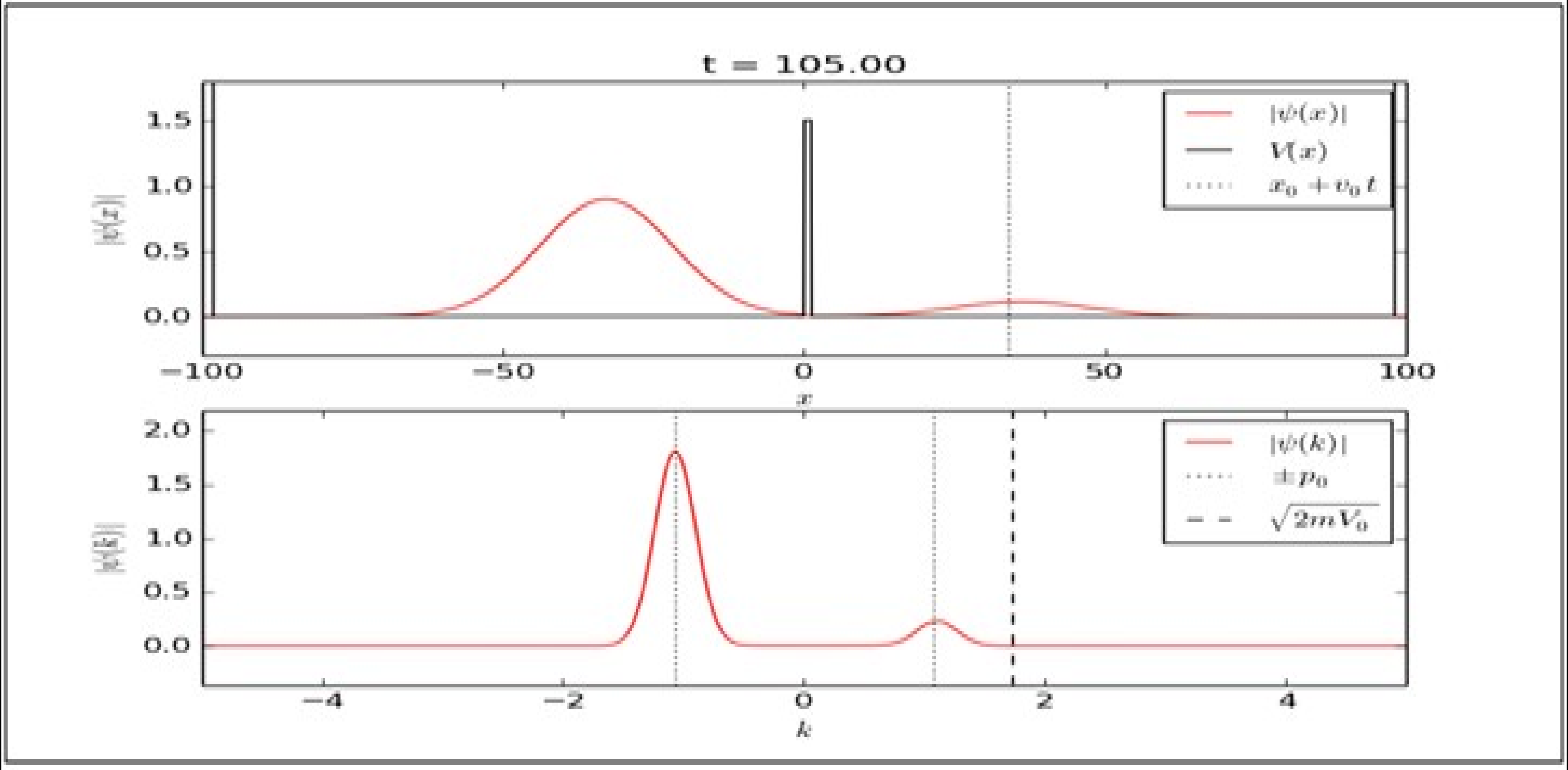


The solid line in the above panel in each of these images represents the potential barrier. The barrier is high enough for a classical particle to not penetrate it.

However, a quantum particle can pass through this barrier, leading to a non-zero probability of finding the particle beyond the barrier as seen in these images.

This is known as the ‘quantum tunneling effect’.

Evolution of the system with time…



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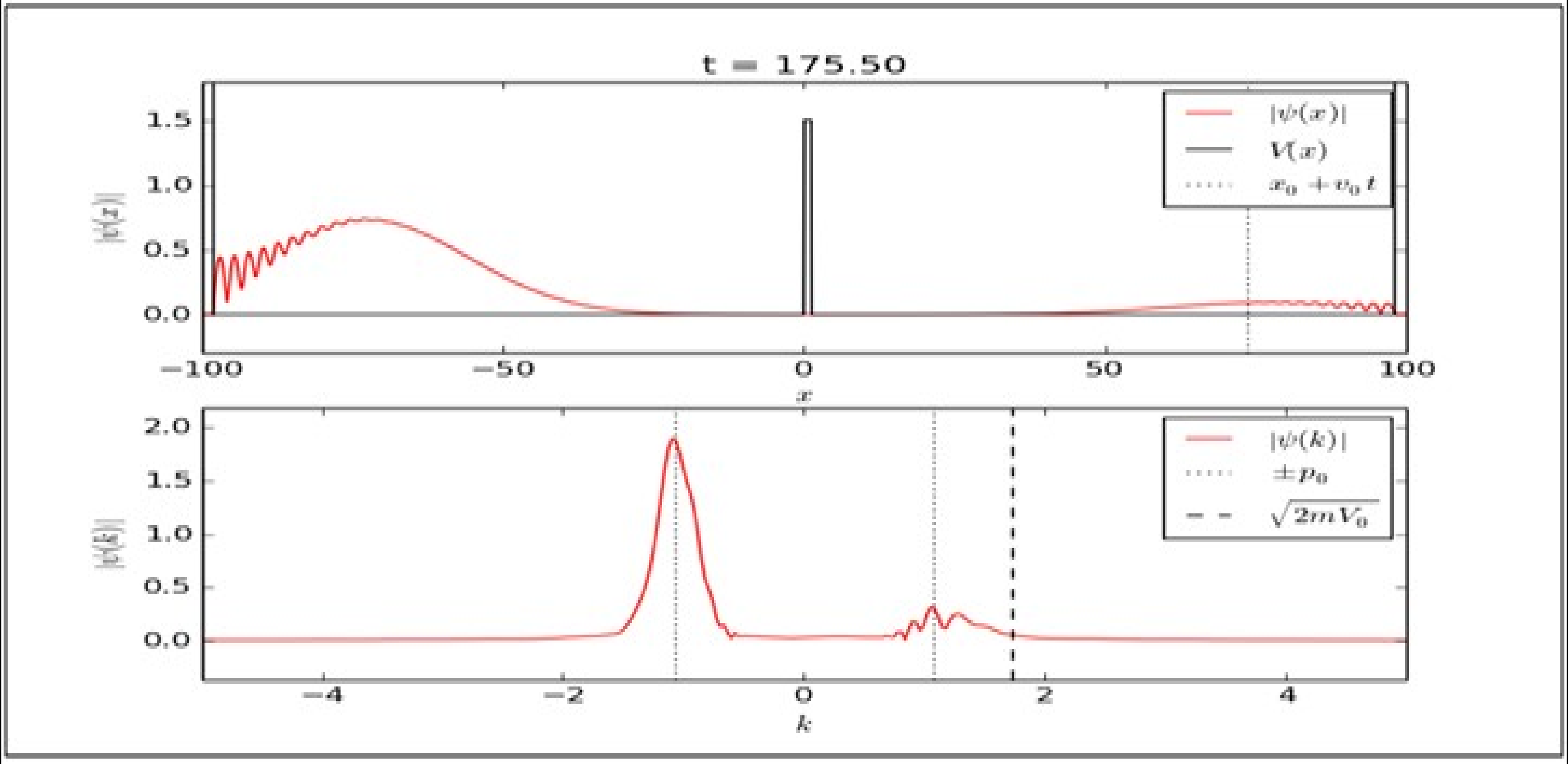

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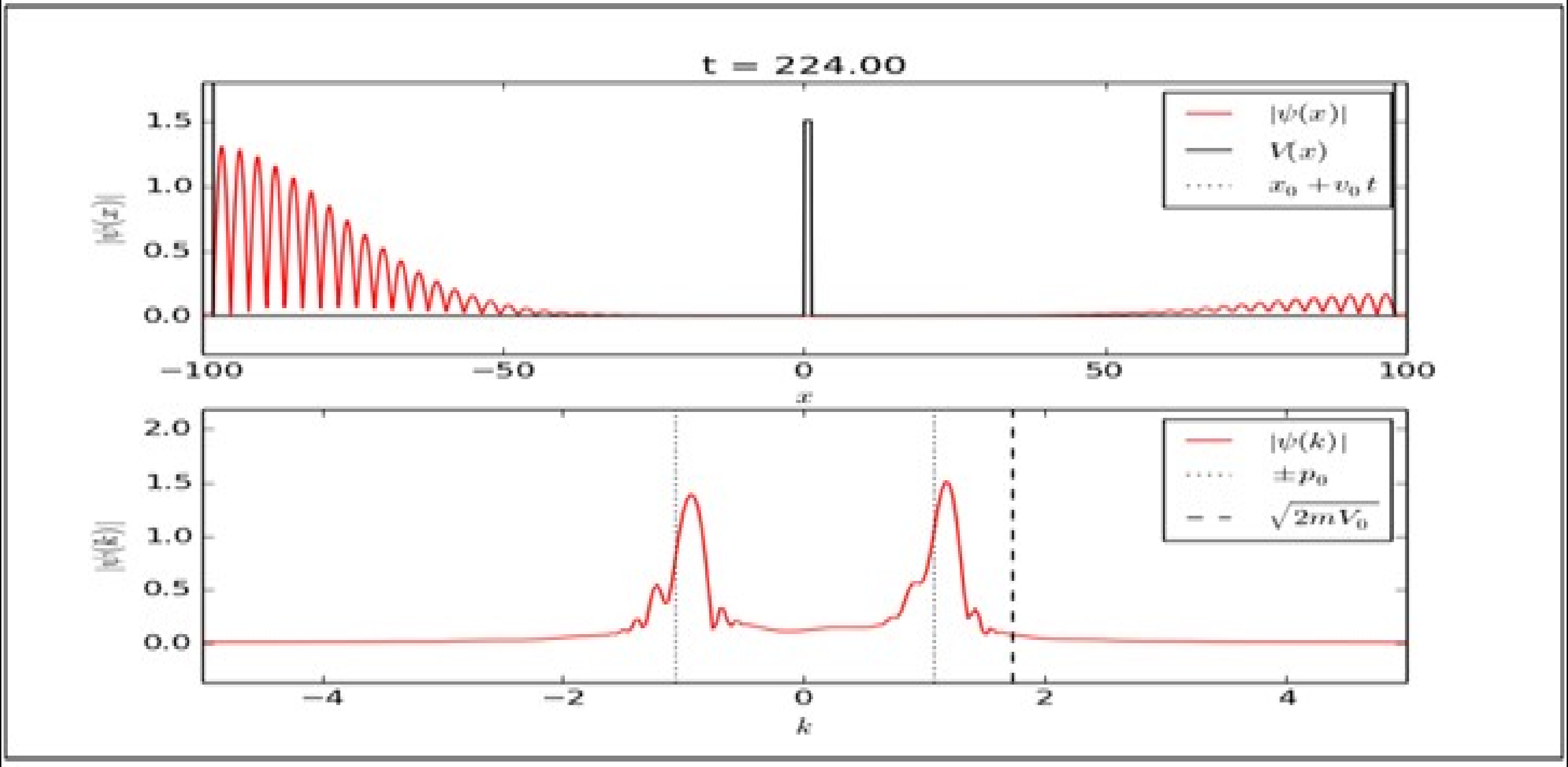

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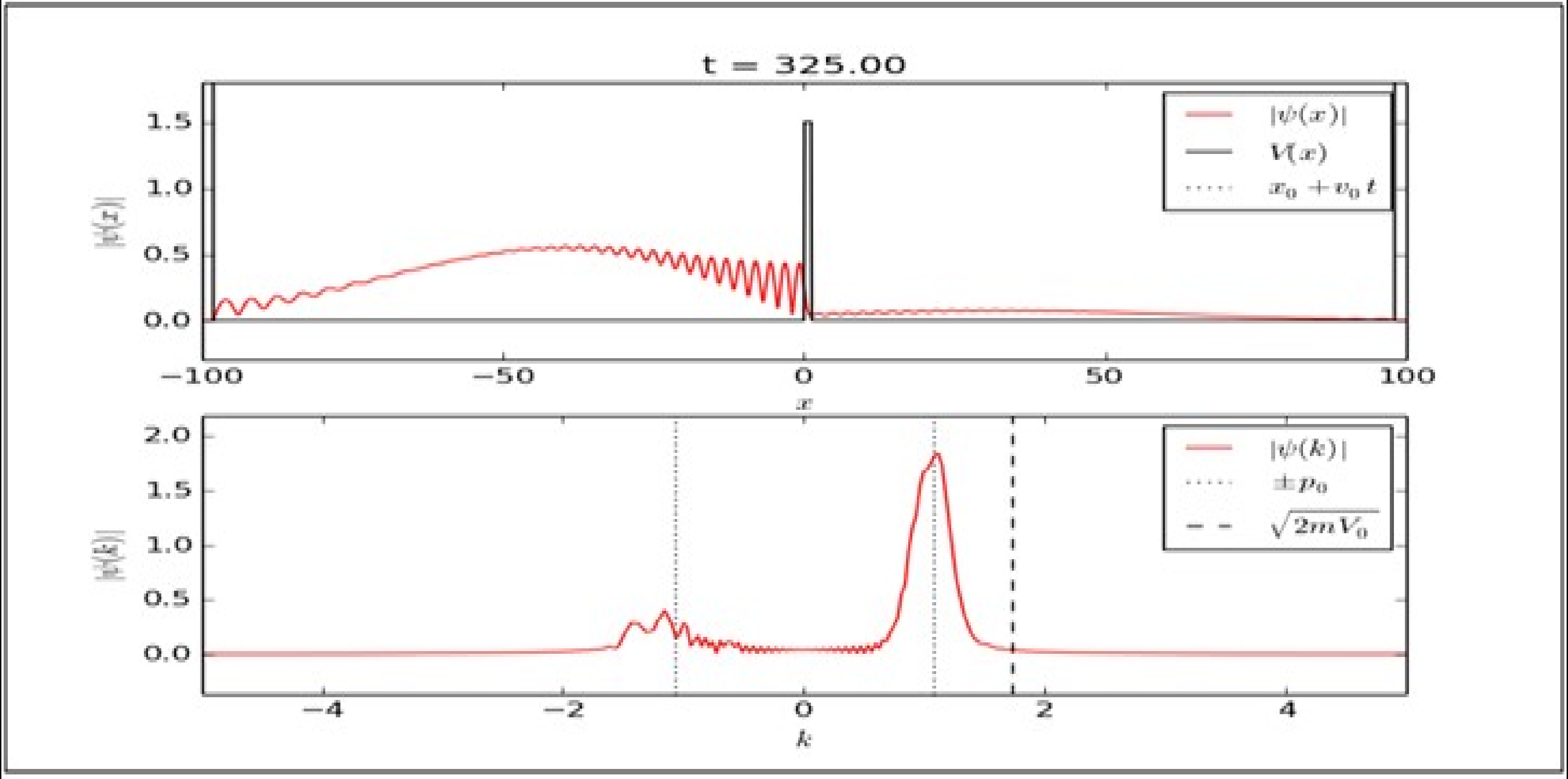
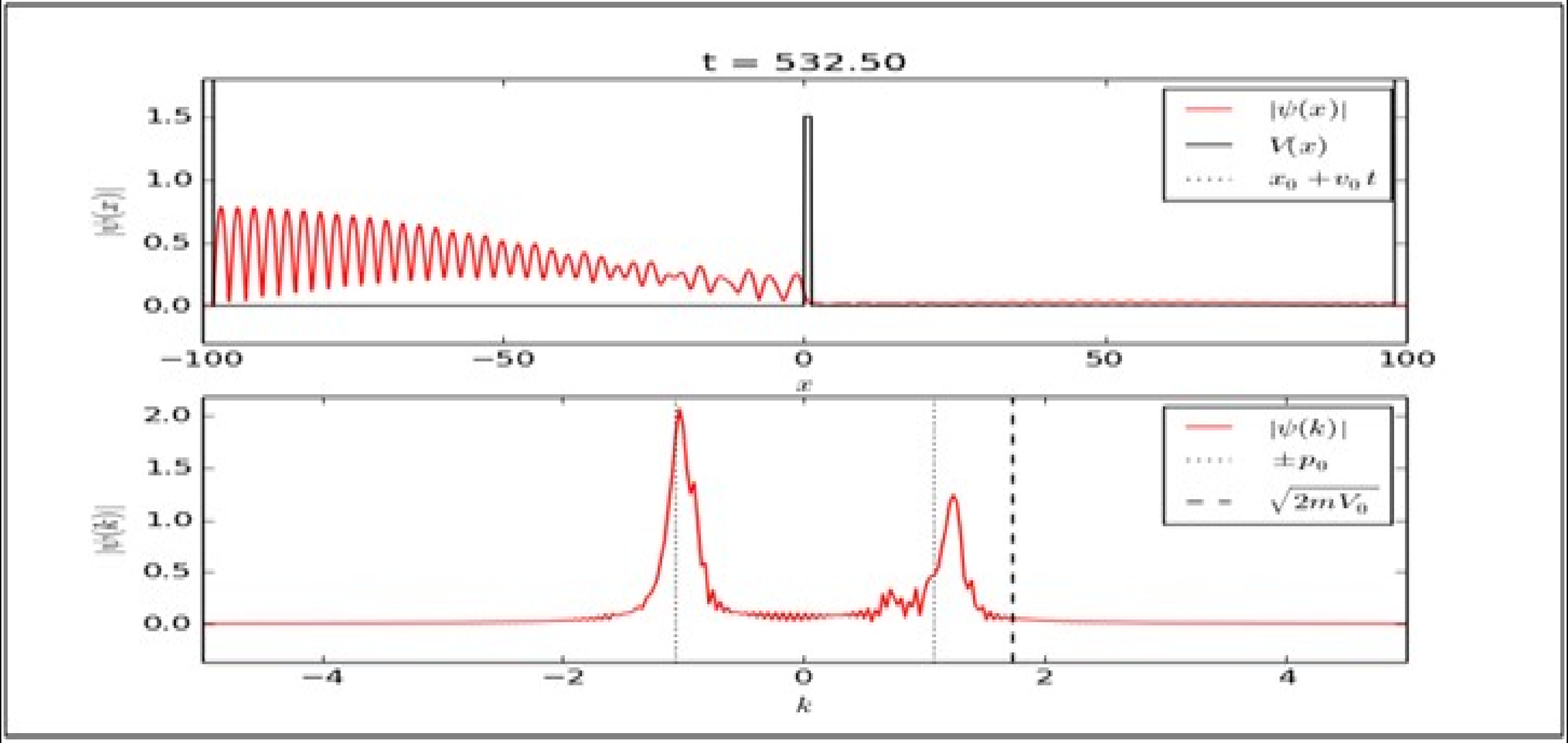


Evolution of the system with time…



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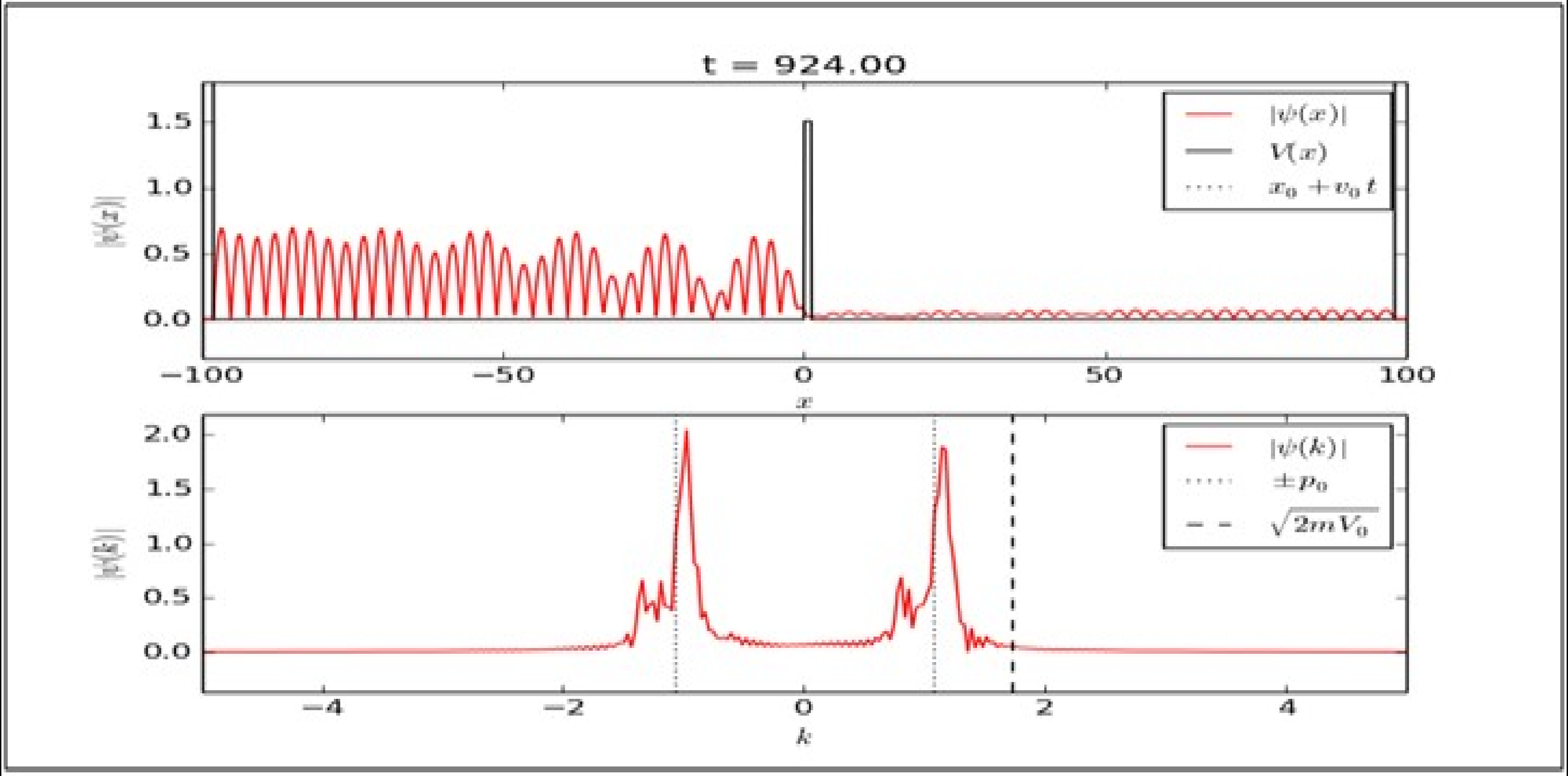

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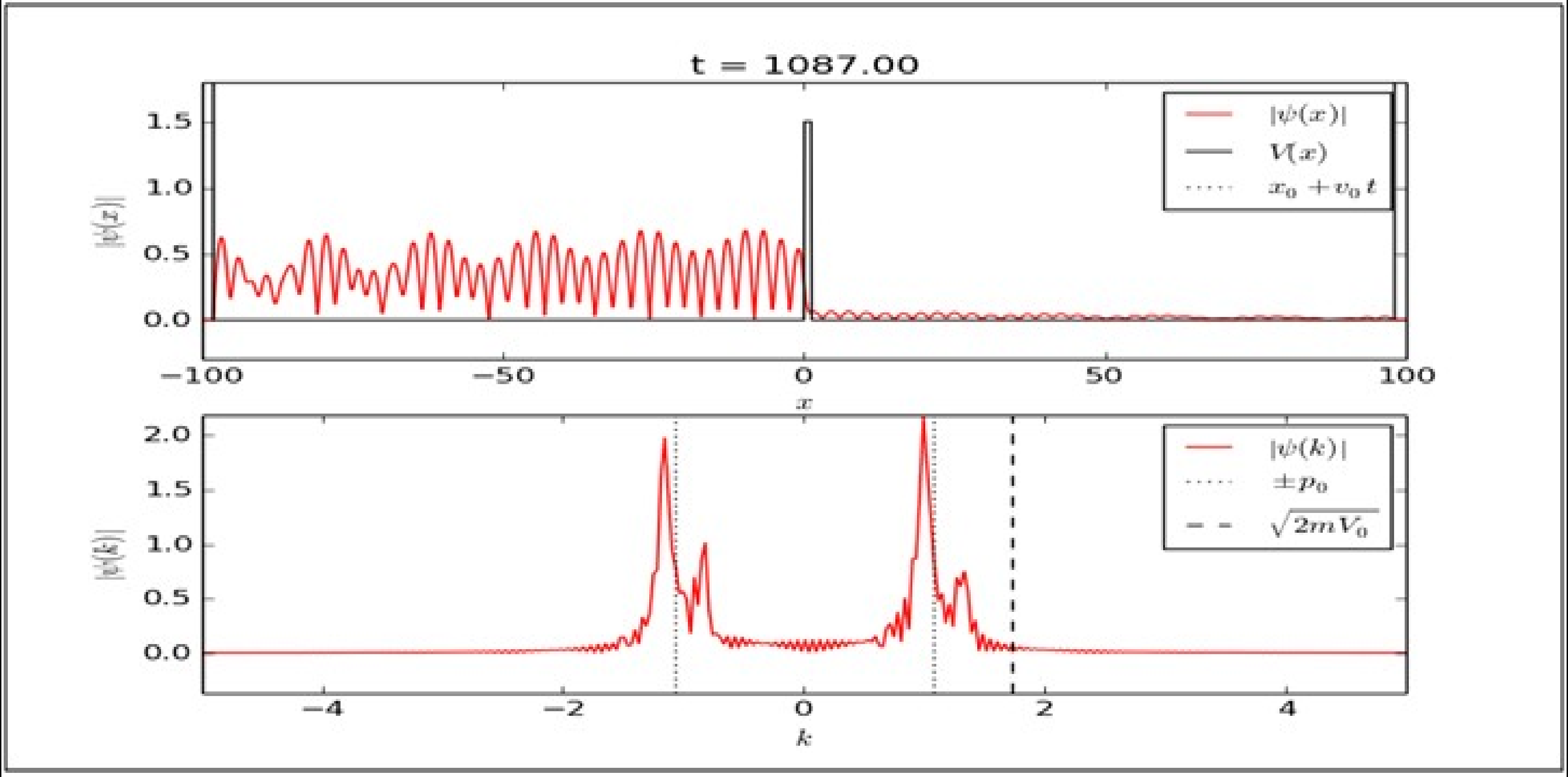

The particle ‘most probably’ resides inside the ‘box’ formed by the potential barrier. As time goes by, the particle collides with the walls of this ‘box’ and is set in a to and fro motion from wall to wall. The two peaks in the bottom panel correspond to the average momentum of the particle.

References

- *Introduction to Quantum Mechanics* by David Griffiths
- Python 2.7 Documentation (references for the code)
- *Numerical Methods for Physics* by Alejandro Garcia
- Wikipedia

Thank you